Submissions

Soltionic solutions generated by quantum groups

Alexander Zuevsky, Academy of Science of the Czech Republic, Mathematics, Czech Republic

Abstract: We review the quantum group technique in construction of quantum soliton solutions to the affine Toda models. Various approaches are illustrated on the main example, the sine–Gordon equation.

View 1

Simulation of frequency dependence of dielectric susceptibility for description of director reorientation dynamics of nematic LC

Dmitrii Vakulin, National Research University of Information Technologies, Mechanics and Optics, Center "Information Optical Technologies", Russian Federation

Abstract: Simulation of the liquid crystal behavior in an external electric field allows to determine the characteristics of the LC device for specific control signal. The reorientation of director tilt angles is described by the Frank-Oseen elasticity theory, by the Leslie-Ericksen hydrodynamics theory and also by Maxwell system of electromagnetic equations. Due to the fact that it is difficult to obtain analytical solution of dependencies polar and azimuthal angles on time it is necessary to use numerical methods. The numerical solution allows to determine the characteristics of the LC device for specific control signal, but it does not allow to solve the inverse problem. It is determining the necessary parameters of the control signal. To solve this problem, we obtained an approximate analytical solution of the dynamics equations of the director reorientation under the electric field for arbitrary values of the elastic constants and boundary conditions. The results of numerical simulation of the director reorientation under the electric field in hybrid-oriented structure of a dual-frequency nematic liquid crystal were obtained. It is shown that results of analytical solution are in good agreement with the results of computer simulation and experiment in case of small deformations of the LC layer and used approximations.

View

A novel method for determining the mean-field directly from the single particle matter density

Shalom Shlomo, Texas A&M University, Cyclotron Institute, United States
Mason Anders, Texas A&M University, Cyclotron Institute, United States
Igal Talmi, The Weizmann Institute of Science, Department of Elementary Particle, Israel

Abstract: We present a novel method, using the single particle Schrodinger equation, to determine the central potential directly from the single particle matter density and its first and second derivatives. As an example, we consider the experimental data for the charge density difference between the isotones 206Pb – 205Tl, deduced by analysis of elastic electron scattering measurements and corresponds to the shell model 3s1/2 proton orbit, and determine the corresponding single particle potential (mean-field). We also present results of least-square fits to parametrized single particle potentials. The 3s1/2 wave functions of the determined potentials reproduce fairly well the experimental data within the quoted errors. The fair agreement with fitted potentials may be an indication that effects of short range correlations on charge distributions due

to shell model wave functions are not significant. More accurate experimental data, with uncertainty smaller by a factor of two or more, may answer the question how well can the data be reproduced by a calculated 3s1/2 wave function.

View

A Finsler Geometry Modeling of the Liquid Crystal Elastomer

Hiroshi Koibuchi, National Institute of technology, Ibaraki College, Mechanical and Systems Engineering, Japan
Andrey Shobukhov, Lomonosov Moscow State University, Faculty of Computational Mathematics and Cybernetics, Lab for Mathematical Modeling in Physics, Russian Federation

Abstract: Liquid crystal elastomer (LCE) is a rubbery material composed of polymer chains that consist of liquid crystals (LC). LCE is well known to undergo a shape transformation from the isotropic to the anisotropic phase. This shape transformation is caused by the nematic transition of the LC included in the LCE. However, the mechanism of this transformation is unknown because the interaction of LC with the bulk polymers is too complex. In this presentation, we extend the two-dimensional Finsler geometry model for membranes[1] to a three-dimensional model for LCE. The Finsler geometry model for LCE is a coarse grained one: the Guassian bond potential S_1 is obtained by extending the one for membranes, which is originally obtained by a simple extension of the Guassian bond potential for the linear chain polymer model. The continuous Hamiltonian, which contains S_1 and the curvature energy S_2, is discretized using a three-dimensional rigid sphere composed of tetrahedrons. We study the shape transformation as a phase transition between the isotropic and anisotropic phases and report the results of the transition order, obtained by the Monte Carlo simulations. [1] H. Koibuchi and H. Sekino, Physica A {\bf 393}, 37-51 (2014).

View

Generating fractal time series sequentially

Sy-Sang Liaw, National Chung Hsing University, Physics, Taiwan

Abstract: There exist a few methods for generating time series of a given fractal dimension. But none of them produces series sequentially. For example, the Random Midpoint Displacement method begins with the two end points of the intended series and feeds in points in between repeatedly. The spectral method prescribes a set of points satisfying a power law and makes a Fourier Transform to obtain the intended fractal series. Sequentially generating a fractal series of dimension 1.5 is easy, simply by simulating a one-dimension random walk step by step. It is also straightforward to generate a series of random numbers one by one to yield a fractal series of dimension 2.0. Unfortunately, fractal time series of a given dimension other than 1.5 and 2.0 have never being generated in a sequential manner. Real time series are recorded one data at a time, that is, sequentially. Many of them are fractals, and their dimensions could be 1.5, 2.0, or others, or even scale-dependent. How do these real systems generate its sequential data with a prescribed fractal dimension? In this report, we present a multi-scale N-step algorithm for generating fractal sequences sequentially. The algorithm predefines the probability, which is obtained in advance from random sequences we generated with a given fractal dimension, for upward change at any time as a function of the N changes in previous N steps. Sequences generated from this N-step algorithm have a monofractal dimension up to certain time scale but change into a random-walk sequence with fractal dimension 1.5 at larger scales. We find that by applying the probability function at several time scales simultaneously each with an appropriate weight on determining the change of the sequence at any time step, we are able to generate

monofractal sequences of quite a long length useful for any practical purpose.

View

DEMO of a virtual paper

Alfred Toms, University of Rome, Department of Physics, Italy
Jack Taylor, University of Rome, Department of Physics, Italy

Abstract: Test abstract

View

On the analysis of photo-electron spectra in extreme light

Phuong Mai Dinh, University Paul Sabatier (Toulouse 3), Laboratory for Theoretical Physics of Toulouse, France

Abstract: The progress in laser technology over the last decades has opened up new avenues for the exploration of properties of clusters and molecules. A laser pulse is characterized by its frequency but also by the laser intensity as well as the laser time profile. While for years the variations of these parameters were heavily constrained by technology, the last two decades, and even more so the last years, have seen tremendous increases in the range of attainable parameters. This is true for intensity~: since the 1990's, it can reach huge values which can lead to very large energy deposits and possibly violent disintegration of the irradiated species. But this is also true for the tuning of the time profile which can now be tailored up to time scales of the order of magnitude of electronic motion and even below. This allows the follow up of the detail of electronic dynamics at its own ``natural" time. The latest breakthroughs were attained in terms of laser frequency with the ongoing possibility of reaching very large frequencies up the X domain. This opens up new possibilities of imaging which are progressively being explored. Benefiting from the development of various coherent light sources and experimental setups, photo-electron spectra (PES) are widely used as a valuable tool to analyze the structure and dynamics of electronic emission in atoms, molecules or solids. One usually identifies the peaks observed in a PES with the mere density of states. However, this labelling can be cumbersome, or can simply fail, when several laser frequencies are used, as in a complex combination of an IR femtosecond pulse and a UV attopulse train. In this talk, we will first explain how time-dependent density functional theory in real time and real space can be used to compute PES. Then we will present a new interpretation of PES patterns in terms of spectral distributions of electronic dipole, monopole, and quadrupole moments, giving a relevant picture for the analysis of PES, especially in involved experimental setups.

View

Calculating Hurst exponent and fractal dimension of neutron monitor data in a single parallel algorithm

Arman Kussainov, al-Farabi Kazakh National University, Physics and Technology, Kazakhstan
Sain Kussainov, K.I. Satpaev Kazakh National Technical University, , Kazakhstan

Abstract: We implemented an algorithm for simultaneous parallel calculation of the Hurst exponent H and the fractal dimension D for the time series of interest. Parallel programming environment was provided by OpenMPI package installed on three machines networked in the virtual cluster and operated by Debian Wheeze operating system. We applied our program for a comparative analysis of week and a half long, one minute resolution, six channels data from neutron monitor. To ensure a faultless functioning of the written code we applied it to analysis of the random Gaussian noise signal and time series with manually introduced self-affinity features. Both of them

expected to have the well-known values of H and D. All results are in good correspondence to each other and supported by the modern theories on signal processing thus confirming the validity of the implemented algorithms. Our code could be used as a standalone tool for the different time series data analysis as well as for the further work on development and optimization of the parallel algorithms for the time series parameters calculations.

Acknowledgements: This research was supported by grant #2532/GF3 provided by the Education and Science Control Committee of the Ministry of Education and Science of the Republic of Kazakhstan to the author at the National Nanotechnology Open Laboratory.

View

The Geometrical Meaning of Time in the Presence of Matter

Asher Yahalom, Ariel University, Electrical & Electronic Engineering, Israel

Abstract: It is stated in many text books that the any metric appearing in general relativity should be locally Lorentzian i.e. of the type gμv = diag(1,−1,−1,−1) this is usually presented as an independent axiom of the theory, which cannot be deduced from other assumptions. The meaning of this assertion is that a specific coordinate (the temporal coordinate) is given a unique significance with respect to the other spatial coordinates. It was shown that the above assertion is a consequence of requirement that the metric of empty space should be linearly stable and need not be assumed [1-6]. In this work we remove the empty space assumption and investigate the consequences of matter on the stability of Lorentzian space-time. Bibliography [1] Asher Yahalom "The Geometrical Meaning of Time" ["The Linear Stability of Lorentzian Space-Time" Los-Alamos Archives - gr-qc/0602034, gr-qc/0611124] Foundations of Physics http://dx.doi.org/10.1007/s10701-008-9215-3 Volume 38, Number 6, Pages 489-497 (June 2008). [2] Asher Yahalom "The Gravitational Origin of the Distinction between Space and Time" International Journal of Modern Physics D, Vol. 18, Issue: 14, pp. 2155-2158 (2009). DOI: 10.1142/S0218271809016090. [3] Asher Yahalom "Gravity and the Complexity of Coordinates in Fisher Information" International Journal of Modern Physics D, Vol. 19, No. 14 (2010) 2233–2237, © World Scientific Publishing Company DOI: 10.1142/S0218271810018347. [4] Asher Yahalom "The geometrical meaning of time - the emergence of the concept of time in the general theory of relativity" a chapter in a book "Advances in Classical Field Theory", Bentham eBooks eISBN: 978-1-60805-195-3, 2011. http://www.bentham.org/ebooks/9781608051953/index.htm. [5] Asher Yahalom "On the Difference between Time and Space" Cosmology 2014, Vol. 18. 466-483. Cosmology.com. [6] Asher Yahalom "The Geometrical Meaning of Time - Some Cosmological Implications" Proceedings of 3rd International Conference on Mathematical Modeling in Physical Sciences (IC-MSQUARE 2014), 28–31 August 2014, Madrid, Spain. Journal of Physics: Conference Series (IOP Publishing), Volume 574, 012061, 2015. doi:10.1088/1742-6596/574/1/012061.

View

EFFECT OF DRYING TEMPERATURE ON CHEMICAL, PROPERTIES AND DIFFUSIVITY OF AVERRHOE BELIMBI

Nor Azni Shahari, Universiti Teknologi MARA, Mathematics, Malaysia

Abstract: In recent years, many fruits dried product have been developed in response to a strong demand by the customer. This fruit have a different composition and hence different moisture diffusivity (D) and during drying, Fick's Law of diffusion that describes the movement of liquid water was used to calculate this diffusivity. However diffusivity has strong effects on the material drying characteristic and must be determined. In this paper, Fick's Law of diffusion with different

kind of boundary conditions was solving using separation of variable (SOV). In order to get the value of D, result obtained using SOV will be compared with the result from the drying of belimbi at temperature of 40°C, 50°C and 60°C. Although the results show that difference between the values of diffusivity for different temperature is relatively small, but the difference in total time requires for drying is totally bigger between 3-7 hours. It show that diffusivity is important measurement and should be considered in the modeling of the drying process. The chemical properties of belimbi slices in terms of vitamin C, total ash and antioxidant activity with different air temperature and pre-treatment were also investigated. Higher drying temperatures gives less drying time, a lower vitamin C and antioxidant activity but greater total of ash, whilst pre-treatment can increased vitamin C and antioxidant activity. The results show that pre-treatment and the drying temperature are important variable to improve mass and heat transfer as well as the belimbi chemical properties.

Acknowledgements: This work was supported by Ministry of Education, Malaysia under Grant Nos 600-RMI/RAGS 5/3 (147/2014). and Universiti Teknologi MARA, Malaysia.

View

Computational chemistry insights on the REDOX Behaviour of Cr and W Fischer carbenes

Petrus van Rooyen, University of Pretoria, Chemistry, South Africa

Abstract: An electrochemical study of a series of Fischer carbene complexes containing a hetero-aryl group showed that Cr and W carbenes exhibit different electrochemical behaviour. The Cr carbenes is oxidized in two one electron oxidation processes, namely Cr(0) to Cr(I) and Cr(I) to Cr(II). On the contrary, Fischer carbene complexes of wolfram is directly oxidized from W(0) to W(II). The first reduction process observed for both W- and Cr-carbenes, is a one electron process. A density functional theory (DFT) computational chemistry study of the electronic structure of the Cr- and W-carbenes, showed that the oxidation is metal based and the reduction is located on the carbene ligand. The DFT calculations further showed that the Cr(II) species is a triplet and the W(II) species a closed shell singlet. DFT calculated ionization potential and electron affinity, relates linearly to the experimental oxidation and reduction potential respectively. Similarly the DFT calculated energy of the HOMO and LUMO of the neutral carbenes, relates linearly to the experimental oxidation and reduction potential respectively. These mathematical relationships obtained can be used to predict experimental measured potentials of related Fischer carbene complexes.

Acknowledgements: The South African National Research Foundation (JC), the Central Research Fund of the University of the Free State, Bloemfontein (JC) and the University of Pretoria (ML and PHvR) for financial assistance.

View

A DFT and structural investigation of the conformations of Fischer carbene complexes

Marilé Landman, University of Pretoria, Chemistry, South Africa

Abstract: A set of different Fischer carbene complexes of group VI and VII metals, with varied heteroatom or metallocenyl and heteroaromatic substituents on the carbene carbon atom, were studied. Density functional theory as well as single crystal diffraction techniques were employed to investigated the most stable conformation of these complexes. The complexes studied, [M(CO)4L{C(X)Z}], with L = PPh3 or CO, X = ethoxy (-OCH2CH3) or amino (-NH2 or NHCy) substituents as the heteroatom carbene substituents, Z = 2-furyl (-C4H3O), 2-thienyl (-C4H3S), 2-

(N-methyl)pyrrolyl (-C4H3NCH3) or cymantrenyl as the second carbene substituent had their substituents varied systematically to give complexes,. The conformations of the complexes, in particular the relative orientations of the heteroatoms in the molecule (syn vs. anti), E/Z isomerism in the aminocarbene complexes and cis/trans isomerism in the ligand substituted complexes as well as various combinations of these aspects, were studied. In general, it was found that the most stable conformation theoretically as well as in the solid state for most of the complexes preferred the syn conformation. The Z-isomer is generally preferred over the E isomer while the cis is more predominant than the trans isomer. Using DFT and NBO calculations, explanations for the preferred conformations were explored. It was concluded that both steric and electronic factors influence the conformations of the carbene complexes, with the extent of contribution of these two factors varying for each of the different carbene substituents.

Acknowledgements: The University of Pretoria for financial assistance.

View

A Fast Greedy Sparse Method of Current Sources Reconstruction for Ventricular Torsion Detection

Shiqin Jiang, Tongji University, School of Electronics and Information Engneering, China

Abstract: A fast greedy sparse (FGS) method of reconstructing cardiac equivalent current sources with 61-channel magnetocardiogram (MCG) data are developed for noninvasive detection and quantitative analysis of individual left ventricular torsion. The cardiac magnetic field inverse problem is solved based on an equivalent distributed source model and distributed current sources are reconstructed by the FGS algorithm. The results demonstrate that one or two dominant current source with larger strength can be identified efficiently. Then, the twisting movement of the left ventricle during systole is examined on the basis of x, y and z coordination curves and angle change of reconstructing dominant current sources. The advantages of this method are noninvasive, visible, with higher sensitivity and resolution. It also may detect cardiac systolic and ejection dysfunction in clinic.

Acknowledgements: Research supported by the National Natural Science Foundation of China (60771030), the National High-Technology Research and Development Program of China (2008AA02Z308), the Shanghai Science and Technology Development Foundation (08JC1421800), the Open Project of State Key Laboratory of Function Materials for Information (Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences).

View

Filtering in Stochastic Systems with Continuous Time over Observations with Memory in The Presence of Anomalous Noise.

Olga Rozhkova, Tomsk Polytechnic University, Lenina 30, 634050, Tomsk, Russia, department of the higher mathematics, Russian Federation

Abstract: We have carried out the synthesis of the optimal in the mean-square sense unbiased filter, for estimation of the state vector, when in the observation channel with memory the anomalous noises with unknown mathematical expectation act in addition to the action of regular noises. The synthesis has been carried out for linear stochastic system with continuous time. For optimal unbiased filter, in the mean-square sense, in the case of anomalous noises action in the observation channel with memory we have proved insensitivity of filter to inaccurate knowledge of matrix of anomalous noise intensity and its equivalence to truncated filter constructed only over nonanomalous components of an observation vector.

View

Virtual Laboratories in Physics with Autogenerated Parameters

Maksim Maksimov, St Petersburg State University, Physics, Russian Federation

Abstract: The paper deals with a virtual laboratory system, which in particular can be used to test knowledge through research. The participant can prefer which tools to operate and what actions should be taken. For the major part of tasks, there are copious ways to obtain the correct solution. One of the most important features of the system that distinguish this one among other simulation packages and educational systems is the pseudo-random physical parameters generation technique. The technique supports constraints and relationships between variables. As a result, it provides correctness and equal complexity of the generated task. The system can be very complex and is highly customizable by internal script system executed on server-side. The system is used as a part of distolymp Learning Management System with about 40 thousand participants per year.

View

Theoretical study of a 0.22THz quasi-optical gyrotron

Xuesong Yuan, University of Electronic Science and Technology of China, School of Physical Electronics, China

Abstract: The fully numerical calculation method for a quasi-optical gyrotron has been investigated in this paper. In this method, the analytical solution to different modes in the quasi-optical interaction cavity is replaced by the numerical solution based on electromagnetic simulation results. A 0.22THz quasi-optical gyrotron with HE06 mode has been investigated by using this method and simulation results show that this approach has a significant advantage of developing terahertz gyrotrons.

View

Pseudo Magic Squares

Ana Lucia Baccon, Universidade Estadual de Ponta Grossa, Matemática e Estatística, Brazil

Abstract: In this paper we introduce the concept of pseudo magic squares (ps-squares). More precisely, we relax the constraints on the numbers to be distinct between themselves and, based on this new definition, we show that this set has a group structure. Additionally, we generalize this concept, i.e., starting from a group we derive a generalized ps-square that also has a group structure. Furthermore, starting from a commutative ring with unity, we construct a ps-square having also a ring structure.

Acknowledgements: GGLG thanks CNPq for partial financial support.

View

The Coulomb interaction in one dimensional quantum mechanics: a distributional approach

José Lunardi, State University of Ponta Grossa, Mathematics and Statistics, Brazil

Abstract: Marcos Calçada1, José T Lunardi1, Luiz A Manzoni2, Wagner Monteiro3 and Marciano Pereira1 1Department of Mathematics & Statistics, State University of Ponta Grossa. Ponta Grossa, PR, Brazil 2Department of Physics, Concordia College. Moorhead, MN, USA 3Graduate Program in Mathematics, Department of Mathematics, Federal University of São Carlos. São Carlos, SP, Brazil In this work we propose a distributional approach to formulate in a mathematically consistent way the interaction between a quantum particle and a Coulomb potential –γ/|x|, (γ Є R) in one dimensional quantum mechanics. From basic mathematical and

physical requirements we specify the most general distribution to play the role of the interaction term in the Schrödinger equation; in this way we extend to the long-range Coulomb interaction a distributional approach formerly introduced to model singular zero range interactions. We discuss the role of symmetries in specifying particular choices of the Coulomb interaction and compare our results with those obtained in the context of the method of self-adjoint extensions.

View

Contact symmetries of constrained systems and the associated integrals of motion

Nikolaos Dimakis, Universidad Austral de Chile, Instituto de Ciencias Fisicas y Mathematicas, Chile

Abstract: The conditions for the existence of contact symmetries (polynomial in the velocities) of constrained systems that are described by quadratic Lagrangians is presented. These Lagrangians are mainly used in the construction of mini-superspace cosmological systems. In the literature, one usually adopts a gauge condition (mostly for the lapse N) prior to searching for symmetries. However, this is an unnecessary restriction that may lead to a loss of symmetries and consequently to the respective integrals of motion. A generalization of the usual procedure rests in the identification of the lapse function N as an equivalent degree of freedom and the according extension of the infinitesimal generator. As a result, conformal Killing tensors (with appropriate conformal factors) can define integrals of motion (instead of just Killing tensors used in the regular gauge fixed case). An example of a relativistic particle in a pp-wave space-time and under the influence of a quadratic potential is illustrated.

Acknowledgements: This work is supported by FONDECYT postdoctoral grant no. 3150016

View

Classification method for heterogeneity in monoclonal cell population

Sachiyo Aburatani, National Institute of Advanced Industrial Science and Technology, Biotechnology Research Institute for Drug Discovery (BRIDD), Japan
Kosuke Tashiro, Department of Systems Life Sciences, Graduate School of Systems Life Sciences, Kyushu University, Japan
Satoru Kuhara, Department of Systems Life Sciences , Graduate School of Systems Life Sciences, Kyushu University, Japan

Abstract: In recent years, monoclonal cell population is known to be composed of some heterogeneous sub-populations, thus our analyzed data is variously mixed and complicated. To gain clear insights into the mechanism of cellular system, the biological data of homogeneous cells should be obtained. In this study, we developed a method based on Latent Profile Analysis (LPA) combined with Confirmatory Factor Analysis (CFA) to divide the mixed data into some classes depend on their heterogeneousness. In general cluster analysis, the number of measured points is constraint, thereby the data can be classified into groups less than the number of samples. By our developed method, the measured data can be divided into groups by their latent effects without constraint. Our method is useful to clarify the all type of omics data, transcriptome, proteome and metabolites.

View

Canonical quantisation via conditional symmetries of the (closed) FLRW model coupled to a scalar field

Adamantia Zampeli, University of Athens, Physics, Greece

Abstract: In this talk, we study the classical, quantum and semiclassical solutions of some axisymmetric cosmologies coupled to a massless scalar field. The Lagrangian of these

minisuperspace models is singular and the application of the theory of Noether symmetries is modified to include the conditional symmetries of the corresponding (weakly vanishing) Hamiltonian. These are found to be the simultaneous symmetries of the supermetric and the superpotential. The quantisation is performed adopting the Dirac proposal for constrained systems. The innovation in the approach we use is that the integrals of motion related to the conditional symmetries are promoted to operators together with the Hamiltonian and momentum constraints. These additional conditions imposed on the wave function render the system integrable and it is possible to obtain solutions of the Wheeler-DeWitt equation. Finally, we use the wave function to perform a semiclassical analysis following Bohm and make contact with the classical solution. The analysis starts with a modified Hamilton-Jacobi equation from which the semiclassical momenta are defined. The solutions of the semiclassical equations are then studied and compared to the classical ones in order to understand the nature and behaviour of the classical singularities.

