

Summaries of all articles

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Combination of the approaches of AMT tags database and labeling of oxygen isotope ^{18}O for quantitative analysis of human urine proteome

Mass spectrometric approaches of quantitative analysis of proteins and peptides imply the usage of isotopic labels. In this paper, we use a simple and cheap technique for peptide labeling of human urine proteome with oxygen-18 by hydrolysis in water $H_2^{18}\text{O}$. Quantitative analysis with the usage of ^{18}O combined with the earlier made data base of accurate mass and time tags of human urine proteome that gives the high descriptiveness of the approach without tandem mass spectrometry application. Within the bounds of the urgent problem of search and identification of the biomarkers on the basis of the comparative analysis of the expression of different genes the new approach to the calculation of the correct ratio of labeled to nonlabeled concentrations is developed. The offered correction of peak abundances in mass-spectra is based on the concept of averaged (hypothetical) amino acid «averagine». The availability of this approach for wide application in proteomics is demonstrated in model experiments.

Keywords: quantitative proteomics, mass spectrometry, accurate mass and time tags data base, isotopic labeling, oxygen 18, urine proteome.

G.N. Vladimirov, A. Kharchenko, R.M. Heeren, E.N. Nikolaev

Modeling of ion motion in orbitrap with accounting for space charge and electric field imperfections

The three-dimensional code based on a PIC algorithm modified for simulation of ion motion in orbitrap is used to investigate the effects of frequency shifts and electric field imperfections. The values of frequency shifts for a different amount of charge in ion clouds are obtained. The analytical description of the electric field imperfections by additional terms of the electric potential is proposed. The influence of imperfections on the ion cloud stability in these fields is investigated.

Keywords: mass-spectrometry, orbitrap, particle in cell, space charge.

P.A. Ryumin, I.A. Boldin, D.M. Avtonomov, E.N. Nikolaev

Simulation of ion clouds dynamics in arbitrarily shaped ion traps and ion transport devices using the capacitance method

We use the capacitance method to find the electric field with accounting of ion-ion interaction and ion-image interaction inside arbitrarily shaped mass spectrometric devices. The idea of the method is to replace the real electrodes, on the surface of which electric charge is induced by the ions inside, with a number of pointlike charges (capacitors). Their charges are computed given the condition that the surfaces of the electrodes are equipotential. We simulate ion clouds motion inside a Kingdon trap (Orbitrap) using the capacitance method combined with the Particle-In-Cell approach with the number of capacitors simulating the electrodes 1600.

Keywords: computer simulation, ion dynamics, capacity method, orbitrap, image charge.

A.P. Alekhin, I.P. Grigal, S.A. Gudkova, Y.Y. Lebedinskii, A.M. Markeev, A.A. Chouprik

Atomic layer deposition of ternary $\text{Hf}_x\text{Al}_{1-x}\text{O}_y$ dielectrics with high permittivity

The $\text{Hf}_x\text{Al}_{1-x}\text{O}_y$ thin film (~ 4 nm) atomic layer deposition process using the liquid-phase organometallic Hf precursor — $\text{Hf}[\text{N}(\text{CH}_3)(\text{C}_2\text{H}_5)]_4$ is developed. This process allows us to obtain $\text{Hf}_x\text{Al}_{1-x}\text{O}_y$ thin films in a wide range of Al concentration: 24–85 atomic percent. The $\text{Hf}_x\text{Al}_{1-x}\text{O}_y$ films reveal the structure of amorphous solid solution. The optimal composition $\text{Hf}_{0,76}\text{Al}_{0,24}\text{O}_y$ with rather high permittivity $k_{\text{high-}k} = 10,5$ and low leakage current density $1,8 \cdot 10^{-5} \text{ A/cm}^2$ at 5 MV/cm is found. The thermal annealing of $\text{Hf}_{0,76}\text{Al}_{0,24}\text{O}_y$ results in the increase of SiO_x intermediate layer and thus in the reduction of leakage current density by roughly an order of magnitude and the reduction of effective permittivity k_{eff} (by ~ 30 %) in $\text{Hf}_{0,76}\text{Al}_{0,24}\text{O}_y/\text{Si}$ structure.

