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# BOOK OF ABSTRACTS



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### How the Tonality of Tweets Impact on the Price and Return of Bitcoin?

A. Nepp, <u>M. Abramov</u>

Ural Federal University, Ekaterinburg, Russia

The main part of people's life is social media today, they spend too much time to communicate with each other. In case of medias the information spreads like wildfire. The Twitter is one of the most popular social media, which has a big popularity among investors on the global market and the market of Bitcoin is not an exclusion. Before the start of this investigation, we have analyzed the following articles: "Quantifying Sentiment with News Media across Local Housing Markets" by Cindy K Soo (2018), the author looks at how the sentiment index explains the changes of property's price on the USA market. "Buying on rumors: how financial news flows affect the share price on Tesla" by Nadine Strauss, Christopher Holmes Smith (2019), they investigates how the tonality impacts on the price of Tesla and reaction of the market. Furthermore, we examined the article: "What drives the Bitcoin price? A factor augmented error correction mechanism investigation" by Lukasz Goczek and Ivan Skliarov (2019). They show us what are reasons of movements Bitcoin's price. Another investigation by Dehua Shen, Andrew Urquhart, Penfgei Wang: "Does Twitter predict Bitcoin?," these authors investigated how posts in case of Twitter impact on the market of Bitcoin. Finally, Tiran Rothman has examined how social medias impact on the behavior of investors on the Bitcoin marketin the article: "Trading the Dream: Does Social Media Affects investors activity?" (2019). This paper adds to the growing literature of Bitcoin by examining how the tonality of tweets impact on the Bitcoin's market especially on the price and return of Bitcoin. We used the volume of tweets collaborating with Google Trends and Coronavirus tweets. The historical data was obtained from the Twitter for the period from 2013 to 2020 by the hashtag "Bitcoin" and "Coronavirus," using the Twitter API. This data was analyzed by sentiment analysis (positive, neutral and negative), for this analyze we have used the ready libraries of data code, which based on the Nodge js platform.

### Stable Regularized Algorithms for Solving the Inverse Gravimetry Problem in the Case of Multilayered Medium

#### E. Akimova, V. Misilov

Ural Federal University & N.N. Krasovskii Institute of Mathematics and Mechanics, UrB RAS, Ekaterinburg, Russia

M. Sultanov

Khoja Akhmet Yassawi International Kazakh-Turkish University, Turkestan, Kazakhstan

The paper is devoted to developing of the stable regularized algorithms for solving the structural inverse gravimetry problem for the case of multilayered medium. The structural problem consists in finding several interfaces between layers with constant densities using known gravitational field. The problem is described by a nonlinear integral equation of the first kind; it is ill-posed. The regularized variant of this equation is proposed for the case of multiple surfaces. For solving the regularized equation, we use the steepest descent method and conjugate gradient method. To reduce the amount of calculation and execution time, we use the technique for approximate calculating the Jacobian matrix. The idea is to drop out small elements, so that the approximated matrix has the band structure. The model problem of reconstructing three surfaces using quasi-real data is considered. The numerical experiments are conducted to study the performance of the proposed gradient methods.

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#### Inversion and Symmetries of the Star Transform

G. Ambartsoumian

Dept of Mathematics, University of Texas at Arlington, TX, USA

The star transform is a generalized Radon transform mapping a function of two variables to its integrals along "star-shaped"trajectories, which consist of a finite number of rays emanating from a common vertex. Such operators appear in mathematical models of various imaging modalities based on scattering of elementary particles. The paper presents a comprehensive study of the inversion of the star transform. We describe the necessary and sufficient conditions for invertibility of the star transform, introduce a new inversion formula, discuss its stability properties and demonstrate its efficiency on numerical examples. As an unexpected bonus of our approach, we prove a long-standing conjecture from algebraic geometry about the zero sets of elementary symmetric polynomials.

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### Effect of Marginal Propensity to Save on Limit Cycle Parameters of Goodwin's Model with "Only Floor" in Induced Investment

#### A.O. Antonova

National Aviation University, Kyiv, Ukraine

S.N. Reznik

Institute for Nuclear Research, National Academy of Sciences of Ukraine, Kyiv, Ukraine

#### M. D. Todorov

Dept of Mathematics and Statistics, San Diego State University, CA, USA & Faculty of Applied Mathematics and Computer Science, Technical University of Sofia, Bulgaria

According to S. Sordi [1], under certain conditions the limit cycles solutions of Goodwin's business cycle model [2] are possible even if the induced investment function is bounded only above or only below (that is, has a ceiling or a floor). These conditions are given by the inequalities

$$r > \epsilon + s\theta$$
,  $s_{\min} < s < 1$ ,  $s_{\min} = \theta^{-1}(\sqrt{r} + \sqrt{\epsilon})^2$ ,

where r is the acceleration coefficient,  $\varepsilon$  and  $\theta$  are the time-lag of the dynamic multiplier and the time-lag between investment decisions and the resulting outlays, respectively, s < 1 is the marginal propensity to save.

As an example, in [1] is considered following Goodwin's equation for national income y(t)

$$\epsilon\theta\ddot{y} + (\varepsilon + \theta s)\dot{y} - \varphi(\dot{y}) + sy = 0 \tag{1}$$

with the "only floor" model of piecewise linear accelerator

$$\varphi = \begin{cases} \varphi(t) = \text{const}, & \dot{y} < \varphi_f r^{-1} \\ r \dot{y}, & \dot{y} \ge \varphi_f r^{-1} \end{cases}$$

and such parameter values r = 2,  $\theta = 1$ ,  $\varepsilon = 0.6$ . In this case, the range of possible values of s for which the limit cycles of equation (1) exist is limited by the inequalities 0.409 < s < 1.

We investigated the dependencies of the Goodwin cycle parameters on the marginal propensity to save for the above parameters and  $\varphi_f = -3$ . The results are shown in the table below.

0.9	6.12	-2.22	6.92
0.8	6.99	-2.62	11.84
0.7	8.26	-3.12	23.44
0.6	10.36	-3.78	62.76
0.5	15.07	-4.66	431.58

Here T is a period of limit cycle,  $y_{\min}$  and  $y_{\max}$  are minimal and maximal values of income. Sordi's results correspond to s = 0.6. Table 1 shows that when s tends to a critical value, you need to abandon the "only floor" model or assume that with a decrease in s decreases  $|\varphi_f|$ , too.

#### References

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[2] R.M. Goodwin, *Econometrica* **19**, 1–17 (1951).

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#### Differential Equations Involving the Schwarzian Derivative

<u>Yu. Bozhkov</u>, P. Ramos da Conceicao Institute of Mathematics, Statistics and Scientific Computation, University of Campinas, Campinas - SP, Brazil

We review the symmetry properties of differential equations involving the Schwarzian derivative. We propose and study new differential equations and systems determined by their Lie point symmetry groups, which generalize the Kummer-Schwarz equation and the Krichever-Novikov equation.

### Improved Interior Tomography Reconstruction Based on Prior Knowledge

E. Bridges

Dept of Electrical and Electronic Engineering, University of Surrey, UK

G. Ambartsoumian

Dept of Mathematics, The University of Texas at Arlington, TX, USA

 $\underline{L. \ Florescu}$ 

Centre for Vision, Speech and Signal Processing, University of Surrey, UK

We address the interior problem of computed tomography that occurs when projection data is only available for a region in the interior of the sample. In this case, the projection data is not enough to accurately reconstruct the attenuation function even in the interior domain. We introduce an algorithm for correcting the interior tomography reconstruction, which is based on prior knowledge in the interior domain. This correction algorithm is then evaluated by performing numerical experiments with the Shepp-Logan phantom for various amounts of data loss, noise levels in the available projection data, and positions and values of the attenuation coefficient known a priori. A good performance of the algorithm based on prior knowledge at one point is demonstrated in the case of noiseless data. In the presence of noise in the projection data, improvements in the reconstructed attenuation function are obtained based on prior knowledge in a subregion of the interior domain. The numerical experiments also demonstrated that the correction algorithm is robust to errors (patient variations) in the values of the attenuation coefficient used as prior knowledge.

### Optimization of Adaptive Control of Business Planning Processes Based on the Network of Economic and Mathematical Modeling

#### A. Shorikov

#### Ural Federal University & Institute of Mathematics and Mechanics UB RAS, Ekaterinburg, Russia

#### $\underline{E. Butsenko}$

#### Ural State University of Economics, Ekaterinburg, Russia

The article discusses the optimization of adaptive control of business planning processes in the face of uncertainty. The results of the work are based on a new method for optimizing adaptive project control using network economic and mathematical modeling. In the process of implementing the method, an optimal adaptive control strategy for the implementation of business planning is formed, the optimal time for its implementation and the optimal schedule for the project as a whole, corresponding to the optimal adaptive control strategy, are calculated. The paper describes a new optimization network economic and mathematical model that takes into account the possibility of adaptive control of the implementation of the business project under consideration, and proposes a new method for solving this problem. The description of the practical implementation of the proposed method for solving this problem is given on a specific example of a business project for opening a catering business. The results obtained in the work show a high degree of effectiveness of the developed new method. Further development of this direction may be associated with the development of a computer-based intelligent system for optimizing adaptive control of business planning processes and the creation of appropriate tools to support managerial decision-making in the implementation of business planning processes by business entities in the face of information uncertainty.

### Intelligent Software System for Optimizing Adaptive Control of Investment Projecting Processes

A. Shorikov

Ural Federal University & Institute of Mathematics and Mechanics UB RAS, Ekaterinburg, Russia

E. Butsenko

Ural State University of Economics, Ekaterinburg, Russia

V. Tyulyukin

Ural State University of Economics & Ural Federal University, Ekaterinburg, Russia

The article describes the functionality of an intelligent software system developed by the authors to optimize adaptive control of investment projecting processes in the face of uncertainty. The results are based on a new method for optimizing adaptive project control using network economic and mathematical modeling. The developed intelligent system is designed to automate the modeling of investment projecting processes and optimize adaptive decision-making control during their implementation on the basis of network economic and mathematical modeling, as well as methods and tools for developing intelligent software systems. This system takes into account the existing specific technical and economic conditions and information support. The results obtained in this work can serve as the basis for creating intelligent instrumental systems for supporting managerial decisionmaking in the implementation of investment projecting processes in the context of information uncertainty and risks.

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### Reduction Dynamics for Soliton Stripes, Vortices, and Vortex Rings in Quantum Superfluids

#### R. Carretero-González

Nonlinear Dynamical Systems Group, Dept of Mathematics and Statistics, and Computational Science Research Center, San Diego State University, San Diego, CA 92182-7720, USA

Motivated by recent experimental advances in the imaging and manipulation of Bose-Einstein condensates (BECs), we showcase some results pertaining the reduction of the original (higher dimensional) dynamics into a much more manageable low-dimensional dynamical system. In particular, we will show how a "soup" of interacting trapped BEC vortices in (quasi-)2D geometries is reduced to a set of couple ODEs that is able to predict bifurcations in the original PDE and the experiment. We will also present a dynamical reduction, based on adiabatic invariants, for a wide variety of solitonic stripes embedded in 2D space (including dark, bright, dark-bright stripes). Finally, we will also explore some extensions of the dynamical reduction for 3D vortex rings which are formed when a vortex filament (a "twister") is looped back onto itself creating a close ring that carries vorticity.

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### Soft Hydraulics: Mathematical Modeling of Flows in Deformable Conduits

V. Anand, I. C. Christov, T. C. Shidhore, X. Wang

School of Mechanical Engineering, Purdue University, West Lafayette, IN, USA

The viscous resistance of hydraulic conduits of non-circular cross-section can be obtained from exact unidirectional flow solutions of the steady Stokes equations. In the last decade, however, experiments at the microscale involving internal flows in channels with soft (compliant) boundaries has presented surprises due to the inherent fluid-structure interactions between flow and deformation. These problems have numerous applications in soft robotics and microfluidics. We discuss new mathematical results on calculating the nonlinear hydrodynamic resistance for the coupled problem, starting from the basic equations of continuum (fluid and solid) mechanics. Via a perturbation approach, the Stokes equations are coupled to the appropriate governing equations of a linearly elastic body. In the distinguished limit of a long and slender geometry, the leading-order flow and elasticity problems are solved analytically. Furthermore, we are able to perform this calculation for a number of relevant geometries. For example, our mathematical theory can handle rectangular microchannels sealed by (thin) elastic films, as well as those created by via replica molding (resulting in thick structures as the walls). Model problems in cylindrical coordinates are treated via shell theory, including viscoelastic effects. Important, the mathematical theory is shown to rationalize previous experimental measurements, and it compares favorably to three-dimensional, two-way coupled direct numerical simulations of fluid-structure interactions.

### Stability of Special Discontinuities in Solutions of the Generalized KdV-Burgers Equation

#### A. Chugaynova

#### Steklov Mathematical Institute of RAS, Moscow, Russia

Nonstationary solutions to the Cauchy problem for a model equation with a complex nonlinearity, dispersion, and dissipation is studied. The stability of special discontinuities propagating through a medium layer with varying parameters is analyzed numerically. In the frame of this problem new nonstationary solutions of the generalized KdV-Burgers equation are found.

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### Solidification Simulation and Casting of an Impeller designed for a Thermochemical Treatment Furnace

M. R. Condruz, O. Dumitrescu, T. Frigioescu, R. Carlanescu

National Research and Development Institute for Gas Turbines - COMOTI, Bucharest, Romania

#### C. Dumitru, A. Ghinea

SC Uttis Industries SRL, Romania

The present study was focused on solidification simulation and casting of an impeller designed for a thermochemical treatment furnace. Starting from a CAD model, the solidification simulation was realized using ProCAST software. The simulation goal was to determine where shrinkage defects emerge in order to improve the model, so the casting process will be realized in optimum conditions and a cast product will be obtained with a defect degree as small as possible. The simulation results showed that shrinkage defects are found at the impeller's hub, but this section will machined to fit the steerer's shaft. Due to application requirements, a CrNiMoN stainless steel was selected for impeller manufacturing, it being a material resistent to high temperatures in corrosive environments. The impeller was manufactured by sand casting using an exothermic feeder head. After solidification, the feeder was mechanically removed and at its base a closed shrinkage macroporosity was observed, result predicted by the solidification simulation. Due to the defect location, it was removed during further processing (by machining). Except for the shrinkage porosity, only some small open holes at impeller's surface were observed which are acceptable for sand cast parts. Based on the current study resulty it was concluded that the simulation results are in a good agreement to the experimental results.

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### Rarefied Gas between Two Coaxial Cylinders. The Effect of Pulsating Motion of the Inner Cylinder at the Cylinders Axis. Acoustic Waves Modeling

P. Gospodinov, <u>D. Dankov</u>, V. Roussinov, M. Mironova Institute of Mechanics, BAS, Acad. G. Bonchev, bl. 4, 1113 Sofia, Bulgaria

On the basis of our previous studies in the flow modeling of rarefied gas between coaxial cylinders under pulsating radial motion and pulsating temperature (one-dimensional problem), the energy transfer in the system of gas - surrounding cylinders is studied at the cylinders axis pulsating of the inner cylinders (twodimensional problem). The energy transfer is modeled with continuous model based on Navier-Stokes-Fourier equations of motion and a statistical DSMC model. The obtained results show how the external mechanical disturbances at the cylinder axis direction influence on the gas flow. These results make it possible to assess the gauge sensitivity under external mechanical disturbances.

### Boundary Conditions Influence on the Behavior of the Casimir Force: A Case Study via Exact Results on the Ginzburg-Landau Type Fluid System with a Film Geometry

D. Danchev, V. Vassilev, P. Djondjorov

Institute of Mechanics, BAS, Akad. G. Bonchev St., Block 4, 1113 Sofia, Bulgaria

The thermodynamic Casimir force in a fluid system depends on the conditions the bounding surfaces exert on either the confined fluid, or binary liquid mixture. This influence is described by imposing proper boundary conditions on the order parameter describing the fluid. We study the force dependence explicitly on the example of the Ginzburg-Landau  $\Phi^4$  model via exact results and series expansions of the corresponding order-parameter profiles. We consider the (+,+), (+,-), Dirichlet-Dirichlet and Neumann-Neumann boundary conditions and a combination of them. We focus on a system with a film geometry close to its bulk critical point in which the order parameter satisfies one of the above mentioned boundary conditions. Solving the corresponding boundary-value problem of one nonlinear differential equation in terms of Weierstrass and Jacobi elliptic functions we report analytic representation of the Casimir force. We study the behavior of the force depending on both the temperature and an external ordering field acting on the system. Our results are in a full agreement with the general arguments of the finitesize scaling theory. We confirm the expectation that the force is attractive if the boundary conditions are the same on each boundary and repulsive otherwise.