View

A Mathematical Model for the Temperature Profile of a Diesel Engine Exhaust Gas

José Ricardo Sodré, Pontifical Catholic University of Minas Gerais, Department of Mechanical Engineering, Brazil

Abstract: This work presents a heat transfer model for the exhaust gas of a diesel power generator to determine the gas temperature profile in the exhaust pipe. The numerical methodology to solve the mathematical model was developed using a finite difference method approach for energy equation resolution and determination of temperature profiles considering turbulent fluid flow and variable fluid properties. The simulation was carried out for engine operation under loads from 0 kW to 40 kW. The model was compared with results obtained using the multidimensional Ansys CFX software, which was applied to solve the governor equations of turbulent fluid flow. Results for the temperature and velocity profiles in the exhaust pipes shows a good proximity between the mathematical model developed and the multidimensional software.

View

Ultrashort Pulse Interaction with Intersubband Transitions of Semiconductor Quantum Wells

Ioannis Katsantonis, University of Patras, Physics Department, Greece
Elias Stathatos, Technological - Educational Institute of Western Greece, Electrical Engineering Department, Greece
Emmanuel Paspalakis, University of Patras, Materials Science Department, Greece

Abstract: In recent years various optical effects have been studied, both theoretically and experimentally, when intersubband transitions of semiconductor quantum wells interact with electromagnetic fields. In some of these studies the Rabi flopping and the coherent propagation of ultrashort far-infrared electromagnetic pulses that interact with a two-subband system in a symmetric semiconductor quantum well structure, taking into account the effects of electron-electron interactions, have been presented. All these studies have shown that at certain electron densities the electron-electron interactions make the intersubband transitions to behave quite differently from atomic transitions. Here, we revisit the problem of coherent ultrashort pulse propagation in a two-subband system in a symmetric semiconductor quantum well structure, performing calculations beyond the rotating wave approximation (RWA) and the slowly varying envelope approximation (SVEA) and taking into account the effects of electron-electron interactions. The interaction of the quantum well structure with the electromagnetic fields is studied with modified, nonlinear, Bloch equations. These equations are combined with the full-wave

Maxwell equations for the study of pulse propagation, so the coupled Maxwell-nonlinear Bloch equations are solved computationally beyond the RWA and SVEA. We present results for the pulse propagation and the population inversion dynamics in the quantum well structure for electromagnetic pulses with different pulse areas at the entrance of the medium and for different electron sheet densities.

Acknowledgements: This research has been co-financed by the European Union (European Social Fund - ESF) and Greek national funds through the Operational Program “Education and Lifelong Learning” of the National Strategic Reference Framework (NSRF) - Research Funding Program: Archimedes III. We thank Professors A. F. Terzis and M. M. Sigalas for useful discussions and help.

View

Size Effects in Elastic Thin Plates

Ruojing Zhang, Tongji University, Institute of Applied Mechanics, China

Abstract: It is well known that any material has a characteristic length (material length) which is depends on the microstructures of the material. The material length of metallic materials has the scale in microns. When the size of plates is getting smaller and is close to the characteristic length of the materials, their bending rigidity becomes larger than might be expected from the classical elasticity. This phenomenon is referred to as the scale effects or size effects. In the present paper, the couple stresses are introduced to model the size effect in elastic thin plates. An extended equation is developed which is available for the bending problem of the plate whose thickness is close to the material length. A comparison with micropolar theory of plates is made.

Acknowledgements: Supporting by the China National Science Foundation (Grant No. 11072178 and 11172214) is gratefully acknowledged.

View

Monte Carlo Software to Investigate ITO compounds

Zoubir HACHOUN, université Djillali Bounaama de khemis miliana , Sciences de la nature et de la vie et sciences de la terre , Algeria

Abstract: Z. Hachoun1,2 ; A Ouerdane 1,3 ; M.Bouslama 3, M.Ghaffour 3, A.Abdellaoui 3, A .Ali benamara2 1 Université de Khemis Miliana, Route de Theniet El Had 44225 KH-Miliana W. Ain Defla Algeria 3 LabMat Ecole Nationale Polytechnique d’Oran Mnaouer Oran 31000 ; Algeria 2 Université Hassiba Benbouali de Chlef. Algeria hachoun_zoubir @yahoo.fr ; ouerdanea@yahoo.fr (mailto:ouerdanea@yahoo.fr) Abstract: Computational background and program code enable us to study the interaction of electron beam with some Insulator transparent oxides (ITO) such as In2O3 and SnO2 compounds used in many technological applications .One of the most successful software in this field is Casino of acronym derived from the words “Monte CArlo SImulation of electroN trajectOry in the solid“. In our case it is based on the interaction process between incident electrons and the targets In2O3 or SnO2 to generate the X-rays signals so recorded [1]. The program of the CASINO simulation allowed us to scan the profile of the In2O3 oxide grown on InP and SnO2 grown on SiO2 substrate. The evolution of the X-rays intensities was monitored by the variation of electron beam energy. For instance, at the energy 4 keV we recorded the emission X-rays from the oxygen of In2O3 on InP and SnO2 grown on SiO2 respectively on fig.1a and fig1.b. The variation of the intensity and the location of peaks for each sample, displayed the morphology of point of view size and spacing of In2O3 and SnO2 microstructures. We note that these microstructures grew near each other for different spacing which might be related to the material structure due to the compactness and the chemical composition in agreement with the results

given by others authors[1,2]. The increase of the energy of the electron beam led to the increase of the intensity of the emission X-rays for both sample. Furthermore Casino software enables us to know the maximum depth reached by the electron beam into the compounds matrice as mentioned by fig.3. The variation of Zmax with the electron beam energy was depicted with accuracy in order to avoid the damage of the ITO compounds[3].

Acknowledgements: To Doctor A. Ouerdane and Professor A. Ali Benamara

View

Development of a Galactic Magnetic Field Model and its application in identifying sources of Ultra-High-Energy Cosmic Rays in Northern Sky.

Pantea Davoudifar, Research Institute for Astronomy and Astrophysics of Maragha (Riaam) , Astroparticle Physics, Iran (Islamic Republic of)
Keihanak Rowshan Tabari, Research Institute for Astronomy and Astrophysics of Maragha (RIAAM), Astroparticle Physics , Iran, Islamic Republic Of

Abstract: New physical conditions were applied to our previous Galactic Magnetic Field model. The relative motion of a Galactic source were also considered. We simulated the propagation of Ultra-High-Energy particles under the influence of Galactic Magnetic Field. In this research the particles were originated from millisecond pulsars located in the northern sky. Considering the relative motion of Galactic sources for a proper time interval, sample test images of millisecond pulsars were produced using cosmic rays of energies ranged in 1018-1019, 1019-1020, and 1020-1021 eV. The results were compared with our previous ones. For each part of the sky considering the structure of Galactic Magnetic Field, the source location and its relative motion to the observer, one may use these images as a guide to find possible sources of the Ultra-High-Energy Cosmic Ray' events. Consequently, a possible method of identifying the sources of these particles were introduced. Some physical limits were discussed.

View

Excitation properties of two-dimensional electron gases in quantum Hall states

Tao Yang, Northwest University, Institute of Modern Physics, China

Abstract: The superfluid, superconducting systems and Bose-Einstein condensates (BECs) share the same underlying mechanism arising from macroscopic occupation of a single quantum state. The quantum Hall (QH) effect can be explained by the condensation of the Chern-Simon composite bosons. However, due to the different types of interactions, the excitation properties of these systems would be quite distinct. In this paper we try to relate the phenomenon of the current induced quantum Hall breakdown (QHBD) with the dynamical excitations from the point view of the composite particle theory, in which the two-dimensional (2D) electron gas in QH systems can be regarded as a boson gas by attaching an odd number of magnetic flux quanta to each electron. We obtain the equation of motion of the composite bosons in the mean field limit, which is similar to the 2D Gross-Pitaevskii equation for condensates, and get the dispersion relations of the collective excitations in the QH states for different situations. We study vortex excitations in the QH states which are related to the current induced QHBD, and compared this situation with the vortex excitations induced when a BEC superfluid passes an impenetrable obstacle.

View

TensorPack: a Maple-based software package for the manipulation of algebraic expressions of tensors in general relativity.

Peter Huf, Deakin University, School of Information Technology, Australia

John Carminati, Deakin University, School of Information Technology, Australia

Abstract: In this paper we: (1) introduce TensorPack, a software package for the algebraic manipulation of tensors in covariant index format in Maple; (2) demonstrate the use of the package with the an orthonormal tensor proof of the theorem =0 => =0 for dust. TensorPack is based on the Riemann and Canon packages (R. Portugal, S.L. Sautú, Applications of Maple to General Relativity, Comput. Phys. Commun., 105, (1997) 233-53; J.M. Martín-García, R. Portugal, L.R.U. Manssur, The Invar Tensor Package, Comput. Phys. Commun. 177 (2007) 640-648) and uses their functions to express tensors in an indexed covariant format. TensorPack uses a string representation as input and provides functions for output in index form. It then extends the functionality to basic algebra of tensors, substitution, covariant differentiation, contraction, raising/lowering indices, symmetry functions and other accessory functions. The output can be merged with text in the Maple environment to create a full working document with embedded dynamic functionality. Following a description of the package, we demonstrate the use of the package by duplicating the proofs for the shear-free theorem for dust as based on Senovilla et al. 1997 (Senovilla, JMM, Sopuerta, C.F., & Szekeres, P. 1998, 'Theorems on shear-free perfect fluids with their Newtonian analogues', Gen.Rel.Grav, vol. 30, pp. 389-411). In this current paper we also present a second version of the proof using the software by employing tensor conditions for vorticity. The package offers potential for manipulation of indexed algebraic tensor expressions in a flexible software environment.

Acknowledgements: We are grateful to J. Senovilla and C. Sopuerta for providing details of some of the more difficult sections of their proofs. We are also grateful to the authors of the Riemann and Canon packages.

View

The difficult birth of silicene and the debut of germanene

Guy Le Lay, Aix-Marseille University, CNRS-PIIM, France

Abstract: Both Europe and the USA, have already invested millions of dollars in the field of two-dimensional (2D) materials, launching such programs as the European Commission's €1 billion Graphene Flagship Project, or the US National Science Foundation's (NSF) Emerging Frontiers in Research and Innovation (EFRI) 2-Dimensional Atomic-layer Research and Engineering (2-DARE) initiative. The field of 2D materials beyond graphene, notably novel elemental ones like silicene, germanene and phosphorene, is accelerating at a rapid pace. Typically, in Europe, all members of this family have been included in the “Science and technology roadmap for graphene, related two-dimensional crystals, and hybrid systems” [1]. The first silicene field-effect transistors operating at room temperature have been fabricated in concert by an American team in Austin and an Italian team in Milano, member of the 2D NANOLATTICES research project funded by the 7th Framework Program of the European Commission –Future and Emerging Technologies (FET) [2]. The synthesis of silicene on a silver substrate has been published for the first time in 2012, in this context [3], and, similarly, that of germanene, on a gold template, in 2014 [4]. In this talk, I will recall how these novel synthetic 2D materials made their debut in Marseille, despite a major obstacle placed on their way [5]. [1] Ferrari, A.C. Nanoscale 7, 4587–5062 (2015). [2] Tao, L. et al., Nature Nanotechnology 10, 227-231 (2015). [3] Vogt, P. et al. Phys. Rev. Lett. 108, 155501(2012). [4] Dávila, M. E., Xian, L., Cahangirov, S., Rubio, A. & Le Lay, G. New J. Phys. 16, 095002 (2014). [5] Le Lay, G., De Padova, P., Resta, A., Bruhn, T. and Vogt, P. J. Phys. D: Appl. Phys. 45, 392001 (2012).

View

Ground state of a two-component dipolar Bose-Einstein condensate in

concentrically coupled annular traps

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Abstract: We investigate the ground-state and rotational properties of a rotating two-component dipolar Bose-Einstein condensate, which consists of both dipolar bosonic atoms with magnetic dipole moments aligned vertically to the condensate and one without dipole moments, confined in concentrically coupled annular traps. We identify the states where the two components coexist, or separate, either radially or azimuthally, as a function of the ratio of dipolar to intra-component contact interactions, and of the rotational frequency. It is found that the tunable dipolar interaction can be used to control the location of each component between the inner and outer rings, and to induce the desired ground-state phase. We also discuss the vortex structure of such a two-component system for nondipolar and dipolar cases, and find various interesting vortex structures, such as interlaced honeycomb and octagonal vortex clusters, as well as vortex necklaces.

Acknowledgements: This work was supported by NSF of China under Grants Nos. 11104064, 11174282, 11303030, and 11474282; the NSF for Distinguished Young Scholars of China under Grant No. 61025023; the NMFSEID under Grant No. 61127901; the key project fund of the CAS for the ‘‘Western Light’’ Talent Cultivation Plan under Grant No. 2012ZD02; the Science and Technology Project of Shaanxi Province under Grant No. 2013KJXX-03,; and the Youth Innovation Promotion Association, CAS.

View

Exploring Silicene mono- and multilayers of Silicene with soft X-ray spectroscopy and DFT calculations

Alexander Moewes, University of Saskatchewan, Physics and Engineering Physics, Canada

Abstract: 2012 brought the first reports of a new member of the 2D material family: a hexagonal honeycomb of Si atoms deposited on the Ag(111) surface called “silicene”[1]. The characteristics and stability of freestanding silicene had previously been theoretically explored [2], and there was a strong push to determine if the epitaxial sheets possessed the promising qualities of their hypothetical freestanding counterparts. Initially, the results of angle-resolved photoemission spectroscopy (ARPES) experiments were thought to indicate that epitaxial silicene had a gapped Dirac cone in its electronic structure [1], as would be expected of freestanding silicene with a broken inversion symmetry. This enticing result, however, would be later overturned through a combination of experimental and theoretical techniques [3-5], and it would eventually be concluded that the epitaxial silicene sheet was in fact metallic with a strong cohesion to the underlying Ag(111) face. However, this conclusion would prove controversial [6,7], as the ambiguity of the ARPES data left some room for interpretation as to whether specific electronic features belonged to the epitaxial Si, the Ag substrate, or represented a hybridization between the two. Soft X-ray emission and absorption spectroscopy (XES and XAS) are synchrotron-based experimental techniques for probing the element-specific projected density of electronic states (PDOS) in the valence and conduction bands of a material. When performed in combination at the Si L2,3 emission and Si 2p absorption edges, XES and XAS allowed us to unambiguously show that the Si valence and conduction states were continuous across the Fermi energy; i.e. that the silicene overlayer was indeed metallic [3]. Complementary DFT simulations also showed a large degree of bonding between the Si overlayer and the Ag substrate. This result is an important but unfortunate finding, as it limits the future utility of epitaxial silicene monolayers on Ag(111). If they are to come into use they must be all at once isolated from their substrates, stable and possessing the linear band dispersion that is responsible for the desirable characteristics unique to 2D electronic systems. One suggested way of achieving these characteristics is to produce a

multilayer of silicene on the Ag(111) surface. These materials have been briefly described in the literature, and early indications suggest that they might play host to a Dirac cone structure [8]. However, other reports insist that bilayers and multilayers are inherently unstable, collapsing into bulk Si nanocrystals shortly after the monolayer deposition is complete [9]. Our DFT calculations predict a stable, AA-stacked silicene bilayer on Ag(111) that corresponds nicely to the scanning tunnelling microscopy (STM) bilayer observations. Unfortunately, these same DFT calculations predict a similar electronic structure as that of the monolayers, namely metallic and bound to the Ag(111). However, our XES and XAS measurements indicate a transition to bulk, sp3-hybridized Si beginning shortly after the completion of a monolayer, supporting the low-energy electron microscopy study that first suggested the nucleation of the silicene sheets to bulk crystals [10] (see Figure). In this way, XES, XAS and DFT provide us with a method for evaluating structural models, predicting and measuring electronic characteristics and determining the composition of a particular sample simultaneously. References: 1. P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M.C. Asesnsio, A. Resta, B. Ealet and G. Le Lay. Phys. Rev. Lett. 108, 155501 (2012). 2. S. Cahangirov, M. Topsakal, E. Aktürk, H. Şahin and S. Ciraci. Phys. Rev. Lett. 102, 236804 (2009). 3. N.W. Johnson, P. Vogt, A. Resta, P. De Padova, I. Perez, D. Muir, E. Z. Kurmaev, G. Le Lay and A. Moewes. Adv. Funct. Mater. 24, 5253 (2014) 4. S. Cahangirov, M. Audiffred, P. Tang, A. Iacomino, W. Duan, G. Merino and A. Rubio. Phys. Rev. B 88, 035432 (2013). 5. D. Tsoutsou, E. Xenogiannopoulou, E. Golias, P. Tsipas and A. Dimoulas. Appl. Phys. Lett. 103, 231604 (2013). 6. S. Huang, W. Kang and L. Yang. Appl. Phys. Lett. 102, 133106 (2013). 7. J. Avila, P. De Padova, S. Cho, I. Colambo, S. Lorcy, C. Quaresima, P. Vogt, A. Resta, G. Le Lay, M. C. Asensio. J. Phys.: Condens. Matter 25, 262001 (2013). 8. P. De Padova, P. Vogt, A. Resta, J. Avila, I. Razado-Colambo, C. Quaresima, C. Ottaviani, B. Olivieri, T. Bruhn, T. Hirahara, T. Shirai, S. Hasegawa, M. C. Asensio and G. Le Lay. Appl. Phys. Lett. 102, 163106 (2013). 9. A. Acun, B. Poelsma, H.J.W. Zandvliet and R. van Gastel. Appl. Phys. Lett. 103, 263119 (2013). 10. N.W. Johnson, D. Muir, E.Z. Kurmaev, and A. Moewes. (under review).

View

DFT analysis of the interface between silicene and Ag(111). Toward a possible covalent functionalization

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Abstract: The (3x3) silicene on (4x4) Ag(111) surface is investigated by means of density functional theory calculations [1]. We focus on the nature of the interactions between the silicene and the Ag surface, in terms of spatial charge localization. No covalent bonds are formed between the silicene and the Ag surface, but there is an overlap between the charge densities of the bottom Si atoms and the nearest Ag atoms. A clear charge reorganization takes place when bringing together the silicene and the Ag substrate. According to Bader charges calculations, the top Si atoms are slightly positively charged, while the Ag surface plane carries a negative charge. This indicates that an electrostatic interaction exists between the Si top atoms and the below-lying Ag atoms resulting in the first possible explanation of the Ag buckling. In the second part of the talk, the possible fuctionalization of the silicene/Ag system will be addressed [2]. Silicene, which forms sp2-sp3 bonds, is expected to present a higher reactivity than graphene, characterized by sp2 bonds only. However, silicene functionalization, with organic molecules, remains an open question. Within density functional theory, we study the adsorption of benzene, a model organic molecule, on the (3x3) silicene on (4x4) Ag(111) surface. We show the presence of two C-C bonds between the benzene molecule, which adopts a butterfly configuration on the silicene. The silicene lattice is

slightly deformed upon benzene adsorption. A charge transfer occurs from top Si atoms to both molecule and Ag substrate. Finally, we show that the covalent functionalization of silicene is possible. REFERENCE [1] R. Stephan, M.-C. Hanf and Ph. Sonnet, Journal of Physics: Condensed Matter 27 (2015) 015002 (freely available on IOPselect). [2] R. Stephan, M.-C. Hanf and Ph. Sonnet, Phys. Chem. Chem. Phys. (submitted).

Acknowledgements: This work was performed using HPC resources from GENCI-IDRIS and the supercomputer facilities of the Mésocentre de l'Université de Strasbourg (grant 2014).

View

Wave function of the Universe, preferred reference frame effects and metric signature transition

Hossein Ghaffarnejad, Semnan University, Physics, Iran, Islamic Republic Of

Abstract: Non-minimally coupled Brans Dicke (BD) gravity with dynamical unit time-like four vector field is used to study flat Robertson Walker (RW) cosmology in the presence of variable cosmological parameter described in terms of the BD field as $V(\phi)=\Lambda\phi^n.$ Aim of the paper is to seek cosmological models exhibiting with metric signature transition. The problem is studied in both classical and quantum cosmological approach. Solutions of classical dynamical equations lead to nonsingular inflationary scale factor of space time as $R(t)=l_p\cosh(t/l_p)$ where l_p denotes to Planck length. Corresponding Euclidean signature scale factor is obtained directly by changing $t\to it$ as $R(t)=l_p\cos(t/l_p)$ describing re-collapsing universe. Dynamical vector field together with the BD scalar field treats as fluid with time dependent barotropic index $\gamma(t)=p(t)/\rho(t)$ where $p(t)$ and $\rho(t)$ are pressure and density of the fluid. At large scales of the space time we obtain $\gamma(t)\to -1$ corresponding to dark matter dominant of the fluid. Positive values of this parameter is obtained only at the Euclidean regime of the space time and whose value is changed from $-\infty$ to $+\infty$ on the metric signature transition hypersurface $t=0$ where metric is degenerated. Dust and radiation domains of the fluid stands on the Euclidean regime of the space time. Euclidean regime is also contained $\gamma(t)

View

Dynamics of Molecules in Gas Electron Diffraction

Yury Vishnevskiy, Bielefeld University, Chemistry, Germany
Denis Tikhonov, Bielefeld University, , Germany
Yuriy Zhabanov, Ivanovo State University of Chemistry and Technology, , Russian Federation

Abstract: Gas electron diffraction (GED) is a direct method for experimental investigation of structure and dynamics of free molecules. Depending on the applied vibrational model it is possible to determine different types of thermally average molecular structures, equilibrium structure, mean square amplitudes of interatomic vibrations and potential functions of internal motions with high accuracy and precision. One of the latest examples is the investigation of 1,2,3,4,5-pentafluoroferrocene .[1] In our current project we are developing the GED method further to be able to investigate larger molecules. Among other difficulties the calculation of vibrational amplitudes and corrections for interatomic distances is problematic because of size of molecules. To overcome this problem the ab initio molecular dynamics is used. A special code for processing molecular dynamics trajectories and applying quantum corrections has been written. This code has been used in real GED investigations of several 1,2-dicarba-closo-dodecaborane derivatives. To assess the reliability of obtained results the same parameters have been calculated on the basis of harmonic and cubic force fields using first order perturbation theory of Sipachev.[2] For this purpose a program has been written, whose main advantages in comparison

to analogs are ability to handle large molecules and significantly increased computational performance. [1] K. Sünkel, S. Weigand, A. Hoffmann, S. Blomeyer, C. G. Reuter, Yu. V. Vishnevskiy, N. W. Mitzel, JACS, 137, 2015, 126 – 129. [2] V. A. Sipachev, J. Mol. Struct., 693, 2004, 235 – 240.