Keywords: atomic layer deposition, thin dielectric films, HfO_2 , Al_2O_3 , HfAlO , structural and chemical properties, leakage currents, electrical characterization.

Y.S. Buranova

Study of cobalt-filled nanotubes by the transmission electron microscopy method

The objective of this research is to study the special features of carbon nanotubes grown in a gasostatic extruder with cobalt filler. Analysis of the crystallographic properties of cobalt filler is promising due to the special features of cobalt nanoparticles. The peculiarity of this research is using a gasostatic extruder for nanotubes synthesis, because this device is not practically used for this purpose. Electron microscope analysis shows the presence of nanotubes with cobalt particles in the test samples. Cobalt is more often found in FCC and HCP modifications. Also, cobalt carbide and nanotubes with differently deformed structures are found. Four different orientations of FCC cobalt particles against the tube's axis are established, viz. [100], [110], [111], [112]. Additional directions are due to twinning in the FCC lattice. In the HCP lattice [001], [110] and [1–14], orientations are established. The formation of three cobalt phases in nanotubes is connected with the carbon exhalation from the melt in the gasostatic extruder.

Keywords: carbon nanotubes, nano-sized cobalt, electron microscopy, deformation structures, graphite.

U.Y. Dziom, A.F. Shevchun, M.R. Trunin

«Whispering-gallery» modes for surface impedance measurements of superconducting crystals

We discuss the possibility and example of application of «whispering-gallery» modes of a cylindrical sapphire resonator to surface impedance measurements of superconducting single crystals with typical dimensions $1 \times 1 \times 0,1 \text{ mm}^3$.

Keywords: resonant methods, surface impedance, magnetic field, dielectric resonator, «whispering-gallery».

G.N. Freyberg

Spontaneous flow of distilled water in solution VWXbe through a drafty highly porous membrane

We present an experimental installation and the experimental results of a spontaneous flow of distilled water in solution VWXbe through a drafty highly porous hydrophobic membrane. The model calculations allow us to explain its nature and refer this process to an osmotic process.

Keywords: highly porous hydrophobic membrane, vacuum, pressure saturated flow of water vapour, spontaneous flow, osmotic process.

A.N. Besedina, N.V. Kabychenko

Investigation of the seismic oscillations in the long-period range of spectrum

The possibility of recording low-frequency oscillations in microseismic noise before earthquakes is considered. The characteristic period of fluctuations of the earth crust block can be moved to the low-frequency part of spectrum reaching values of the periods of hundreds of seconds when the zone of the earth crust transfers to a metastable state. For detection of such long-period oscillations in microseismic noise, special filtration methods are to be used. A correction scheme of the seismographs characteristics, for instance, geophone GS-20DX, which increases its frequency range to the lower frequency limit up to 0.5 Hz from the initial value of 10 Hz, is suggested.

Keywords: earthquake, seismic vibrations, long-period oscillations.

M.N. Golenko, N.N. Golenko

Entrainment and vorticity effects during wind-driven coastal upwelling and downwelling by the example of the South-East Baltic

When considering flow dynamics during wind-driven coastal upwelling or downwelling main attention is focused on the geostrophic alongshore flow and cross-shore ekman transfer. At the same time, the essential components of these processes are the entrainments (compensative flows) of the deep and respectively cool waters onto the surface towards the shore during upwelling and of near surface coastal waters into the deep layers out of shore during downwelling. The structure of the entrainment and the nature of the forces it is produced by are investigated in this paper. The investigations are carried out on the base of numerical modeling for the region of the South-East Baltic. The relationship between the term $U \frac{\partial U}{\partial x}$ and the other terms in the Navje-Stoks equation suggests that the entrainment is driven by nonlinear advection expressed in the term $U \frac{\partial U}{\partial x}$. The contribution of the nonlinear centrifugal forces into the quasigeostrophic balance on the surface layer of the area considered is also studied. For this purpose we analyze the local to planetary vorticity ratio $Ro = \frac{V \left(\frac{\partial V}{\partial x} - \frac{\partial U}{\partial y} \right)}{fV}$ called the Rossby Number.