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### Problem of Parametric Optimization of Cross-Sections in Bent Rod Corroding Elements: Method of Solution

#### D.G. Zelentsov, O.A. Liashenko, O.R. Denysiuk

Dept of Information Systems, Ukrainian State University of Chemical Technology, Dnipro, Ukraine

The paper focuses on the problem of finding optimal cross-section sizes of bent rod (beam) elements exposed to aggressive media. A new method for solving the optimization problem of this class is proposed. It is necessary to determine crosssection dimensions of a beam, which would ensure that its cross-section area would be minimal, and for a given period of operation it would retain its bearing capacity. The influence of an aggressive medium causes the destruction of a surface layer of metal and, consequently, changes in size of structural elements. Mechanical stresses significantly accelerate the corrosion process. A model of corrosion deformation in this case includes differential equations describing accumulation of geometric damage and including stress functions, and a system of mechanical equations for calculating stress-strain state. When modeling the process of corrosion deformation in real structures, it is possible to solve the system of differential equations only numerically. The authors analyze existing approaches to solving such problems. Based on the analysis, a fundamentally different approach, which significantly decrease computational costs, is proposed. The paper considers the problem of vector optimization based on two criteria: the minimum area and the perimeter of a cross-section at the moment of exhaustion of load-bearing capacity. The target function includes a weight factor? that takes into account the influence of the crosssection perimeter. The proposed method is based on an assumption that there is only one value of the coefficient ? that ensures that solutions of the problem in both traditional and new statements coincide. To compare these results correctly, it is necessary that a cross-section is represented in both statements by a set of rectangular fragments both at the initial moment of time and at the moment corresponding to the limit state, so a model of a corroding equivalent cross-section is used.

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### Modeling Dynamic Patterns from COVID-19 Data Using Randomized Dynamic Mode Decomposition in Predictive Mode and ARIMA

#### D. A. Bistrian

#### Dept of Electrical Engineering and Industrial Informatics, Politehnica University of Timisoara, Hunedoara, Romania

#### G. Dimitriu

Dept of Medical Informatics and Biostatistics, Grigore T. Popa University of Medicine and Pharmacy, Iasi, Romania

#### I. M. Navon

Dept of Scientific Computing, Florida State University, Tallahassee, FL, USA

In this paper we aim to develop a mathematical tool for modeling and medium term prediction of the evolution of the new Corona virus (Covid-19) dynamics using real data provided by existing World Health Organization (WHO) data bases. Epidemiological strategy with the new Corona virus struggle must achieve two main concepts: developing a tool for modeling the evolution of the disease and developing a tool for prediction of disease spreading. Thus modeling and prediction of disease spreading represents challenging and actual topics in epidemiology.

In the context of application of interdisciplinary techniques for modeling the new Corona virus dynamics and effects, the guiding line of this paper is motivated by the efficiency of reduced order modeling in problems arising in epidemiology, where data are provided by statistical tools or are collected during the pandemic manifestation. We refer to this data as discrete or non-intrusive data. Prediction from the non-intrusive data of disease spreading, susceptible individuals, infected and recovered individuals require a faithful mathematical model. The intent of this paper is to undertake efficient techniques to build a mathematical model that simulates the evolution of the strongly nonlinear behavior of the Covid-19 virus dynamics and to define a new mathematical and numerical methodology for studying dominant and coherent patterns in this dynamic.

In the present work we address the investigation of epidemiologic dynamics through the perspective of reduced order modelling (ROM) using Randomized Dynamic Mode Decomposition (rDMD). The objective of rDMD is to build a model of smaller dimension from raw data, to decrease the computational burden while leading to a controlled loss of accuracy. To asses predictions from the non-intrusive data of disease spreading an additional key innovation in the paper consists in forecasting the DMD-ROM model in time using autoregressive integrated moving average (ARIMA) models, using a sliding time window technique also referred to as adaptive DMD.

The proposed mathematical model is applied for the first time on Covid-19 infectious disease data. The key-benefits of the proposed methods are as follows: dynamic patterns of infectious disease spread are obtained, the information provided by the mathematical model can be useful for allocating vaccine resources for the year, sending surveillance teams to monitor the disease and timing the interventions to leverage natural disease dynamics. Processing epidemiological data concerning Corona virus disease by scientific tools presented in this paper can help relevant actions such as: allocating intervention resources, avoiding redundancy in surveillance team deployment and designing effective immunization campaigns. Quantitative modeling and analysis plays a key role in understanding disease spread and optimally applying intervention resources to maximize the probability of success for eradication. A quantitative evaluation of the spatial modes computed from the DMD decomposit-ion and a rigorous error analysis for the reconstruction of data are performed.

#### Stability Analysis of Gyroscopic System

A. U. Dominic

Dept of Mathematics, Akwa Ibom State University, P.M.B. 1167 Uyo, Nigeria

In this work, a stability theorem for determining the stability or otherwise of a gyroscopic system is developed. A Lyapunov function is obtained by solving the arising Lyapunov matrix equation. The Lyapunov function is then used to obtain response bounds for displacements and velocities both in the homogeneous and inhomogeneous cases. Examples are given to illustrate the efficacy of the results obtained.

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### Efficient Quasi-Monte Carlo Sampling for Quantum Random Walks

E. Atanassov, M. Durchova

Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria

Quantum random walks are the natural counterpart of the classical random walk, arising when quantum effects are taken into consideration. Many Monte Carlo methods use the classical Brownian motion as a building block. Although it appears naturally in various problems of computational physics, it is also used extensively in the stochastic models used for pricing of financial assets. When quantum random walks are used instead, more complex behaviors can be observed. However, the simulation of a quantum random walk requires more computational resources. By using low-discrepancy sequences instead of pseudorandom numbers, one may hope to decrease the statistical error of the simulation. Another approach for improved efficiency is to use the power of computational accelerators, which are suitable for problems, where a well-ordered sequence of computations is to be performed repeatedly. In our work we concentrated on using GPGPU computing in order to speed-up the operations involved in the generation of the low-discrepancy sequence as well as the subsequent sampling of the quantum random walks. In this work we explain our sampling algorithm and demonstrate its efficiency on model problems from the domain of option pricing.

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### Determination of the Structural Requirements of $\mu$ -Opioid Receptor Ligands with Docking

T. Dzimbova, F. Spundzhi, R. Mavrevski, N. Pencheva, P. Milanov

Neofit Rilski South-West University, Blagoevgrad, Bulgaria

The  $\mu$ -opioid receptor (MOR) is an important target in the search of novel analgesics. The MOR agonists, such as morphine, remain the most powerful analgesics available to relieve postoperative and cancer pains. However, these compounds produce adverse effects, including development of tolerance and physical dependence, sedation, constipation, some respiratory depression, nausea, and vomiting. These unwanted effects significantly diminish the patients' quality of life. Thus structural requirements of binding to this receptor attract considerable scientific attention. Different classes of compounds were synthesized and biologically tested as ligands of the receptor with different effects. The aim of the present study is with a help of docking and subsequent analysis to determined structural requirements for the ligands. Ligand preparation was done with Avogadro software. Docking was performed with GOLD 5.2 using all functions available in the program. In vivo biological effects of the compounds were previously tested and already published. Binding to the receptor of four groups of compounds (arginine, kyotorphin, Melanocyte-inhibiting factor - 1 and RGD analogues) was analyzed and specific binding sites were determined. The main finding according to the results of docking and in vivo tests was that there was a relationship between the size of the molecule and the presence of specific functional groups capable to bind the receptor stronger. Smaller molecules could enter binding site of the receptor easily and could form the ligand-receptor complex with lower energy, which is associated with stronger and prolonged effect. Docking and subsequent mathematical analysis could be promising tools in design of new and potent ligands of  $\mu$ -opioid receptor.

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### Mathematical Modeling of the Impact of a Pulse Seismic Source on Geological Media

#### E. Efimov

Siberian Federal University, 660041 Krasnoyarsk, Russia

#### O. Sadovskaya, V. Sadovskii

#### Institute of Computational Modeling SB RAS, 660036 Krasnoyarsk, Russia

Present research is aimed at identification of the optimal operating conditions of an electromagnetic pulse seismic source. It is proposed to compare the amplitudefrequency characteristics and evaluate the seismic efficiency for different values of the source platform area and for various types of a pulse load.

An original software complex for multiprocessor computing systems of cluster architecture was used for computational modeling of wave processes in a geological blocky-layered medium. Used mathematical model of the dynamics of geomedia is able to account elastic, viscoelastic and elastic-plastic properties of soils. In order to reduce computational costs, a plane-layered soil structure with uniform layers is considered, which allows us to move on to a two-dimensional axisymmetric problem. The numerical algorithm is constructed using the two-cyclic splitting method with respect to spatial variables. One-dimensional systems of equations obtained after splitting are solved numerically using conservative finite difference schemes based on the ideas of grid-characteristic methods.

A numerical estimation of seismic efficiency was carried out taking into account the artificial dissipation of energy, which occurs when approximating non-divergent terms. It is proposed to compute the energy fluxes on grids of different scales with the further application of the Runge formula, which allows us to refine the solutions and significantly reduce the artificially dissipated energy. The parameters of seismic efficiency and amplitude-frequency characteristics obtained using computer simulation are in good agreement with experimental data and satisfy the requirements for the seismic source.

Acknowledgements. This work is supported by the Krasnoyarsk Mathematical Center and financed by the Ministry of Science and Higher Education of the Russian Federation in the framework of the establishment and development of regional Centers for Mathematics Research and Education (Agreement No. 075-02-2020-1631).

### Simulation of Silicon Solar Cell Radiation Effects with GEANT4

#### A. Fedoseyev, S. Herasimenka

#### Regher Solar LLC, Tempe, AZ, 85284, USA

In this paper we present the approach to numerical simulation of the radiation effects in Silicon solar cells with on GEANT4 software [1]. In a past, we have developed a family of predictive model for radiation induced effects by high energy electrons in a silicon solar cell structure using a number of software tools (ITS software, SRIM [2,3], and CASINO [4]) [5,6]. Selective results from some of these models are used for comparison with the GEAMT4 simulation results.

Improvements to solar cell radiation hardness are critical for power generation applications in for long-term NASA space missions. When solar cells are used in outer space or in Lunar environment, they are subject to bombardment by high-energy particles, which induce a degradation referred to as radiation damage. Research, review, and analysis of solar-cell radiation-effects, models in literature have been conducted, and physics-based models have been selected and tested in our previous work.

GEANT4 is a software toolkit for the simulation of the passage of particles through matter. It is used by large number of experiments and projects in a variety of application domains, including high energy physics, astrophysics and space science, medical physics and radiation protection. Over the past several years, major changes have been made to the toolkit in order to accommodate the needs of these user communities, and to efficiently exploit the growth of computing power made available by advances in technology. Indeed, GEANT4 simulation has become mission-critical in fields such as high energy physics and space science. GEANT4 has both electron and proton radiation models, in distinction to the software mentioned above.

The overall objective of our research is to enable GEANT4 simulation capabilities available for accurate solar cell radiation effects to improve the solar cell efficiency and radiation hardness, by the proper choice of the solar cell material composition, and design to mitigate radiation effects and solar cell degradation. GEANT4 low energy "semiconductors" component has been tested for more accurate simulation of radiation effects in the low energy range from 0.1eV to 10MeV, compared to the standard GEANT4 distribution for high energy physics.

These results show that GEANT4 can be used for Simulation of silicon solar cell radiation effects. We have successfully conducted the accurate electron irradiation experiments with Geant4, that were not possible with IAS, SRIM, and CASINO software.

#### References

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### Finite Element Method Stabilization Supersonic Flows with Flux Correction Transport Method

#### A. Fedoseyev

#### Ultra Quantum Inc., Huntsville, AL, USA

In this paper we present the development of a stabilized finite element method (FEM) for numerical simulations of supersonic and hypersonic flows using the Flux Correction Transport (FCT). The instabilities observed in numerical solutions for supersonic flows reflect the fundamental problems of the finite element method, and cannot be avoided within the finite element approach implemented in the code. The papers published for scalar transport [1], and for compressible flow problem [2] provide a break-through for this problem, resulting in algorithms of increased stability and performance, by implementing this on the level of the matrix of the algebraic linear system, resulting from PDE discretization in the FEM.

The finite element method that we use, is a Galerkin method with local basis functions, and is at least a second-order approximation method. Due to this nature, the construction of a low-order approximation to introduce more viscosity and suppress instabilities (like in finite-difference method or in finite volume method) cannot be done easily in the frame of the finite element method. That is why Streamwise Upwind Petrov Galerkin (SUPG) and Generalized Petrov Galerkin (GPG) methods remained the only means to stabilize the numerical solution in the finite element method codes.

While SUPG and GPG have been efficient numerical models to stabilize the numerical solution in the finite element method codes for many flow problems, SUPG and GPG do not work well for supersonic and hypersonic flows.

Flux Limiters have shown their efficiency to deal with this problem in finitevolume methods, but these Flux Limiters cannot be carried to finite-element method explicitly (or at all). For 30 years since the introduction of FTC by Boris and Book [3], finite element developers have been unable to bring this important and efficient feature into finite element codes. Apparently this explains a very limited use of the finite element method for hypersonic flows (due to a poor numerical stability of the solution).

The idea behind the FCT method by Kuzmin is remarkably simple. First, the difference between conservative approximations of high- and low-order is decomposed into a sum of antidiffusive fluxes. Next, each flux is multiplied by a solution-dependent correction factor that was determined by a flux limiter. The limited flux is added to the low-order solution which is assumed to be nonoscillatory. The purpose of the flux limiter is to ensure that no new maxima or minima can form, and existing extrema cannot grow. That is, the limited antidiffusive correction must be a local extremum nonincreasing or, loosely speaking, local extremum diminishing (LED).

In this work we describe the implementation of the finite element method with the Flux Correction Transport (FCT), present the examples and comparisons for supersonic and hypersonic flows simulations. From the results it follows that one can perform finite element simulations with CFL=1 or more (up to 20) and get numerically stable long time solutions, with a 30X speed increase compared to maximum possible CFL=0.03 for methods without FCT.

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### Application of Markov Chains for Studying of Particulate Matter (PM10) Air Contamination for the City of Ruse, Bulgaria

#### I. Georgiev, I. Zheleva, M. Filipova

Angel Kanchev University of Ruse, Bulgaria

Dust is a major atmospheric air pollutant. Its harmful health effect depends mainly on the size and chemical composition of the suspended dust particles, on the other chemical compounds adsorbed on their surface, including mutagens, DNA modulators, etc., as well as on the area of the respiratory system in which they are deposited.

Air pollution by particulate matter (PM10 – particulate matter with a diameter between 2.5 and  $10\mu$ m) is going up recently in Ruse region, Bulgaria. The sources of dust on the territory of Ruse region, Bulgaria are industry, transport and domestic heating by solid fuel. PM10 levels for Ruse mark a significant increase during the autumn-winter period compared to the levels during the spring-summer period. The biggest peak of PM10 levels for the autumn-winter period is usually observed in January months. It is in January that the number of days in which there is exceedance of the limit values of the PM10 levels is maximum observed.

This paper attempts to apply Markov chain models to forecast the behavior of Particulate Matter (PM10) air contamination of the city of Ruse, Bulgaria.

A Markov chain is a stochastic model describing a sequence of possible events in which the probability of each event depends only on the state attained in the previous event. Research has reported the application and usefulness of Markov chains in a wide range of topics such as physics, chemistry, biology, medicine, music, game theory and sports.

This study aims to explore the Markov chains to study the behavior of PM10 air contamination in Ruse, Bulgaria. For this we use the official data for PM10 daily measurements from Bulgarian Ministry of environment and water for the period 2017-2019. Probability results from the Markov chain models are presented and commented in the paper.

**Keywords:** PM10 air contamination in Ruse, Bulgaria, Markov chain model, forecast.

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### Distortion Compensation of IN 625 Parts Manufactured by Selective Laser Melting

T. Frigioescu, G. Matache, T. Badea

National Research and Development Institute for GasTurbine - COMOTI, Bucharest, Romania

D. Ionita

SC Tecnital SRL, Romania

Metallic powder bed-based methods are the most studied additive manufacturing (AM) techniques. During the manufacturing process, the high-power laser melts the metallic powder according to a 3D CAD design, but due to the high thermal gradient induced between the melting and solidification process a material



Figure 1. Nozzle design: a) initial model; b) compensated model

thermal contraction is registered. Thereby, a deformation compensation should be applied for the additive manufactured metallic parts. Parts deformation compensation involves performing a thermostructural numerical simulation where the process parameters are used as boundary condition. Using the resulting geometry for the AM process it should provide a part with nominal designed values.

The study was focused on geometric compensation of metallic parts manufactured from IN 625 using LASERTEC 30SLM machine. The compensation simulation was performed on a nozzle and a mandrel part using ANSYS Additive Print software. Conventional and compensated designs were used for the manufacturing process. The resulted parts were 3D scanned and results were compared with the 3D CAD models as is presented in Figure 1 where the red color represents positive dimensional deviations, blue color represents the negative dimensional deviation while green color represents the areas with no deviation. It was determined that applying the distortion compensation increases significantly the part's precision.

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Keywords: Selective laser melting, distortion compensation, 3D scanning

J. Genoff

Technical University of Sofia, branch Plovdiv, 4000 Plovdiv, Bulgaria

The CESTAC method and its software implementation CADNA have shown to be effective tools in the analysis of floating-point numerical errors caused by inappropriate computational precision. This paper presents: First, a sophisticated investigation of some properties of the CESTAC method that originate from the stochastic arithmetic at its theoretical core and concern the stochastic reliability and reproducibility of the test runs and their results. Then, second, in pursuit of more reliability and reproducibility, a rather unusual idea is proposed and explored – to replace the stochastic arithmetic with a deterministic one, but every otherwise single numeric value should now be replaced by more than one value with different finite precisions. Such an approach leads to several consequences, but the most crucial of them is the necessity of simultaneous support of all representing values when arithmetic operations are performed. Here arises a really hard logical problem, which is successfully solved. A software implementation of the proposed method in CADNA-like style is also presented, along with much and various experimental data.