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View

Interaction ions matter by TRIM Monte Carlo code to analyze Semiconductor Surface behavior

Abdallah Ouerdane, Université Djilalli Bounaama de Khemis Miliana, Sciences des matériaux faculté des Sciences et de la technologie, Algeria

Abstract: A Ouerdane *,** Z. Hachoun*; M.Bouslama **, M.Ghaffour **, A.Abdellaoui **, *Université de Khemis Miliana, Route de Theniet El Had 44225 KH-Miliana W. Ain Defla Algeria ** LabMat Ecole Nationale Polytechnique d'Oran Mnaouer Oran 31000 ; Algeria ouerdanea@yahoo.fr (mailto:ouerdanea@yahoo.fr) Abstract: Computational background and program code are reported to study the interaction of ions beam with the semiconductor surfaces. Ziegler et al. [1] have developed a good simulation methods TRIM (Transport and Range of Ion in Mater) and SRIM (Stopping and Range of Ion in Mater) to characterize the interaction of the ions irradiated or targeted gas and solids samples [2] In our study the Ar+ ions bombardment is achieved according to the normal incidence with the surface of atoms of the target with the possibility to form vacancies on irradiated area of some III-V compounds as InP, InSb and InN. concerning the effect of Ar+ InSb, allowing us to affirm the formation of nanostructures Fig.1 gives the TRIM spectra :(the number of vacancy as function of the depth) or the ions Ar+ at the for three compounds which enables us to deduce a range projectile of about Rp =28 Á , Rp=22Á , Rp=19Á respectively for InN InP and InSb compound at energy set at 300 eV. Using TRIM only, we could not determine the size (height and periodicity) of these features so we use the Sigmund simulation method which depends on the sputtering yield Y (Ɵ, E) (the number of atoms removed per incident ion), where Ɵ is the incident angle, formed by the direction of the incident ion beam and the surface of the target, and E the ion incident energy [3]. Also it depends on the nuclear stopping cross section computed by the SRIM simulation method which is based on the interaction process between the Ar+ ions of different energies and the matter.. The Sigmund theory is a successful theory describing the sputter yield Y(Ɵ,E) in the linear cascade regime[4].The energy dependence of the sputter yield) is complex because it defines the three regimes of sputtering, i.e. the direct knock-on, linear cascade and spike sputter regimes [5]. The ion energy used in this study is usually the one associated with the linear cascade regime. The bombardment-induced topography can be quantitatively described in terms of a noisy Kuramoto–Sivashinsky partial-differential equation [5] which is extremely complicated. The analytical solution has been obtained for simplified form, giving to the height h(x, y, t) of the roughness surface of the target as function of the bombarded ion energy E, the fluence ɸ and the sputtering yield Y (0, E) .Using SRIM 2008, we plot successively the spectra corresponding to the variation of the stopping range Sn and the sputter yield Y (0, E). However, our aim is to know the nanodots height h(x,t) formed by Ar+ and the spatial periodicity for the studied III-V compounds According to our result in Fig.2., the roughness amplitude h(x, t) of the nanostructures due to Ar+ ion bombardment is about 20Å and 30 Å 35 Å for InSb and InP and InN respectively at 300 eV incident ion, energy and 45 mn of sputter time. In another hand, according to Bradley- Harper and Johan .B. Malherbe et al; the wavelength or the spacing between bombardment-induced ripples depend on the ion flux J (number of ion by cm2), the sputter yield of the bombarding ions Y(0,E) ,the density of III-V compounds InP and InSb of energy deposition E, the surface diffusion parameter; the range

projectile Rp of energy deposition E computed in.fig.8 for the thee compounds respectively. Using all these parameters, we compute the values of for each compound.

Acknowledgements: To the Prof.Bouslama and Y.Al-Dury

View

State transition induced by higher-order effects and background frequency

Zhan-Ying Yang, Northwest University, School of Physics, China

Abstract: The state transition between the Peregrine rogue wave and W-shaped traveling wave induced by higher-order effects and background frequency is studied. We find that this intriguing transition, described by an exact explicit rational solution, is consistent with the modulation instability (MI) analysis that involves a MI region and a stability region in a low perturbation frequency region. In particular, the link between the MI growth rate and the transition characteristic analytically demonstrates that the localization characteristic of transition is positively associated with the reciprocal of the zero-frequency growth rate. Furthermore, we investigate the case for nonlinear interplay of multilocalized waves. It is interesting that the interaction of second-order waves in the stability region features a line structure rather than an elastic interaction between twoW-shaped traveling waves.

View

A Frontier orbital energy approach to redox potentials

Jeanet Conradie, University of the Free State, Chemistry, South Africa

Abstract: The prediction of the oxidation and reduction potentials of molecules is important in many research areas. A review of relationships obtained between frontier orbital energies (HOMO and LUMO energies in eV) and the calculated ionization potential (IP in eV) or adiabatic electron affinity (EA in eV) and experimental oxidation and reduction potentials for selected series of beta-diketones, rhodium-beta-diketonato and metal-tris-beta-diketonato complexes is presented. The good linear relationships obtained for related series of complexes show that the oxidation and reduction potentials of these complexes can be predicted by their DFT-calculated energies: beta-diketones: Epc (V vs. Fc/Fc+) = -0.63 ELUMO – 3.63 R2 = 0.99 Epc (V vs. Fc/Fc+) = 0.62 EA – 2.39 R2 = 0.84 Fc-containing beta -diketones: E0' (V vs. Fc/Fc+) = -0.24 EHOMO – 1.15 R2 = 0.92 E0' (V vs. Fc/Fc+) = 0.098 IP - 0.40 R2 = 0.87 Fe(beta -diketonato)3: E0' (V vs SCE) = -0.59 ELUMO – 2.74 R2 = 0.96 E0' (V vs SCE) = 0.71 EA – 1.94 R2 = 0.94 Mn(beta -diketonato)3: (Epc + Epa)/2 vs SCE/V = -0.76 ELUMO – 2.75 R2 = 0.98 (Epc + Epa)/2 vs SCE/V = 0.83 EA – 1.95 R2 = 0.91 Rh(beta -diketonato)(P(OPh)3)2: Epa (V vs. Fc/Fc+) = -1.50 EHOMO – 7.81 R2 = 0.85 Rh(beta -diketonato)(CO)(PPh3): Epa (Rh in V vs. Fc/Fc+) = -0.45 EHOMO – 2.11 R2 = 0.89 Epa (Rh in V vs. Fc/Fc+) = 0.29 IP – 3.65 R2 = 0.97 Rh(beta -diketonato)(cod): Epa (Rh in V vs. Fc/Fc+) = -0.35 EHOMO – 1.31 R2 = 0.90 Epa (Fc in V vs. Fc/Fc+) = -0.39 EHOMO-1 – 1.52 R2 = 0.99

Acknowledgements: This work has received support from the Norwegian Supercomputing Program (NOTUR) through a grant of computer time (Grant No. NN4654K), the South African National Research Foundation, HPC Warehouse Facility and the Central Research Fund of the University of the Free State, Bloemfontein.

View

Modeling of intense charged particle bunch dynamics in external magnetic fields

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Matter States, Russian Federation
Mikhail Saratovskyh, National Research Nuclear University MEPhI, Department of Physics of Extreme Matter States, Russian Federation

Abstract: The program module CAMFT is developed to calculate the intense charged particle bunch dynamics in external magnetic fields. The program is based on the accurate solution of the motion equation for each particle of the intense bunch that allows to exclude the problems typical for PIC-method. The program is written on C++ and uses OpenMP 2.0 for parallelization, so one can simulate the behavior of the bunch with intensity about 109-1010 particles. Visual C++ and library Qt 4.8.3 of qtcreator are used for the result visualization. Dynamics of the bunch with arbitrary phase distributions in magnetic fields of arbitrary geometry may be studied by means of the program. The actual CAMFT version is checked while accelerating structure with racetrack geometry simulated. Modified CAMFT version is checked for ITEP Heavy-Ion Prototype mass-spectrometer.

View

A software tool based on the Surface Evolver for precise location of tumours as a preoperative procedure to partial mastectomy

Valério Ramos Batista, Federal University of ABC, CMCC, Brazil
Marcelo do Nascimento, Federal University of Uberlandia, Faculty of Computing, Brazil
Antonio Elias Fabris, University of São Paulo, IME, Brazil

Abstract: We present a fast and reliable program that gives precise location of breast tumours for a partial mastectomy. Our program is fully implemented in the Surface Evolver, which is a general-purpose simulator of physical experiments. By starting from the mammograms that show a tumour one takes its 2D coordinates in each view (CC and MLO). These coordinates, together with some measurements of the patient's breast, are given as input to our simulator. From this point on the simulator reproduces all main steps of taking mammography with a virtual transparent breast that matches the patient's. The virtual mammography procedure is graphically displayed on the computer screen, so that users can track the virtual tumour inside the breast. As output we have the coordinates of the tumour position when the woman lies on the operating table for the surgery. With these coordinates the surgeon can make a small incision into the breast and reach the tumour for its removal. The whole structure of the breast is preserved after a simple plastic correction.

View

Gauss Runge-Kutta methods for general relativistic long-term integrations

Jonathan Seyrich, University of Tuebingen, Faculty of Math and Science, Germany

Abstract: In simulations of possible sources of gravitational waves, long-term integrations of general relativistic binary systems are required. For this purpose, we show that the structure preserving Gauss Runge-Kutta schemes are efficient and accurate integrators for various systems such as extreme mass ratio inspirals (EMRIs) described by the Mathisson-Papapetrou equations, EMRIs described by a Hamiltonian approximation and post-Newtonian systems.

View

Algorithmic improvements to an exact region-filling technique

Valério Ramos Batista, Federal University of ABC, CMCC, Brazil
Antonio Elias Fabris, University of São Paulo, IME, Brazil

Abstract: We present many algorithmic improvements in our early region filling technique, which in

a previous publication* was already proved to be correct for all connected digital pictures. Ours is an integer-only method that also finds all interior points of any given digital picture by displaying and storing them in a locating matrix. Our filling/locating program is applicable both in computer graphics and image processing. (*A programme to determine the exact interior of any connected digital picture, Aditi International Journal of Computational Mathematics 3, 1-23, 2014).

View

Computational neuroanatomy: mapping cell-type densities in the mouse brain, simulations from the Allen Brain Atlas

Pascal Grange, Xi'an Jiaotong-Liverpool University, Department of Mathematical Sciences, China

Abstract: The Allen Brain Atlas of the adult mouse (ABA) consists of digitized expression profiles of thousands of genes in the mouse brain, co-registered to a common three-dimensional template (the Allen Reference Atlas). Since its publication in 2007, this brain-wide, genome-wide data set has triggered a renaissance in neuroanatomy. Its voxelized version (with cubic voxels of side 200 microns) is available for desktop computation in MATLAB. On the other hand, brain cells exhibit a great phenotypic diversity (in terms of size, shape and electrophysiological activity), which has inspired the names of some well-studied cell types, such as granule cells and pyramidal cells. However, no exhaustive taxonomy of brain cell is available. A genetic classification of brain cells is being undertaken, and some cell types (including granule cells and pyramidal cells), have been chraracterized by their transcriptome profiles (the quantity of mRNA corresponding to each gene is measured in microdissected cells of a given type, using microarrays). However, given a cell type characterized by its transcriptome, it is not clear where else in the brain similar cells can be found. The ABA can been used to solve this region-specificity problem in a data-driven way: rewriting the brain-wide expression profiles of all genes in the atlas as a sum of cell-type-specific transcriptome profiles is equivalent to solving a quadratic optimization problem at each voxel in the brain. However, the estimated brain-wide densities of 64 cell types published recently were based on one series of co-registered coronal in-situ hybridization (ISH) images per gene, whereas the online ABA contains several image series per gene, including sagittal ones. In the presented work, we simulate the variability of cell-type densities in a Monte Carlo way by repeatedly drawing a random image series for each gene and solving the optimization problem. This yields error bars on the region-specificity of cell types. For instance, granular cells appear very specific to the cerebellum, which the distribution of densities of pyramidal neurons is less peaked.

Acknowledgements: Microarray data were made available by Ken Sugino, Benjamin Okaty and Sacha B. Nelson. The Allen Atlas data were analysed under the guidance of Michael Hawrylycz and Lydia Ng.

View

Human-Computer Interfaces Applied to Numerical Solution of the Plateau Problem

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Valério Ramos Batista, Federal University of ABC, CMCC, Brazil
Antonio Elias Fabris, University of São Paulo, IME, Brazil

Abstract: In this work we present a program in Matlab to solve the Problem of Plateau numerically, and the program will include human-computer interfaces. The Problem of Plateau has applications in areas of knowledge like, for instance, Computer Graphics. The solution method will be the same one of the Surface Evolver, but the difference will be a complete graphical interface with the user. This will enable us to implement other kinds of interface like ocular mouse, voice, touch, etc. To date, Evolver does not include any graphical interface, which restricts its use by the scientific

community. Specially, its use is practically impossible for most of the Physically Challenged People.

View

Mie-type potential from a multiparameter exponential model: Bound state solutions in D-dimensions

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Álvaro Menéndez, Escuela Superior de Física y Matemáticas IPN, Dep. Física, Mexico
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Abstract: The Mie potential is an important model of molecular interaction very useful in describing diatomic molecules. This is due that Mie potential comprises a repulsive part at short distances and an attractive part for large distances. As a consequence, one of their particular cases, the Lennard-Jones potential, has been extensively used in many branches of physics and chemistry. In this work, exact analytical solutions of the D-dimensional Schrödinger equation with the Mie-type potential are presented. i.e without using any approximation scheme to the centrifugal term. These eigenfunctions and eigenvalues are obtained as a particular case of the exactly solvable Schrödinger equation for a class of multiparameter exponential-type potential. That is, we propose a transform from an exponential-type potential to an inverse power law. As useful application of our approach, the bound state solutions for the Kratzer-Fues and Coulomb potentials are obtained as specific cases from the proposal.

View

A new method for constant-NPT molecular dynamics

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Abstract: The well-established molecular dynamics simulation methods for constant-NPT ensemble systems such as the Andersen-Nosé-Hoover method and their variants are known to alter the dynamic properties of the molecules under consideration, because their equations of motion are modified by the coupling with the thermostat or the barostat. To circumvent this artifact, we propose a new molecular dynamics simulation method, which models the actual role played by the movable thermal wall that disturbs only the molecules near the wall of the simulation box. We test the efficiency of our algorithm in attaining the target temperature and pressure, and the conformity of the calculated equilibrium and dynamic properties to those of a constant-NPT ensemble system.

View

Principal component analysis for determination of polymorphic forms of ranitidine hydrochloride

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Kornelia Lewandowska, Institute of Molecular Physics of the Polish Academy of Sciences, Poznan, Department of Molecular Crystals, Poland
Magdalena Paczkowska, Poznan University of Medical Sciences, Department of Pharmaceutical Chemistry, Poland
Andrzej Miklaszewski, Poznan University of Technology, Institute of Materials Science, Poland
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Abstract: Ranitidine hydrochloride is a histamine type 2 receptor antagonist. It is widely used for the treatment of stomach ulcers [1]. Raniditine hydrochloride exists in two polymorphic forms (I and II). Its polymorphism is connected with the tautomerism of a nitroethenediamine moiety (the presence of enamine, nitronic and imine groups). The polymorphic forms of ranitidine differ in their physical stability, solubility and bioavailability [2]. Previous studies have shown the possibility of applying principal component analysis (PCA) to ensure the required selectivity of determination of the polymorphic forms of ranitidine by using Raman spectroscopy in a binary mixture with and without excipients [3]. However, the application of PCA has so far been investigated as part of experimental research involving one particular analytical technique. The aim of this work was to propose a method for classifying ranitidine hydrochloride samples in terms of the polymorphic forms constituting them with the support of results of theoretical analysis. The classifications were conducted basing on PCA of X-ray diffraction (XRD) patterns as well as Fourier transform infrared and Raman spectra. The objective was to develop a method requiring almost no experimental data due to the application of ab initio molecular modeling to provide reference spectra of a given polymorphic form. The quantum chemical calculations were done with the Hartree-Fock method and density functional theory implemented in Gaussian 09. The results of applying PCA for the different spectroscopic methods were compared to those obtained with XRD as reference. In the approach adopted for this work, the dataset consisted of two reference theoretical spectra of pure polymorphic forms and the investigated spectra of samples with mixed forms. The data were rearranged so that the spectral peaks were viewed as values projected on the base while the classes of samples (pure form I, pure form II, mixture) as loadings of the dimensions of the new base. That data arrangement enabled the scores of values to express the ability of a given peak to differentiate between the polymorphic forms, which was invaluable for a further analysis and description of the spectra, whereas the Euclidean distance between the termination points of the loadings of the contaminated and of the pure samples allowed classification of the contents of a given sample as mostly polymorphic form I or polymorphic from II. A comparison of PCA of the spectra obtained by the investigated spectroscopic methods indicated a superior performance of the XRD patterns, where the features differentiating the polymorphic forms of ranitidine hydrochloride were the most visible. This study demonstrated that FT-IR and Raman spectroscopies subjected to PCA provide spectra which also allow distinguishing between polymorphic forms I and II in ranitidine hydrochloride samples, without exposing them to X-radiation. 1. Canadian Pharmacists Association (2000), Ranitidine HCl, Webcom limited, Toronto: 1772–1774. 2. Mirmehrabi M et all. (2004), Inter. J. Pharm., Solubility, dissolution rate and phase transition studies of ranitidine hydrochloride tautometric forms, 282: 73–85. 3. Pratiwi D. et all. (2002) Eur. J. Pharm. Biopharm. Qualitative analysis of polymorphic mixtures of ranitidine hydrochloride by Raman spectroscopy and principal components analysis, 54: 337–341.

Acknowledgements: This research was supported in part by PL-Grid Infrastructure. This study was supported by SONATA grant from the National Science Centre Poland DEC-2013/09/D/N27/02525.

View

Pattern formation in non-eqilibrium spinor polariton condensates

Florian Pinsker, University of Oxford, Atomic and Laser Physics, United Kingdom

Abstract: Polariton condensates are a hot topic in physics as they combine properties of lasers, atomic Bose-Einstein condensates and semiconductor physics. As such they provide a rich basis for physical phenomena. Among them are the emergence of nonlinear excitations such as solitons, quantum vortices and antiferromagnetic spin splitting in optical lattices. I this work I particularly provide the theoretical basis for a new phenomenon: non-equilibrium bright solitons

and half-bright solitons. Those become feasible within attractive polariton condensates, which should be accessible experimentally thanks to Feshbach resonances [Nat. Phys. 10, 500-504 (2014)] allowing the active control over interactions between polaritons. Their mathematical description however is quite challenging. It turns out that a system of partial differential equations defines a condensate wave function, which completely describes the relevant aspects of the physical system in a certain parameter regime. This set of partial differential equations is quite involved and only few mathematical statements have been made so far. One aim of this paper is to employ the non-conservative Lagrangian formalism for polariton theory research and to compare the results with a state-of-the-art numerical analysis. This Lagrangian formalism includes the non-equilibrium properties due to the finite lifetime of polaritons forming the system. The developed theory enables us to make a variety of statements about bright solitons and half-bright solitons within a non-equilibrium system. On the other hand have numerical studies of phenomena observed in polariton condensates proven to be a reliable instrument even for predicting new types of states. By those means we can elucidate the rich phenomenology related to bright solitons which could inspire and guide future experimental investigations on polariton condensates.

Acknowledgements: Erwin Schroedinger Fellowship, EPSRC doctoral prize fellowship

View

Reactivity of silicene towards atoms and molecules

Thierry ANGOT, Aix-Marseille University, , France

Abstract: Silicene is a recent synthetic low-dimensional allotrope of silicon with a honeycomb structure similar to graphene. Silicene is attracting a lot of attention because of its fundamental possibilities as well as its potential compatibility with microelectronics technologies. Yet, fundamental knowledge about silicene is still in its infancy and to contribute to the actual state of the art, we have undertaken an experimental work dedicated to studying the reactivity of silicene with respect to organic materials hydrogen atoms. We have investigated the interaction between silicene and atomic hydrogen. Focusing on the Si-H vibrational modes, we demonstrate that depending on the film thickness, the reactivity the silicene films are different. We also discuss the isotopic exchange. Finally we evidence an etching of the surface upon adsorption. We also have studied the effect of a strong electron acceptor organic molecule on the electronic properties of silicene grown on Ag(111). Indeed, similarly to graphene, a multilayer film of silicene appears to be intrinsically n-type doped. A possible issue to circumvent this intrinsic doping is to adsorb strong electron acceptor molecules that will act as a p-type dopant. With that aim, we have combined several surface sensitive techniques to study the adsorption of 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ) on silicene-($\sqrt{3}\times\sqrt{3}$)R30°. We demonstrate that while there are strong modifications on the vibrational modes of the molecules, suggesting a strong charge transfer from the silicene to the molecule, there is unexpectedly no significant modification of the silicene's valence band.

View

Silicene and Germanene on Ag(111) and AlN/Ag(111) substrates

Athanasios Dimoulas, National Center for Scientific Research DEMOKRITOS, Institute of Nanoscience and Nanotechnology, Greece

Abstract: It is widely accepted that silicene can be grown on Ag(111) single crystal substrates forming a buckled honeycomb lattice with a (3x3) superstructure with respect to (1x1) silicene (or 4x4 with respect to (1x1) Ag(111)) [1]. The electronic band structure of silicene though is under

debate since it is not clear whether a Dirac cone [1] similar to that of graphene exits also in silicene. We provided the first evidence by ARPES [2] that silicene on Ag creates a surface metallic state with a steep, linear dispersion near the K point of Ag surface Brillouin zone and a saddle point near the M point, resembling the pi band dispersion of graphene. The data were subsequently confirmed by others [3]. Although Dirac Fermions are not confirmed, our work indicates that silicene, hybridizing with Ag turns the surface band structure of Ag into a graphene-like structure which opens the way to engineer new graphene-like systems using appropriate hybrid metal/semiconductor interfaces. Realizing germanene has proven to be considerably more difficult. First attempts with deposition of Ge on Ag(111) shows that Ge/Ag ~ 1/3 coverage resulted in an ordered Ag2Ge surface alloy with a sqrt3 R 30o superstructure and a rich cone-like bandstructure [4]. In essence this system is similar to that of silicene on Ag supporting the assumption that graphene-like surfaces could be created in certain semiconductor/metal interfaces as a result of hybridization, giving this asumption more general validity. Following the recent success in synthesizing germanene on Pt(111) [5] and Au(111) [6], we provide evidence that germanene can also be created on non-metallic substrates such as 2D hexagonal AlN [7] epitaxially grown on Ag (111) substrates. More specifically, electron diffraction and high resolution synchrotron XAFS data indicate [8] that Ge-Ge bonds are formed on AlN which are shorter than that in bulk Ge and very close to free-standing germanene predictions. Although the electronic band structure of this germanene /AlN configuration still needs to be determined, the possibility to grow germanene on non-metallic or even insulating substrates creates huge prospects for applications in electronics. References: [1] P. Vogt et al., Phys. Rev. Lett. 108, 155501 (2012); [2] D. Tsoutsou et al., Appl. Phys. Lett. 103, 231604 (2013); [3] Mahatha et al., Phys. Rev. B 89, 201416(R) (2014); [4] E. Golias et al., Phys. Rev. B 88, 075403 (2013); [5] L. Li et al., Adv. Mater. 26 4820 (2014); [6] M. E. Davila et al., New J. Phys. 16, 095002 (2014); [7] P. Tsipas et al., Appl. Phys. Lett. 103, 251605 (2013); [8] E. Xenogiannopoulou et al., ImagineNano 2015 conference, Bilbao, (2015)

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View

Germanene: A new 2D-material with high potential for nano-electronics

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Guy Le Lay, Aix-Marseille University, CNRS-PIIM, France

Abstract: Presently, two-dimensional materials are one of the most active areas of nanomaterials research. Here we report the structural stability, and electronic properties of monolayer configurations of a novel synthetic germanium allotrope that does not exist in nature i.e., germanene [1]. The discovery of graphene, a one-atom-thick honeycomb carbon sheet, can be considered as a defining point in the research and development of stable, truly 2D material

systems [2]. This new materials exhibit unusual electrical and mechanical properties, that have been the subject of much research and have inspired the study of other 2D materials such as silicene [3], germanene [1], phosphorene [4], stanene... Nowadays, silicene is a fact and has already formed the gate of transistor devices [5], while single layer germanene has been synthesized recently on different substrates, namely Pt(111), Au(111) and also Al(111) [6,1,7]. In our particular case, we have grown in situ an atom-thin, ordered, two-dimensional multi-phase film through germanium molecular beam epitaxy using a gold (111) surface as a substrate. Its growth is similar to the formation of silicene layers on silver (111) templates. One of the phases, forming large domains, as observed in scanning tunneling microscopy, shows a clear, nearly flat, honeycomb structure. Thanks to thorough synchrotron radiation core-level spectroscopy measurements and advanced density functional theory calculations we can identify it as a $\sqrt{3} \times \sqrt{3}$ R(30°) germanene layer in conjunction with a $\sqrt{7} \times \sqrt{7}$ R(19.1°) Au(111) supercell. Hence, compelling evidence of the synthesis of the germanium-based cousin of graphene on gold has been presented [1]. We have performed further studies on the formation of multilayer germanene trying to understand the initial interaction with the substrate and then the multilayer structure. One can anticipate a strong impact of both single and multi layer germanene because of the expected very high mobilities of the carriers, the potential optical applications, the predicted robust two-dimensional topological insulator character, nearly up to room temperature, resulting from the large effective spin-orbit coupling opening the way to the Quantum Spin Hall Effect, the possibility of very high Tc superconductivity, and, last but not least, the practicability of direct integration in the current electronic industry. [1] M.E. Dávila, L. Xian, S. Cahangirov, A. Rubio and G. Le Lay, New J. Phys., 16, 095002 (2014). [2] K. Geim, K. S. Novoselov, Nature Materials 6, 183 (2007). [3] P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M.C. Asensio, A. Resta, B. Ealet, G. Le Lay, Physical Review Letters 108, 155501 (2012). [4] A. Castellanos-Gomez, L. Vicarelli, E. Prada, J. O. Island, K. L. Narasimha-Acharya, S. I Blanter, D. J. Groenendijk, M. Buscema, G. A. Steele, J. V. Alvarez, H. W. Zandbergen, J. J. Palacios and H. S. J. van der Zant, 2D Materials 1, 025001 (2014) [5] L. Tao, E. Cinquanta, D. Chiappe, C. Grazianetti, M. Fanciulli, M. Dubey, A. Molle and D. Akinwande, Nature Nanotechnol. 10, 227 (2015). [6] L. Li, S.-Z Lu, J. Pan , Z. Qin, Y.-Q. Wang, Y. Wang, G.-Y. Cao, S. Du, H.-J. Gao, Adv. Mater., 26, 4820 (2014). [7] M. Derivaz et al., To be published.