Keywords: wind-driven coastal upwelling and downwelling, alongshore geostrophic flow, entrainment, current space structure, nonlinear advection, centrifugal forces, Rossby Number, numerical modeling.

E.A. Dorofeev, D.I. Ignatyev, A.N. Khrabrov

Application of artificial neural networks for simulation of unsteady aerodynamic characteristics

The conventional approach to the simulation of the unsteady aerodynamic characteristics using the aerodynamic derivatives does not provide the required precision of the results at high angles of attack due to the significant dynamical effects caused by the dynamics of flow separation and vortices breaking. A possibility of artificial neural networks application for simulation of the unsteady aerodynamic characteristics within a wide range of the angles of attack in the case of delta wing harmonic oscillations is shown. A short definition of the artificial neural networks is presented. Given in the present paper is the description of methods of mathematical simulation of the unstable aerodynamic characteristics. Mathematical models describing the results of dynamical experiments with forced oscillations obtained at different frequencies are presented. Hysteresis of the aerodynamic characteristics is simulated on an example of the delta wing.

Keywords: artificial neural networks, delta wing, unstable aerodynamic characteristics, high angles of attack, hysteresis.

V.P. Legostaev, A.V. Subbotin, S.N. Timakov, A.V. Zykov

On stability of the precession motion of a rotating ring-shaped membrane with central rigid insertion

One of the problems of angular maneuver guidance by a large rotating solar sail with central rigid insert is considered. According to Lyapunov's method, the stability of the stationary form of the sail at the regular precession of the membrane rotation axis is proved. The stationary form is found both by the method of direct integration of the nonhomogeneous partial differential equation and the Fourier decomposition method of the computed analytical solution on normal mode (Heine's local functions). In accordance with Voigt's hypothesis, the asymptotic stability of the sail's stationary form in case of the structural damping is proved.

Keywords: stability of motion, spacecraft, solar sail.

M.V. Mikhailov, I.I. Larkov

Solution of the relative navigation problem with use of ASN measurements

This paper describes operations of ASN-M satellite navigation hardware installed onboard the ISS. ASN-M performs solving the problem of ISS autonomous navigation. The functioning of satellite navigation software ASN-M is modeled by the mathematical simulation of the ASN navigation receiver. The analysis of perturbing factors' influence on the formed state vector accuracy is conducted using flight data modeling. The algorithms of ASN measurements' filtering are presented. These algorithms perform both the continuous generation of the ISS current state vector and increasing its accuracy. It is shown that the dynamic filtration of the measurements improves the accuracy of the relative position vector up to 0.5–1 m.

Keywords: control, motion, navigation, approach, system, space, station.

V.V. Ryzhakov, M.V. Ryzhakov

Development of the mathematical model of the estimation system of gas medium polycomposition and its parameter estimation algorithm according to the full-sized experiment

In this paper, we develop the mathematical model of the multichannel simultaneous estimation system of gas medium polycomposition, which is a system of interconnected transformation functions of separate channels on all components of the gaseous medium, which takes into account linear and nonlinear components of output data. The offered model allows us to consider the assemblage of experimental data and increase the precision of the medium composition estimation. The developed algorithm of model parameters definition realizes a repetitive process on the basis of the introduced systems of the conditional equations, which allows obtaining the demanded calculation accuracy with the essential simplification of corresponding procedures.

Keywords: mathematical model, gaseous medium, components, a multichannel system, transformation function, algorithm, a repetitive process, computing procedures.

A.I. Bachurin

Conceptual approach to the formation of innovation policies diversity oriented to the matching of supply and demand for innovations

The paper considers the problem of a lack of approach to the study of holistic diversity of modernization and innovation development policies that is one of the reasons of fragmentariness and low effectiveness of innovation management. The subject area is researched and its conceptual framework is synthesized: logic schemas of innovations and policies and its lines, as well as a model variety of policies based on methods of supply and demand for innovations matching.