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### Comparison of Heuristic Algorithms in Solving a Specific Model of Transport Task Using Mixed Integer Linear Programing

I. R. Georgiev, D. Grozev, V. Pavlov, E. Veleva A. Kanchev University of Ruse, Bulgaria

This report looks at a specific model of transport task. An often-used option for determining the cost value is analyzed. The optimization model used is related to solving a large-scale NP problem. A comparison of different heuristic algorithms has been made to solve the specific task. An application was developed in Matlab to solve the task of the various algorithms under consideration.

Key words: Transport Task, mixed integer optimization, heuristic algorithms

#### **Riemann-Hilbert Problem, Integrability and Reductions**

V. S. Gerdjikov

Institute of Mathematics and Informatics, BAS, 1113 Sofia, Bulgaria & Dept of Applied Mathematics, National Research Nuclear University MEPHI, Moscow, Russia

R. Ivanov

School of Mathematical Sciences, Technological University Dublin - City Campus, Kevin St., Dublin, Ireland

#### A. Stefanov

#### Institute of Mathematics and Informatics, BAS, 1113 Sofia, Bulgaria

The present report is based on our paper [1] and paper is dedicated to integrable models with Mikhailov reduction groups  $G_R \simeq \mathbb{D}_h$  [2]. Their Lax representation allows us to prove, that their solution is equivalent to solving Riemann-Hilbert problems, whose contours depend on the realization of the  $G_R$ -action on the spectral parameter. New examples of Nonlinear Evolution Equations (NLEE) with  $\mathbb{D}_h$ symmetries are presented. In particular we derive a new integrable version of the Heisenberg ferromagnet equations with Hamiltonian:

$$H = \frac{1}{2} \int \left( \frac{1}{4} \underline{S}_x^2 - 4a \sum_{ij} \underline{S}_i \underline{S}_j \right) dx$$

where a is a constant and  $A_{ij}$  is a symmetric matrix.

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### On Asymptotic Regimes of Manakov Solitons in Adiabatic Approximation

V. S. Gerdjikov

Institute of Mathematics and Informatics, BAS, 1113 Sofia, Bulgaria & Dept of Applied Mathematics, National Research Nuclear University MEPHI, Moscow, Russia

M. D. Todorov

Dept of Mathematics and Statistics, San Diego State University, CA, USA & Dept of Applied Mathematics and Computer Science, Technical University of Sofia, Bulgaria

In [1,2,3,4] we analyze the dynamical behavior of the N-soliton train in the adiabatic approximation of the perturbed Manakov model:

$$i\frac{\partial \vec{u}}{\partial t} + \frac{1}{2}\frac{\partial^2 \vec{u}}{\partial x^2} + (|u_1|^2 + |u_2|^2)\vec{u} = i\vec{R}[\vec{u}],\tag{2}$$

where  $i\vec{R}[\vec{u}]$  are various perturbative terms. They describe gain/loss effects

$$iR[u] = i\left(\gamma u + \beta(\vec{u}^{\dagger}, \vec{u})u + \eta(\vec{u}^{\dagger}, \vec{u})^{2}\vec{u}\right) + V(x)\vec{u}.$$

as well as effects of several types of external potentials, e.g.,  $V(x) = A\cos(\Omega x + \Omega_0)$ .

We show that the evolution of the N-soliton train is described by a perturbed complex Toda chain (PCTC). The soliton trajectories given by PCTC fit excellently to the trajectories, obtained by solving numerically the perturbed Manakov model (2) for a wide class of initial soliton parameters. The method can also be extended to other physically important equations such as Sassa-Satsuma equation.

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### The A-Body Exactly Solvable Pairing Interaction from an Engineering Point of View

V. Gueorguiev

Institute for Advanced Physical Studies, Montevideo Str., Sofia 1618, Bulgaria & Ronin Institute for Independent Scholarship, Montclair, NJ, USA

The oblique basis method is reviewed from engineering point of view related to vibration and control theory. Examples are used to demonstrate and relate the oblique basis in nuclear physics to the equivalent mathematical problems in vibration theory. The mathematical techniques, such as principal coordinates and root locus, used by vibration and control theory engineers are shown to be relevant to the Richardson-Gaudin pairing-like problems as well as the A-body exactly solvable pairing in nuclear physics.

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### Numerical Method for Solving the Problem of Pricing an American Put-Option

V.V. Shaydurov, <u>L.V. Gileva</u>, A.A. Efremov Institute of Computational Modeling of SB RAS, Krasnoyarsk, Russia

In the field of stochastic financial mathematics, the problem arises of modeling the pricing of urgent options. Since it is not possible to obtain an exact solution for such models, numerical methods are used. Along with traditional finite-difference methods, a class of hybrid approximations has been developed where the Lagrange approach is used to approximate the motion operator whilst the finite-difference method in Euler variables is used for the elliptic operator. In the present talk, a numerical method is described that is based on a combination of Lagrangian approximation with the finite element method, which is applied to solving the problem of pricing an American sales option (put-option).

The function to be determined depends on two variables and its domain is subdivided into two parts by an a priori unknown internal boundary. In one subdomain the function is a solution of the initial boundary value problem for a parabolic equation; and in the other one it is a linear function of the space variable. The position of the internal boundary at an arbitrary instant of time is defined by the condition providing continuity of the solution derivative with respect to the space variable.

We carefully studied the smoothness of the solution of this problem and found out the degree of unlimited growth of the second order derivatives of the solution in a neighborhood of the point at which the solution has singularity. This information was used to refine the grid in each variable in order to achieve the usual order of convergence, in contrast to uniform grids when the order of convergence is significantly reduced.

Acknowledgements. This work is supported by the Russian Science Foundation with Project 20-61-46017.

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### Two-Step Time Series Analysis for Air Pollution in Relation to Weather Conditions: Case Study of Nessebar, Bulgaria

### S. Gocheva-Ilieva, D. Voynikova, <u>A. Ivanov</u>, M. Stoimenova Paisii Hilendarski University of Plovdiv, Bulgaria

Air pollution is a major problem in many urban areas in Bulgaria, harmful to the human health. In this study, based on a large number of observations for particulate matter 10 micrometers or less in diameter (PM10) and concomitant meteorological conditions, the task of mathematical modeling of the time series and predicting the level of future concentrations is set. As a case study, data about the town of Nessebar, a typical seaside city, were used. The collected data are daily averaged for the period February 2015 – March 2018. Using the autoregression moving average (ARIMA) method, models of the considered time series are built. To obtain more realistic forecasts, the methodology is implemented in two steps. The first step is to build univariate ARIMA models for any of the meteorological variables and to predict their future values. In the second step, the calculated forecasted values are applied to construct ARIMA PM10 models and to estimate the forecasts of this pollutant for a short time of 3 days ahead. The obtained models agree well to the known observed values. The proposed approach can be applied to other type of pollutants. It does not depend on additional forecasts from other sources and allows the development of a software application to predict future levels of pollution depending on the meteorological hazards.

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### Nonstandard Finite Difference Method with Higher Order Accuracy

F. Alalhareth, <u>M. Gupta</u>, H.V. Kojouharov, S. Roy, J.M. Slezak University of Texas at Arlington, TX, USA

We are proposing a new class of nonstandard finite difference methods (NSFD). NSFD methods provide an efficient way to solve many problems numerically appearing in engineering and science and also known to provide several advantages over classical techniques. Our proposed methods are shown to be elementary stable and higher order accurate. Finally, we validate our methods using numerical simulations.

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### Scalability Study of Different MPI Algorithms for a Predator-Prey Model with SEIR Epidemic Disease

S.-M. Gurova, E. Atanassov, T. Gurov, and A. Karaivanova

Institute of Information and Communication Technologies, BAS, Acad. G. Bonchev str. 25 A, Sofia, Bulgaria

In this work, the authors investigate the scalability of different MPI approaches for solving a nonlinear system of ODEs by Euler's method. The system describes SEIR (Susceptible-Exposed-Infectious-Recovered) epidemic disease in the prey where the predator-prey interaction is given by Lotka - Volterra type. The different coefficients of the system are grouped in four groups: (i) migration coefficients; (ii) natural mortality coefficients; (iii) mortality by disease and predation and (iv) specific coefficients describing infection rate, incubation rate, recovery rate and etc. As a preproduction process all coefficients grouping in the above 4 groups are discretized with a fix step in a given interval. Thus, a huge number of equilibrium points is received. The parallel algorithms allow us to receive a large number of solutions of the system of ODEs. Using these solutions we can select those equilibrium points in which the dynamics of population is stable and the disease is controlled. A lot of parallel tests were done on three HPC systems: ARGO (DIT-UA), ARIS (GRNET), and Avitohol (IICT). The numerical results show that the scalability depends on the architecture of the HPC system and type of the parallel algorithm.

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### On Dynamics of Vortex Pair in Stratified Fluid

#### V. Gushchin and I. Smirnova

#### Institute for Computer Aided Design of RAS, Moscow, Russia

The problem of the dynamics of the vortex pair in stratified liquid is considered. The pair is two vortexes arranged symmetrically relative to the vertical axis, but with the opposite direction of rotation, so that it begins to rise upwards. This task was previously considered for the case of a homogeneous liquid, where the movement of the pair and its interaction with the free surface was studied.

Stratification is a picnocline model. A homogeneous layer is near the surface, under it a sharp gradient and further in the depth the stratification is linear. Salinity is chosen as a stratifying component, just as it can be implemented in the laboratory. The task is described by the Navier-Stokes equations in the Boussinesq approximation. To solve the problem, the SMIF method is used, of course, the finite different scheme of which has such properties as the second order of approximation on spatial variables, minimal scheme dissipation and dispersion, performance in wide range of Reynolds and Froude numbers and, most importantly, when solving wave processes are a property of monotony.

The dynamics of such a pair are studied depending on its geometric sizes, the intensity of the vortexes and the depth of their initial immersion.

### Efficient URA-Based Numerical Solvers for $(A^{\alpha} + qI)u = f$ , $\alpha \in (0, 1), q \ge 0$

#### S. Harizanov

#### Institute of Information and Communication Technologies & Institute of Mathematics and Informatics, BAS, Sofia, Bulgaria

This talk is devoted to finding a numerically efficient procedure for solving large-scale fractional algebraic equations of the type  $(A^{\alpha} + qI) u = f$ , where  $A \in \mathbb{R}^{n \times n}$  is a sparse symmetric positive-definite matrix, I is the identity matrix,  $\alpha \in (0, 1)$ , and  $q \geq 0$ . Such problems appear for example in fully discrete approximations of static or time-dependent sub-diffusion-reaction problems.

The matrix  $A^{\alpha}$  is dense, therefore its derivation and direct usage are extremely impractical in terms of both memory storage and computational cost. Instead, we use (k, k)-univariate uniform rational approximations (URA) elements  $r(\xi; \alpha)$ of the function  $\frac{1}{\xi^{\alpha}+q}$ ,  $\xi \in [1, +\infty)$ , and compute an approximate solution  $\tilde{u} = r(A; \alpha)f$  in a very cheap way via solving k non-fractional linear systems of the type  $(A - d_i I) u = f$ ,  $d_i < 0$ , where  $\{d_i\}_1^k$  are the poles of  $r(\xi; \alpha)$ . Thus, the computational complexity of the proposed technique is only a scalar multiple of the computational complexity of the corresponding solver for the non-fractional sparse algebraic equation (A + qI) u = f.

In theory, the optimal choice for  $r(\xi; \alpha)$  is the element of best approximation (BURA), which leads to the smallest error  $||u - \tilde{u}||_{\ell^2}$ , depending only on the univariate uniform approximation error  $||r(\xi; \alpha) - \frac{1}{\xi^{\alpha} + q}||_{C[1,\infty)}$  and not on the condition number  $\kappa(A)$ . However, the derivation of the BURA element for large q and small  $\alpha$  is a severely numerically instable and computationally expensive process, even though it is a pre-processing step and needs to be done only once in life time. In this talk, we propose various alternatives of the BURA approach, which rely on a priori information on the spectral radius of the matrix A and we provide numerical examples, that those alternatives behave better in practice.

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### Which Bug Bugs You More? Microbiome Competition and Toxin Interference

M. Hohn, A. Radunskaya

Dept of Mathematics, Pomona College in Claremont, CA, USA

H. Kojouharov

Dept of Mathematics, University of Texas, Arlington, TX, USA

M. D. Todorov

Dept of Mathematics and Statistics, San Diego State University, CA, USA & Faculty of Applied Mathematics and Computer Science, Technical University of Sofia, Bulgaria

The last decade has seen a surge of interest in understanding the functional relationships between the elements that make up the diverse ecology of the gut microbiome. This ecological web includes bacteria, viruses and microbes that enter and leave living bodies. They affect metabolism and stimulate the immune system, affecting directly or indirectly most physiological functions. Mathematical modeling has recently begun to play a role in our understanding of the functioning of the microbiome, and how the microbiome is affected by the outside world. Various types of animal models give insight into the gut microbiome. For example, consider the importance of the insect gut microbiota as an invisible third faction in the chemical arms race that has given rise to a large portion of Earth's terrestrial diversity. In this talk, we present a mathematical model that describes the spatial dynamics of several competing bacteria populations along with a toxin that inhibits the growth of one of bacteria populations. The model consists of a system of four non-linear partial differential equations describing the interactions of the bacteria as they flow through the digestive tract. The model simulations and analysis give insight into possible mechanisms to explore in future laboratory experiments.

### Preliminary Analysis of Construction and Demolition Waste Management in Bulgaria

#### M. Filipova, I. Zheleva, D. Hvarchilkova

#### Angel Kanchev University of Ruse, Bulgaria

Construction and demolition waste (C&DW) (CDW) consists of unwanted material produced directly or incidentally by the construction or industries. This includes building materials such as insulation, nails, electrical wiring, shingle, and roofing as well as waste originating from site preparation such as dredging materials, tree stumps, and rubble. CDW is generated by activities such as construction and/or partial or complete demolition of buildings and urban infrastructure. Within the EU, different definitions apply to this group of waste making it difficult to carry out comparative analyses between countries. In some countries even ground leveling materials are classified as construction waste.

In C&DW may present some hazardous components such as asbestos, tar, radioactive components, polychlorinated biphenyls, lead, electrical elements containing mercury, insulating materials containing dangerous substances, *etc.* Removing hazardous components of any waste is important in order not to pollute recyclable materials.

The biggest part of the C&DW waste consist of bricks, concrete, gypsum, wood, glass, metals, plastics, solvents, asbestos and excavated earth. It is one of the heaviest and bulkiest wastes which are generated in each country in the European Union. Many of these components can be recycled. To date, about 54% of construction waste is recycled in the Republic of Bulgaria, but the national targets imposed by the Waste Framework Directive require 70% of CDW to be materially utilized by 2020. For some species, such as metals, the share also has to reach 90%. Each construction of a building over  $700m^2$  in Bulgaria must have a construction waste management plan (CDWMP) developed.

There is a possibility to recycle many elements of construction waste. Different types of construction and demolition waste are subject to specific recycling and recovery methods. Methods for recycling and subsequent recovery of construction waste vary according to the type of waste. For the most part of C&DW (about 80% by mass), they are inorganic and non-toxic and subject to re-use or recycling. The degree of recyclability of the construction waste depends on several factors – the share of the different types of waste, the degree of pre-treatment (sorting), the pollutant with harmful or hazardous substances, which depends on the processes of waste generation. Building design and practice also have an impact. Waste related to the renovation and rehabilitation of buildings has a less favorable profile, as they are most often mixed, generated over an extended period, in relatively small quantities and by different owners, posing challenges for their recycling.

In this paper a preliminary analysis of CDW management in Bulgaria is presented, using official data from Bulgarian National Statistical Institute.

In Bulgaria for the period 2013-2017, there is an almost threefold decrease in the amount of non-hazardous construction waste generated. During the same period, hazardous construction waste also decreased by over 50%. In 2016, 54% recycling of construction and demolition waste (CDW) was achieved with the aim of achieving a minimum of 70% by 2020 according to the Waste Management Framework Directive (Directive 2008/98 / EC). On this basis, amendments to the Waste Management Act (WMA) were introduced and the Ordinance on construction waste management and input of recycled construction materials (NUSOVRM) was prepared. New standards for the quality of construction materials used have been modified and introduced. In order to reduce landfill recycling, financial incentives are provided by municipalities. Some of the public-funded construction sites require a mandatory percentage of recycled waste, depending on the type of site. Specific targets (for construction waste codes) introduced for recovery for each construction - for example 85% for concrete and reinforced concrete waste, 90% for metals.