View

Effective Hamiltonian and Band Structure of Phosphorene in the Presence of External Strain, Electric Field, and Magnetic Field

Lok Lewyanvoon, The Citadel, School of Science and Mathematics, United States

Abstract: The method of invariant is used to derive effective Hamiltonians in the presence of strain and external fields for phosphorene. All the unknown parameters up to the appropriate order have been identified. The zero-field band structure is confirmed to be quadratic in the wave vector. The results for phosphorene are compared to graphene and silicene. In particular, we found that the band energies change quadratically with a perpendicular electric field but linearly with an external perpendicular magnetic field, whereas both behaviours are linear for silicene. The band structure and deformation potential parameters have been determined by fitting to density-functional theory calculations. Peculiarities related to the structural anisotropy of phosphorene are pointed out.

View

Controlled Interaction of a Four-Level Quantum Emitter with a Plasmonic Nanostructure

Emmanuel Paspalakis, University of Patras, Materials Science Department, Greece

Efthymios Kallos, University of Patras, Materials Science Department, Greece
Vassilios Yannopapas, National Technical University of Athens, Department of Physics, Greece

Abstract: Recently, there is increasing interest in the study of the interaction of quantum emitters (such as atoms, molecules and semiconductor quantum dots) with plasmonic nanostructures. The large fields and the strong light confinement associated with the plasmonic resonances enable strong interaction between the electromagnetic field and the quantum emitters near plasmonic nanostructures. Also, the quantum emitter can be used for the controlled optical response of the coupled quantum – plasmonic system. In this work, we present new theoretical results on the controlled dynamics of a four-level quantum emitter coupled to a plasmonic metamaterial, specifically a periodic two-dimensional array of metal-coated dielectric nanospheres. Two external electromagnetic fields with a fixed relative phase are applied to the system and are used for the control of the dynamics of the quantum system. For the study of the system's dynamics, we combine the density matrix approach for the quantum emitter with ab initio electromagnetic calculations for the plasmonic metamaterial. We then present results for the time evolution of the probabilities (populations) of the different levels of the quantum emitter in both the presence and the absence of the plasmonic nanostructure. Also, in the presence of the plasmonic nanostructure, we consider different distances of the quantum emitter from the plasmonic nanostructure and different materials for the metal of the metal-coated dielectric nanospheres.

Acknowledgements: This work was implemented within the framework of the Action "Supporting Postdoctoral Researchers" of the Operational Program "Education and Lifelong Learning" (Action's Beneficiary: General Secretariat for Research and Technology), and was co-financed by the European Social Fund and the Greek State (Program Nanokallos PE3_26).

View

Silicene on ultrathin Pb layers

Mariusz Krawiec, Maria Curie-Sklodowska University, Institute of Physics, Poland
Agata Podsiadły-Paszkowska, Maria Curie-Sklodowska University, Institute of Physics, Poland

Abstract: Using density functional theory we study structural and electronic properties of silicene on ultrathin Pb layers. A special emphasis is put on formation of silicene due to Pb quantum size effect (QSE) states. Several possible silicene superstructures have been found featuring QSE-dependent binding energies, much lower than in the case of Ag(111) substrate. The linear dispersion of silicene bands and possible energy gap opening as a function of Pb layers is also discussed.

View

Silicene: state-of-the-art, opportunities, and specific issues

Eugenio Cinquanta, IMM-CNR, Laboratorio MDM, Italy

Abstract: Silicene, a honeycomb-like Si lattice, has been so far a fascinating theoretical surmise [1] with no experimental counterpart as due to the natural sp3 hybridization of Si bonding. Being an atomically thin layer of silicon, silicene attracts an enormous interest as emerging research material for the semiconductor technology roadmap and for its intrinsic affinity with the ubiquitous silicon technology. Artificially forcing the silicene lattice was firstly made possible in the epitaxial growth of a Si monolayer on Ag(111) substrates [2]. However, unlike graphene, silicene self-organizes in regularly buckled lattices with periodic atomic arrangements as due to the commensurate match with the hosting Ag substrate [3]. This structural complexity results in an interplay of sp2 and sp3 bonding which causes the silicene lattice to degrade under environmental conditions. On the other hand, the strong hybridization with the substrate dramatically influences

the electronic properties of silicene therein suppressing the emergence of Dirac cones. The stability and the interaction with the substrates are the two bottlenecks for the “portability” and the exploitation of silicene in device platforms. Here we discuss effective methods to address both issues and subsequently integrate a silicene layer in a field effect transistor, together with an overview of the optical properties of the two-dimensional Silicene/Ag(111) interface [5, 6]. [1] S. Cahangirov, et al., Phys. Rev. Lett. 102, 236804 (2009). [2] P. Vogt, et al., Phys. Rev. Lett. 108, 155501 (2012). [3] D. Chiappe, et al., Adv. Mater. 24, 37, 5088 (2012). [4] L. Tao, Nat. Nanotech. 10, 227–231 (2015). [5] E. Cinquanta, et al. J. Phys. Chem. C 117, 16719 (2013). [6] E. Cinquanta, et al. Ultrafast charge dynamics at the two-dimensional Silicene/Ag(111) interface, in preparation (2015).

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View

Resonances in electron collisions with small biomolecules using the R-matrix method

Jonathan Tennyson, University College London, Physics and Astronomy, United Kingdom

Abstract: Resonances (long-lived temporary states) of low-energy electrons in collisions with molecules inside the body are thought to lead to DNA strand-breaks. A series of studies have been performed characterising the resonances features in a variety of small biomolecules using first principles quantum mechanical calculations based on use of the R-matrix method. These calculations identify both shape resonance, where the electron is temporarily trapped in a low-lying unoccupied orbital of the target, and Feshbach resonances which involve trapping of the electron with simultaneous excitation of the target. A review of the current status of this work will be presented at the meeting.

View

Numerical analysis of the effect of the kind of activating agent and the impregnation ratio on the parameters of the microporous structure of the active carbons

Mirosław Kwiatkowski, AGH University of Science and Technology, Faculty of Energy and Fuels, Poland

Abstract: The paper presents the results of the research on the application of the LBET class adsorption models with the fast multivariant identification procedure as a tool for analysing the microporous structure of the active carbons obtained by chemical activation using potassium and sodium hydroxides as an activator. The proposed technique of the fast multivariant fitting of the LBET class models to the empirical adsorption data was employed particularly to evaluate the impact of the used activator and the impregnation ratio on the obtained microporous structure of the carbonaceous adsorbents.

Acknowledgements: The research is led within the AGH University of Science and Technology in Krakow grant No. 11.11.210.217.

View

Application of the clustering-based LBET class adsorption models to the analysis of the microporous structure of silica membranes

Mirosław Kwiatkowski, AGH University of Science and Technology, Faculty of Energy and Fuels, Poland

Abstract: This paper presents the application research results of the clustering-based LBET class adsorption models as a tool for the analysis of the porous structure of silica membranes. This research provides information on possible significant advantages that can be drawn while applying the new proposed method of microporous structure description in comparison with the conventional approaches. Furthermore, the obtained calculation results and additional information from adsorption isotherms analysis using LBET class models as well as their interpretation are shown. In particular, in the presented method it is possible to easily acquire not only information regarding the values of the obtained structure parameters, but also, more importantly, precise information on the reliability of these parameter calculations.

Acknowledgements: The research is led within the AGH University of Science and Technology in Krakow grant No. 11.11.210.217.

View

Enhancement of Excitonic Resonances with Plasmonics and Periodicity

Ergun Simsek, George Washington University, Electrical Engineering, United States

Abstract: The electromagnetic waves scattered and absorbed by the multilayered structures having atomically thin layered materials can be enhanced by metal nanoparticles' plasmonic resonances and periodicity. In this work, we show that this enhancement can be accurately calculated using analytical methods specifically developed for multilayered media. Analytical methods’ accuracy and efficiency is compared against experimental results found in the literature and commercially available full wave electromagnetic solvers, respectively.

View

Spinning particles moving around black holes: integrability and chaos.

Georgios Loukes-Gerakopoulos, Charles University in Prague, Institute of Theoretical Physics, Czech Republic

Abstract: The motion of stellar compact objects around supermassive black holes, which lie in the center of galaxies, can be approximated by the motion of spinning test particles. The equations of motion describing such systems are in general non-integrable, and therefore, chaotic motion should be expected. In this presentation we shall focus on a canonical Hamiltonian formalism where the spin of the particle is included only up to the linear order. We shall discuss the motion of a particle in the case that the spacetime background is of a non-rotating black hole and in the case the background is of a rotating black hole.

View

Multiscale physics of radiation damage and ion beam cancer therapy

Andrey V. Solov'yov, MBN Research Center, MBN Research Center, Germany

Abstract: The multiscale approach to the molecular level assessment of radiation damage in biological targets consequent to irradiation by ions was designed in order to qualitatively and quantitatively describe the effects that take place when energetic ions interact with living tissues, e.g. the Relative Biological Effectiveness (RBE) of radiation [1]. A road towards the understanding physical aspects of ion-beam cancer therapy on the molecular level revealed that this problem has many temporal, spatial, and energy scales, while the main events leading to the cell death happen on a nanometer scale. The multiscale approach is interdisciplinary, phenomenon-based and, having started some years ago, passed several milestones making discoveries on different scales, for review see [1]. Thus, in addition to the traditional pathways of biodamage often related to secondary electrons and free radicals production in cells after irradiation [2], the multiscale

approach also considers a new efficient pathway of DNA damage caused by the nanoscopic shock waves created by the strong local heating in the vicinity of the ion tracks due to the energy deposited by ions [3]. It allows also to evaluate radio-sensitisation effects caused by metal nanoparticles and other radio-sensitising molecular species [4]. This work is especially active now within the currently running European project ITN-ARGENT [5]. References [1] E. Surdutovich, A.V. Solov'yov, Eur. Phys. J. D, Colloquium paper, v.68, p.354-(1-30) (2014) [2] P. de Vera, R. Garcia-Molina, I. Abril, A.V. Solov'yov, Physical Review Letters 110,148104 (2013) [3] E. Surdutovich, A. Yakubovich, and A.V. Solov'yov, www.nature.com / Scientific reports, 3, 1289 (2013) [4] A.V. Verkhovtsev, A. V. Korol, A.V. Solov'yov, Physical Review Letters, 114, 063401 (2015) [5] http://www.itn-argent.eu/

Acknowledgements: Support of this work by the COST Action Nano-IBCT and the Marie Curie ITN-ARGENT is gratefully acknowledged.

View

Theoretical investigation of the ultrafast dissociation of ionized biomolecules immersed in water

Rodolphe Vuilleumier, Ecole normale supérieure and UPMC, Chemistry, France
Marie-Anne Hervé du Penhoat, UPMC, IMPMC, France
Marie-Françoise Politis, Université d'Evry val d'Essonne, LAMBE, France
Marie-Pierre Gaigeot, Université d'Evry val d'Essonne, LAMBE, France
Ivano Tavernelli, Zurich IBM Research, , Switzerland

Abstract: Irradiation by swift ions, such as in hadron therapy or following irradiation by cosmic rays, have a sizeable probability to lead to double ionization events. These double ionization events are very energetic and may be more damageable than other primary events. This is in line with the increase of lethality of soft x-rays when their energy allows for core excitation of carbon atoms, thus producing localized bouble ionization through Auger effect. We have studied the very early stages following double ionization events, from sub-fs to few 10's of fs, of the coupled ion and electron dynamics in complex molecular environments: liquid water, water clusters, and solvated bio-molecule such as uracil and a sugar. To this end, we have performed time-dependent density functional theory based first-principle molecular dynamcs simulations in the Ehrenfest approximation.

Acknowledgements: M.-A. Hervé du Penhoat, M.-F. Politis, M.-P. Gaigeot, P. Lopez-Tarifa, M. Alcami, F. Martin and I. Tavernelli

View

The role of the environment in DNA damage by low-energy electrons

Jorge Kohanoff, Queen's University Belfast, Atomistic Simulation Centre, United Kingdom

Abstract: DNA damage caused by irradiation has been studied for many decades. Motivations include assessing the dangers posed by radiation, and understanding radiotherapies and how to improve their efficiency in combating cancer. A full description of the irradiation process involves multiple size and time scales. It starts from the interaction of radiation (either electromagnetic or particles) with the biological medium causing ionization and more generally electronic excitation. This is followed by the propagation of the newly created species, notably electrons and radicals, which scatter inelastically with other components of the medium, e.g. water, proteins, ions, DNA. Follows a stage of chemical diffusion of these species, until these become solvated and inactivated by the medium, or they chemically react with other species by making or breaking bonds, especially in DNA. Low-energy electrons produced by ionization play an important role in

this damage. This has been shown experimentally more than a decade ago using plasmid DNA samples [1]. By performing similar experiments on analogues of DNA components and water, it was proposed that electronic resonances around 10 eV are responsible for fragmentation via dissociative electron attachment (DEA) processes. Since then, a significant body of work has been carried out to elucidate the role of DEA. In particular, it was shown that damage can be produced by very low-energy electrons well below the ionization threshold (as low as 1 eV or lower). At QUB we have embarked in a comprehensive study of the role of the environment in favouring or preventing the damage produced to DNA by low-energy electrons. In this presentation I will describe our efforts aiming at understanding the behaviour of DNA components in a realistic, physiological-like environment. This is being done by first-principles molecular dynamics simulations in condensed phase models of increasingly complex DNA fragments solvated in water and in the presence of proteins [2-6]. Perhaps the most interesting conclusion is that the condensed phase environment offers a large variety of mechanisms to protect DNA from strand breaks, which do not operate in the gas-phase or microsolvated environments. References: [1] B. Boudaiffa et al., Science 287, 1658 (2000). [2] M. Smyth and J. Kohanoff, Phys. Rev. Lett. 106, 238108 (2011). [3] M. Smyth and J. Kohanoff, J. Am. Chem. Soc. 134, 9122 (2012). [4] M. Smyth, J. Kohanoff and I. Fabrikant, J. Chem. Phys. 140, 184313 (2014). [5] Bin Gu, M. Smyth and J. Kohanoff, Phys. Chem. Chem. Phys. 16, 24350 (2014). [6] M. McAllister, M. Smyth, Bin Gu, G. Tribello and J. Kohanoff, to be submitted.

Acknowledgements: I would like to thank my collaborators Maeve Smyth, Maeve McAllister, Bin Gu, Lila Bouessel du Bourg, Alberto Fraile, Ilya Fabrikant and Gareth Tribello. The calculations have been carried out in HECToR and ARCHER supercomputers, through the allocation given by EPSRC to the UKCP consortium.

View

Resonances in electron collisions with small biomolecules using the R-matrix method

Jonathan Tennyson, University College London, Physics and Astronomy, United Kingdom

Abstract: Resonances (long-lived temporary states) of low-energy electrons in collisions with molecules inside the body are thought to lead to DNA strand-breaks. A series of studies have been performed characterising the resonances features in a variety of small biomolecules using first principles quantum mechanical calculations based on use of the R-matrix method. These calculations identify both shape resonance, where the electron is temporarily trapped in a low-lying unoccupied orbital of the target, and Feshbach resonances which involve trapping of the electron with simultaneous excitation of the target. A review of the current status of this work will be presented at the meeting.

View

Post-quantum attacks on key distribution schemes utilising weakly stochastic sources

Colin Wilmott, Nottingham Trent University, Mathematics, United Kingdom

Abstract: It has been established that the security of quantum key distribution protocols can be severely compromised were one to permit an adversary to possess a very limited knowledge of the random sources used between the communicating parties. While such knowledge should always be expected in realistic experimental conditions, the result itself opened a new line of research to fully account of real-world weak randomness threats to quantum cryptography. Here we expand of this novel idea by describing key distribution schemes that are provably secure against general attacks by a post-quantum adversary before then discussing the possible security

consequences for such schemes under the assumption of weak randomness.

View

Simulation of conductivity of polymer films on metal surface

Olga Maksimova, Cherepovets State University, Ministry of Education and Science of the Russian Federation, Russian Federation
Maksimov Andrei, Cherepovets State University, Chair of Physics, Russian Federation

Abstract: In this paper, protective properties of polymer films are analyzed. The simulation is performed by means of the Monte-Carlo method on the basis of three-dimensional lattice model of polymer system with orientational interactions. Initially, configuration of polymer system is calculated by the Metropolis algorithm taking into account the characteristics of the internal structure (constants of intermolecular interactions etc.), temperature regime and metal quality. Further, for the study of conductivity, the motion of charged particles within the proposed lattice model is investigated on the basis of the calculated configuration. The interaction energy of the oxygen atom with eight neighboring links of polymer chains and electric double layer on the metallic surface is accounted. The direction of movement of charged particles is calculated by the Monte-Carlo method according to the energy advantage of its position. This method allows to calculate the number of charged particles passing through the polymer film and reaching the metal sheet surface. The dependences of conductivity on temperature, film thickness, and distance between molecular layers are obtained. It is shown that there is an optimum density for the given film thickness at which it possesses protective properties. The adequacy of the developed mathematical models and calculated dependences are verified by comparison with laboratory data and production testing.

Acknowledgements: This work was supported by the Ministry of Education and Science of the Russian Federation, project №1715 (contract № 2014/267).

View

Knowledge-Based Framework: its specification and new related discussions

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Rodrigo Zaniolo, University of São Paulo, Institute of Mathematics and Computer Science, Brazil
Kalinka Castelo Branco, University of São Paulo, Departament of Computer System, Brazil

Abstract: Unmanned Aerial Vehicle is a common application of critical embedded systems. The heterogeneity prevalent in these vehicles in terms of services for avionics is particularly relevant to the elaboration of multi-application missions. Besides, this heterogeneity in UAV services is often manifested in the form of characteristics such as reliability, security and performance. Different service implementations typically offer different guarantees in terms of these characteristics and in terms of associated costs. Particularly, we explore the notion of Service-Oriented Architecture (SOA) in the context of UAVs as safety-critical embedded systems for the composition of services to fulfil application-specified performance and dependability guarantees. So, we propose a framework for the deployment of these services and their variants. This framework is called Knowledge-Based Framework for Dynamically Changing Applications (KBF) and we specify its services module, discussing all the related issues.

View

Pseudo Magic Squares

Giuliano La Guardia, State University of Ponta Grossa, Mathematics and Statistics, Brazil

Abstract: A magic square of order n is an n x n square (matrix) whose entries are distinct

nonnegative integers such that the sum of the numbers of any row and column is the same number, the magic constant. In this paper we introduce the concept of pseudo magic squares, i.e., magic squares defined over the ring of integers, without the restriction of distinct numbers. Additionally, we generalize this new concept by introducing a group (ring) structure over it. This new approach can provide useful tools in order tofind new non-isomorphic pseudo magic squares.

Acknowledgements: This research was partially supported by the Brazilian Agencies CAPES and CNPq.

View

MICROSCALE THERMAL CONVECTION

Roger Khayat, University of Western Ontario, Mechanical & Materials Engineering, Canada

Abstract: When the geometrical gap is of the same order of magnitude as the mean free path of the fluid, the Navier-Stokes-Fourier equations become inapplicable. Conditions of validity of non-Fourier effects are reviewed and examined for the convection of a thin fluid layer. In this case, the fluid possesses a relaxation time, reflecting the delay in the response of the heat flux and the temperature gradient. The constitutive equation for heat flux is frame invariant, of the upper-convected type. It is found that a fluid in microgeometry can exhibit oscillatory convection, not predicted for Fourier convection in large gap.

View

Scaling laws of turbulence intermittency in the atmospheric boundary layer: the role of stability

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R. Cesari, Istituto di Scienze dell'Atmosfera e del Clima (ISAC-CNR), , Italy
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Abstract: Bursting and intermittent behavior is a fundamental feature of turbulent fluid flows [Frisch, 1995], especially in the vicinity of solid obstacles, such as walls or the ground. This is associated with the complex dynamics of turbulent energy production and dissipation, which can be described in terms of coherent motion structures. These flow structures are generated at random times and remain stable for relatively long life times, after which they become suddenly unstable and a rapid of decay of the motion structure occurs. This intermittent behavior is described as a birth-death point process of self-organization, i.e., a sequence of crucial events randomly occurring in time determining the emergence and decay of self-organization. This process is here investigated by means of the Inter-Event Time (IET) distribution and of the correlation among events. In particular, we investigate the time intermittency of turbulent transport associated with the birth-death of self-organized coherent structures in the atmospheric boundary layer. The IET distribution associated with self-organization is typically a power-law decay with an asymptotic power exponent, known as complexity index [Paradisi et al., 2012] and characterizing the complexity of the system, i.e., the ability to develop self-organized, metastable motion structures. We use a robust method, based on the diffusivity scaling of some event-driven random walks, for the estimation of the system's complexity [see Paradisi et al., 2012 for a brief account of the method]. The method has been applied to turbulence velocity data in the atmospheric boundary layer and a neutral condition is compared with a stable one. We find that the complexity index associated with intermittency is lower in the neutral case with respect to the stable one. As a consequence, the crucial birth-death events are more rare in the stable case, and this could be associated with a less efficient transport dynamics.

View

The Generalized Susceptibility of Dislocation Segment in Nondissipative Crystal

Victor Dezhin, Voronezh State Technical University, Mathematics and physical and mathematical modeling, Russian Federation

Abstract: Igor Bataronov, Voronezh State Technical University, Department of higher mathematics and physical and mathematical modeling, Russian Federation Victor Dezhin, Voronezh State Technical University, Department of higher mathematics and physical and mathematical modeling, Russian Federation Abstract: Oscillations of a dislocation segment under the action of external forces are considered. Obtain expressions for the matrix elements, which are expressed through the matrix of the generalized susceptibilities dislocation oscillators. Elimination of non-physical features in the region of large wave numbers to perform the analysis within the Peierls dislocation model. An expression for the low-frequency asymptotic behavior of diagonal and non-diagonal elements of the matrix of generalized susceptibilities dislocation oscillators are obtained.