Keywords: novelties, innovations, modernization, innovation policy, innovation development, variety, typology, strategic planning and management, demand, supply.

I.S. Guz

Training a monotone ensemble of classifiers using empirical risk minimization

The method for training monotone classifiers using an empirical risk minimization principle is introduced in this paper. Based on this method, a monotone ensemble of several independently trained classifiers is constructed. The classification quality of a monotone ensemble of classifiers depending on the number and type of algorithms it uses is researched using practical problems.

Keywords: monotone classifier, monotone corrector, classification quality of classifier ensembles.

F.A. Druzhinin, V.V. Tokarev

Engineering designing and financing of innovations — engineering optimum

We continue to study the joint solution of physical and financial feasibility of the innovation designs considered in [1]. The transition from the stream dynamical description to volumetric static description of the problem, which allows us to obtain the analytical solution and reveal the qualitative features of an engineering and financial engineering problem reduced to the classical problem of mathematical programming, is realized. The engineering problem is intentionally free from market financial restrictions, so its solution gives the upper bound of the efficiency of the innovation project, which can be identified with national economy activity.

Keywords: financial flow and capacity, discount corrections, engineering optimum, mathematical programming, sequential optimization.

V.A. Dykhta, S.P. Sorokin, G.N. Yakovenko

Control systems: extremality, optimality and identification conditions of the algebraic structure

A new class of Lyapunov- type functions dependent on the canonical state variables of the differential system of extremality conditions is introduced. These functions, being strongly and weakly monotone along trajectories of the system, extend the applicability of control theory methods that use solutions of the Hamilton-Jacobi inequalities and equation. Applying this class of functions for positional and optimization control problems is proposed. We also discuss mathematical models of controlled systems, which are based on groups and Lie algebras. We consider a procedure that allows using the «test» influence on the system to identify structural properties.

Keywords: maximum principle, extremality conditions, extremals, Hamilton–Jacobi inequalities, sufficient optimality conditions, identification systems, Lie groups and algebras, algebraic structure.

V.V. Karachik, N.A. Antropova

Construction of polynomial solutions of some boundary value problems for Poisson equation

The polynomial solution of the third boundary value problem for Poisson equation in a unit ball is found. The explicit representation of harmonic functions in the Almansi decomposition is used.

Keywords: third boundary value problem, Poisson equation, polynomial solution, Almansi decomposition.

B.G. Kukharenko

Study of the nonlinear dynamics system based on transient time series

The transient time series of nonlinear dynamic system variables are studied. Using the numerical solutions of the Duffing model as an example, spectral estimation features by the Prony method and the Hilbert transform are demonstrated. The amplitude-frequency dependency is defined for a numerical solution representing a free nonlinear oscillation. The defined dependency provides an opportunity to identify the nonlinear dynamical system.

Keywords: nonlinear dynamical system, transient time-series, spectral analysis, the Prony method, Hilbert transform, Duffing model, backbone curves, dynamical system identification.

A.V. Minaev

Criteria and methods for the estimation of social business projects

In this research, we try to estimate the social effect of social business projects. For this purpose, we classify types of the social effect on the basis of social business projects existing in Russia. For each such class, we offer the methodology of estimating the social effect size. On the basis of this analysis we offer selection techniques by the investor of social business projects.

Keywords: social business, social project, social effect, project evaluation, project selection.

N.I. Khokhlov, I.B. Petrov

Grid-characteristic method for modeling of seismic waves

This paper describes a method for simulating the propagation of elastic waves in a deformed solid. Love and Rayleigh seismic waves in three dimensions are numerically calculated. The results are in good agreement with theory. The potentialities of the developed software package are shown by the simulation result of the passage of elastic waves through a ground object. A possible destruction pattern is obtained under the Mises condition.

Keywords: grid-characteristic method, Rayleigh waves, Love waves, dynamics of deformable solids, modeling, systems of hyperbolic equations.

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The experience of the joint MIPT–Intel educational laboratory

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MIPT Experience in Selection, Vocational Guidance and Motivation to Scientific Work of Young People Gifted in Physics and Mathematics