**Keywords.** Construction and demolition waste (CDW), preliminary analysis, CDW management in Bulgaria.

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### The Power Estimation of Some Parametric Criteria of Time Series Trends

V. Myrhorod, <u>I. Hvozdeva</u>, Ye. Derenh

Odessa Maritime Academy National University, Ukraine

Trend criteria are widely used in diagnostic systems of technical objects conditions. The intensity of the false alarm flow (errors of the first kind) is the main characteristic of such criteria. On the other hand, trend criteria, like other statistical criteria for hypotheses distinguishing, should also be evaluated by their power. Such evaluation requires the trend statistics analysis at alternative hypothesis accepting, that is a trend presence in the sample. As a rule, in this case the trend statistics are non-stationary, which makes it difficult to obtain their characteristics. However, for a number of important practical cases, such analysis can be performed with some assumptions made. The adoption of generating data statistical model in the form of the sum of a linear trend and a stationary random component is the first of these assumptions. The possibility of samples obtaining of decisive statistics on some final analysis window is the second assumption. When practical problems solving the requirements for high performance are set for the trend criteria, therefore, the trend should be detected at the initial stage of its development, where it is still described by a linear function. The power of the trend criteria was estimated by the method of analytical estimates and statistical modeling. The criteria of cumulative sums, Fisher, student's differences of means, Hald-Abbe and the correlation criterion were selected for the analysis. Empirical dependencies of these criteria powers on the development rate of a linear trend are constructed. The proposed approach allows selection of the applied trend criteria by their power for the considered statistical model of data generating. As a result, it becomes possible to make a reasonable choice of such criteria and increase the reliability of diagnostic conclusions about the technical conditions of objects.

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### Gaining Control over Cytokine Storm in COVID-19: In silico Perspective

N. Ilieva, E. Lilkova

Institute of Information and Communication Technologies & Institute of Mathematics and Informatics, BAS, Sofia, Bulgaria

P. Petkov, L. Litov

Faculty of Physics, St. Kliment Ohridski University of Sofia, Bulgaria

N. Todorova

Institute of Biodiversity and Ecosystem Research, BAS, Sofia, Bulgaria

M. Rangelov

Institute of Organic Chemistry with Centre of Phytochemistry, BAS, Sofia, Bulgaria

SARS-CoV-2 is an enveloped positive-sense, single-stranded RNA virus that causes severe respiratory syndrome in humans. The current COVID-19 pandemic accounts so far for over 8 million infected people and close to half a million deaths worldwide. To devise therapeutic strategies to counteract SARS-CoV-2 infection it is crucial to develop a comprehensive understanding of how the virus hijacks the host and inactivates its immune response during the course of the infection. This knowledge is indispensable for developing new drugs, alongside with repurposing existing ones.

In the acute phase of Covid-19 the impact of the virus on the immune system escalates into a state of overreaction, the so-called cytokine storm, which according to clinical data is the main contributor towards a fatal outcome of the disease. It is triggered by an overproduction of proinflammatory cytokines, particularly IL-6 and IFN $\gamma$ .

Aiming at finding means to prevent the development of a cytokine storm, we conduct *in silico* investigations of the inhibitory action on IL-6 and IFN $\gamma$  activity of LMWH oligosaccharides, thus revealing their potential as anti- in amatory drugs.

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### Hybrid Boosted Trees and Regularized Regression for Studying Ground Ozone and PM10 Concentrations

A. Ivanov, M. Stoimenova-Minova, S. Gocheva-Ilieva

Paisii Hilendarski University of Plovdiv, Bulgaria

The problem of atmospheric air pollution is of great concern to human health, the clean environment and the climate, and is an actual topic in environmental research. The major pollutants of air are PM10, PM2.5, SO2, ozone (O3) and more. For each geographical region, there are specific sources of pollution, as well as conditions for the containment of harmful emissions into the air for longer periods of time. Bulgaria is a member state of the European Union in which low air quality is permanently reported, against the statutory limits in European legislation. Significant exceedances of regulatory limits have been measured for many of the major air pollutants. This paper focuses on the application and comparison of two machine learning methods – Boosted trees and regularized regression to investigate the influence of meteorological, atmospheric and other factors on air quality based on empirical data. Hybrid type models have also been built and tested. A new approach is applied to investigate the effect of sample size on model quality and to evaluate the optimal sample size. The modeling process uses daily average ozone and PM10 emissions data in the city of Rousse, Bulgaria, measured at licensed automated stations, under the control of the European Environment Agency in Bulgaria. As a result, validated models with high statistical goodness-of-fit indicators such as coefficient of determination, root mean square error, etc., and for embedded models – Akaike information criterion (AIC) were obtained. The best selected models show very good agreement with the measured data in the order of 90%. Short-term forecasts for future pollution have been
made. There is a slight preference for boosted trees models over those generated by regularized regression.

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# Coriolis Effect for Internal Ocean Waves – Hamiltonian Approach

R.I. Ivanov

School of Mathematical Sciences, Technological University Dublin, Ireland

A derivation of the Ostrovsky equation for internal waves with methods of the Hamiltonian water wave dynamics is presented. The internal wave formed at a pycnocline or thermocline in the ocean is influenced by the Coriolis force of the Earth's rotation. The Ostrovsky equation arises in the long waves and small amplitude approximation and for certain geophysical scales of the physical variables.

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## Distribution Sensitive Estimators of the Index of Regular Variation Based on Ratios of Order Statistics

<u>P. Jordanova</u>

Faculty of Mathematics and Informatics, K. Preslavski University of Shumen, Bulgaria

M. Stehlik

Department of Statistics and Actuarial Science, The University of Iowa, Iowa City, IO, USA & Institute of Statistics, Universidad de Valparaíso, Valparaíso, Chile & Department of Applied Statistics, Johannes Kepler University, Linz, Austria

The ratios of central order statistics seems to be very useful for estimating the tail of the distributions and therefore, quantiles outside the range of the data. In 1995 Isabel Fraga Alves investigated the rate of convergence of three semiparametric estimators of the parameter of the tail index in case when the cumulative distribution function of the observed random variable belongs to the max-domain of attraction of a fixed Generalized Extreme Value Distribution. They are based on ratios of specific linear transformations of two extreme order statistics. In 2019 we considered Pareto case and found very simple and unbiased estimator of the index of regular variation. Then, using the central order statistics we showed that this estimator has many good properties. Moreover, we observed that it is asymptotically equivalent to one of Alves's estimators and proved unbiasedness, asymptotic consistency, asymptotic normality and asymptotic efficiency. Here we use central order statistics and a parametric approach and obtain distribution sensitive estimators of the index of regular variation in some particular cases. Then, we show that they are unbiased, or asymptotic consistent and asymptotically normal. The paper finished with a brief simulation study.

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# Determination of the Heat Dissipation Power of Components in the Electronic Unit Using the Readings of the Built-in Temperature Sensors

#### E. Karepova, Yu. Shan'ko, V. Derevyanko, D. Nesterov

### Institute of Computational Modeling of SB RAS, 660036 Krasnoyarsk, Russia

We propose an approach for constructing a data-based thermal model for an electronic unit (EU). The model describes the relationship between the heat dissipation of electronic components and temperatures of several points in the EU. The model allows calculating the heat dissipation powers of the electronic components using the real-time readings of the build-in temperature sensors in the EU.

Assumed that the EU can operate in several modes. Each mode corresponds to a set of active electronic components dissipating certain heat which lead to some temperature distribution over the EU. It is also assumed that there is a system of temperature sensors on the EU, which readings are available for processing in the real-time.

A series of trial data is used to construct the model. The trial data are obtained from temperature sensors under conditions when each electronic component is heated separately. After construction, the model is used to determine in the realtime heat dissipation powers of components in the EU. We can determine the operation mode of the EU using our classifier which was obtained earlier. In addition, some failures of the operation modes can be detected.

The proposed approach was tested experimentally on the EU heat simulator. The EU is a rectangular aluminum frame, on which printed circuit boards with high-power transistors is installed to simulate the operation of real electronic components. Heat from the transistors is removed from the EU through the flat bottom surface of the frame. The test bench is used to investigate thermal operating modes of the EU both in the atmosphere and in a vacuum. The test bench is a vacuum chamber with a heat removing base that maintains the temperature, and with a temperature sensing system at control points of the EUs and environment.

In the work, the data-based thermal model of the EU simulator is built. The experiments showed that the model gives a good estimate of the dissipated heat power of the electronic components.

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## Anomalous Effective Diffusivity of Hydrogen in bcc-Fe from RPMD Simulations

I. Katzarov

Institute of Metal Science, Equipment and Technologies with Hydro- and Aerodynamics Centre, "Acad. A. Balevski", BAS, Sofia, Bulgaria & King's College London, UK

N. Ilieva

Institute of Information and Communication Technologies, and Institute of Mathematics and Informatics, BAS, Sofia, Bulgaria

L. Drenchev

Institute of Metal Science, Equipment and Technologies with Hydro- and Aerodynamics Centre, "Acad. A. Balevski", BAS, Sofia, Bulgaria

According to the current understanding, the devastating effects of dissolved hydrogen (at the level of some atomic parts per million, appm) on the toughness of high strength steel are due to either the loss of cohesive strength (the HEDE hypothesis) or the enhanced localised plasticity (the HELP hypothesis). Atomistic modeling of a hydrogen interstitial in  $\alpha$ -iron is a challenging task because of the time scale required to measure the dislocation motion and H diffusivity but most importantly, because of the necessity to account for nuclear quantum effects (NQEs) that are neglected in the classical molecular modeling approaches.

The state-of-the-art method to include NQEs in the calculation of properties of condensed phase systems is the *path integral molecular dynamics* (PIMD), which is a classical molecular dynamics in an extended phase space. The computational cost – about an order of magnitude longer computing time – is worth for obtaining quantum phase space averages, making thus feasible PIMD simulations with thousands of atoms and the use of *ab initio* electronic structure calculations to propagate the dynamics for small systems.

Within the framework of *ring-polymer molecular dynamics* (RPMD) simulation technique we show that quantum effects in influence noticeably the dislocation mobility even at room temperature, in particular we observe increase of hydrogen drag at extremely high H concentrations and increase of the rate of dislocation detachment from the H atmosphere at lower concentration.

Acknowledgements. This research was supported in part by the Bulgarian Science Fund under Grant KP-06-N27/19/17.12.2018, the Bulgarian Ministry of Education and Science (contract D01205/23.11.2018) under the National Research Program "Information and Communication Technologies for a Single Digital Market in Science, Education and Security (ICTinSES)," approved by DCM \$577/17.08.2018, and the European Regional Development Fund, within the Operational Programme "Science and Education for Smart Growth 20142020" under the Project CoE "National Center of Mechatronics and Clean Technologies" BG05M20P001-1.001-0008-C01.

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# Nonhomogeneous Boundary Value Problem for a Clamped Rectangle: Exact Solution

#### A. P. Kerzhaev

### Institute of Earthquake Prediction Theory and Mathematical Geophysics, RAS, Moscow, Russia

This paper presents an exact solution to the nonhomogeneous boundary value problem of the theory of elasticity for a clamped rectangle. First, a solution to the nonhomogeneous problem for an infinite strip with clamped sides is constructed. Then, a solution for the rectangle is added to this solution, with the help of which the boundary conditions at the ends are satisfied. To solve the nonhomogeneous problem in the clamped strip, Papkovich's generalized orthogonality relation is used. The solution in the rectangle is represented in the form of series in Papkovich-Fadle eigenfunctions, the coefficients of which are determined by simple formulas. The final formulas are simple and can easily be used in engineering.

## Invariant Transformations Preserving Geodesic Quasi-Einstein Spaces

V. Kiosak

Odessa State Academy of Civil Engineering and Architecture, Ukraine

A. Savchenko

Kherson State Agrarian University, Ukraine

S. Khniunin

Odessa Maritime Academy National University, Ukraine

Authors investigate transformations of quasi-Einstein spaces when these spaces continue to admit non-trivial geodesic mappings despite being transformed. The first pair is represented by quasi-Einstein space and relevant space corresponding to the first by non-trivial geodesic mapping. The latter pair is formed by transformation of the former. The tensor characteristic of the resulting spaces is found. The results facilitate the modeling of quasi-Einstein spaces when treating a trajectory of testing particles.

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## Influence of Permeable Boundaries on the Linear Stability of a Convective Flow Caused by a Nonlinear Heat Source

M. Zigunovs, A. Kolyshkin, and I. Iltins

Dept of Engineering Mathematics, Riga Technical University, Latvia

Stability of a convective flow in a tall annulus caused by nonlinear heat sources is considered in the paper. The walls of the annulus are permeable. The base flow is a superposition of a steady flow in a vertical direction due to nonlinear heat sources and a steady flow in the radial direction through the walls of the annulus. Linear stability problem is solved numerically by a collocation method. Numerical results show that radial inward or outward flow has a stabilizing influence on the convective flow in the vertical direction while the increase of the Frank-Kamenetsky parameter destabilizes the flow.

## Cryptographic Analysis of Digital Image Encryption Algorithm

#### K. Kordov

## Dept of Computer Informatics, Konstantin Preslavsky University of Shumen, Bulgaria

In this paper, Stefanski chaotic map is used for constructing a Pseudo-random generator. The proposed scheme is implemented for digital image encryption algorithm. The proposed algorithm is designed for securing gray-scale and color images. For proving the security of encryption, extensive cryptographic analysis is performed and the results are presented in this paper. The empirical cryptographic tests include Random tests, Key-space Analysis, Key sensitivity Analysis, Visual Analysis, Histogram Analysis, Entropy Analysis and Correlation Analysis.

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## Text Encryption Algorithm for Secure Communication

## K. Kordov

### Dept of Computer Informatics, Konstantin Preslavsky University of Shumen, Bulgaria

In this paper, a new encryption algorithm is presented, designed for secure text message communication. The proposed cryptographic system is based of pseudorandom generator, constructed with two chaotic maps. For security level determination, extensive cryptographic analysis is performed. The evaluation of the presented cryptographic scheme includes the results of statistical testing, key-space analysis, frequency analysis, common correlation analysis, entropy analysis, key sensitivity analysis and speed performance. The results are presented and explained in this paper.

# The Finite-Difference Solving the Planning Problem of Oncoming to a Given State

V. S. Kornienko, V. V. Shaydurov

Department of Computational Mathematics, Institute of Computational Modeling of Federal Research Center KSC SB RAS, Krasnoyarsk, Russia

Mean field games theory provides an adaptation of statistical physics "mean field" theory to cases in which the physical particles are replaced by agents who mutually interact in various strategic situations. It leads to optimization problem formulated as coupled pair of parabolic partial differential equations of the Kolmogorov (Fokker-Planck) and Hamilton-Jacobi-Bellman types. A wide range of problems, which are able to formulate in Mean Field terms, leads to growing interest in searching of efficient numerical methods for these problems. Here a finite-difference analogue of the differential problem formulated in terms of this theory for solving the task of oncoming to a given state is presented. The development of mean field games in the form of transport problems can have a large impact on the further development of forecasting problems and minimizing estimated costs. The use of monotonous numerical schemes based on Semi-Lagrangian approximation allows getting close rapidly to the solution of a discrete problem that has all the properties of a continuous one. In contrast with other studies in this field, rough approximations to a given target with the help of penalty functions are not used here. Instead, we only specify the direction and step in which minimization should be performed, that give more natural conditions to minimize total consumption.

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## Spatial Orientation of Nanoparticle Pairs under Uniform Laser Field

#### V. Kornienko

## Siberian Federal University, & Department of Computational Mathematics, Institute of Computational Modeling of Federal Research Center KSC SB RAS, Krasnoyarsk, Russia

#### A. Tsipotan, V. Slabko

#### Siberian Federal University, Krasnoyarsk, Russia

It is known, that under external fields system tend to occupy a position corresponding to the minimum potential energy of their interaction with the field. External electromagnetic field induces polarization on each particle, and the interaction of these polarization tend to line up particles along the direction of the external field, which is counteracted by thermal motion. As a result of these two processes, a certain equilibrium distribution of the spatial orientations of the nanoparticles is established. It has a statistical nature and depends on the mechanism of interaction of nanoparticles with an external field. The orientation of the particles in an alternating field is associated with certain relaxation times, which depend on the viscosity and temperature of the medium and on the geometric structure of the samples. Earlier in [1], the fundamental possibility of the formation of multiparticle nanostructures step-by-step from a preliminary preformed pair of particles was presented. It was shown that such a formation with high probability can be performed during a single laser pulse (10 ns). However, in order to estimate the total assembly time of the structure, it is also necessary to take into account the relaxation time for the preformed pair of particles and the orientation distribution for such pairs.

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## Random Forest Models of 305-Day Milk Yield for Holstein Cows in Bulgaria

#### A. Yordanova, H. Kulina

### P. Hilendarski University of Plovdiv, Bulgaria

In the field of stock breeding the research of the factors which influence the highest levels of the productivity (for example milk yield) is of significant importance both for the selection of animals and for determining the conditions of their raising. This article researches the influence of 11 exterior traits of the Holstein Friesian breed of cows on the average milk yield for 305 days. The purpose of this work is to demonstrate the possibilities of the method Random Forest method for building models with high enough statistical traits to determine the main exterior traits of the animals influencing the milk yield. From a sample of 97 cattle observations from 4 farms in Bulgaria two models were built to study the dependence of 305 dairy milk yield of the Holstein Friesian cow breed in terms of 12 independent variables -11 exterior traits and the farm where the animals are raised. The first model is based on 11 independent variables for exterior traits, and the second is based on the same 11 independent variables as the farm has been added. Both models describe about 95% of the data and identify and agree on the main exterior traits that affect the milk yield – udder width, chest width, tarsal (hock) joint development and gait. The models are compared with the published CART models of the same data set.