View

A random field approach to the Lagrangian modeling of turbulent transport in vegetated canopies

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Rita Cesari, CNR, ISAC, Italy

Abstract: We present an application of a Lagrangian Stochastic Model (LSM) (Olla and Paradisi, 2003) to turbulent dispersion in a turbulent boundary layer over complex terrain, where turbulent coherent structures are know to play a crucial role. In particular, we investigate the case of a vegetated canopy by using semi-empirical parameterizations of turbulence profiles in the region inside and above a canopy layer (Hsieh et al., 2003). The LSM is based on a 4-dimensional Fokker-Planck (4DFP) equation, which extends the standard Thomson87 Lagrangian approach to turbulent transport (Thomson, 1987; see also Duman et al., 2014). The 4DFP model is derived by means of a Random Field description of the turbulent velocity field. The main advantage of this approach is that not only the experimental Eulerian one-point statistics, but also the Eulerian two-point two-time covariance structure can be included explicitly in the LSM. At variance with the standard Thomson87 approach, the 4DFP model allows to consider explicit parameterizations of the turbulent coherent structures as it explicitly includes both spatial and temporal correlation functions. In order to investigate the effect of the turbulent geometrical structure on a scalar concentration profile, we performed numerical simulations with two different covariance parameterizations, the first one isotropic and the second anisotropic. We show that the accumulation of scalars near the ground is due to the anisotropic geometrical properties of the turbulent boundary layer.

View

Effect of a Surface Asperity at the Nanoscale

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Abstract: Influence of a surface irregularity on stress distribution in a subsurface and on stress concentration has been widely analyzed at the macrolevel. For example, stress concentration coursed by roughness of a surface and interface has been recently examined in works [1–3]. At

the same time, it was observed [4] that mechanics of nanostructured elements, including nanoparticles, nanowires, nanobeams and nanofilms as well as heterogeneous materials containing nanoscale inhomogeneous defers notably from the general one. Unlike bulk material elements, the nanostructures have elastic properties which are highly depend on their size. This size dependency of properties at the nanoscale can be understood by incorporating the effect of surface stress (e.g. [5–8]). The intent of this work is to examine the effect of surface and bulk elastic parameters, surface stress and nanosized asperity shape on stress concentration and local stress distribution at a solid surface. We consider the 2-D model of semi-infinite elastic solid having a surface asperity at the nanoscale and subjected to remote tensile loading. It is assumed that, according to Young-Laplace law [9], the traction at the boundary is expressed in terms of surface stress which is intrinsic to nanometer size structures. In order to find the surface stress we take into consideration the condition of surface and bulk inseparability. To solve the boundary value problem, we use Gurtin-Murdoch surface elasticity model [9] containing constitutive equations for the surface linear elasticity with two elastic parameters and residual surface stress [10]. The way of deriving an analytical solution of the problem presented is similar to that which has been applied recently to a number of problems at the macrolevel [e.g. 1–3, 11, 12]. This advanced method is based on Goursat-Kolosov complex potentials, Muskhelishvili representations and the boundary perturbation technique. Two special processes peculiar exclusively to our method of solving such problems are used. The first is constructing an algorithm of obtaining any-order approximation in the boundary perturbation method. The second consists in a unique approach to the boundary value problems taking into account surface stresses. This approach leads to the solution of the singular integro-differential equation either in surface stress [5, 6] or in expansion coefficients of surface stress in each-order approximation. We consider surface asperities distributed at regular intervals with the ratio of maximum nanometer size deviation from the plane surface to the period. For this case, the algorithm for obtaining an analytical solution of the integral equation in the form of Fourier series has been derived. Numerical results have been obtained for the first-order approximation. The different shape of the curved surface is considered: from wavy sinusoidal surface to periodically distributed surface defects such as grooves and convexities. The influence of surface elasticity, surface shape and relative size of asperities on stresses at the surface has been analyzed for aluminum material. In particular, the size-effect is discovered. It becomes apparent in stress dependence on a period of surface roughness if the values of this period have the order of 10 nanometers. REFERENCES [1] Grekov M., Kostyrko S. Int. J. Eng. Sci. 89 (2015) 61. [2] Grekov M., Kostyrko S. J. Appl. Math. Mech. 77 (2013) 79. [3] Vikulina Yu., Grekov M., Kostyrko S. Mech. Solids. 45 (2010) 778. [4] Wang J., Huang Z., Duan H., Yu S., Feng X., Wang G., Zhang W., Wang T. Acta Mechanica Solida Sinica. 24 (2011) 52. [5] Grekov M., Yazovskaya A. J. Appl. Math. Mech. 78 (2014) 172. [6] Vikulina Yu., Grekov M. Vestnik St. Petersburg University. Mathemetics. 45 (2012) 174. [7] Eremeyev V., Altenbach H., Morozov N. Dokl. Phys. 54 (2009) 531. [8] Goldstein R., Gorodtsov V., Ustinov K. Phys. Mesomech. 13 (2010) 318. [9] Gurtin M., Murdoch A. Arch. Rational Mech. Anal. 57 (1975) 146. [10] Duan H., Wang J., Karihaloo B. Advances in Applied Mechanics. 42 (2009) 1. [11] Grekov M. J. Appl. Math. Mech. 75 (2011) 476. [12] Grekov M., Morozov N. Mordern Analysis and Applications. Ser. Operator Theory: Advances and Applications. Basel: Birkhauser. 191 (2009) 127.

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View

First-principles study of migration of Carbon and native defects in GaN

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Abstract: GaN has proved to be a suitable material in optoelectronic and power electronics applications. Defects, both point [1] and extended ones [2], affect the electronic properties of devices. Among them, carbon is a relevant and easily incorporated defect in GaN. For example, carbon and oxygen complexes are attributed to cause the yellow lumines- cence of GaN [3]. In addition, impurity diffusion is usually mediated by native defects. Hence, the study of migration of defects is essential in evaluating the performance of devices. The migration energy of Carbon and native defects in wurtzite GaN is investigated using DFT calculations. The Minimum Energy Path (MEP) and the migration barriers of these defects were obtained using the Nudged Elastic Band (NEB) method with the climbing image modification (CI-NEB) [4]. [1] S. Limpijumnong and C. G. Van de Walle, ‘‘Diffusivity of native defects in GaN,’’ Phys. Rev. B, vol. 69, p. 035207, Jan 2004. [2] M. Matsubara, J. Godet, L. Pizzagalli, and E. Bellotti, ‘‘Properties of threading screw dislocation core in wurtzite GaN studied by Heyd-Scuseria-Ernzerhof hybrid functional,’’ Applied Physics Letters, vol. 103, no. 26, pp. –, 2013. [3] D. O. Demchenko, I. C. Diallo, and M. A. Reshchikov, ‘‘Yellow luminescence of gallium nitride generated by carbon defect complexes,’’ Phys. Rev. Lett., vol. 110, p. 087404, Feb 2013. [4] G. Henkelman, B. P. Uberuaga, and H. Jonsson, ‘‘A climbing image nudged elastic band method for finding saddle points and minimum energy paths,’’ The Journal of Chemical Physics, vol. 113, no. 22, pp. 9901–9904, 2000.

View

Simulations of a epidemic model with parameters variation analysis for the dengue fever

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Abstract: Kermack and McKendrick proposed in 1927 the SIR model, precursor in mathematical epidemiology. It proposes to divide a population into three classes of individuals: susceptible, infected and recovered. The model uses a differential equations system fed with parameters that characterize the dynamics of those classes. The dengue fever is a viral disease transmitted by the vectors Aedes aegypti and Aedes albopictus mosquitoes and presents the peculiarity of being caused by four viral strains. This makes possible an infection of the same population by more than a viral strain simultaneously; thus, there is a situation where cross-immunity among subtypes virus is observed. The dengue fever is characterized by recurrent epidemics, mainly in large cities, where control actions have been shown inefficient facing the disorganized population increase and basic sanitation problems. This recurrence is the motivational factor for using a model that includes seasonal parameters. This work presents modifications in the traditional epidemiologic model SIR by inserting parameters and classes that simulate real conditions of the biological epidemical scenario in question. It presents a mathematical model that supports the presence of two disease strains, the possibility of a temporary cross-immunity and the seasonal influence. Finally, a huge attention is given to a study about the influence of the parameters associated with the epidemic in the epidemiological behavior of the population in question. Results of those studies are generated, illustrated, interpreted and discussed in their mathematical and biological sense.

View

Investigating ionisation cluster size distribution due to sub- 1 keV electrons in view of Heisenberg’s uncertainty principle

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Andrew Nisbet, University of Surrey, , United Kingdom

Abstract: High levels of cellular damages upon exposure to irradiation are thought to be initiated by low energy secondary electrons, typically of energies of a few hundreds eV. It is commonly agreed that the radio-sensitive region within a cell is a volume equivalent to a strand of DNA of 10 base pairs. This is defined as cylindrical dimensions of 2.3 nm in diameter and 3.4 nm in length. The complexity of damages, such as double or single DNA strand breaks, caused by low energy secondary electrons, is associated with the probability of the number of ionisation events occurred within the volume. Most computational studies of radiation transport are achieved by Monte Carlo methods based on event-driven simulations, such as GEANT4-DNA and PARTRACK, where each particle is treated as a classical object with precisely known position and energy. However, as the wavelengths of low energy electrons become comparable with the length scale of the radio-biologically sensitive volume, each event particle should be treated quantum mechanically where the Heisenberg's uncertainty principle is followed. Whilst shown in this paper that individual low energy electron interactions are not suitable to be treated by 'classical' transport methods, the uncertainties associated with the ionisation distribution simulated by GEANT4-DNA codes are examined in light with the Heisenberg's uncertainty principle. Here, given that the volume of interest in the simulation of ionisation cluster size distribution is non-point-like; particular attention is given to the validity of using 'classical' transport methods in simulations of ionisation cluster size distributions.

View

Testing General Relativity on Cosmological scales

Athina Pouri, National and Kapodistrian University of Athens, Research Center for Astronomy and Applied Mathematics, Physics, Greece

Abstract: In order to test the validity of General Relativity (GR) on cosmological scales, it has been proposed that measuring the so called growth index, γ, could provide an efficient way to discriminate between scalar field dark energy models which admit to general relativity and modified gravity models. Using the clustering properties of the Luminus Red Galaxies and the growth data we attempt to place tight constraints on the growth index γ and thus testing possible departures from GR.

View

Influence of anisotropy on percolation and jamming of linear k-mers on square lattice with defects

Yuri Tarasevich, Astrakahan State University, Applied Mathematics and Computer Science, Russian Federation

Abstract: By means of the Monte Carlo simulation, we study the layers produced by the random sequential adsorption of the linear rigid objects (k-mers also known as rigid or stiff rods, sticks, needles) onto the square lattice with defects in the presence of an external eld. The value of k varies from 2 to 32. The point defects randomly and uniformly placed on the substrate hinder adsorption of the elongated objects. The external field affects isotropic deposition of the particles, consequently the deposited layers are anisotropic. We study the influence of the defect concentration, the length of the objects, and the external field on the percolation threshold and the jamming concentration. Our main findings are 1) the critical defect concentration at which the percolation never occurs even at jammed state decreases for short k-mers (k < 16) and increases for long k-mers (k > 16) as anisotropy increases, 2) the corresponding critical k-mer concentration

decreases with anisotropy growth, 3) the jamming concentration decreases drastically with growth of k-mer length for any anisotropy, 4) for short k-mers, the percolation threshold is almost insensitive to the defect concentration for any anisotropy.

Acknowledgements: The reported study was partially supported by Russian Foundation for Basic Research, research project No. 14-02-90402 Ukr a and the Ministry of Education and Science of the Russian Federation, project no 266.

View

Modelling irradiation by EM waves of multifunctionalized iron oxide nanoparticles and subsequent drug release

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Abstract: We present a multiscale and multiphysics model of the irradiation by electromagnetic waves of radiofrequency of iron oxide nanoparticles functionalized by drug-releasing polymers used as new multifunctional therapeutic compounds against tumors. We compute ab initio the thermal conductivity of the polymer chains as a function of the length, model the unfolding of the polymer after heat transfer from the nanoparticle by molecular mechanics, and develop a multiscale thermodynamic and heat transfer model including the surrounding medium (water) in order to model the drug release.

Acknowledgements: Région Pays de la Loire, GENCI-CURIE, CRIHAN

View

SEVIRI Cloud mask by Cumulative Discriminant Analysis

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Abstract: The novel method of Cumulative Discriminant Analysis (CDA) is applied to the cloud detection of SEVIRI satellite observations. SEVIRI (Spinning Enhanced Visible and Infrared Imager) is an imager on board of the geostationary satellites launched within Meteosat Second Generation (MSG) programme. We want to exploit its high temporal resolution (one Earth scene every 15 minutes) in order to develop a very accurate cloud mask. The methodology is based on a series of statistics related to the cloud properties. The cumulative distribution functions of these statistics is analyzed using CDA, and a statistical scheme is developed to discriminate clear from cloudy scenes. Results have been compared with the SEVIRI cloud mask provided by EUMETSAT (European Centre for the Exploitation of Meteorological Satellite), selected as reference, in order to tune and validate the discrimination algorithm. We have investigated ten statistics: the brightness temperature from the eight SEVIRI infrared channels (from 3.9 μm to 13.4 μm) and two brightness temperature differences at different infrared wavelengths. We trained the statistics on a selected region, the Basilicata area located in the south of Italy, and in different time periods, the first decade of each month of 2012, in order to take into account the seasonal variability. Moreover

we developed the study considering land and sea surface and distinguishing between daytime or nighttime, in order to consider both the daily variability and the dependence from the surface type. After that we carried out the validation of the scheme using SEVIRI observations acquired in the second decade of each month in 2012. The results show a very good agreement with the reference cloud mask.

View

Using Botnets to provide security for safety critical embedded systems - a case study focused on UAVs

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Paulo Rogério de Mello Cardoso, Centro Universitário Senac, , Brazil
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Abstract: The use of unmanned aerial vehicles (UAVs) has been growing not only in military applications, but also in civilian. UAVs have enormous potential for use, which mostly still are unexplored. For the use of UAVs in the airspace, not only Brazilian new studies on methods of analysis and technologies should be incorporated into navigation systems, control among others, promoting security mechanisms for these aircraft. Implement security mechanisms using a platform with operating systems and botnet to simulate such attack Distributed Denial of Service (DDoS) in UAVs is an important task when it is aimed at containment and mitigation of attacks on this type of platform.

View

Numerical Simulations of Isothermal Collapse and the Relation to Steady-State Accretion

Rhameez Sheldon Herbst, University of the Witwatersrand, Computational and Applied Mathematics, South Africa

Abstract: In this paper we present numerical simulations of collapsing, spherically symmetric clouds. The focus of the collapse is on the core bounce which is related to the ratio of free-fall to sound travel times. In the second part of this work we present analytical solutions for steady-state accretion of isothermal in one dimension. The analytical solutions are shown to match the numerical simulations in the late stages of collapse.

Acknowledgements: Many thanks go to my supervisors Prof C. Harley and Prof E. Momoniat

View

Inferring microarray relevance by enrichment of chemotherapy resistance-based microRNA sets

Hasan Ogul, Baskent University, Computer Engineering, Turkey

Abstract: Inferring relevance between microarray experiments stored in a gene expression repository is a helpful practice for biological data mining and information retrieval studies. In this study, we propose a knowledge-based approach for representing microarray experiment content to be used in such studies. The representation scheme is specifically designed for inferring a disease-associated relevance of microRNA experiments. A group of annotated microRNA sets based on their chemotherapy resistance are used for a statistical enrichment analysis over observed expression data. A query experiment is then represented by a single dimension vector of

these enrichment statistics, instead of raw expression data. According to the results, new representation scheme can provide a better retrieval performance than traditional differential expression-based representation.

View

ab initio Molecular Dynamics study of the hydrogen bond in the acetic acid cyclic dimers

BENMALTI Mohamed el Amine, Université Abdelhamid Ibn Badis-Mostaganem, Chemistry, Algeria

Abstract: Both ab initio molecular dynamics simulations based on the Born-Oppenheimer approach and ab initio B3LYP/6-31G+(d) calculations have been carried out to determine the energies and vibrational properties of acetic acid dimer. The two IR spectrum of the acetic acid dimer in the gas phase obtained from the two methods are compared to our previous spectrum calculated by a quantum approach [Mohamed el Amine Benmalti, Paul Blaise, H. T. Flakus, Olivier Henri-Rousseau, Chem Phys, 320(2006) 267-274.]. The theoretical model is taking into account the strong anharmonic coupling. The aim of this work is to show which method of calculation gives better understanding of the interpretation of the infrared spectra for acetic acid dimer.

View

Structure evolution of silicene on Ag(111)

Noriaki Takagi, The University of Tokyo, Department of Advanced Materials Science, Japan

Abstract: Two-dimensional (2D) materials nowadays offer intriguing issues because of their exotic properties leading to future applications from electronic and optical devices to green technology devices. Silicene, the 2D honeycomb lattice of Si atoms, has recently emerged as a rising star. In the last few years, challenges to realize silicene have been performed on solid substrates. Silicene grown on Ag(111) is the most surveyed both theoretically and experimentally so that the knowledge has been integrated very rapidly. Here we focus on the geometric and electronic structures of silicene grown on Ag(111) and discuss several puzzles that we solved and that remain to be solved.

View

The lattice model of ions dynamics in dipole environment in high-frequency external field

Pavel Stishenko, Omsk State Technical University, Chemical Technology an Biothecnology, Russian Federation

Alexander Myshlyavtsev, Omsk State Technical University, , Russian Federation

Abstract: The molecular model of ions kinetics in dipole environment in alternating external field was investigated with Kinteic Monte Carlo method. The model was proposed in [EPL, 106 (2014) 46004] as a molecular-level explanation of the anomalously high liquid water conductivity in case of high-frequency current, called Debye relaxation. Elaboration of this model in an approximate kinetic theory framework have shown that for quantitative agreement of the model with experiments reqires much higher concentration of ions in a water than it is generally accepted. With Kinteic Monte Carlo simulations it is possible to directly meassure conductivity of the sample for different freequencies of external field and for different ion's concentration. That would clarify the necessary magnitude of ion's concentrationa and validate the model of Debye relaxation.

View

Fractal fragmentation and small-angle scattering

Eugen Anitas, Joint Institute for Nuclear Research, Bogoliubov Laboratory of Theoretical Physics, Russian Federation

Abstract: The small-angle scattering form factor of a three-dimensional idealized fragmentation model based on the concept of renormalization is calculated. The system consists of randomly oriented microscopic fractal objects whose positions are uncorellated. It is shown that in the fractal region, the form factor is characterized by a succesion of maxima and minima superimposed on a simple power-law decay, and whose scattering exponent coincide with the fractal dimension of the scatterer. The present analysis of the scattering form factor allows us to obtain the fractal iteration number. The results could be used to obtain additional structural information about systems obtained through fragmentation processes at microscale.

View

On the integrability of evolving membranes

Adrian Sotomayor, Antofagasta University, Mathematics, Chile
Alvaro Restuccia, Antofagasta University, Physics Department, Chile
Luis Cortés Vega, Antofagasta University, Mahematical Department, Chile

Abstract: We analyze an integrable sector of the space of solutions of the four dimensional (super) membrane theory, where the target space is locally Minkowskian and hence a solution of the Supergravity equations. By performing a duality transformation we relate it to the 1+1 Born-Infeld integrable equation

View

Regularization of ill-posed problems in Banach space

Matthew Fury, Penn State Abington, Mathematics, United States

Abstract: We investigate regularization for the abstract Cauchy problem du/dt = Au, 0lomorphic semigroup on a Banach space X and x is an element of X. The problem is generally ill-posed as solutions do not depend continuously on the initial data. For example, letting -A be the Laplacian yields the backward heat equation. Although proximity to a solution may be lost when the initial data is perturbed, we prove that a known solution of the problem may be estimated via a small change in the operator A which yields an approximate well-posed problem. Research in this field has produced many effective approximations in both Hilbert space and Banach space including Lattes and Lions' quasi-reversibility method. Recently, as regularization has been sought for non-linear problems, authors have investigated perturbations with a less severe error order. For example, Bousetilla and Rebbani introduce a modified quasi-reversibility method where the approximate operator is defined by a logarithmic function. With this approach, we prove that the abstract Cauchy problem may be regularized via continuous dependence on modeling, that is a small change to the operator yielding a small change in the corresponding solutions. The theory applies to partial differential equations, particularly the backward heat equation. In future work, we intend to extend our study to non-linear ill-posed problems in Banach space.

View

Impact of the Protective Forest Barriers Close to the Highway on Concentration of PM10 and PM2.5

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Hynek Reznicek, CTU Prague, Dept. of Technical Mathematics, Czech Republic
Viktor Sip, CTU Prague, Dept. of Technical Mathematics, Czech Republic

Abstract: The article is devoted to the numerical simulation of the distribution of PM10 and PM2.5 particles emitted from the highway. The mathematical model is based on the Navier-Stokes equations for viscous incompressible turbulent flow simplified by the Boussinesq approximation. The transport equation for the passive pollutant is added. Resulting set of equations is then solved by the AUSM MUSCL scheme in the finite volume formulation. The time integration is performed by the BDF method of the second order with artificial compressibility in dual time. The atmosphere is supposed to be neutrally stratified. This scheme is used for modelling of process of distribution and deposition of the pollutants emitted from the highway. Various types of the protective forest barriers are studied in order to reduce dustiness in the selected regions.

View

Study of deformed quasi-periodic Fibonacci two dimensional photonic crystals

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Abstract: Quasiperiodic photonic crystals are not periodic structures. These structures are generally obtained by the arrangement of layers according to a recursive rule. Properties of these structures make more attention the researchers especially in the case when applying defects. Indeed, the photonic crystals with defects present localized modes in the band gap leading to many potential applications such light localization. The objective of this work is to study by simulation the effect of the global deformation introduced in 2D quasiperiodic photonic crystals. Deformation was introduced by applying a power law, so that the coordinates y of the deformed object were determined through the coordinates x of the non-deformed structure in accordance with the following rule: y = x1+k. Here k is the coefficient defining the deformation. Therefore, the objective is to study the effect of this deformation on the optical response of 2D quasiperiodic photonic crystals, constructed by Fibonacci generation. An omnidirectional mirror was obtained for adequate Fibonacci iteration a part of visible spectra.

View

The intracellular potential relief profile of nanosized crystals of superionic conductor LaF3

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Abstract: The results of quantum-chemical calculations Profile intracell potential relief along which an ion moves in the interstitial F1 in nanolattices superionic crystal LaF3, having dimensions of 3.5 × 2.0 × 2.2 nm ("three-dimensional" grille) and 27 × 0.7 × 0.8 nm ("quasi-one" lattice) with greater dimension along the lattice constant along the lattice constant are presented. It was found that the "three-dimensional" lattice effective value Em barrier to the movement of ions in the insulating phase LaF3 is 0.37 eV, and the energy Ea disorder is 0.16 eV. It is shown that in the superionic phase the barrier Em reduced several times to the value of 0.15 eV, whereas the amount of energy Ea disorder, which determines the state of F1 interstitial ion is reduced to 0.04 eV.

Calculations of the potential profile for threadlike ("quasi-one") lattice shown that the effective value of the superionic state barrier Em varies from 0.38 to 0.23 eV, and the amount of energy Ea disorder varies from 0.22 eV to 0.04 eV for different types of jumps ions F1. In the same phase of the dielectric value Em reduced to 0.22 eV, and the value of Ea is 0.08. It is shown that for both types of grids for some configurations of fluoride ion energy value of Ea disorder does not exceed 1-2.5 kT, which is one of the basic conditions for the formation of a highly conducting phase in the crystal LaF3.