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## Transonic Flow Oscillations and Bifurcation over a Flat-Sided Wedge with a Blunt Trailing Edge

#### A. Kuzmin

#### Dept of Fluid Dynamics, St. Petersburg State University, Russia

An advanced design of turbine blades involves an injection of coolant flow through a slot in the blunt trailing edge to ensure a thermal protection of the blade and downstream turbine stages. The thermal protection and flow behavior in the wake were studied numerically and experimentally in a number of papers. In particular, the *AIAA* 2019-0881 paper by A. Martinez-Cava *et al* addressed subsonic, transonic and supersonic flows over a symmetric flat-sided profile, focusing on the nature and development of oscillations in the wake. The obtained timeaveraged flow fields were symmetric about the longitudinal axis (the x-axis). Meanwhile, airfoils with flat or nearly flat sides are known to admit non-symmetric regimes at zero angle of attack in a band of transonic free-stream Mach numbers. The asymmetry is caused by instability of the shock wave interaction with a flow acceleration region located downstream. In the present paper we study numerically the 2D turbulent transonic flow over a flat-sided symmetric wedge similar to the profile examined in AIAA 2019-0881. Solutions of the Reynolds-averaged Navier-Stokes equations are obtained with a finite-volume solver of second-order accuracy on fine computational meshes. The solutions demonstrate essential oscillations of the turbulent transonic flow in the wake and aft region. In addition to the oscillations, computations reveal flow bifurcation and transitions to asymmetric regimes with either positive or negative lift in a band of the inflow Mach number at zero angle of attack. A jet injection in the wake does not eliminate the flow bifurcation, though attenuates the high-frequency oscillations.

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## On Some Classes of Growth Functions and Their Links to Reaction Network Theory

#### M. Lazarova

Faculty of Applied Mathematics and Informatics, Technical University of Sofia, Bulgaria

#### S. Markov

Institute of Mathematics and Informatics, BAS, Sofia, Bulgaria

#### A. Vassilev

### Faculty of Mathematics and Informatics, Sofia University St. Kliment Ohridski University of Sofia, Bulgaria

In this work we study some characteristics of sigmoidal growth functions that are solutions to dynamical systems induced by reaction networks. In addition, the studied dynamical systems are close to the Gompertzian and logistic type growth models [1,2]. Apart from the growing species, the considered reaction networks involve an additional decaying species interpreted as environmental food resource [3]. Using reaction network theory approach [4], we formulate several generalizations of the classic logistic model, borrowing ideas from the Gompertz model as well. We are studying monotonicity order-preservation properties of the model solutions using graphical visualizations.

**Keywords.** Dynamic growth model, dynamical system, reaction networks, logistic model, Gompertz model, sigmoidal growth functions.

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## Self-Association of Antimicrobial Peptides in Solution: Formation Patterns

T. Lazarova, P. Petkov, L. Litov

Faculty of Physics, St. Kliment Ohridski University of Sofia, Bulgaria

E. Lilkova

Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria

N. Ilieva

Institute of Information and Communication Technologies & Institute of Mathematics and Informatics, BAS, Sofia, Bulgaria

Antimicrobial peptides (AMPs) are small proteins with a molecular weight below 10kDa, 6–100 residues long, mainly cationic and with an amphiphilicnature. They are a key element in the primary host defense against microbial invasions in all eukaryotes. AMPs present a remarkable structural diversity, being grouped in four major classes:  $\alpha$ -helical,  $\beta$ -stranded, mixed and extended. The special class of cyclotides (the cyclic AMPs) is beyond the scope of the present study. AMPs exhibit rapid and efficient antimicrobial toxicity against a range of pathogens – Gram-positive and Gram-negative bacteria, fungi, parasites, and some viruses. Despite the millions of years of co-evolution, bacteria have failed so far to develop even limited resistance against their action. All this makes AMPs a promising therapeutic alternative to the conventional antibiotics in the face of dramatically increasing bacterial (multi-drug) resistance. The antimicrobial action of AMPs is not completely understood, neither is their behavior in bodily liquids prior to attacking the target membrane scrutinised. Thus, it is not known when they adopt their biologically active secondary structure and if certain collective phenomena take place. By means of molecular-dynamics simulations we demonstrate on several examples (bombinin H2, indolicidin, but also newly isolated peptides from the mucus of the garden snail *Cornum Aspersa*) that particularly extended AMPstend to self-associate in clusters and this process also drives their convergence into the biological fold.

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## **Conformal-Flat Kahlerian Spaces**

O. Lesechko

Odessa State Academy of Civil Engineering and Architecture, Ukraine

O. Latysh

Odessa National University Maritime Academy, Ukraine

#### T. Spichak

Kherson State Maritime Academy, Ukraine

A research on Kahlerian spaces had started long time prior to the work of Kahler which gave them their name. T.A. Shirokov was the first to study them. He treated conformally flat Riemannian spaces which contain covariantly constant obliquely symmetrical affinor. We continued the research of T.A. Shirokov, taking into account conformally flat Kahlerian spaces. We proved that there is no conformally flat Kahlerian space that differs from flat with over four dimensions. We study geodesic properties and define a type of metric for four-dimensional spaces. The special cases of these spaces are constructed as an example. We conduct an analysis in tensor shape without limitations on a sign of a metric tensor.

## In Silico Indications for Human Interferon Gamma Inhibition by Heparin

E. Lilkova

Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria

N. Ilieva

Institute of Information and Communication Technologies & Institute of Mathematics and Informatics, BAS, Sofia, Bulgaria

P. Petkov, L. Litov

Faculty of Physics, St. Kliment Ohridski University of Sofia, Bulgaria

M. Rangelov

Institute of Organic Chemistry with Centre of Phytochemistry, BAS, Sofia, Bulgaria

Interferon gamma (IFN $\gamma$ ) is a pleiotropic cytokine with a key role in the immune system signaling and modulating of innate and adaptive immune responses to viral and some bacterial pathogens. During some infections, including SARS and COVID-19, elevated blood levels of the cytokine have been associated with a life-threatening condition – cytokine storm syndrome (CSS), that if not recognized and treated promptly, could progress to mul- tiple organ failure and death. A potential suitable treatment for CSS is the inhibition and elimination of circulating hIFN $\gamma$ .

Heparin, a natural glycosaminoglycan, and its low molecular weight derivatives (LMWH) are widely used clinically as anticoagulants. In addition, heparin is known to bind to hIFN $\gamma$  and limit its circulatory half-life.

Here we report preliminary results of a computational study of the interaction of hIFN $\gamma$  and LMWH oligosaccharides based on 350ns long molecular dynamics simulations. The interaction is very strong and binding occurs on a few tens of ns timescale. In addition, the formed complexes are extremely stable. It is noteworthy that the interaction site in not just limited to the flexible C-termini of hIFN $\gamma$ , but also includes the upstream nuclear localization sequence of the molecule.

Acknowledgements. This work is partially supported by the Bulgarian Ministry of Education and Science (contract D01205/23.11.2018) under the National Scientific Program "Information and Communication Technologies for a Single Digital Market in Science, Education and Security (ICTinSES)," approved by DCM  $\ddagger 577/17.08.2018$  and by the Bulgarian Science Fund (Grant DN 11/20/22.12.2017). Computational resources were provided by the BioSim HPC Cluster at the Faculty of Physics by the St. Kliment Ohridski University of Sofia and the Avitohol Supercomputer at BAS.

### Parallel Algorithms for Processing Digital 3D Images

S. Harizanov, <u>I. Lirkov</u>

Institute of Information and Communication Technologies, BAS, Acad. G. Bonchev str., bl. 25A, 1113 Sofia, Bulgaria

This talk is devoted to the development of computationally efficient numerical algorithms for 3D digital image processing with application in Virtual Material Design and Non-destructive Testing of composite material. A general framework is proposed for the case of Computed Tomography (CT), consisting of two steps. Firstly, each of the 2D radiographic projections, generated by the acquisition device, is independently pre-processed in order to significantly decrease the image noise level and additionally enhance the image edges/details. Secondly, the generated 3D volume reconstruction of the pre-processed CT data is segmented into multiple classes, depending on the chemical composition of the scanned specimen. Based on this segmentation, various important physical macro-characteristics of the material, such as porosity, elasticity, ductility, thermal and electrical conductivity, magnetic and fluid permeability, *etc.*, can be computer simulated.

The algorithms, implemented in both steps are based on nonlinear convex optimization, thus are iterative and possess low theoretical convergence rate. Hence, they are impractical if realized in a sequential fashion, especially for processing high-resolution industrial CT data, where the voxels could be billions. However, both algorithms allow high level of parallelism and can be run on high-performance computing machines. In this talk, we experimentally investigate the performance of those algorithms on HPC computer system.

Acknowledgements. The research is a continuation of a joint work with Stanislav Harizanov. It is financially supported by the National Scientific Program "Information and Communication Technologies for a Single Digital Market in Science, Education and Security (ICTinSES)," contract No DO1-205/23.11.2018, financed by the Ministry of Education and Science in Bulgaria.

#### Heat Surce Control During Additive Processes

M. Zagirnyak, E. Kobilskaya, V. Lyashenko

Kremenchuk Mykhailo Ostrohradskyi National University, Ukraine

#### A. Salenko

I. Sikorsky Polytechnic Institute, National Technical University of Ukraine, Kyiv, Ukraine

Additive Manufacturing is one of the fastest growing technologies in many industries, including medicine, machine, airplane, rocket and others. The essence of the technology lies in the sequential formation of layers of molten plastic thread heated in the extruder, in the heated area, according to 3D data embedded in the printer program. 3D printing technology (additive manufacturing) is a process in which objects are formed layer by layer on an operating platform through computeraided design and manufacturing. One of the major problems that limiting the widespread use of additive manufacturing technology is the low quality of layer-bylayer padding of the thread on the heated area with a 3D printer. A mathematical model of the temperature field of a polymer filament, which is melted in an extruder according to FDM technology (fused deposition modeling), is considered Fused deposition modeling (FDM) is an additive manufacturing (AM) process in which a physical object is created directly from a computer-aided design (CAD) model using layer-by-layer deposition of a feedstock plastic filament material extruded through a nozzle. The mathematical model of the temperature field of the polymer filament is considered as a boundary value problem for the equation of thermal conductivity with the addition of corresponding boundary and nonlocal integral conditions in a moving cylindrical medium, which is heated in a restricted region by external heat sources.

The introduction of a nonlocal integral condition made it possible to consider the control problem of the temperature field of the filament at the outlet of the extruder, which allows to improve the physical and mechanical properties of the parts obtained by the FDM technology. The problem is solved numerically by reducing the boundary-value problem in a continuous domain to a difference problem in a separable (discrete) domain. The temperature distributions of the polymer filament at the outlet of the extruder under different conditions of the additive manufacturing are constructed.

## Numerical Modeling of Exchange Coupling Control in System of Donor and Quantum Dot Pairs

#### E.A. Levchuk, <u>L.F. Makarenko</u>

### Dept of Applied Mathematics and Computer Science, Belarusian State University, 4 Independence Ave., 220030 Minsk, Belarus

System of a single donor and electrically defined quantum dot is proposed as a possible realization of a qubit for solid-state quantum computer. In such proposals, two-qubit operations are implemented via exchange interaction between neighboring qubits, which can be controlled with external fields.

In this work, numerical simulation of exchange coupling in the system of nearsurface donor and quantum dot pairs is carried out. Exchange energy under the effect of external magnetic and electric fields has been calculated using unrestricted Hartree-Fock method. Fourier transform and finite element methods have been used to solve the problem for the Poisson equation.

The dependencies of exchange energy on geometric parameters and external fields have been obtained. It has been found that magnetic field can increase exchange energy of neighboring donors by several order, while it is impossible for electric field, as relocation of electronic density takes place at large electric fields. Thus, magnetic field is more preferable for exchange coupling control as it changes exchange energy in a wider range, while electric field of the gate can be used for more accurate tuning of exchange coupling. It has been shown that in the case when donor centers are located near the semiconductor surface, exchange energy is more sensitive to the gate field, which means that exchange coupling control in such systems differs significantly from the case of bulk donors.

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### **Invariant Transformations Preserving Geodesic Lines**

### $\underline{L. Makarenko}$

Odessa National University Maritime Academy, Ukraine

#### O. Lesechko, L. Sokolova

Odessa State Academy of Civil Engineering and Architecture, Ukraine

In order to solve the problem of cardinality of class of spaces that permit nontrivial geodesic mappings, there were invariant transformations preserving geodesic lines introduced into consideration. The initial condition is a presence of two spaces permitting non-trivial geodesic mappings. Then, using them, one constructs a new pair of pseudo-Riemannian spaces that have common geodesic lines. This row is infinite and never intersects. The developed methods can be applied for modelling of real processes.

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# On Biorthogonal Approximation of Solutions of Some Boundary Value Problems on Shishkin Mesh

#### E. Kulikov, <u>A. Makarov</u>

#### Saint-Petersburg State University, Russia

Singular perturbation boundary value problems are widely studied in applied problems of physics and engineering. However, their solutions are rarely possible to construct in an explicit form, so numerical methods of solving such problems are actively studied. Functions that are the explicit or approximate solution of this problem have huge boundary layer components; therefore, the application of classical interpolation methods leads to significant errors. This paper considers a piecewise-uniform Shishkin mesh, which allows improving the quality of approximation in the boundary layer. A local approximation scheme is implemented, minimal splines are used as basis functions, and the coefficients are calculated as de Boor-Fix type functional values, which are biorthogonal to minimal splines. The results of numerical experiments are presented. They show that the discussed approximation method allows getting accurate approximations of functions that are the solutions of singular perturbation boundary value problems, in comparison with previously published works.

## Relegation Classifier: A Machine-Learning Approach for Optimizing Analysis Significance in the Physical Sciences

<u>M. McCracken</u>, K. George

Washington & Jefferson College, PA, USA

Use of machine learning (ML) models to classify signal and background instances in discrete datasets is a critical component of many analyses in fields such as particle physics and astrophysics. In these applications, maximizing the statistical significance of signal events in a resulting data sample is often paramount to maximizing classification accuracy, the typical figure of merit for model optimization. However, accuracy and statistical significance can in fact be in tension in applications where signal and background are inseparable in some regions of the input feature space. Statistical significance can also be compromised in uses where the signalto-background ratio is dramatically different for training and application datasets, as is the case in searches for rare physical phenomena. We present the relegation classifier, a novel approach to binary and multi-class problems that optimizes a neural network to predict into an expanded category space using a loss function that explicitly combines prediction accuracy and statistical significance. This approach provides the model with freedom to ignore regions of the input space in which events from multiple classes are impossible to separate without overfitting. We demonstrate the application of the relegation approach to simulated particle-physics datasets, as well as a toy-model dataset that allows us to tune signal fraction and signal-background separability. We compare the relegation approach performance to those of logistic regression and softmax classification.

## The Boundary Value Problem of the Theory of Elasticity in a Rectangle: an Exact Solution

I. Menshova, A. Kerzhaev

Institute of Earthquake Prediction Theory and Mathematical Geophysics, RAS, Moscow, and Bauman Moscow State Technical University, Russia

T. Shulyakovskaya

Schmidt Institute of Physics of the Earth, RAS, Moscow, Russia

#### Xiankun Zeng

Qingdao University of Technology, and Collaborative Innovation Center for Engineering Construction and Safety in the Blue Economic Zone of Shandong Higher Education Institutions, Qingdao, China

An exact solution is constructed for the boundary value problem of the theory of elasticity in a rectangle, in which two opposite (horizontal) sides are free, and normal stresses are given on the other two (the ends of the rectangle) (evensymmetric deformation relative to the central axes). The solution is constructed in the form of expansions in Papkovich-Fadle eigenfunctions. The expansion coefficients are determined by simple closed formulas. Examples are considered. Comparison with the exact solution for a half-strip is given.

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## A New Coupled-Cluster Derived Equation of State of Infinite Neutron Matter

#### S. Mishev

New Bulgarian University, Sofia, Bulgaria

We present formulae and estimates on the correlations due to single and double clusters of neutrons and in particular how they modify pressure-density relationship (the equation of state - EoS) of degenerate neutron Fermi gas. We show that the new terms are non-negligible at densities higher than the nuclear saturation density ( $\rho > \rho_0$ ) and gradually vanish in environments with  $\rho < \rho_0$ . The presented corrections to the EoS are vindicated by the latest NICER findings found, *e.g.*, in Refs. [1,2].

Acknowledgements. This work is partially supported by the Bulgarian National Science Fund under Contract No. DFNI/KP-06-PN-38/12.

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## The Role of Institutional Factors in the Process of Public Mental Health Formation

### A.N. Nepp, <u>N.A. Musatova</u> Ural Federal University, Ekaterinburg, Russia

To date, according to the World Health Organization, one of the top priorities of healthcare both globally and on a national level is prevention of suicides which annually cause more than 800,000 deaths (WHO, 2015). This fact determines the relevance of scientific research connected with theoretical and methodological justification and empirical evidence of institutional factors influence on the suicide dynamics followed by development of practical recommendations based on the research results. Cardiovascular disease (Choi et al, 2014) and mental disorders (Wynter, Smith, 2017; Cohen, 1985) are most susceptible to institutional factors influence. In the analysis of scientific research it has been identified that enough attention is paid to the relationship of public health to hereditary factors (Wills, Sherris, 2008) and to government spending on health care (Schell *et al*, 2007; Kennelly et al, 2003; Gravelle et al, 2002). It is to be noted that Beckfield (2010) considers opening up of political institutions to be an institutional factor for research and determines the importance of further research into the concept of "neoliberalism" as a condition for public health improvement. According to some researchers, politicians should take into account all the consequences of their proposals, for example, reducing or ignoring crime, as they can affect health care (Christian R. Eiler, 2017), senior citizens' health (Mathis et al, 2016), including their mental health (Foster et al., 2016). However, the above-mentioned research shows no empirical evidence of suicide rates being affected by such institutional factors as political stability, efficiency of legal framework and the Internet and social networks penetration. As a hypothesis for the study, we made several assumptions:

1. Political stability growth and efficient legal framework reduce the number of suicides;

2. An increase in the number of the Internet and social networking sites users has a negative effect on suicide rates growth.

As part of research to confirm our hypothesis and substantiate the effects of political stability, law and the Internet and social networks development on suicide rates we have used the model fixed effects. The results can be of use to national policy when reforming health care system to improve public mental health.

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## Molecular Dynamics Study of the Adsorption and Aggregation of Linear Alkyl Benzene Sulfonate

F. Mustan, A. Ivanova, S. Tcholakova

### Faculty of Chemistry and Pharmacy, St. Kliment Ohridski University of Sofia, Bulgaria

Linear alkyl benzene sulfonate (LAS) is a popular surfactant used in industry as a stabilizer of different cosmetics and detergent formulations. The properties of LAS are well studied by different experimental methods but the explanation of some of the observed phenomena, e.g., specificity of counterions binding, requires more detailed investigations at the molecular level.  $\langle br \rangle > In$  the current study, we describe computationally the adsorption and aggregation processes of LAS. We construct three systems with LAS molecules randomly placed in water with different thickness of the aqueous phase in the absence and in the presence of calcium cations (Ca2+). The surfactants are allowed to adsorb at the vacuum/water interface. All models are simulated with atomistic molecular dynamics for up to 20 and 100 ns. It is found that depending on the thickness of the water layer the processes of adsorption and aggregation are in competition. In the smallest systems, the adsorption is dominant and dense adsorption layers are formed. In the largest models, the aggregation is dominant. In the layers with middle water slab thickness, the adsorption is preferred at short simulation times but after that stable aggregates are formed in the bulk in conjunction with non-dense adsorption layers. With respect to the effect of Ca2+, it is found that independently on the thickness of the aqueous phase the aggregation is much faster than in the system without Ca2+ and larger micelles are formed. These results are in very good agreement with the experimentally observed precipitation of LAS in the presence of Ca2+. The reason for this strong interaction between LAS and Ca2+ is explained with the dehydration of both the hydrophilic head of the surfactant and Ca2+.

### Three-geodesic Mappings of Spaces of Affine Connectivity

O. Nazerenko

Odessa State Academy of Civil Engineering and Architecture, Ukraine

S. I. Kadievskaya

Odessa State Academy of Civil Engineering and Architecture, Ukraine

H. Wright

K. D. Ushynsky South Ukrainian National Pedagogical University, Odessa, Ukraine

Here, we applied three-geodesic mappings of spaces of affine connectivity in order to model processes that are running under energetic regimes without influence of outer forces processes that run under energetic regimes with beforehand defined outer forces. Parallel transport is generalized as a transport of Fermi-Walker. When a tangent vector is transported by method of Fermi-Walker along a curve, the latter is geodesic line, when a vector relates to curve of the first curvature, then the curve is an almost geodesic line, when a vector relates to the second curvature, then the curve is a three-geodesic line. We obtained a special form of main equations of theory of three-geodesic mappings of spaces of affine connectivity with torsion.

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## 3D Mathematical Model of the Human Body: Analytical Results

G. Nikolova and D. Dantchev

Institute of Mechanics, BAS, Acad. G. Bonchev St. bl. 4, 1113 Sofia, Bulgaria

In the current study, we present a 3D mathematical model of the human body for evaluation of the mass-inertial characteristics of all segments of the body. Specific realization of the model is proposed based on anthropometric data for Bulgarian population provided by the representative anthropological investigation of 5290 individuals (2435 males and 2855 females) of the Bulgarian population at the age between 30-40 years [1]. Using the proposed model, after deriving the corresponding analytical expressions needed for the geometrical bodies used in the modeling, we provide analytical expressions and estimate numerically the massinertial characteristics of all of the segments of the body: their mass, center of mass, the volume, and the principal moments of inertia. The comparison between our model results and data reported in literature for other Caucasian shows an overall good agreement, thus supporting the validity of the described method. The model is applicable in medicine, rehabilitation robotics, sports, ergonomics, computer simulations, *etc.* 

Acknowledgements. The financial support by the Bulgarian National Science Fund: Contract DN-07/5 "Study of anthropometric and mass-inertial characteristics of the Bulgarian men and women via mathematical models of the human body" is gratefully acknowledged.

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## Modified Method of Fuzzy Recognition of Proteins in Electrophoresis in Population Genetics

V. Olevskyi, O.V. Olevskyi

Ukrainian State University of Chemical Technology, Dnipro, Ukraine

Yu. Olevska

Dnipro Polytechnic National Technical University, Ukraine

N. Ausheva

Igor Sikorsky Polytechnic Institute – National Technical University of Ukraine, Kyiv, Ukraine

We propose the development of a previously created method for fuzzy recognition of proteins by gel electrophoresis of earthworm tissues in population genetics. In case when several proteins have close masses, their traces on the electrophoregram intersect. The visually determined boundaries of the fuzzy membership function carrier are unjustifiably narrowed, as can be seen in the dependence of the boundaries on the mass of the protein. Therefore, it is necessary to clarify the coordinates of the carrier of the fuzzy membership function for each of them.

The methodology developed by us involves the construction of an experimental membership function on a narrowed carrier, the approximation of it by selected curve (Gauss or Bezier) and, then, the adjustment of the boundaries of the carrier by extrapolating the approximants until the membership function reaches a predetermined level. The effectiveness of the application of the technique in studying the effect of laser radiation on changing the genotype of a worm population is shown

## Monte Carlo Methods for Sensitivity Studies of Large-Scale Air Pollution Model

#### Tz. Ostromsky, I. T. Dimov, V. Todorov

Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria

Sensitivity studies are nowadays applied to some of the most complicated mathematical models from various intensively developing areas of application. Such a sophisticated model in the area of air pollution modeling is the Danish Eulerian Model, a powerful large scale air pollution model with a long development history. Over the years it was used successfully in different long-term environmental studies for the European region. In this talk we discuss some performance-critical achievements in the parallel optimization and a systematic approach for sensitivity analysis of the latest version of the Danish Eulerian Model, UNI-DEM, A comprehensive experimental study of Monte Carlo algorithms based on Latin Hypercube Sampling and Adaptive approach for multidimensional numerical integration has been done. The algorithms have been successfully applied to compute global Sobol sensitivity measures, corresponding to the influence of several input parameters on the concentrations of some of the air pollutants of highest importance. In this work some results of the global sensitivity study of the UNI-DEM are presented. One of the most attractive features of UNI-DEM is its advanced chemical scheme – the Condensed CBM IV, which consider a large number of chemical species and numerous reactions between them, of which the ozone is one of the most important pollutants for its central role in many practical applications of the results. Different efficient stochastic algorithms for multidimensional integration have also been applied on a further stage of the sensitivity studies. We make a comparison with two adaptive Monte Carlo algorithms and a special type of Latin Hypercube Sampling. The numerical tests show that the Monte Carlo algorithms under consideration are efficient for the multidimensional integrals under consideration and especially for computing small by value sensitivity indices.

**Keywords:** Air pollution model, supercomputer, parallel computing, sensitivity analysis, Monte Carlo algorithm, Latin Hypercube.

Acknowledgements. This work is supported by the Bulgarian National Science Fund under Project DN 12/5-2017, "Efficient Stochastic Methods and Algorithms for Large-Scale Problems" and under Project KP-06 M32/2-17.12.2019 "Advanced Stochastic and Deterministic Approaches for Large-Scale Problems of Computational Mathematics."

### Modeling the Competition between Three Languages

### S. Paekivi and A. Rekker

### School of Natural Sciences and Health, Tallinn University, 29 Narva Road, 10120 Tallinn, Estonia

Languages can be viewed as entities competing among each other over speakers, with less advantageous ones eventually dying out. Through such a process, approximately 90% of the worlds languages are predicted to go extinct in the current century [1, 2]. Motivated by this prognosis, the past two decades has seen a surge of interest in the modeling of language competition dynamics, with emphasis being put on systems of two competing languages. The Abrams and Strogatz model (ASM) proposed by in 2001 in Ref. [3] is generally cited as inspiration for the latter. Considering the existence of multi-ethnic regions and the rising effect of globalization (the spread of globally prevalent languages) however, it is also of interest to know the properties of competition between three distinct language groups. We present such a model, as a generalization of the ASM to a threestate variant and find analytical expressions for its stationary points and report their stability criteria, for the case of a power-law type transition function. We present a framework to describe the models dynamics for any distribution of initial speakers and in particular, some interesting phenomenon arising from the interplay of system and language parameters.

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## Electromagnetic Modeling and Simulation of Microwave and mm-Wave Devices Based on Liquid Crystal Compounds

N. C. Papanicolaou, M. A. Christou

Dept of Mathematics, University of Nicosia, 46 Makedonitissas Ave, CY-2417 Nicosia, Cyprus

A. C. Polycarpou, M. Nestoros, R. Tchema

Dept of Engineering, University of Nicosia, 46 Makedonitissas Ave, CY-2417 Nicosia, Cyprus

Tunable devices and materials have always been extremely important for a variety of applications in the optical as well as the m-wave and mm-wave bands. With the arrival of 5G communications networks, the need for compact, lightweight devices is imperative. Liquid Crystals (LC) are anisotropic and tunable, and these properties make them an attractive proposition for use in portable devices and communication hubs. In this paper, three such LC-based devices capable of operating in the 5 GHz and 30 GHz (5G) bands are presented: A frequency-agile patch antenna, a variable phase shifter, and a steerable leaky wave antenna operating at a single frequency.

In all cases, tunability is achieved via the application of a low-voltage external electric bias field to the LC-cell. This affects the dielectric properties of the crystal by re-orienting its molecules, the macroscopic orientation of which is denoted by a unit vector called the director. The dielectric properties of the LC-cell are characterized by its relative permittivity tensor, which is a function of the directors' orientation. The latter is determined at every point of the cell by solving a coupled system of PDEs numerically. The obtained relative permittivity tensor is input into a High-Frequency Full-Wave Electromagnetic Simulator based on the Finite Element Method. Finally, the simulation results are analyzed and the performance and capabilities of the applications are discussed.

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## Modeling of the Transport Work of Taxi Vehicles in Ruse

<u>V. Pavlov</u>, I. Zheleva, E. Veleva A. Kanchev University of Ruse, Bulgaria

This report explores the transport performance of taxi-cars operating on the territory of Ruse. The problem is interpreted as a mass service system with failures for a non-static input stream of request and a variable number of serving channels. After the collected and processed statistics for received requests, the input stream is modeled as a periodic non-linear function. The main parameters of the survey are: density of refusals, average number of taxi drivers occupied during the day and intensity of serviced requests. The subject of the study is one full working day of 24 working hours. For the calculation of the parameter values a MatLab application was created.

Key words: Queue theory, incoming flow, taxi cars, refusals

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# Plane Stress State of a Multilayer Fibrous Composite Differently Resistant to Tension and Compression

### I. Petrakov, V. Sadovskii

Institute of Computational Modeling of SB RAS, Krasnoyarsk, Russia

The paper devoted to the plane stress state of a multilayer fiber composite plate. Polymer-based composite reinforced by thin carbon fibers is used as the material for the plate. Each layer of the plate is a unidirectional fibrous composite. This type of composite material has different tensile and compression moduli, since the fibers having high tensile stiffness and low stiffness upon compression.

Generalized rheological method is used: a rheological scheme was composed and the constitutive equations were constructed using the cone of permissible deformations projection of the strain tensor according to the norm, consistent with the tensor of additional elastic moduli. The projection is calculated using the Uzawa algorithm. The elastic moduli of a unidirectional composite under tension and compression were obtained from experimental data. Hooke's law was written for a unidirectional composite in the coordinate system associated with the orientation of the fibers, and in the system obtained by rotation around an axis perpendicular to the reinforcement plane. The elastic moduli of the layered composite used in the constitutive equations are determined from the elastic moduli for each layer using the Voigt and Reis averaging formulas. The problem of plane static loading was solved numerically using the finite element method with the obtained constitutive equations. As a result, a mathematical model of a multilayer fibrous composite material was created and the problem of static loading of a plate of a multilayer fibrous composite in a plane stress state was solved.

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## Investigating the Effects of Manifold Mixup on Transfer Learning

L. Petrov

New Bulgarian University, Sofia, Bulgaria

Deep learning is currently state of the art at learning complex representations from training data. However, on test time, the generalization abilities of neural networks can sometimes fail to predict correctly, while at the same time doing so with high confidence. One reason for this is the fact that after training, the latent representation of data might become highly non-linear, with very good ability of the model to predict the training examples, but with poor generalization to test examples. One way to control for this, is a regularization method called manifold mixup. The technique interpolates between the representations of data points on training time. This encourages models to build more flat representations, casting different classes of data further apart, while building broader, low-confidence margins between them. This prevents the network from being overly certain when generalizing to unseen examples. One field where it is important to build strong models with good generalization abilities, especially with scarce data, is transfer learning. We propose the usage of manifold mixup when fine-tuning pretrained neural network models on new data sets, and we investigate the effect of this regularization technique on transfer learning.

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### Integrable Discretizations for Classical Boussinesq System

## Liu Qing Ping

Dept of Mathematics, School of Science, China University of Mining and Technology, Beijing

In this talk, we propose and study integrable discrete systems related to the classical Boussinesq system. Based on elementary and binary Darboux transformations and associated Bäcklund transformations, both full-discrete systems and semidiscrete systems are constructed. The discrete systems obtained from elementary Darboux transformation are shown to be the discrete systems of relativistic Toda lattice type appeared in the work of Suris (1997) and the ones from binary Darboux transformations are two-component extensions of the lattice potential KdV equation and Kac-van Moerbeke equation. For these discrete systems, their different continuum limits, various interesting reductions and Darboux-Bäcklund transformations are considered. Some solutions such as discrete resonant solitons are also presented.

This is a joint work with Wenhua Huang and Lingling Xue.

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# Infinitesimally Small Deformation Which Preserves Geodesic Lines

<u>T. Podousova</u>, V. Dumanska Odessa State Academy of Civil Engineering and Architecture, Ukraine

# A. Ugol'nikov

## Military Academy, Odessa, Ukraine

The authors have proven that regular straight circular cylinder permits a nontrivial infinitesimally small deformation, which preserves geodesic lines and any equal-area parts of the surface, which is unequivocally defined by aforehand fixed non-zero function of a variable and two constants. Tensor fields were found in evident form. Every deformation of this type can be interpreted as a momentless stressed condition of cylindrical shell with a certain surface stress.

# A Sufficient Condition for Solvability and Stability of a Cantilever Timoshenko Beam Type System Embedded in an Elastic Medium

# S. Popov, V. Vassilev Institute of Mechanics, BAS, Sofia, Bulgaria

The paper we suggest, deals with a generalised Timoshenko type system of four equations, whose coefficients are supposed to be smooth functions, depending on the spatial variable only. The aim of this survey focuses on establishing some sufficient condition for well-posedness of the problem and proving periodicity behaviour of the existing solution when the system take into account the elastic medium. The technique, we develop in order to derive the aforementioned results, consists of introducing some Sobolev spaces and studying the properties of the system operator, when it is embedded in them. Moreover there is a natural comparison between the local density of the energy conservation law of the physical clamped Timoshenko beam system and the correspondent inner product of the basic pivot space, where we are interested in studying the main properties of the abstract system operator. By this way, it is proven that the system operator is maximal monotone onto the basic pivot space, moreover it results to be an antiself-adjoint one. Hence, as a consequence, it is proven that the whole spectrum of the regarded operator consists only of completely imaginary isolated points with an unique accumulation point.

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## Application of Leiko Network for Construction of Scans

#### I. Potapenko

Odessa I.I. Mechnikov National University, Ukraine

#### S. Bykova, I. Ogorodnichuk

Odessa State Academy of Civil Engineering and Architecture, Ukraine

Isoperimetric extremal of a turn on surfaces in three-dimensional Euclidean space is a curve along which the condition kg = cK is true, here kg – geodesic curvature without taking into account a sign, K – full (Gaussian) curvature of a surface, c – isoperimetric constant. Regular network on a surface with non-zero Gaussian curvature is called Leiko network, when every line of any of a pair of single-parametric families creating a network is an isoperimetric extremal of a turn. Moreover, isoperimetric constant is the same for every two lines of a single family. If certain conditions of algebraic nature are true for Christoffel symbols, it is a necessary and sufficient condition in order to define a regular mesh on the surface of non-zero Gaussian curvature as a Leiko network. Application of Leiko network helped to authors in solving a problem of scanning of tent shell of negative Gaussian curvature that is created by rotation of parabola's branch around an outer vertical axis. The proposed method permits to minimize corrections of edge effect that appears due to incomplete filling of a surface by a network.