View

Analysis of paramagnetic centers for threevalent iron in aluminosilicates

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Abstract: The processes of minerals formation in geological environments are poorly understood because of their complexity and diversity. A complex multi-stage evolution of each natural minerals leads to the formation of various defects in the crystal lattice, i.e. to deviations from the ideal crystal structure. This presentation deals with the local defects in the minerals-silicates, which were formed as in the process of their growth, as under the influence of ionizing radiation. It is known that local defects, formed during the minerals growth are stable. Passing through the crystal lattice the ionizing radiation (e.g., elementary stream defined by the energy particles, gamma rays, etc.) interacts with it. The effects of radiation on the mineral can be expressed by heating of the crystal, breaking of some chemical bounds, redistribution of free electrons between lattice ions and impurities, and by formation of short-lived isotopes of chemical elements. The irradiation of the mineral outputs a crystalline structure of the energy balance and, thereby, contributes to the formation of defects within the structure. This type of defects is unstable. It is determined by the degradation of mechanical, electrical and other properties of silicates which limits their use. Unfortunately, there are no reliable criteria for identification of defects with natural and radiation background. To a large extent this is due to insufficient knowledge of the nature of point defects in aluminosilicates. The paper presents the results of investigation of the radiation-induces defects in fluorine aluminosilicates from the Volyn-field [Al2 (SiO4)-F, O (H)] by the Electron Paramagnetic Resonance (EPR) method. The studies were conducted on the spectrometer “Bruker” ER 220D, in the temperature range 77-300 K, in X-frequency band. Three types of EPR spectra of single centers were obtained. Their angular dependence was also investigated. The obtained EPR spectra correspond to the model of the paramagnetic ion Fe3+ in the high-spin state S=5/2. Three types of paramagnetic centers were found: one with cubic-symmetry and two with orthorhombic-symmetries. The parameters of the spin-Hamiltonian are given in the table. ---------- ---------- g- factor | ΔH – the width of EPR line (Oe) | a- the constant of the fine structure (sm^{-1}) ---------- ---------- 2,004 | 64 | 113.10^{-4} ----------

---------- 2.022 | 68 | 616.10^{-4} ---------- ---------- 2.040 | 103 | 697.10^{-4} ---------- ---------- The models of point defects forming in minerals as a result of neutron irradiation were given. It was shown that in tetrahedral complexes of SiO4 the substitution of silicon by the magnetic ion (Al, Fe, Cr, V) displacing from the tetrahedron center occur. The cause of the off-center position effect of the ions was discussed.

View

Enhanced 4D-PET contrast-oriented seed-based automatic segmentation algorithm: minimizing heterogeneity impact on volume accuracy.

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Abstract: The aim of this work is to evaluate the performance of a contrast-oriented (COA) seed-based segmentation algorithm for tumor delineation in retrospectively gated (4D-)PET images of lung cancer lesions. In order to identify the main degrading factors, we analyze the dependence of volume accuracy with respect different parameters and therefore, an enhanced version of the algorithm is proposed and evaluated. For the analysis, the algorithm is applied in 4D-PET acquisitions for 8 lung cancer patients. The consensus of three manual contours is established as the gold standard. With the Dice Similarity Coefficient we measure the volume accuracy of the algorithm with respect to the gold standard (DSCA) and moreover, we measure the variability among the 3 experts (DSCE). DSCA/DSCE is employed to evaluate the dependence of algorithm response with respect: lesion activity concentration (ATmean),homogeneity (1/COVT) and volume (VT), derived from the consensus; background activity concentration (Bgmean) and homogeneity (1/COVBg), derived from the volume surrounding the lesion; and target-to-background ratio (TBR). In the enhanced algorithm, the mean activity derived from the segmented volume is applied as an input for a new threshold-volume computation. For its evaluation, the 3 patients with statistically significant discrepancy between DSCA and DSCE are employed. The analysis results in an average of algorithm volume accuracy over the patients, DSCA=0.71±0.08, that is within the variability obtained among experts, DSCE=0.78±0.07. However, DSCA/DSCE has shown a linear correlation with ATmean,1/COVT and VT : r=-0.827, r=0.750 and r=0.714, respectively. The proposed method has reported and average volume accuracy improvement of 25± 3%. In conclusion, the initial algorithm has shown good performance on average, but degrading response for increasing lesion volume, activity and heterogeneity. The enhanced version has shown to minimize this effect in a preliminary evaluation. It motivates a future validation with a larger number of patients to confirm the improvement and to identify the values of activity, heterogeneity and volume for its automatic application.

View

Theoretical and spectroscopic studies of the multipole-ordered ground states of actinide dioxides

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Abstract: The electronic properties of actinide-based materials have been the focus of extensive investigations, and especially the hidden-ordered ground states forming at low temperatures proved to be an extremely challenging research subject. The richness of 5f-electron physics can

be attributed to the multiple degrees of freedom activated through the simultaneous presence of strong spin-orbit coupling and on-site Coulomb interactions. These conditions are in particular met in the actinide dioxides, which have provided a treasure trove of a rich variety of multiorbital physics over many years. Here, the results of ab-initio calculations of their ground states within the LDA+U framework are used to describe the behaviour of the different active electric and magnetic multipoles. In agreement with experimental observations, the nonmagnetic state of plutonium dioxide is computed to be insulating, whereas those of uranium and neptunium dioxides require symmetry breaking to reproduce the insulator ground states, a condition which is met with magnetic phase transitions. The magnetic properties of the latter compounds in the ordered phase are studied by mean-field random phase approximation calculations, emphasizing the importance of multipolar superexchange interactions. Finally, the main findings of these theoretical analysis are discussed against the results of inelastic neutron scattering experiments. Together, these provide a consistent description of the hidden-order phase of neptunium dioxide in terms of higher-rank magnetic multipole ordering and emphasize that quadrupolar waves constitute a major component of the dynamics of uranium dioxide.

View

The Approximate Bayesian Computation methods in the localization of the atmospheric contamination source

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Abstract: In many areas of application, a central problem is a solution of the inverse problem, especially estimation of the unknown model parameters to model the underlying dynamics of a physical system precisely. In this situation, the Bayesian inference is a powerful tool to combine observed data with prior knowledge to gain the probability distribution of searched parameters. We have applied the modern methodology named Sequential Approximate Bayesian Computation (S-ABC) to the problem of tracing the atmospheric contaminant source. The ABC is technique commonly used in the Bayesian analysis of complex models and dynamic system. Sequential methods can significantly increase the efficiency of the ABC. In the presented algorithm, the input data are the on-line arriving concentrations of released substance registered by distributed sensor network from OVER-LAND ATMOSPHERIC DISPERSION (OLAD) experiment. The algorithm output are the probability distributions of a contamination source parameters i.e. its particular location, release rate, speed and direction of the movement, start time and duration. The stochastic approach presented in this paper is completely general and can be used in other fields where the parameters of the model bet fitted to the observable data should be found.

View

Decarbonization of Methane Bubbles in a Liquid Metal medium: A Multi-physics Investigation with Detailed Chemistry and Interfacial Fluid Mechanics

Kian Mehravaran, IASS-Potsdam, E3 Cluster, Germany

Abstract: Decarbonization of Methane via injection of Methane bubbles in a catalytic medium such as liquid tin holds certain promise in the area of Hydrogen production as it is a CO2-free approach to combustion. In this study, numerical solutions to the conservation equations of energy and concentration are sought in spherical coordinates, with the assumption of polar and azimuthal symmetry. Moreover, the fluid mechanics of the rising and deforming bubble is captured by detailed, 3-D, VOF calculations and linked with the energy and concentration calculations. A comprehensive kinetic mechanism is considered for Methane, including the catalytic surface reaction at the interface of the bubble and the liquid metal. Multi-component diffusion is considered for the calculation of the diffusion velocities of individual species. The resulting system

of ODEs are solved by the CVODE stiff system of ODEs solver. Validation of the solution for constant properties and no chemical reaction has been performed and the results match the analytical solution of the diffusion equation to within a few percentages. Experiments are performed as well and in a heated, liquid-tin column. Apart from the overall agreement seen in the values of Hydrogen mole fraction, there is a surprisingly well match between the measured and predicted values of the minor species Ethene.

View

Recent advances in wave and circulation modeling for the coastal-ocean predicting systems

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Abstract: The ocean wave and circulation modelling has shown impressive developments, both on the theoretical aspects as in the quality of the results available to users. The state-of the art development of the WAM wave model for forecasts applications at operational services and for hind-casts and climate assessments for the North Sea and the German Bight is presented. The ocean waves control the exchange of energy, momentum, heat, moisture, gas, etc. between the ocean and the atmosphere in the earth system. Therefore this study addresses also the coupling between wave and circulation models. This topic reflects the increased interest in operational oceanography to reduce prediction errors of state estimates at coastal scales. The uncertainties in most of the presently used models result from the nonlinear feedback between strong tidal currents and wind-waves, which can no longer be ignored, in particular in the coastal zone where its role seems to be dominant. A nested modelling system is used to producing reliable now- and short-term forecasts of ocean state variables, including wind waves and hydrodynamics. Issues of downscaling, data assimilation, atmosphere-wave-ocean couplings and ecosystem dynamics in the coastal ocean are discussed. The synergy between observations and models is increased on the road to improving the ocean state estimate and predictions in the coastal areas and generating up-to-date information, products and knowledge. Sea state reconstructions and climate scenarios computations have created a huge interest to use the data in industrial applications.

View

DEVELOPMENT OF A SUPPORT VECTOR MACHINE-BASED IMAGE ANALYSIS SYSTEM FOR FOCAL LIVER LESIONS CLASSIFICATION IN MAGNETIC RESONANCE IMAGES

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Abstract: Purpose: The design and implementation of a computer-based image analysis system employing the support vector machine (SVM) classifier system for the classification of Focal Liver Lesions (FLLs) on routine non-enhanced, T2-weighted Magnetic Resonance(MR) images. Materials and Methods: The study comprised 92 patients; each one of them has undergone MRI performed on a Magnetom Concerto (Siemens). Typical signs on dynamic contrast-enhanced MRI and biopsies were employed towards a three class categorization of the 92 cases: 40-benign FLLs, 25-Hepatocellular Carcinomas(HCC) within Cirrhotic liver parenchyma and 27-liver metastases from Non-Cirrhotic liver. Prior to FLLs classification an automated lesion segmentation algorithm based on Marcov Random Fields was employed in order to acquire each FLL Region of

Interest. 42 texture features derived from the gray-level histogram, co-occurrence and run-length matrices and 12 morphological features were obtained from each lesion. Stepwise multi-linear regression analysis was utilized to avoid feature redundancy leading to a feature subset that fed the multiclass SVM classifier designed for lesion classification. SVM System evaluation was performed by means of leave-one-out method and ROC analysis. Results: Maximum accuracy for all three classes (90.0%) was obtained by means of the Radial Basis Kernel Function and three textural features (Inverse-Different-Moment, Sum-Variance and Long-Run-Emphasis) that describe lesion's contrast, variability and shape complexity. Sensitivity values for the three classes were 92.5%, 81.5% and 96.2% respectively, whereas specificity values were 94.2%, 95.3% and 95.5%. The AUC value achieved for the selected subset was 0.89 with 0.81 – 0.94 confidence interval. Conclusion: The proposed SVM system exhibit promising results that could be utilized as a second opinion tool to the radiologist in order to decrease the time/cost of diagnosis and the need for patients to undergo invasive examination.

View

A two-class population balance equation model for the flocculation of microalgae

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Abstract: Microalgae such as Chlorella spp. are unicellular photosynthetic aquatic organisms useful for biomass production. A major challenge in downstream processing of microalgae lies in separating the microalgae from their growth medium, that is, the harvesting process. The cost and energy demand for harvesting microalgae could be significantly reduced if the cells could be pre-concentrated by flocculation. Several ways to flocculate microalgae are available, ranging from flocculation induced by chemicals or by an electric field, to bio-flocculation and spontaneous autoflocculation. A bimodal flocculation describes the flocculation process in which both microflocs and macroflocs change their relative mass fraction and develop a bimodal floc size distribution with two peaks in the mass or volumetric size distribution. Modeling of this phenomenon has been attempted using a two-class population balance equation (PBE) in order to fully understand the kinetics of the microalgal flocculation process.

View

APPLICATION OF CFD TO HYDROGEN DEFLAGRATION IN A VENTED ENCLOSURE

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Abstract: Hydrogen is a very promising alternative fuel which is expected to play a significant role in the near future. However, significant safety issues are associated with it. In the case of an accidental release, hydrogen mixes with air and can form a flammable mixture over a wide range of concentrations. In the present work, CFD simulations of hydrogen deflagration in a medium scale vented room are performed. The room is filled with homogeneous hydrogen-air mixture of 18% v/v. The combustion model is based on the turbulent flame speed concept. The turbulent flame speed is a modification of Yakhot's equation, in order to account for all the main physical mechanisms which appear in hydrogen deflagrations. Special attention is given to the modeling of

the external explosion. The overpressure time series inside and outside of the enclosure are compared with the experimental results. The flame front position is also compared with the experimental data. Good agreement with the experiment is observed.

View

Trans-dimensional Monte Carlo sampling for structure decoupling: an application to geophysical inverse problems

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Abstract: Trans-dimensional (trans-D) algorithms have been recently introduced to the earth sciences to solve inverse problems without having to impose a fixed spatial structure to the model parametrization (e.g. a fixed number of layers in a 1D structure). Trans-D algorithms are usually implemented in a Bayesian framework, i.e. where the solution is a full probability density function of the unknown parameters, rather than a single “best-fiting” model. This posterior probability density function is usually approximated by sampling the parameter space with Markov chain Monte Carlo (McMC) algorithms, where the sampled models are asymptotically distributed as the target distribution (i.e. the posterior probability distribution). It has been demonstrated that trans-D algorithms contain an in-build “Occam's razor”. Thus, they show a parsimonious behavior, i.e. between two models that explain equally well the data, the model with fewer parameters will have a higher posterior probability. This fact guarantees that the model complexity is completely dictated by data and not by subjective choices (like damping and smoothing parameters), avoiding the introduction of any artifacts. Trans-dimensional algorithms can be easily used for joint inversion of different data-set using a “Hierarchical Bayes” approach. Solving the joint inverse problem using a “Hierarchical Bayes” approach allows one to estimate the magnitude of the data error for each data-set thus avoiding the use of subjective weights to “balance” the contribution of each data-set to the solution. In the simplest case of joint inversion, two different observables concur to the reconstruction of the same physical parameter. In more complex cases, two observables are used to investigate the structure of two physical parameters, sharing the same structure. In the latter cases, however, some difficulties arise if the two observables display very different resolving power. In this case, the structure of the target solution might be twisted toward one observable, introducing non resolved (i.e. over-complex) structure for the other investigated parameters. In this study, we develop a trans-D algorithm for joint inversion of two different data-sets to reconstruct the 1D structure of two different physical parameters. The 1D structure for the two parameters can be completely coupled (i.e. the two physical properties share the same layering) or completely decoupled, or a mixture. In this way, the “parsimony” of the trans-D algorithm produces common discontinuities (a “coupled” structure) for portions of the 1D profile where the two observables displays similar resolving power, while the two reconstructed 1D structures will be different (i.e. the two structure are “decoupled”) where the two observables have different resolving power. The algorithm is tested using a classical geophysical inverse problems. We apply the trans-D algorithm to a simple “changepoints” problem. We analyse the time-variation of S-wave splitting parameters (delay time and fast-axis directions) during a seismic sequence to highlight when such parameters changed in time.

View

Study of properties of the symmetry in hybrid symmetrical quasi-periodic photonic

crystals

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Abstract: The light propagation through a one-dimensional symmetric photonic structure which is mad of two dielectric materials of different refractive indices, which are arranged in a quasi-periodic sequence (Bg27/Sv4/Bg27) determined by the symmetric Silver mean (Sv4) distribution embedded between two Bragg structures (Bg27), is studied using the transfer matrix method (TMM). The focus lies on the investigation of the influence of symmetry of the structure as well as the dependence of the transmission on the frequency, the angle of incidence of the light striking the structure and the symmetrical deformation of the structure. Deformation was introduced by applying a power law, so that the coordinates y of the deformed object were determined through the coordinates x of the non-deformed structure in accordance with the following rule: y = x1+k. Here k is the coefficient defining the deformation. A comparison will be made with a symmetrical periodic structure having the same number of layers. All results were discussed in relation with the k values. Indeed in the case of low k values near zero a monochromatic filter was obtained and in the case of relatively high values an omnidirectional mirror was obtained.

View

Computational Models of an Inductive Power Transfer System for Electric Vehicle Battery Charge

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Abstract: One of the issues to be solved for electric vehicles (EVs) to become a success is the technical solution of its charging system. In this paper, computational models of an inductive power transfer (IPT) system for EV battery charge are presented. Based on the fundamental principles behind IPT systems, 3 kW single-phase and 22 kW three-phase IPT systems for Renault ZOE are designed in MATLAB/Simulink. The results obtained based on the technical specifications of the lithium-ion battery and charger type of Renault ZOE show that models are able to provide the total voltage required by the battery. Also, considering the charging time for each IPT model, they are capable of delivering the electricity needed to power the ZOE. In conclusion, this study shows that the designed computational IPT models may be employed as a support structure needed to effectively power any viable EV.

View

Movement of a vortex filament near oscillating pinning centers in the hard superconductor

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Abstract: A problem on vortex behavior near oscillating pinning centers in the type III superconductors is considered. The oscillations can be caused by different reasons, for example, by the acoustic oscillations of a superconductor crystalline lattice. It is shown that under the

assumption of strong external action, movement of a vortex filament can be described by a parabolic problem with a free boundary. In this case, an unknown free boundary is a-priory represented by the set of points, in which a transition from superconducting to normal state and vice versa occurs. A number of statements on the qualitative properties of a free boundary are derived from the general theory of such problems; thus, the properties of a phase boundary “superconductor - non-superconductor” are considered. The revealed mathematical regularities of free boundary behavior are transferred to the diffusion processes of superconducting carriers during vortex movement, carrier birth and annihilation.

View

Computational approach to study FFLO phases in nanoscale superconductors

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Abstract: Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phases [1] arise in superconductors under high magnetic fields from the imbalance of the populations of electrons with spin up and spin down caused by strong Zeeman spin splitting of the quasi-particles states. Nevertheless for these states to be realized, superconductivity must not be, firstly, destroy by orbital pair breaking, thus, orbital pair breaking must be smaller than Pauli pair breaking for them to be observed. FFLO phases were predicted to exist in unconventional superconductors with layered structure or with large effective mass, which suppress the effect of orbital pair breaking. The orbital pair breaking is naturally weaker in nano-superconductors, for which higher magnetic fields are, thus, accessible, increasing the possibility of finding stable FFLO phases in them. To study the presence of FFLO phases in nanoscale superconductors, we solve the generalized Bogoliubov-de Gennes (BdG) equations in a disc geometry. Generalized BdG equations take into account Zeeman spin interaction, and are composed of two sets of standard BdG equations (with an extra Zeeman spin term) connected through a common order parameter. This order parameter is defined as a sum of contributions of both sets of equations. To solve the generalized BdG equations in the disc geometry, we employ a method similar to the one previously developed to solve Ginzburg-Landau equations [2]. First, the one-electron generalized momentum operator (in magnetic field) is projected into the space defined by the eigenfunctions of the Laplacian operator, which is further used as a basis for generalized BdG problem. The generalized BdG equations are solved self-consistently with the BCS equation for the order parameter from which the spatial distribution of the latter in an applied magnetic field is obtained. We will discuss solutions for both standard and generalized BdG equations. We also note that the method used here can be extended to general 2D forms like it was recently proposed to solve Ginzburg-Landau equations in arbitrary planar geometries [3]. [1] P. Fulde, R. Ferrel, Phys. Rev. 135, A550 (1964) ; A. I. Larkin, Y. N. Ovchinnikov, Sov. Phys. JETP 20, 762 (1965) [2] L. F. Chibotaru, A. Ceulemans, M. Morelle, G. Teniers, C. Carballeira, V. V. Moshchalkov, J. Math. Phys. 46, 095108 (2005) [3] P. J. Pereira, V. V. Moshchalkov, L. F. Chibotaru, Phys. Rev. E 86, 056709 (2012)

View

Effect of loading history on visco-elastic properties of a polymer

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Abstract: Rheology of polymer gels exhibit visco-elastic behaviours. These properties can be described and analysed involving generalized calculus. Complexity of their behaviour involves fractional order of constitutive equations, as shown by Das(2011), Heymans and Bauwens(1994), Dutta Choudhury et al.(2012).Non-linearity is introduced through a generalized calculus approach by incorporating a non-integer order time derivative in the viscosity equation. A strain hardening

proportional to the time lag between the two loading steps is also incorporated.We have modelled viscoelastic effect of polymers and their memory effect of loading by introducing memory kernel during solving constitutive equation of stress-strain. This model reproduces the three salient features observed in the experiment, namely - the memory effect, slight initial oscillations in the strain as well as the long-time solid-like response. Dynamic visco-elasticity of the sample is also reported.

View

Modelling of poro-visco-elastic biological systems.

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Abstract: Michael Gasik, Aalto University Foundation School of Chemical Technology, Department of Material Science and Engineering, Finland Yevgen Bilotsky, Aalto University Foundation School of Chemical Technology, Department of Material Science and Engineering, Finland The research of mechanical properties of poro-visco-elastic biomaterials is an important task, especially for tailoring the best conditions for ingrowth and healing of implants. In this work we analysed the behaviour of biomaterials under different static and dynamic loading regimes, in "dry" and "wet" conditions. Retrieved data revealed nonlinear relations between applied force and resulting deformation, with time and frequency dependence. These features were described by a nonlinear model, which reasonably fits mentioned peculiarities. The simplified model was validated with numerical simulations using COMSOL software. Upon validation it allows incorporation of the experimental data obtained by biomechanical spectroscopy towards prediction of biomaterials behaviour in "in vitro" conditions, with the purpose to extrapolate to clinically-relevant environment.

View

Modeling of microaccelerations of spacecraft indoor environment caused by thermal impact

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Abstract: The article deals with modeling of microaccelerations of spacecraft indoor environment caused by thermal impact while spacecraft enters and leaves the Earth's shade. “NASTRAN” was used for modeling. There were got the own deformation shapes of large elastic elements of spacecraft. The homogeneous plates were used as elastic elements for modeling.

View

Effects of Magnetic Field and Hall Current to the Blood Velocity and LDL Transfer

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Abstract: The magnetic field and Hall current effects have been considered on blood velocity and concentration of low-density lipoprotein (LDL). It is important to observe those effects to the flowing blood in a stenosed artery. The analysis from the obtained results may be useful to some clinical procedures, such as MRI, where the radiologists may have more information in the investigations before cardiac operations could be done. In this study, the uniform magnetic field and Hall current are applied to the Newtonian blood flow through an artery having a cosine-shape stenosis. The governing equations are coupled with mass transfer and solved employing a finite difference Marker and Cell (MAC) method with an appropriate initial and boundary conditions. The

graphical results of velocity profiles and LDL concentration are presented in this paper and the results show that the velocity increases and concentration decreases as Hall parameter increased.

View

Multilayer Silicene on Ag(111) and √3×√3-Ag/Si(111)-7×7

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Abstract: Multilayer silicene [1-5], the silicon equivalent of multilayer graphene, was produced in ultra high vacuum (UHV) on silver (111) surfaces. These films grow in consecutive flat terraces, after the initial formation of the 3×3 reconstructed first silicene monolayer, which is in a 4×4 coincidence super cell with respect to the silver (111) unit cell. All terraces have a honeycomb √3×√3R(30°) surface symmetry, with respect to 1×1 silicene, as detected in Scanning Tunnelling Microscopy (STM) and Low Energy Electron Diffraction patterns (LEED). The √3×√3R(30°) symmetry was first observed by Wu's group [6, 7]. They attributed this structure to the first and/or bilayer silicene, although it arises from second, third and all upper silicene layers [1-5]. Currently there is a scientific debate on the possibility that the multilayer silicene is indeed thin film of bulk-like silicon [8-10]. Thick epitaxial multilayer silicene films were obtained either on Ag(111) 5 or √3×√3R(30°)-Ag/Si(111)-7×7 and studied by LEED, Auger electron spectroscopy, X-ray diffraction, energy dispersive X-ray reflectivity, Fourier transform infrared as well as Raman spectroscopy. The temperature for both substrates during the silicon growth, strongly influences the nature of these films, by passing amorphous, multilayer silicene and bulk Si(111). These results are of crucial interest for applying silicene in the well-established silicon based nowadays-widespread electronics, taking into account that the first FET single layer silicene was successfully realized [11]. [1] P. De Padova et al., Appl. Phys. Lett. 102, 163106 (2013). [2] P. De Padova et al., J. Phys. : Condens. Matter, Fast Track Commun. 25, 382202 (2013). [3] P. Vogt et al., Appl. Phys. Lett. 104, 021602-1-5 (2014). [4] E. Salomon et al., J. Phys.: Condens. Matter, 7, 185003 (2014). [5] P. De Padova et al., 2D Materials 1, 021003 (2014). [6] B. Feng et al., Nano Lett. 11, 3507 (2012). [7] L. Chen et al., Phys. Rev. Lett. 109, 056804-1-5 (2012). [8] T. Shirai et al. Phys. Rev. B 89, 2414031- 2414035 (R) (2014). [9] J. Chen et al., Arxiv 1405.7534. [10] J. Mannix et al., ACS Nano, 8, 7538 (2014). [11] L. Tao et al.,Nat. Nanotech. DOI: 10.1038/NNANO.2014.325.

View

Modification of silicene via oxidation, hydrogenation and halogenation

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Abstract: Graphene and silicene are two elemental 2D materials discovered so far, consisting of single sheet of C and Si atoms, respectively. Both graphene and silicene host Dirac fermion state that induces exotic spintronic and optoelectronic properties. To explore these effects, in many cases it requires a control of the electronic state, for examples, doping or opening a gap at the Dirac point. Chemical adsorption is an effective method to modify the electronic property of graphene, where a dramatic band-gap opening was observed upon graphene hydrogenation. Theoretical calculations also suggested intriguing properties in chemically modified silicene, for examples, large gap (~3 eV) opening, interesting ferromagnetic and optoelectronic properties. Here we present our experimental works on the surface chemistry of silicene by oxidation, hydrogenation and halogenation. We found interesting long range ordered phases in hydrogenated and halogenated silicene, revealing the reaction nature of silicene with these two adsorbates. Moreover, we found that hydrogenation can help us to disclose the seemingly

complicated superstructures of clean silicene on Ag, and to find out the intrinsic structure of the underlying silicon network.

View

Synthesis of Germanene

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Abstract: We have investigated the growth of Pt on Ge(110) using scanning tunneling microscopy and spectroscopy [1]. The deposition of several monolayers of Pt on Ge(110) followed by annealing at 1100 K results in the formation of three-dimensional eutectic GePt nanocrystals. Upon cooling down these eutectic GePt nanocrystals phase separate into pure Ge2Pt and Ge phases. The Ge segregrates towards the surface and forms a germanene layer. The germanene honeycomb lattice is composed of two hexagonal sub-lattices that are displaced vertically by 0.2 Å. The nearest-neighbor distance of the atoms in the honeycomb lattice is 2.5±0.1 Å, i.e. very close to the predicted nearest-neighbor distance in germanene. The differential conductivity (dI/dV) versus energy data reveals a V-shaped dependence with a non-zero minimum that is located just above the Fermi level.

View

Methods to create required dynamic properties of a spacecraft using its orientation schemes

Ksenya Potienko, Samara State Aerospace University named after academician S.P. Korolev, Radio department, Russian Federation

Abstract: The following article deals with problem to meet the microacceleration requirements for conducting of technological processes on board of a spacecraft. Different methods of spacecraft orientation are analyzed here to solve this problem.

View

Novel graphene wrapped WO3 photocatalyst using for water pollutant degradation

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Abstract: The present study reported the synthesis of graphene wrapped WO3 nanocomposites using a one-step hydrothermal process. The synthesized nanocomposites were used to degrade dyes in pollutant water. The results showed WO3 nanopellets dispersed uniformly on the graphene surface. Moreover, the photocatalytic degradation efficiency of the prepared nanocomposites enhanced signifincantly compared to the neat WO3. The study offers a new way to degrading dye effluent in the industrial waste water at high degradation speed.

View

Density functional theory study on the doping and surface chemistry of hydrogenated silicene

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Abstract: When silicene is hydrogenated (i. e., passivated by hydrogen), a bandgap occurs so that

it becomes a semiconductor. Analogous to all the other semiconductors, doping is highly desired to realize the potential of hydrogenated silicene (H-silicene). In the framework of density functional theory (DFT), we have studied the doping of H-silicene with boron (B) and phosphorus (P). The concentration of B or P ranges from 1.4% to 12.5%. It is found that the doping of B or P enables the indirect-bandgap H-silicene to be a semiconductor with a direct bandgap. With the increase of the concentration of B or P, both the valence band and the conduction band shift to lower energies, while the bandgap decreases. Both B- and P-doping lead to the decrease of the effective mass of holes and electrons in H-silicene. For both B- and P-doped H-silicene a subband absorption peak may appear which blueshifts with the increase of the dopant concentration. Organic surface modification may be critical to the practical use of H-silicene. It is intriguing to know if organic surface modification seriously impacts the structural, electronic and optical properties of H-silicene. We focus on four organic surface modification schemes (hydrosilylation, alkoxylation, aminization and phenylation) with the experimentally demonstrated surface coverage of about 33%. The geometrical structures, band structures and optical absorption of organically surface-modified H-silicene have been compared with those of silicene and H-silicene in the frame work of DFT. It is found that organic surface modification leads to the increase of the buckling distance of silicene, while causing the angles of bonds in the honeycomb structure of silicene to decrease. Although the initial hydrogenation makes silicene become an indirect-bandgap semiconductor, the subsequent organic surface modification schemes further change the band structure of silicene. Hydrosilylation, phenylation, alkoxylation and amination all give rise to the reduction of the bandgap of H-silicene. Hydrosilylated and phenylated H-silicene are indirect-bandgap semiconductors, while alkoxylated and aminated H-silicene are direct-bandgap semiconductors. Changes of the optical absorption induced by organic surface modification are well correlated to the corresponding changes of the band structure.

View

Regular and Chaotic Dynamics in the Gross-Pitaevskii Equation by an External Potential

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Abstract: Many theoretical and experimental studies have been performed on nonlinear properties in Bose-Einstein Condansate (BEC). It is well known that BEC is described by Gross-Pitaevskii Equation (GPE) with an external potential. GPE has rich numerical and analytic solutions for different optical lattice because of the interatomic interactions. In this work, we construct an external potential that accelerates the atoms in the x direction with tilted force. Then the regular and chaotic behaviours of GPE are presented with Poincare sections in phase space.

View

An energy method for the Cauchy problem for the Helmholtz equation

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Abstract: The Cauchy problem for the Helmholtz equation appears in various applications and is severely ill-posed. For solving the problem, we present a method that consists of minimizing an energy-like error functional. For this, we first introduce an artificial boundary in the interior of the domain. This addition of the interior boundary allows us to derive a bilinear form that gives us a proper framework for the formulation of the problem as an optimization problem. Numerical results that confirm the convergence of the proposed method are also presented.

View

A TECHNIQUE FUNCTIONAL BASED ON THE EUCLIDEAN ALGORITHM WITH APPLICATIONS TO 2-D ACOUSTIC DIFFUSERS

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Abstract: The main objective of this work is to build, based on the Euclidean algorithm, a functional technique, which allows to discover a direct proof of Chinese Remainder Theorem. Also, we given its properties as applications to 2-D acoustic and Diffractal diffusers. The novelty of our technique is its functional algorithmic character, which improves ideas as well as results of the author and his collaborator in a previous work.

View

Computation of the Mutual Inductance between Air-Cored Coils of Wireless Power Transformer

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Abstract: Wireless power transfer system is a modern technology which allows the transfer of electric power between the air-cored coils of its transformer via high frequency magnetic fields. However, due to its coil separation distance and misalignments, a maximum power transfer is not guaranteed. Based on a more efficient and general model available in the literature, rederived mathematical models for evaluating the mutual inductance between circular coils with and without lateral and angular misalignments are presented. Rather than presenting results numerically, the computed results are graphically implemented using MATLAB codes. The results are compared with the published ones and clarification regarding the errors made are presented. In conclusion, this study shows that power transfer efficiency of the system can be improved if a higher frequency alternating current is supplied to the primary coil, the reactive parts of the coils are compensated with capacitors and ferrite cores are added to the coils.

View

A model for anomaly classification in intrusion detection systems.

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Abstract: The Intrusion Detection Systems (IDS) constitute an important security layer for computer systems. IDSs are traditionally divided into two types according to the detection methods they employ, namely (i) misuse detection and (ii) anomaly detection. Anomaly detection have been widely used and its main advantage is the ability to detect new attacks. However, the analysis of anomalies generated can become expensive, since they often have no clear information about the malicious events they represent. In this context, this paper presents a model for automated classification of alerts generated by an IDS that performs its detections by anomaly. The main aim is the classification of the information provided in the alert of an anomaly in well-defined taxonomies of attacks. Some common attacks to computer networks were considered and we

achieved important results that can equip security analysts with best resources for their analyzes.

View

Investigating Color Models for Cellular Segmentation of White Blood Cells

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Abstract: Quantitative analysis of white blood cells in blood smear images offers important information about health conditions of patients to pathologists. Image processing techniques can be used to aid experts in detection of diseases and orientation to effective treatments. Identification of white blood cells is essential for their classification, making analysis even more accurate. This paper presents a method for detection of WBC applied on different channels of RGB, HSI, L*a*b and YIQ models. The best result was obtained with the channel H from HSI color model, wherein regions of interest were selected by the Otsu's thresholding method. A postprocessing step was applied using morphological operations, removal of small objects and region filling. The proposed system was tested on 367 images for analysis of its performance through Jaccard and Accuracy metrics, reaching results of 87.49% and 98.91%, respectively. Different channels of color models, already used in other studies in the literature, showed inferior results compared with the obtained in this work.

View

Evaluation of the Magnetic Fields and Mutual Inductance between Circular Coils Arbitrarily Positioned in Space

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Abstract: This paper presents the evaluation of the magnetic fields and mutual inductance between circular coils arbitrarily positioned in space. Firstly, based on an advanced and relevant model available in the literature, MATLAB code is implemented to evaluate the mutual inductance between circular coils arbitrarily positioned with respect to each other. The computed results are compared with the numerical results previously published in the literature and a detailed clarification regarding the huge computational errors made are presented. In the second part, a complex and relevant model available in the literature for evaluating the magnetic fields due to a circular coil is presented. Based on the useful information, the model for computing the magnetic fields between two circular coils is formulated. The computed results are validated with experimental measurements. The comparison of the results shows that the developed model and the experimental measurements conducted are accurate and effective.

View

Analysis of Stomata Distribution Patterns for Quantification of the Foliar Plasticity of Tradescantia Zebrina

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Abstract: Here we propose a method for the analysis of the stomata distribution patterns on the surface of plant leaves. We also investigate how light exposure during growth can affect stomata distribution and the plasticity of leaves. Understanding foliar plasticity (the ability of leaves to modify their structural organization to adapt to changing environmental resources) is a fundamental problem in Agricultural and Environmental Sciences. Most published work on quantification of stomata has concentrated on descriptions of their density per unit of leaf area, however density alone does not provide a complete description of the problem and leaves several unanswered questions (e.g. whether the stomata patterns change across various areas of the leaf, or how the patterns change under varying observational scales). We used two approaches here, to know, Bouligand-Minkowski descriptors and complex networks, as a means to provide a description of the complexity of these distributions. In the experiments, we used 18 samples from the plant Tradescantia Zebrina grown under three different conditions (4 hours of artificial light each day, 24 hours of artificial light each day, and natural light) for a total of 69 days. The network descriptors were capable of correctly discriminating the different conditions in 88% of cases, while the fractal descriptors discriminated 83% of the samples. This is a significant improvement over the correct classification rates achieved when using only stomata density (56% of the samples).

View

Numerical investigation of light localization in generalized Thue-Morse 1D photonic crystal

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Abstract: We theoretically investigate the spectral and light localization properties in one dimensional (1D) generalized Thue Morse quasi-periodic photonic structures. Here, we consider generalized Thue Morse sequences GTM(m,n,l) with inflation scheme L→L^m H^n H→H^n L^m Equivalently GTM (m,n,l) can be constructed as: S_0=L, S¯_0=H S_(l+1)=S_l^m S¯_l^n S¯_(l+1)=S¯_l^n S_l^m Theoretical analysis is performed by TMM (Transfer Matrix Method) algorithm to study the optical properties by simulating the electric field intensity. This method provides an analytical approach for calculation of wave propagation in multilayer media. We have shown that by varying m and n simultaneously in the generalized Thue-Morse structure, the electric field intensity varies according to the parity of these parameters and also according to the peak positions. We show that the whole structure GTM(m,n,l) has an interesting application for well selection pairs (m, n) values. So, the light localization depends strongly with m, n and l and for appropriate values maximum light localization was obtained

View

Gravitational mass and Newton’s universal gravitational law under relativistic conditions

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Abstract: We discuss the predictions of Newton’s universal gravitational law when using gravitational, mg, rather than the rest masses, mo, of the attracting particles. According to the equivalence principle, the gravitational mass equals the inertial mass, mi, and the latter, which can be directly computed from special relativity, is an increasing function of the Lorentz factor, gamma, and thus of the particle velocity [1]. For gravitationally bound rotating composite states, the ratio of the thus computed gravitational force for gravitationally bound rotational states to that corresponding to low (gamma=1) particle velocities is shown to be of the order of (mPl/m¬o)2 where mPl is the Planck mass [1]. The same result, within a factor of two, is obtained via the use of the derivative of the effective potential of the Schwarzschild geodesics of GR. It is shown that the predictions of this relativistic Newtonian gravitational law are in good agreement with the predictions of GR for some macroscopic systems as well. [1] C.G. Vayenas, S. Souentie, A. Fokas, Physica A, 405, 360-379 (2014)

View

Design of phononic-crystals by tailored graphene-like structures

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Abstract: With the ongoing development of state-of-the-art fabrication techniques phononic-crystals have attracted a lot of interest lately [1]. The concept dates back to the 90's [2,3] when it was shown that acoustic wave propagation in elastic media exhibits a band gap and certain frequencies are completely blocked. Adjusting the phononic band gap has become one important goal in the study of phononic crystals for the design of new acoustic wave devices, but also for the next generation thermoelectric devices. Motivated by recent developments in achieving highly defined patterns in hybrid graphene - hexagonal boron nitride (G-hBN) materials [4,5] we investigate here the possibility of tuning the phononic band structure. Graphene and hBN are two structurally very similar materials, with a lattice mismatch of less than 2%, which makes them ideal to form binary composites. However, they have different electronic properties, graphene being a semimetal, while hBN a large band gap semiconductor. We consider periodic arrays of G-hBN, as 2D infinite planes and finite width nanoribbons, and analyze the phononic band gap tuning by changing the shapes of the G-hBN domains, by employing DFT calculations. Hollow graphene structures and allotropes of graphene [6] provide alternative routes for achieving 2D materials with tunable properties. The nanoribbon structures are investigated with a particular focus on reducing the phononic heat conductivity, which implies a larger figure of merit and therefore an improved thermoelectric conversion. [1] N. Zen, T. A. Puurtinen, T. J. Isotalo et al., Nature Communications 5, 3435 (2014). [2] M. Sigalas and E.N. Ecconomou, Elastic and Acoustic Wave Band Structure, Journal of Sound and Vibration, 158, 377-382 (1992). [3] M.S. Kushwaha, P. Halevi, L. Dobrzynski and B. Diafari-Rouhani, Acoustic Band Structure of Periodic Elastic Composites, Phys. Rev. Lett. 71, 2022-2025 (1993). [4] Li Song, Lijie Ci, Hao Lu et al., Nanolett. 10, 3209 (2010). [5] Yongji Gong, Gang Shi, Zhuhua Zhang et al., Nature Communications 5, 3193 (2014). [6] A. L. Ivanovskii, Russ. Chem. Rev. 81, 571 (2012).

View

Using UAVs and digital image processing to quantify areas of soil and vegetation

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Abstract: Unmanned aerial vehicles (UAVs) are becoming a very popular tool for remote sensing and crop monitoring. They are more easily deployed, cheaper and can obtain images with higher spatial-resolution than satellites. Some small, commercial UAVs can obtain images with spatial-resolution as low as 1.5cm per pixel. This opens up the range of possible remote sensing and monitoring applications. Moreover, they can cover large areas in very little time, such as 50 ha in about 20min, which makes UAVs the ideal tool for monitoring large farms and plantations. On the other hand, it is important to know precisely the area covered by farms in order to avoid invasion of other properties or preserved areas, and also to detect flaws in the plantation area. However, it is difficult to measure planted areas in some cases, such as Eucalyptus crops. Therefore, this paper aims to evaluate the use of UAV imagery for precise area measurement in Eucalyptus crops. We developed an image-processing algorithm to segment regions of soil, low biomass and high biomass and tested it on a Eucalyptus plantation in the city of Lençóis Paulista -SP, Brazil. Results show that the area quantification is very accurate especially for bare soil regions and this method can be used to estimate areas in other scenarios.

View

Use of Genetic Algorithm for the Selection of EEG Features

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Abstract: Algorithm (GA) is a popular optimization technique that can detect the global optimum of a multivariable function containing several local optima. GA has been widely used in the field of biomedical informatics, especially in the context of designing decision support systems that classify biomedical signals or images into classes of interest. The aim of this paper is to present a methodology, based on GA, for the selection of the optimal (or nearly optimal) subset of features that can be used for the efficient classification of Event Related Potentials (ERPs), which are recorded during the observation of correct or incorrect actions. ERPs are a special category of electroencephalographic (EEG) signals, which are recorded from various locations on a subject's scalp when the subject is presented with external stimuli or events. In our experiment, ERP recordings were acquired from sixteen (16) healthy volunteers who observed correct or incorrect actions of other subjects. The brain electrical activity was recorded at 47 locations on the scalp. The GA was formulated as a combinatorial optimizer for the selection of the combination of electrodes that maximizes the performance of the Fuzzy C Means (FCM) classification algorithm. In particular, during the evolution of the GA, for each candidate combination of electrodes, the well-known Σ-Φ-Ω features were calculated and were evaluated by means of the FCM method.

The proposed methodology provided a combination of 24 electrodes, with classification accuracy 90.6%. Thus, GA can be the basis for the selection of features that discriminate ERP recordings of observations of correct or incorrect actions.

View

MATHEMATICAL MODELING OF MULTIPLE SHOCK INITIATION IN HETEROGENEOUS EXPLOSIVES USING A MESOSCOPIC REACTION RATE MODEL

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Abstract: To understand and predict the physics of explosive materials, numerical models are utilized to simulate various scenarios. Various hazard and vulnerability scenarios for explosives involve multiple shock compression. In the present study, a kind mesoscopic model for shock ignition of solid heterogeneous is examined in order to demonstrate its availability to account for the desensitization by multiple shocks in explosives. Since the mesoscopic model is based on the assumption of the elastic viscoplastic pore collapse mechanism, and the desensitization mechanism is also described usually in connection with the closure of pores, the ability of the mesoscopic model to predict the desensitization effects must be analyzed. For this purpose, the mesoscopic model has been numerically modeled and implemented in hydrodynamic code LS-DYNA as a user defined equation of state. For verification, the double shock, reflected shock and detonation quenching experiments have been modeled. The numerical results show that the model can reproduce various features of the previously reported experiments involving the double shock desensitization of solid explosives.

View

Numerical Analysis of Thirring Model under White Noise

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Abstract: Today, the effects of noise on dynamical systems are an attractive area of research. The noise acts as a driving term in the equations of motion in nonlinear systems. In this work, we present conformally invariant pure spinor nonlinear Thirring model. Thirring model describes Dirac fermions in (1+1) space-time dimensions with local current-current interaction. This model has rich dynamic of the quantization of relativistic quantum field theories. We investigate the response of Thirring oscillator to white noise by constructing Poincaré sections in phase space.

View

Early breast cancer detection method based on a simulation study of single-channel passive microwave radiometry imaging

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Abstract: Microwave radiometry (MWR) for noninvasive temperature imaging is based on near-field power reception and has been proposed for early cancer detection by estimating the internal body temperature distribution [1]. The measurement of a radiometer (also known as brightness temperature - Tb) is considered to emanate as the weighting average over the antenna's field of view, of the real core temperature (T) multiplied by a weighting function (W); W depends on the antenna properties as well as tissue characteristics [2]. The aim of the present study is to provide a methodology for detection and visualization of alterations in internal body temperature, based on single channel microwave radiometer imaging. In order to obtain Tb measurements a simulation study was conducted that modeled a./ the human breast, as an hemisphere of homogeneous tissue, b./ the temperature distribution (T) by means of a Butterworth function, and c./ the antenna characteristics (W) according to [3]. Moreover, a simulated lesion was employed of variable size and position, to provide for slight temperature changes inside the breast. The inverse problem solution, meaning finding the temperature distribution T from the simulated data Tb, was approached by assuming that the temperature distribution is the mixture of distributions with unknown parameters. The values of the parameters values were determined by means of the least squares method in conjunction with the singular value decomposition method. The proposed method was validated in a variety of scenarios by altering the lesion size and location, the radiometer position with and without presence of noise. The method proved capable in identifying alterations in different parts of the breast. The visualization was performed with 2-D images in the form of thermal maps, where the temperature distribution in the coronal plane was imaged.
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Acknowledgements: The research activities that led to these work, were co-financed by National Funds and by the European Regional Development Fund (ERDF) under the Hellenic National Strategic Reference Framework (NSRF) 2007-2013, concerning the project "MMRIBTM" with ref. number (12CHN181) within the Bilateral Cooperation between Greece & China action.