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# Hydrodynamics, Heat and Mass Transfer During Crystal Growth in Assembly of "Hele–Shaw" Cells

### A. I. Prostomolotov, N. A. Verezub

Ishlinsky Institute for Problems in Mechanics RAS, Moscow, Russia

The physicochemical processes are studied in a new modification of Bridgman's crystal growth by way of a "cassette" crystallization in the assembly of "Hele–Shaw" cells for producing the polycrystalline bismuth telluride, which is used for thermoelectric applications. The aim was associated with the study of heat and mass transfer processes for the elimination of an instability of polycrystalline growth in the form of dendritic formations. It was established an influence of a crystallization rate on a chemical and phase micro inhomogeneity arising in the polycrystalline bismuth telluride. Negative affects of a large crystallization rate on the thermoelectric and mechanical properties of grown bismuth telluride wafers are discussed.

### **Recent Developments on Integrable Peakon Systems**

Zhijun (George) Qiao

### School of Mathematical & Statistical Sciences, University of Texas Rio Grande Valley, Edinburg, TX, USA

In my talk, I will introduce integrable peakon and cuspon equations and present a basic approach how to get peakon solutions. Those equations include the well-known Camassa-Holm (CH), the Degasperis-Procesi (DP), and other new peakon equations. I take the CH case as a typical example to explain the details. My presentation is based on my previous work (*Communications in Mathematical Physics* 239, 309–341). I will show that the Camassa-Holm (CH) spectral problem yields two different integrable hierarchies of nonlinear evolution equations (NLEEs), one is of negative order CH hierarchy while the other one is of positive order CH hierarchy. The two CH hierarchies possess the zero curvature representations through solving a key matrix equation. We see that the well-known CH equation is included in the negative order CH hierarchy. In particular, the CH peakon equation is extended to the FORQ/MCH and other higher order peakon models with peakon and weak-kink solutions. In the end of my talk, some open problems are also addressed for discussion.

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#### Liouville Correspondences between Integrable Hierarchies

#### Changzheng Qu

Ningbo University, Ningbo 315211, China

It is well-known that the Camassa-Holm-type equations admit several nontrivial proper-ties in contrast with the classical integrable systems. In this talk, we show that a pair of Liouville transformations between the isospectral problems of the mCH and mKdV equations, the isospectral problems of the Novikov and Sawada-Kotera equations, and the isospectral problems of the Degasperis-Procesi and Kaup-Kupershmidt equations relate the corresponding hierarchies, in both positive and negative directions, as well as their associated conservation laws. Combining those results with the Miura transformations relating KdV equation and mKdV equation, and the generalized Miura-transformation relating the Sawada-Kotera and Kaup-Kupershmidt equations, we further construct implicit relationships which associate the CH equation and mCH equation, the Novikov and Degasperis-Procesi equations. These results can be further extended to the cases for the multi-component Camassa-Holm-type systems.

This is a joint work with Prof. Peter Olver, Prof. Jing Kang and Prof. Xiaochuan Liu.

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# Utilization of Dynamical Systems' Multiple Trajectories for Short and Long Terms Time Series Forecasts

#### V. Rayskin

Tufts University, MA and New York Institute of Technology, USA

We propose a dynamical system's approach for time series analysis. The method allows highly accurate short term prediction. In some cases, we can also discuss the global qualitative properties of the dynamics' phase portrait that describe various long term tendencies for of the underlying process that reflect different scenarios of the external influence. We provide examples of the digital platforms' (Homes.mil and Wikipedia.org) traffic prediction. Our short term prediction is more accurate than the traditional time series models (ARIMA, Holt-Winters, *etc.*). The global phase portrait analysis helps to understand the properties of the platforms and suggests the mechanisms of the traffic improvement. We also provide examples of the COVID-19 short term prognosis in multiple countries. Using machine learning technique, we select the countries with similar spread of the virus, and apply the dynamical system's model for the comparison and prediction of the infection's spread. We are developing the technique for the long term trends' estimates for various scenarios of external policies.

## A Pontryagin Maximum Principle Based on Fokker-Planck Approach to Control Traffic Motion

#### S. Roy

University of Texas at Arlington, TX, USA

### A. Dey

Oregon State University, OR, USA

In this work, we investigate a Fokker-Planck (FP) control framework for traffic motion. Such control frameworks arise in the context of crowd control and evolution of stock prices. The FP control strategy is formulated as the minimization of an expectation objective with a bilinear optimal control problem governed by the FP equation. We present theoretical results on existence of optimal control. A new optimization scheme based on the Pontryagin maximum principle is used to solve for the optimal control. Numerical experiments in 2 dimensions demonstrates the efficiency of the proposed framework.

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## Pressureless Euler-Poisson Equations and Exact Thresholds in the Dynamics of Cold Plasma

O. Rozanova, E. Chizhonkov, M. Delova Faculty of Mechanics and Mathematics, Moscow State University, Russia

We consider a quasilinear system of hyperbolic equations that describes plane electrostatic non-relativistic oscillations of electrons in a cold plasma with allowance for electron-ion collisions and show that it is equivalent to the pressureless Euler-Poisson equations with nonzero background density in the presence of relaxation. In 1D case we obtain a criterion for the existence of a global in time smooth solution to the Cauchy problem. It allows to accurately separate the initial data into two classes: one corresponds to a globally in time smooth solutions, and the other leads to a finite-time blowup. The influence of electron collision frequency  $\nu$  on the solution is investigated. It is shown that there is a threshold value, after exceeding which the regime of damped oscillations is replaced by the regime of monotonic damping. The set of initial data corresponding to a globally in time smooth solution of the Cauchy problem expands with increasing  $\nu$ , however, at an arbitrarily large value there are smooth initial data for which the solution forms a

singularity in a finite time, and this time tends to zero as  $\nu$  tends to infinity. The character of the emerging singularities is illustrated by numerical examples.

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## Geodesic Mappings of Compact Quasi-Einstein Spaces

### A. Savchenko

Kherson State Agrarian University, Ukraine

#### V. Kiosak

Institute of Engineering, Odessa State Academy of Civil Engineering and Architecture, Ukraine

### A. Kamienieva

## Odessa National University Maritime Academy, Ukraine

Research on geodesic mappings "in general" is based on the results that were obtained locally. Integral theorems are applied for interpretation of local results for compact Riemannian spaces. Main equations of geodesic mappings theory are applied to quasi-Einstein spaces in linear form. The invariant of a particular type is built in order to apply integral theorem. We found characteristics that are sufficient in order to define unanimously a compact quasi-Einstein space by its geodesic lines.

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# "Mean Field Games" as Mathematical Models of Dynamic Socio-Economical Activity

#### V. Shaydurov and V. Kornienko

Institute of Computational Modeling SB RAS, 50/44 Akademgorodok, & Siberian Federal University, 79 Svobodny, Krasnoyarsk, Russia, & Tianjin University of Finance and Economics, 25 Zhujiang Rd., Hexi District, Tianjin, China

The talk begins with a review of modern mathematical economic models with the "Mean Field Game" structure coming from theoretical physics. They are currently used for the predictive modeling under given control conditions or for optimizing control actions to achieve the desired result. The mathematical model is a pair of parabolic partial differential equations (Fokker-Planck-Kolmogorov and Hamilton-Jacobi-Bellman types with a corresponding set of initial and boundary conditions) for optimizing a given target functional. For this problem, the discretization is applied to obtain systems of nonlinear algebraic equations which are solved in an iterative way to get the best instant benefit for each agent. The authors present the special type of approximation inheriting the basic properties of a differential problem (conjugacy and monotonicity of operators, their boundedness in the corresponding norms) at a discrete level. This mathematical apparatus is used for the quantitative modeling of the distribution or the use of alternative resources, environmental problems, optimization of wages and insurance, network sales, and other socio-economic activities to predict the aggregate behavior of the great mass of agents looking for instant personal benefit.

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# Conformal Mappings Preserving the Curvature of Multi-Dimensional Platforms

T. Shevchenko

Odessa State Academy of Civil Engineering and Architecture, Ukraine

O. Gudyreva

Kherson State Maritime Academy, Ukraine

#### Ju. Fedchenko

Odessa National Academy of Food Technologies, Ukraine

We treat certain generalizations of curvature concept for a pseudo-Riemannian space and carry out an analysis. of some characteristics of aforementioned curvatures. The attention is focused on alterations of special curvatures of a space in the course of conformal mapping. Conformal mapping is called non-trivial if it retains the curvature in respect to three-dimensional platforms but it does not retain the curvature in respect to two-dimensional platforms. We prove that pseudo-Riemannian spaces with dimensions over four do not permit non-trivial conformal mappings. We study some geometrical properties of these spaces. An example of metric is constructed.
### Modified Commutators vs. Modified Operators in a Quantum Gravity Minimal Length Scale

#### D. Singleton

#### Dept of Physics, California State University, Fresno, CA, USA

Phenomenological models of quantum gravity propose modified commutators of the form  $[\hat{x}, \hat{p}] = i\hbar(1 + \beta p^2)$ . These modified commutators are thought to be sufficient to give rise to a minimum length scale. We test this assumption and find that it is the specific modification of the position and momentum operators rather than the modified commutators which determine of there is a minimal length scale or not. This fact – that it is the specific form of the modified operators which determine the existence or not of a minimal length scale – can be used to keep or reject specific modifications of the position and momentum operators in models of quantum gravity.

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# On the Application of Nested Dissection Reordering for Solving Fractional Diffusion Problems Using HSS Compression

D. Slavchev, S. Margenov, I. Georgiev

Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria

The anomalous (fractional) diffusion has a wide application in modeling many physical phenomena including superconductivity phenomena, protein diffusion within cells, diffusion through porous media, *etc.* The Fractional Laplacian is a non-local operator. Thus, after the discretization we get a dense system of linear equations. Using the traditional Gaussian elimination results in computational complexity of  $O(n^3)$ .

The hierarchical compression methods utilize the structure of the matrix to compress it into a sparser approximation. The Hierarchical Semi-Separable (HSS) compression is a derivative method that approximates the off-diagonal blocks as  $A_{ij}, i \neq j \approx U_i B_{ij} V_j$ . If the approximation of  $A_{i\neq j}$  is low-rank, the generator matrices  $U_i, B_{ij}$  and  $V_j$  are much smaller than the non-compressed block  $A_{ij}, i \neq j$ . The diagonal blocks  $A_{ii}$  can be compressed in a similar way and so on recursively. The computational complexity is  $O(r^2n)$ , where r is the maximum off-diagonal rank and, ideally, r approaches  $O(\ln n)$ . The overall complexity of the solver is  $O(r^2n)$ . However, the performance heavily depends on the ordering of the unknowns. In this work we analyze the use of Nested Dissection on the initial mesh to produce a more suitable ordering. Nested Dissection uses a divide and conquer approach to recursively divide the mesh in two and then each halve in two again, and so on recursively.

We assess the use of Nested Dissection reordering for improving the performance and accuracy of a parallel HSS solver from the STRUctured Matrix PACKage (STRUMPACK) for a fractional diffusion problem modeled with the Ritz potential. We compare the results with the results with the original ordering, as well as using a direct Gaussian elimination solver from Intel's Math Kernel Library (MKL).

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# Accounting for Singularities of the Electric Field Acting on a Liquid Crystal

I. Smolekho, O. Sadovskaya, V. Sadovskii

### Institute of Computational Modeling SB RAS, 660036 Krasnoyarsk, Russia

A computational algorithm for modeling the liquid crystals behavior under the action of electric field has been presented in [1]. A liquid crystal layer is placed between periodically disposed short capacitor plates, where electric field is created by appearance of charges. In the exterior part of a layer, the electric field potential satisfies the Laplace equation, whose approximate solution is obtained using the method of straight lines. Inside a layer, the equation taking into account the medium anisotropy is fulfilled. Its solution is constructed by the iterative method using a recurrence relation. On the capacitor plates the potential difference is set. On the remaining parts of the layer boundary, the conditions for the electric potential continuity between the dielectric and air (vacuum) are satisfied together with the condition of electric induction continuity in normal direction. In present work the influence of electric field singularities is analyzed, which arise at the ends of the capacitor plates due to a sharp change in the boundary conditions at these points. Electric potential is represented as the sum of two terms. The first of them is the smooth solution. The second one is the sum of solutions with singularities at the ends of upper and lower capacitor plates. The singular solutions are taken in the form of  $A + B\varphi^{(k)}$ , where constants A and B are found using the least squares method.

The analysis shows that the first partial derivatives of potential are bounded functions. The second derivatives, which influence on the couple forces in the liquid crystal domains, grow near the plates ends inversely with the distance. We incorporate the algorithm of singularity accounting into parallel computational algorithm that simulates the mechanical, temperature, and electrical effects on a liquid crystal [2].

Acknowledgements. This work is supported by the Krasnoyarsk Mathematical Center and financed by the Ministry of Science and Higher Education of the Russian Federation in the framework of the establishment and development of regional Centers for Mathematics Research and Education (Agreement No. 075-02-2020-1631).

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# On the Practical Stability with Respect to Manifolds for Impulsive Control Fractional-Order Systems

#### I. Stamova

University of Texas at San Antonio, TX, USA

In this paper, efficient sufficient conditions for practical stability with respect to manifolds of a class of impulsive control fractional systems of differential equations will be presented.

### On the Pseudo-Riemannian Spaces with Special Structure of a Curvature Tensor

A. Stechun, G. Poletaev, T. Voytik

Odesa State Academy of Civil Engineering and Architecture, Odessa, Ukraine

Specialization of pseudo-Riemannian spaces is a wide-spread method of research. It is conducted via structure of intrinsic objects of spaces. This approach permits studying the relational structures and optimal approximation of real space under study by a model. A curvature tensor is an important intrinsic object of pseudo-Riemannian spaces. Its structure consists in limitations of algebraic or differential order and permits to study geometric properties of pseudo-Riemannian space. Author study geometric properties of pseudo-Riemannian spaces without limitations imposed on signature or sign of metric tensor due to a structure of a curvature tensor. Three types of spaces are defined.

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# On COVID-19 Predictions: Issues on Stability, Model Sensitivity and Precision

M. Stehlík

Statistics & Actuarial Science, University of Iowa, USA Dept of Applied Statistics & Linz Institute of Technology, Johannes Kepler University in Linz, Austria Institute of Statistics, Universidad de Valparaíso, Valparaíso, Chile

We formulate the ill-posedness of inverse problems of estimation and prediction for covid19 growth curves from statistical and mathematical perspectives. These leave us with a plenty of possible statistical regularizations, thus generating plethora of sub-problems. We can mention the as examples stability and sensitivity of peak estimation, starting point of exponential growth curve, or estimation of parameters of SIR model. We also illustrate that several country-specific covariates, like social structure, or air pollution by PM2.5 or PM10, can play crucial way in regularization of the estimators. We will illustrate this on example of Chile, where start of exponential growth, grounded on microbiological-epidemiological model was severely underestimated. Moreover, in a specific country, one can define several social groups which can contribute in a heterogeneous way to whole country epidemiological curves. Moreover, each parameter has its specific sensitivity, and naturally, the more sensitive parameter deserves a special attention. *E.g.*, in SIR (Susceptible-Infected-Removed) model, parameter  $\beta$  is more sensitive than parameter  $\gamma$ . In simple exponential epidemic growth model, *b* parameter is more sensitive than *a* parameter. We provide sensitivity and illustrate it on the country specific data. We also discuss on statistical quality of COVID-19 incidence prediction, where we justify an exponential curve considering the microbial growth in ideal conditions for epidemic. We model number of infected in Iowa State, USA, Hubei Province in China, New York State, USA. All empirical data justifies an exponential growth curve for initial prediction during epidemics. We also discuss peculiarities of covid19 prediction in Chile and Slovak Republic.

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### Hybrid CART-ARIMA Approach for PM10 Pollutant Modeling

#### M. Stoimenova-Minova

#### Paisii Hilendarski University of Plovdiv, Bulgaria

According to the latest data, in many cities in Bulgaria, the levels main air pollutant – particulate matter PM10 continue to be high. The high values of the air pollutant are extremely harmful to human health and the environment. The problem is very pressing all over the world and in many European countries, just as in Bulgarian cities, the threshold limits for air pollution are regularly exceeded. This study applies hybrid CART-ARIMA models to the analysis of concentrations of PM10 in the city of Pazardzhik, which exceed the permissible health and safety threshold. The data are modeled using average daily measurements of PM10 from 5 January 2012 to 15 June 2016, as well as meteorological measurements. The CART method is applied at the first step of building the model. The second step uses the ARIMA method to approximate and smooth over the error in the CART model obtained in the first step. The results demonstrate an 80% fit of the best model with the actual measured air pollutant. The best model is used to forecast particulate matter one day ahead and the result is close to the actual measured concentrations. The proposed approach is an alternative for notifications of forthcoming pollution and its prevention.

### EM and Accelerated EM Algorithms for Statistical Estimation of Multitype Branching Processes

#### A. Staneva, <u>V. Stoimenova</u>

# Faculty of Mathematics and Informatics, St. Kliment Ohridski University of Sofia, Bulgaria

Branching processes form an important and wide subclass of stochastic processes. They have numerous applications in different scientific and practical areas, from biology and cell proliferation through epidemiology, physics and and neutral chain reactions to finance and insurance. Many of them involve multitype modeling. Statistical estimation of the process' characteristics is an important issue in their study. The nature of the models require a big amount of data, which is often impossible to be observed, considering only the total population sizes. In order to obtain the maximum likelihood estimators when the information is not sufficient, we use approximation methods. In our study the EM algorithm serves as an effective instrument for calculation of the estimates when a part of data is hidden. We propose examples of two-type branching processes and a software implementation of the EM algorithm, illustrated via simulations and computational results.

Acknowledgements. The research was partially supported by the Bulgarian National Science Fund, Grant No KP-6-H22/3 and by the financial funds allocated to the St. Kl. Ohridski University of Sofia, grant No 80-10-116/2020.

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### The Impact of Twitter Sentiment Analysis on Stock Prices

# A. Nepp and <u>I. Sukhanova</u> Ural Federal University, Ekaterinburg, Russia

Nowadays social media has become an integral part of everyone's daily life. It changed the way people communicate with each other by giving the opportunity to interact constantly. One tweet can be shared with a millions in an instant. The information spreads extremely fast. This phenomenon increases the importance of social media users' community. Its influence is growing and goes beyond the online environment.

This study aims to examine the impact of the factors that determine the users' trust, measured by polarity of content, likes and retweets, to the company's stock price volatility. We investigated the reaction of users to e-commerce companies' scandals which had received wide coverage by social media. The historical data was obtained from Twitter for the period from 2014 to 2019 for e-commerce who had a social media scandal in these years. Tweets were collected using the name of the company as a keyword. Data set was analyzed for sentiment fluctuations through a lexicon-based Sentiment Analysis. The polarity (negative, positive, neutral) of collected tweets was detected. The received Panel Data was estimated using through OLS, random-effect and fixed-effect approaches.

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# On Strong Duality in Linear Semidefinite and Copositive Programming

### O. Kostyukova

Institute of Mathematics, National Academy of Sciences, Minsk, Belarus

#### <u>T. Tchemisova</u>

#### University of Aveiro, Portugal

Copositive programming deals with optimization over the convex cone of socalled copositive matrices (i.e. matrices which are positive semi-defined on the nonnegative orthant). Copositive problems form a special class of conic optimization problems and have many important applications, including NP -hard problems.

Given a linear copositive programming problem, we derive for it a new extended dual problem which satisfies the strong duality relations and does not require any additional regularity assumptions.

The extended dual problem is based on the recently introduced concept of the set of normalized immobile indices, but neither the immobile indices themselves nor the information about the vertices of the convex hull of these indices is explicitly used.

The obtained strong duality formulations for linear copositive problems have similar structure and properties as that proposed in the works by M. Ramana, L. Tuncel, and H. Wolkowicz, for semidefinite programming.

Acknowledgements. This work was partially supported by state research program "Convergence" (Republic Belarus), Task 1.3.01, and by Portuguese funds through CIDMA – Center for Research and Development in Mathematics and Applications, and FCT – Portuguese Foundation for Science and Technology, within the project UID/MAT/04106/2019.

### Mathematical Modeling of Therapeutic Response to Yttrium-90 for Liver Cancer

#### S. Teerapol

### King Mongkut's University of Technology Thonburi, Bangkok, Thailand

The present paper considers a treatment of liver cancer with the Yttrium-90 radioemvolization, resulting in the necrosis of the liver be destroyed or reduced which is using a Single Photon Emission Computed Tomography-Computed Tomography (SPECT/CT) as diagnostic protocols. Since assessing cancer response to different dose of Yttrium-90, we develop a mathematical model and use it to simulate different dosage and treatment patterns. The model was constructed to focus on the interactions between existing cancer cell, new and developing cancer cell, and Yttrium-90 activity. We find that the treatment of cancer would be far more effective if patients were treated on a higher dose and treated every 1 month, the size of cancer was rapidly decreasing. When compared to actual treatment results in 3 patients, the change in cancer characteristics of the patients are consistent with the model.

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# A Comparison of Advanced Quasi Monte Carlo Methods for Multidimensional Integrals in Air Pollution Modeling

### V. Todorov

Institute of Mathematics and Informatics, and Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria

#### I.T. Dimov, Tz. Ostromsky

#### Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria

Sensitivity analysis of model outputs to variation or natural uncertainties of model inputs is very significant for improving the reliability of these models. Several efficient quazi-Monte Carlo algorithms - van der Corput sequence and Fibonacci based lattice rule have been used in our sensitivity studies of the model output results for some air pollutants with respect to the emission levels and some chemical reactions rates. The algorithms have been successfully applied to compute global Sobol sensitivity measures corresponding to the influence of several input parameters (six chemical reactions rates and four different groups of pollutants) on the concentrations of important air pollutants. The study has been done for the areas of several European cities with different geographical locations. This is the first time when the van der Corput sequence is applied to this problem and a comparison with the low discrepancy of Sobol has been made. The numerical tests show that the stochastic algorithms under consideration are efficient for the multidimensional integrals under consideration and especially for computing small by value sensitivity indices.

Acknowledgements. The work is supported by the Bulgarian National Science Fund under Young Scientists Project KP-06 M32/2-17.12.2019 "Advanced Stochastic and Deterministic Approaches for Large-Scale Problems of Computational Mathematics" and by the National Scientific Program "Information and Communication Technologies for a Single Digital Market in Science, Education and Security (ICT in SES)," contract No DO1-205/23.11.2018, financed by the Ministry of Education and Science in Bulgaria.

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# Determination of Elastic Properties in Metal Parts Made via Additive Manufacturing using Ultrasonic Measurements

<u>A. Toma</u>, T. Badea, R. Carlanescu

National Research and Development for Gas Turbines COMOTI, Bucharest, Romania

C. Rugina

IMSAR, Romania

### M. Soare

Nuclear NDT, Romania

#### D. Ionita

#### SC TECNITAL SRL, Bratasanca, Romania

The scope of this study was to determine the Young's Modulus using US measurements for two probes obtained through additive manufacturing. Young's Modulus of Elasticity can be determined through computations based on measured sound velocities and material density. The Young's Modulus determination was carried out in two different case studies, one performed by a RENAR (Romanian Accreditation Association) certified organization, NUCLEAR NDT, and one performed by COMOTI in cooperation with IMSAR (Solid Mechanics Institute of the Romanian Academy). Both studies carried out were on AM probes manufactured

from INCONEL 625 after the thermal treatment. The paper presents the steps followed: Density determination, Time of Flight determination, Longitudinal and transversal wave sound velocities determination and Young Modulus and Poisson coefficient determination. An comparative analysis between the two data sets were carried out. The results obtained in both case studies are very similar, so the procedure to determine the elastic properties of the metal parts made via additive manufacturing using ultrasonic measurements is validated. The observed small differences of the values could be induced by the probes thickness.

Acknowledgements. This work was carried out within POC-A1-A1.2.3-G-2015, ID/SMIS code: P\_40\_422/105884, "TRANSCUMAT" Project, Grant no. 114/09.09.2016 (Subsidiary Contract no. 3/D.1.1/114/27.11.2017), Project supported by the Romanian Minister of Research and Innovation.

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# A Mini-Review on Non-Destructive Techniques for Additive Manufactured Metal Parts

A. Toma, G. Matache, R. Condruz, R. Carlanescu

National Research and Development for Gas Turbines COMOTI, Bucharest, Romania

#### D. Ionita

SC TECNITAL SRL, Bratasanca, Romania

Worldwide the additive manufacturing technology it is used on large scale, on different fields of application, not only when unique parts are needed. Therefore, the manufacturing process must be carried out based on clear procedure and work instructions, the traceability of the entire process must be assured and acceptance criteria must be settled. A big role on the entire quality verification chain is the tests methods used to characterize the metallic parts fabricated. This article aims to provide an updated mini-review on the NDT approaches used to identify defects related to the powder-based additive manufacturing (AM) technologies. The minireview aim is to provide an overview on different NDT methods suitable for different types of manufacturing related flaws and defects. In the carried out study several characterizes were taken into consideration, such as: laser power, scan speed, layer thickness, spacing of scan lines, powder feed rate, powder size distribution, and surface chemistries. All this process parameters and powder attributes have impact on microstructural features present in AM components (e.g., grain size, texture, etc.) and are the cause to the generation of defects. Also, after reviewing the NDT approaches, a good practice short guide is presented in the paper.

Acknowledgements. This work was carried out within POC-A1-A1.2.3-G-2015, ID/SMIS code: P\_40\_422/105884, "TRANSCUMAT" Project, Grant no. 114/09.09.2016 (Subsidiary Contract no. 3/D.1.1/114/27.11.2017), Project supported by the Romanian Minister of Research and Innovation.

**Keywords:** Non-destructive techniques, metal additive manufactured, 3D scanning.

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## Giant Unilamellar Vesicle Formation: A Protocol Comparison

G. Valchev

Institute of Mechanics, BAS, Acad. G. Bontchev str., bl. 4, 1113 Sofia, Bulgaria

The cell membrane is a dynamic and complex barrier which separates the living cell from its environment. It consists of a high variety of lipids and proteins and is continuously reorganized by the cell, making its in vivo study difficult. Thus one has to use membrane model systems with precisely controlled composition to investigate fundamental interactions of membrane components under well-defined conditions. Giant unilamellar vesicles (GUVs) are well-known model systems, especially because they are easily observable using optical microscopy. In the present work, we give an overview of the existing methods for GUV production and present our efforts on forming single, free-floating vesicles up to several tens of  $\mu$ m in diameter and at high yield.

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### Numerical Modeling of Wave Processes in Multilayered Micropolar Plates and Shells

### M. Varygina

Institute of Computational Modeling of the SB RAS, Krasnoyarsk, Russia

With the appearance of new materials with prescribed properties of internal microstructure such as laminated or fibrous composites, granulated media, powderlike materials, mathematical models of micropolar media acquired special relevance. In this paper, the layer-wise description of the layered structure of micropolar thin bodies is considered. Each layer is seen as an independent plate or shell. Kinematic assumptions for each separate layer are made in the framework of the approximation approach. The compatibility conditions on the interface between two adjacent layers are introduced as additional constraints. The reduction of the three-dimensional problems of elastic micropolar media to the two-dimensional problems is performed using various averaging procedures in the thickness direction. In order to ensure the correctness of the initial boundary value problems, the systems of equations describing multilayered micropolar plates and shells are written in the form of thermodynamically self-consistent systems of conservation laws.

For the numerical analysis of the problems, parallel computational algorithms based on the two-cyclic splitting method in combination with monotone essentially non-oscillatory scheme and implicit finite-difference Crank-Nicolson scheme. Parallelization is performed by the CUDA (Compute Unified Device Architecture) technology. The computation results of wave propagation in multilayered micropolar plates and cylindrical shells are presented.

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### Planar Mappings of Spaces of Affine Connectivity

Yu. Vashpanov, O. Lesechko

Odessa State Academy of Civil Engineering and Architecture, Ukraine

#### O. Olshevska

Odessa National Academy of Food Technologies, Ukraine

Authors treat a certain generalization of geodesic mappings for spaces of affine connectivity with torsion. They obtain equations, which link corresponding tensors of Riemann, Ricci and Weyl of respective spaces and define objects that are invariant in respect to planar mappings.

# Generalized Multiscale Finite Element Method for Neutron Diffusion Equation

A. O. Vasil'ev, D. A. Spiridonov

North-Eastern Federal University, Yakutsk, Russia

A. V. Avvakumov

Kurchatov Institute National Research Center, Moscow, Russia

Construction of multiscale method for neutron diffusion equation is considered. The neuron diffusion approximation is mostly used for reactor analysis. To solve the problem on a fine grid the finite element method is used. The solution on a coarse grid was obtained with the use of the generalized multiscale finite element method (GMsFEM). The main idea is to create local multiscale basis functions that can be used to effectively solve on a coarse grid. Numerical results show that GMsFEM can take into account the small-scale characteristics of the medium and provide accurate solutions.

### Seasonality of the Levels of Particulate Matter PM10 Air Pollutant in the City of Ruse, Bulgaria

#### E. Veleva, I. R. Georgiev

### A. Kanchev University of Ruse, Bulgaria

This paper presents empirical study of the seasonality in air pollution of a Bulgarian city, caused by PM10 (particulate matter 10  $\mu$  micrometers or less in diameter). Different statistics, describing the change of PM10 over time have been considered. The trend and seasonality in the data are modeled using different approaches of time series analysis: regression models, decomposition, seasonal ARIMA models. The results are used to obtain point and interval estimates for future values of PM10 levels.

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# Seasonality of the Levels of Particulate Matter PM10 air pollutant in the city of Silistra, Bulgaria

#### E. Veleva, I. Zheleva, I. Georgiev

A. Kanchev University of Ruse, Bulgaria

This paper presents statistical study of the seasonality in air pollution PM10 (particulate matter with 10 micrometers or less in diameter) of the Bulgarian city Silistra, located near the Danube river. PM10 levels for the Danube region in Bulgaria mark a significant increase during the autumn-winter period compared to the levels during the spring-summer period. Different statistics, describing the change of PM10 over time have been considered. The trend and seasonality in the data are modeled using different approaches of time series analysis: regression models, decomposition, seasonal ARIMA models. The results are used to obtain point and interval estimates for future values of PM10 levels.

# Convective Mass Transfer in Crystallizers of Continuous-Flow with Screw Solution Inflow

N. A. Verezub, A. I. Prostomolotov

Ishlinsky Institute for Problems in Mechanics RAS, Moscow, Russia

### A.E. Voloshin

Shubnikov Institute of Crystallography RAS, Moscow, Russia

The mathematical model is considered for studying the process of growing a mixed crystal from a mixture of two water-salt solutions (salts of cobalt and nickel chlorides). The crystallizer model is equipped by an additional mechanism for screw solution inflows, which provides a high salt saturation and its homogeneity on the growing crystalline facet. The influence of crystallization surface microroughness on the features of its flow around by saturated solution is analyzed. The distributions of salt concentration and supersaturation on a smooth and micro rough crystalline facet are compared.

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# Nonlinear Phenomena in Dynamics of Convection-Coupled Equatorial Waves

M. Rostami University of Cologne, Germany

### <u>V. Zeitlin</u>

Sorbonne University, Paris, France

We demonstrate existence of a new type of coherent structures, equatorial modons, in the dynamics of equatorial waves in planetary atmospheres, show how they arise from localized pressure and wind anomalies in the vicinity of the Equator, and how they are enhanced and maintained by the moist convection. We compare then these structures with observations in the context of so-called Madden-Julian Oscillation in tropics.

### Test and Training Model of a Pyrolysis Unit with Three Vertical Tigels

Dz. Menseidov

Institute of Mechanics, BAS, Sofia, Bulgaria

#### M. Filipova, <u>I. Zheleva</u>

Angel Kanchev University of Ruse, Bulgaria

Pyrolysis is a thermal process in which automatic control is of great importance for the production of final products. This creates a challenge for the development of new technologies and ways of training and preparation of specialists. The creation of a reduced model of an automatic pyrolysis station system is such technology, which will enable learners to get acquainted, through the ongoing process simulation with many possible scenarios. This will increase the level of safety in the pyrolysis station itself during actual operation.

 ${\bf Keywords:} \ {\bf Automatic \ control \ systems, \ pyrolysis, \ education, \ simulation, \ training.}$ 

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# Study of the Efficiency Coefficient of the Steganographic Embedding in Text Containers Using the Letter Replacement Method

<u>S. Zhelezov</u>, T. Stoyanova Dept of Computer Systems and Technologies, Konstantin Preslavsky University of Shumen, Bulgaria

The embedding efficiency is one of the important indicators for the steganographic methods. This article presents a study of this indicator when embedding hidden information in text containers using the letter replacement method. Containers in four different languages were studied and a comparison of the embedding efficiency in each of these languages was made.

# Unification of Some Results via a General Approach to Simulation Functions in *b*-Spaces

 $\underline{\mathrm{K.~Zoto}}$ 

Dept of Mathematics & Computer Sciences, University of Gjirokastra, Albania

A. Sulaj

Faculty of Economics & Agribusiness, Agricultural University, Tirana, Albania

The metric spaces play a significant role in many fields of science. Therefore, in recent decades, these have been generalized by weakening, extending or even removing some axioms from their definition. Thus, due to the numerous applications in both pure and applied mathematics, the interest for studying their topological properties and fixed points is very high. Also, the study of the existence and uniqueness of fixed points in generalized spaces is of great interest. Starting from paper of F. Khojasteh in [1] many results in fixed point theory have been unified by using class of simulating mappings and type of Z-contraction. Recently by authors in [2,3] this class of mappings was extend by defining the notions of  $\Psi$ simulation function, and also types of  $Z_{\Psi}$ -contractions. In this work we define a general class, called  $\Psi$ -s simulation functions, and also types of  $\kappa_{\Psi-z}$ -contractions via new functions in the setting of b-metric-like spaces, covering, extending and unifying a large number of existing research work.

Keywords: Z-contraction;  $\Psi$ -s simulation functions; b-metric-like; fixed point

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