View

A MATHEMATICAL MODEL OF THE DYNAMICS OF QUANTUM THERMAL FLUCTUATIONS

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Abstract: In this paper, we study the problem of fluctuations of observables dependent on the spatial coordinates and time and describing the collective motion in the long-wavelength range. The authors of [1, 2] proposed to consider the dynamics of quantum-thermal fluctuations of the density and drift velocity at equilibrium with respect to the temperature in the framework of the stochastic hydrodynamics, which is a generalization of the Nelson stochastic mechanics [3]. This allows extending the hydrodynamic form of the quantum mechanics to finite temperatures. As a result, the system of equations, which is valid at any temperatures, was obtained for a one-dimensional model taking the diffusion pressure of the warm vacuum into account. Moreover, we have managed to write these equations in the form of the equations of two-velocity hydrodynamics ■((du_ef)/dt=-∂/∂q (vu_ef)-∂/∂q (u_ef^2)/2,@dv/dt=-(2D_qu)/ħ ∂U/∂q+Ξ_T ∂/∂q (u_ef^2)/2,) (1) where uef is the effective diffusion velocity, v is the drift velocity, Dqu is the quantum self-diffusion

coefficient in the cold vacuum at T = 0, Ξ_T is the parameter taking the effective environmental influence into account, and U(q) is the potential energy of the regular action. In this paper, we consider the principal validity of the given hydrodynamic model for describing the evolution of quantum-thermal fluctuations based on the self-diffusion mechanism. We show that this model leads to the parabolic type of equations, which allows using it to describe the dynamics of macroscopic fluctuations unlike the Nelson model leading to equations of the elliptic type describing stationary processes. In the numerical study of system (1), we show that the solution has the form of a perturbation wave running with respect to the spatial coordinate and evolving with time. Thus, we assume that the hydrodynamic approach to the quantum theory allows, in principle, constructing the model of the dynamics of quantum-thermal fluctuations taking the self-diffusion mechanism into account. References Sukhanov A.D. JMP, 2008, v.154 (1). P.185 Sukhanov A.D., Golubjeva O.N. JMP 2009. V.160 (2). P 369. 3. Nelson E. Dynamical theory of Brownian motion. Princeton: Princ. Univ. Press., 1967

View

Design of a decision support system, trained on GPU, for assisting melanoma diagnosis in dermatoscopy images

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Abstract: The purpose of this study was to design a decision support system for assisting the diagnosis of melanoma in dermatoscopy images. Clinical material comprised images of 44 dysplastic (clark’s nevi) and 44 malignant melanoma lesions, obtained from the dermatology database Dermnet. Initially, images were processed for hair removal and background correction using the Dull Razor algorithm. Processed images were segmented to isolate moles from surrounding background, using a combination of level sets and an automated thresholding approach. Morphological (area, size, shape) and textural features (first and second order) were calculated from each one of the segmented moles. Extracted features were fed to a pattern recognition system assembled with the Probabilistic Neural Network Classifier, which was trained to distinguish between benign and malignant cases, using the exhaustive search and the leave one out method. The system was designed on the GPU card (GeForce 580GTX) using CUDA programming framework and C++ programming language. Results showed that the designed system discriminated benign from malignant moles with accuracy higher than 90%, employing morphological and textural features. The proposed system could be used for analyzing moles depicted on smart phone images. This could assist towards early detection of melanoma cases, if

suspicious moles were to be captured on smartphone by patients and be transferred to the physician together with an assessment of the mole's nature.

Acknowledgements: The research activities that led to these work, were co-financed by National Funds and by the European Regional Development Fund (ERDF) under the Hellenic National Strategic Reference Framework (NSRF) 2007-2013, concerning the project "MARK1" with ref. number (ISR_3233) within the Bilateral Cooperation between Greece & Israel action.

View

Mathematical Model for Absolute Magnetic Measuring Systems in Industrial Applications

Marina Ludszuweit, Helmut-Schmidt-University, University of the Federal Armed Forces Hamburg, Department of Mechanical Engineering, Germany

Abstract: Most of the scales for measuring systems are based on incremental and absolute measuring methods. Incremental scales need to initialize a measurement cycle at a reference point. From there, the position is computed by counting increments of a periodic graduation. Absolute methods do not need reference points since the position can be read directly from the scale. The positions on the complete scales are encoded using several incremental tracks with different graduation. We present a new method for absolute measuring using only one track for position encoding up to micrometre range. We use a pattern of trapezoidal magnetic areas, so we can store more complex information than by simple binary patterns. For positioning, we use the magnetic field. Every position is characterized by a set of values measured by a hall sensor array. We implement a method for reconstruction of absolute positions from the set of measured values. We compare different patterns with respect to uniqueness, accuracy, stability and robustness of positioning and discuss how stability and robustness of our measuring method can be described mathematically. We show how they are influenced by different errors during the measurement in real applications and how those errors can be compensated.

View

Numerical study of deformed Hybrid Bragg /Fibonacci sequences One Dimensional Photonic Crystal by transfer matrix method

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Abstract: Photonic crystal structures have attracted great interest in research area and industry field. Photonic crystals are periodic systems that consist in general of separate high dielectric and low dielectric regions. The periodicity or spacing determines the relevant light frequencies. In this paper we describe theoretical analysis by extracting the transmission spectra in the spectral range 0.3-3 μm of deformed one dimensional photonic crystal hybrid Bragg /Fibonacci quarter wave structure by using a transfer matrix method. Deformation was introduced by applying a power law, so that the coordinates y of the deformed object were determined through the coordinates x of the non-deformed structure in accordance with the following rule: y = x1+k. Here k is the coefficient defining the deformation degree. The study configuration is H(LH)7/(FQPS)7. The Fibonacci quasiperiodic structure (FQPS) is generated by the rule Sl+1=Sl.Sl−1. The initial generations S1

and S2 are taken as S1 = H and S2 = L where H and L are two elementary layers with refractive indices nL = 1.45 and nH taken to be varied from 2.34 to 3.7. We show that the whole structure H(LH)7/(FQPS)7 for the third Fibonacci generation has an interesting application as an omidirectional mirror covering the three optical telecommunications wavelengths 0.85 ; 1.3 and 1.55 μm. All results were compared to the periodic Bragg structure which has the same number of layers.

View

Numerical approach for dating of literary works

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Abstract: This paper is about a numerical approach to a problem of dating of literary works based on an author's idiolect analysis. We used literary works with specified date of writing from the Project Gutenberg Literary Archive. The number of dated works was over 20,000, which were used for drawing up of 2-gramms frequency dictionary for each text. The proposed method of dating of literary works is based on comparison of syntactic and stylistic parameters of a text with the same parameters of widely used lexicons of different years. We drew up 2-gramms frequency dictionaries for the period from 1700 to 2010 using Google books Ngramm database. Distribution functions parameters of different frequency dictionaries were compared using various relative entropy metrics (like Kullback–Leibler divergence). Classification was carried out using artificial neural networks. Before the training of the neural network, the entire database was divided into a training and test datasets. The first dataset was used during the training of the neural network, the second dataset - for testing. The results of testing showed good accuracy of dating of literary works. It is offered to use the proposed approach to to establish the date of earlier undated publications or verify existing dates of publications, for example, the works of Molière and Corneille.

View

State of the superconductor in the inhomogeneous external field due to magnetic moment close to surface

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Abstract: We study the state of the bulk superconductor under effect of the external magnetic moment placed near to the surface. To find the order parameter and magnetic vector potential distributions, we solve the Ginzburg-Landau equations using the pseudoviscosity method for the corresponding time-dependent GL (TDGL) equations. The computational complexity of this problem is caused mostly by the memory access sparseness and large volume of the grid due to the three-dimensional geometry. We overcome it by choosing nonuniform grid and GPGPU calculation. Main applications of this work include development of novel spintronic devices and high-Tc superconducting (HTSC) materials with improved transport characteristics.

View

Validating Knowledge Based Framework Through Mission-Oriented Sensors Array and Smart Sensor Protocol

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Rayner Pires, University of São Paulo, Institute of Mathematics and Computer Science, Brazil
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Abstract: Due to the unmanned aerial vehicles versatility, the remarkable and growing use of these aircrafts nowadays has driven not only the expectations of that market values but also the amount of research in several related areas. So these systems require continuous evolution and adaptation. Because the usage of SOA can provide and support the integration between mission and aircraft, we propose and use the Knowledge Based Framework for Dynamically Changing Applications (KBF) in this kind of aircraft. Moreover, using KBF and the Mission-Oriented Sensors Array (MOSA) to decouple the mission from the aircraft control systems, the development of new applications for these vehicles can be benefited. Then, the Smart Sensor Protocol (SSP) allows the connection between MOSA and UAVs with KBF. The results show that it is possible to successfully implement the SSP on a modest hardware, making its implementation feasible in real scenarios. These results support the feasibility of implementing an interface mechanism for coupling of intelligent mission processors in civilian and military UAVs, contributing to the proliferation of these aircrafts.

View

The filamentation of a laser beam as a "labyrinth" instability

Florin Spineanu, National Institute of Laser Plasma and radiation Physics, Plasma and Fusion, Romania

Abstract: Experimental studies have revealed the formation of structures in a transversal plane of a high power (self-guided) laser beam. The structures consist of filaments generated by the transversal modulation competing with the interaction with the inhomogeneous atmospheric refractive index. The pattern of filamentation is similar to a lattice cluster as in a 2D percolation process and appears to be associated to a phase transition. We provide evidence that there is a correlation between this filamentation and the "labyrinth" instability in reaction-diffusion systems. Besides the similarity of the spatial organization in the two cases, we show that the two differential equations that describe the dynamical processes lead to effects that can be mutually mapped. For the laser beam at high power the Non-linear Schrodinger Equation in a regime of strong self-focusing and ionization of the air is solved by robust solitons. For the labyrinth instability a model of activator-inhibitor is solved. A simple, discrete, model of 2D coupled cubic lattice maps clearly exhibits the same tendency of organizing the space in an evolving filament pattern. We discuss the common ground and the possible use of this analytical connection and suggest that the same effect of unstable interface dynamics and gradient flow occurs in these processes.

View

Clustering of the points lying on monotonous curves as a partition into antichains.

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Abstract: Let us consider some set of points on the Cartesian plane. Each point is a part of one of few curves describing the dependency between abscissas and ordinates. In our case these are dependencies between the rock occurrence depth and the oil saturation described by Skelt-Harrison equation. In this work a problem of distributing these points into clusters corresponding to different curves is being investigated. First stage of clustering involves determining the least number of curves demanded to describe all the points and finding points definitely lying on specific curve. These points are used to obtain parameters of the original dependencies described by Skelt-Harrison equation. The final clustering can be naturally performed using restored curves. Conventional clustering methods cannot be applied due to problem specifics. Another issue with

conventional methods is computational complexity, when applied to large amount of data. Sometimes sampling can help to deal with this problem, however in specific case it may also provide a data set, which cannot be clustered. For first stage of clustering an original method based on presenting data points as elements of partial ordered sets with coordinate order is proposed. Thus to solve clustering problem one needs to find all the points which are parts of maximum length chains and to distribute them into corresponding antichains. One can propose obvious algorithm to solve the problem in quadratic time, based on Mirsky's theorem. In this work algorithm of O(n log(n)) complexity is proposed. The algorithm is based on the fact that Dushnik–Miller dimension of the partially ordered set is equal to 2 and can be applied to a wide class of dependencies.

View

Study of Hybrid Bragg /Paper folding/Bragg sequences one dimensional photonic crystal using the transfer-matrix approach

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Yassine Bouazzi, Photovoltaic and semiconductor materials laboratory, National Engineering School of Tunis, University of Tunis El Manar, , Tunisia
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Abstract: In this work, a new type of optical device using photonic band gap materials has been proposed. Indeed, a combination of periodic (PMS) and Paper Folding quasi-periodic one-dimensional photonic multilayer systems (QPMS) were used. SiO2(L) and TiO2(H) were chosen as two elementary layers with refractive indexes nL=1,45 and nH=2,30 respectively. Hence, the study structure is [(PMS)^J][(QPMS)^P][(PMS)^J], which forms an effective Fabry–Perot filter (FPF), where J and P are respectively the repetition number of periodic (PMS) and quasi-periodic (QPMS) stacks. The effect of these two parameters for producing an improved polychromatic filter with high finesse coefficient (F) and quality factor (Q) is presented in details. We use the so-called Transfer Matrix Method (TMM) to numerically investigate the optical properties in the visible range of these hybrid photonic structures. We show that the number and position of resonator peaks are dependent on the QPMS repetition number P and the iteration order of the QPMS generating sequence.

View

QUANTUM DYNAMICS OF BIOLOGICAL PLASMA

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Abstract: A quantum solution of the Fisher–Kolmogorov–Petrovskii–Piskunov equation with convection and linear diffusion is obtained which can provide the basis for the quantum biology and quantum microphysics equation. On this basis, quantum emission of biological systems, separate microorganisms (cells or bacteria), and dust plasma particles is investigated. The possibility arises of creating a generator of hard photons with energy higher than 1000 GeV. Life on the Earth can need relic radiation.

View

Mathematical modeling of thermodynamic and transport properties of H-bonded low-temperature substances

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Abdurakhman Aldiyarov, Kazakh national university, Technical physics, Kazakhstan
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Abstract: The results of modeling of isotopic water mixture clusters in nitrogen and argon cryomatricies are presented. Earlier, our experimental studies of water in cryomatrix have shown that changes in the concentration of an analyte in matrix leads to a splitting of the absorption bands characteristic frequencies of the molecules in the IR spectrum. Moreover the multiplicity of characteristic absorption bands in the IR spectrum remained unchanged during heating of the samples from the condensation temperature to the sublimation temperature of the matrix element. In order to find out what the structure of clusters is responsible for the immutability of the absorption bands in the vibrational spectrum during thermal cycling of the samples computer research of water molecules enclosed in nitrogen and argon cryomatrix by the molecular dynamics simulation was conducted. For this purpose, theoretical studies were carried out using computer software packages, that implement used by us semi empirical and ab initio molecular dynamics methods. As a result of the research, the data must be obtained are of theoretical interest for summarizing the physico-chemical properties of systems, consisting of water molecules, and their combination with inert gases, as well as other atoms for studying the properties of molecular crystals composed of small molecules.

View

Canonical equations of Hamilton for the nonlinear Schrodinger equation

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Abstract: We define two different systems of mathematical physics: the second-order differential system (SODS) and the first-order differential system (FODS). The Newton's second law of motion and the nonlinear Schrodinger equation (NLSE) are the exemplary SODS and FODS, respectively. We obtain a new kind of canonical equations of Hamilton (CEH), which are of some kind of symmetry in form and are formally different with the conventional CEH without symmetry [Goldstein et al., Classical Mechanics, 3rd ed, Addison-Wesley, 2001]. We also prove that the number of the CEHs is equal to the number of the generalized coordinates for the FODS, but twice the number of the generalized coordinates for the SODS. We show that the FODS can only be expressed by the new CEH, but do not by the conventional CEH, while the SODS can be done by both the new and the conventional CEHs. As an example, we prove that the nonlinear Schrodinger equation can be expressed with the new CEH in a consistent way.

View

Constructive Realization of Geometric Integration in Accelerator Physics

Sergei Andrianov, Saint Petersburg State University, Applied Mathematics abd Control Processes, Russian Federation

Abstract: In the paper some of problems of constructive realization of paradigm of geometric integration devoted to long-time evolution of the particle beam in cyclic accelerators are described. Some constructive solutions based on the Lie methods and the Kronecker algebraic operations for

solution of corresponding motion equations are presented. These solutions can be constructed as in a numerical form or in the form of symbolic expressions. In the latter case the corresponding modules can be encapsulated into a special database. This allows realizing parametric studies of the dynamical system using the methods and instruments of computer algebra. Some examples of modeling of real processes are presented.

View

The Wavelet Method for Locating the Critical Point in Glass Transitions

Ayse Humeyra Bilge, Kadir Has University, Faculty of Engineering and Natural Sciences, Turkey

Abstract: The critical point of a sigmoidal curve is defined as the limit of the points where the derivatives of a sigmoidal point reach their global extreme value. Recently we have shown that the location of the critical point is controlled by the phase of the Fourier transform of the sigmoidal curve. In the present work we use data on glass transition to show that the observed crical point agrees with the theoretical prediction. As there is no analytical model for the glass transition curve, we use a wavelet method to compute the Fourier transform. Joint work with Onder Pekcan, Kadir Has University

View

Enzymatic mechanism of serine protease thrombin reconstructed in a computational model

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Yulia Einav, Holon Institute of Technology, Holon, Israel, Faculty of Sciences, Israel

Abstract: Thrombin is a typical serine protease that plays a crucial role in blood clotting and thrombolysis. The negative D189 of the enzyme is crucial for aligning the positive arginine of the substrate in the proper position for hydrolysis. The catalytic activity of thrombin is accelerated by metallic ions, of which Na+ is the most potent. The ion binding site identified by crystal structures is, however, 17 Å apart from the enzyme's active site. This separation could not explain the exact mechanism of Na+ influence. In the present study, based on molecular dynamics simulations, we calculated electrostatic forces and interaction distances and performed a rigorous statistical analysis of these data in order to reconstruct an enzymatic mechanism of thrombin in a computational model. We show that negative D189 of the enzyme can interact either with a Na+ ion or with the positive moiety of the product. The ionic bond created between D189 and Na+ eventually leads to the dissociation of the product from the enzyme and, thus, completion of the catalytic cycle.

View

The Quantum Monte Carlo method in real time to study of the dynamics of weakly interacting Bose-systems.

Iliya Kuznetsov, National Research Nuclear University MEPhI, Department of Physics of Solid State and Nanosystems, Russian Federation

Abstract: The numerical algorithm based on the Quantum Monte Carlo method reformulated in real time to study of the dynamics of interacting quantum systems, is developed. In our talk, we present the application of this approach for the study of non-equilibrium processes in weakly interacting Bose gas: approaching the thermal equilibrium, the formation of a Bose-Einstein

condensate, thermal relaxation in the system of polaritons in a semiconductor sample inside the resonator[1],[2], the dynamics of positronium gas annihilation in the one of the most promising scheme of the gamma-ray laser[3]. 1. Oleg L. Berman, Yurii E. Lozovik, and David W. Snoke. Theory of Bose-Einstein condensation and superfluidity of two-dimensional polaritons in an in-plane harmonic potential. Phys. Rev. B,77:155317, Apr 2008 2. A. Rahimi-Iman, A. V. Chernenko, J. Fischer, S. Brodbeck, M. Amthor, C.Schneider, A. Forchel, S. Hoing, S. Reitzenstein, and M. Kamp. Coherence signatures and density-dependent interaction in a dynamical exciton-polariton condensate. Phys. Rev. B, 86:155308, Oct 2012 3. H. K. Avetissian, A. K. Avetissian, and G. F. Mkrtchian Self-Amplified Gamma-Ray Laser on Positronium Atoms from a Bose-Einstein Condensate. Phys. Rev. Lett. 113: 023904, July 2014

View

Effects of W-boson and neutrino magnetic moment on the differential cross-section of neutrino-electron scattering

Asan Damanik, Sanata Dharma University, Mechanical Engineering, Indonesia

Abstract: We study and consider the W boson and neutrino magnetic moment on the differential cross-section of neutrino-electron scattering in the frame of standard model particle physics. We also discussed some phenomenological implications of the W boson and neutrino magnetic moment on the physics beyond standard model

View

Quantum Mechanics Beyond Coarse Graining

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Michael Zeitlin, IPME RAS, Mathematical Methods in Mechanics Group, Russian Federation

Abstract: We construct some universal picture for re-consideration of base states and generic phenomena, like entanglement, in Quantum Mechanical set-up. Our main goal is related to the analytical continuation of the standard zoo of solutions/base states from trivial ones, like plane waves or gaussians to novel states, possibly realizable, which permit more realistic (re)interpretation of the base folklore of Quantum Mechanics as well as more proper analytical/numerical modeling on the whole qualitative scale from entanglement to decoherence. Definitely, there is a set of experimental features as well as theoretical prerequisites demanding the appearance of new usefulness images. We start from some simple categorification procedure allowing to consider generic states as sheaves but not functions, after that we look for internal hidden symmetries on the level of the underlying "categorified" Hilbert space of extended states. The orbits of these symmetries create the arena where we can model the novel features of our generalization of Quantum Mechanics. The analytical instruments allowing us to model both qualitative and quantitative aspects are Nonlinear Local Harmonic Analysis on the representations of orbits of hidden symmetries of underlying generalized Hilbertian spaces and variational principles which permit the algebraization of the subsequent control of the type of behaviour. It seems that reasonable extension of the zoo of possible (realizable) states can simplify the search of prototypes for realizable quantum devices as well as provide the more realistic (re)interpretation of the long-living standard "quantum folklore".

View

Nonlinearities due to radiating energy on a physical system

Fernando Maass, University of Antofagasta, Physic, Chile

Abstract: We discuss from a physical and mathematical point of view radiating electrical circuits in

forms of the Poynting theorem. We determine the nonlinear differential equation satisfied by the electrical current in the circuit. The nonlinearity of the equation is due to the contribution of the radiated energy. We study the space of solutions of the nonlinear equation. We show that the generic solution presents a “sudden death” behavior in distinction to the exponential decaying solutions of linear systems with energy losses due to the presence of resistance on the circuit. These exists an exponential decaying solution of the nonlinear differential equation, it exists for particular initial data and hence it is not a generic solution. Moreover, it is unstable with respect to small perturbations of the initial conditions.

View

Turbulence modeling using test modes

Madalina Vlad, National Institute of Laser, Plasma and Radiation Physics, Plasma Theory Group, Romania

Abstract: We present an analytical self-consistent approach, which is able to analyze the processes that appear in the nonlinear stage of turbulence. The statistical characteristics of the turbulence and of the transport are evaluated as functions of time. The results concern drift turbulence in confined plasmas, but possible extensions to other physical systems are discussed. The method is essentially based on a combined study of test particle and test modes in turbulent plasmas. We show that the main cause of the nonlinear processes that appear beyond the quasilinear stage of turbulence is trajectory trapping or eddying. The requirements for modeling these processes are deduced. Trapping introduces quasi-coherent aspects in test trajectory statistics, which lead to large scale correlations (inverse cascade), nonlinear damping of the drift modes and generation of the zonal flows.

View

Deterministic particle transport in a micro-pump

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Abstract: The present work was motivated by a micro-pumping device allowing particle sorting depending on their size or mass. A pore periodic lattice filled of liquid and suspended particles is connected at both ends to basins. A periodic pumping is applied leading to a periodic driving flow. Depending on the pressure oscillations (amplitude and frequency) a net motion of the particles appears. This particle drift was interpreted as a ratchet effect called drift ratchet in literature: inertialess advecting particle under Brownian fluctuation in an asymmetric geometry. In contrast, we focus on an axisymmetric deterministic model with particles of small inertia in a creeping flow. The particle drag force is computed using Boundary Element Method and we show that a non-linear ODE governs the particle motion. Path-following method is employed in the parameter space in order to retrace the scenario that leads from trivial periodic solutions to particle transport. Under appropriate conditions, particles may drift and two main transport mechanisms are identified. For very small inertia, quasi-periodic transport occurs. We show that this dynamics is similar to the phase drift during a loss of synchronization of a periodic oscillator under weak external periodic force. In contrast, for moderate small inertia, the transport threshold involves a chaotic dynamics and strange attractors. Finally, we relate the different transport mechanisms with the pore shape and the pumping kind.

View

Radio Resource Allocation on Complex 4G Wireless Cellular Networks

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Abstract: Nowadays users are demanding continuous delivery of increasingly higher data over the Internet, in both wired and wireless networks. Due to its real-time nature, wireless data delivery typically has bandwidth, delay and loss requirements. Moreover, the 3GPP Long Term Evolution (LTE) is the new standard developed to cope with future mobile data and emerging media applications. The generic characteristics of wireless networks are time-varying and their performance is generally inferior to those of wired networks. Therefore, it is still a challenging problem to efficiently provide data delivery service of high quality over 4G LTE Wireless Networks. However, for wireless data delivery in LTE, higher data rate could lead to higher packet loss rate, thus degrading the user's Quality of Experience (QoE). Generally, wireless communication systems should support a large number of users with flexibility in their quality of service (QoS) and Quality of Experience (QoE). The challenges to ensure the fulfillment of these requirements arise from the limited availability of frequency spectrum, and the nature of the wireless channel. To solve this issue, intelligent radio resource algorithms interacting in both the physical and the application layers are critical. Radio resource allocation are categorized into two major classes with different objectives The objective of the first class is to minimize the total transmit power with the constraint on users' data rates whereas in the second class, the objective is to maximize the total throughput with the constraints on the total transmit power as well as users' data rates. In this article we consider the heuristic algorithm which improves step by step wireless data delivery over LTE cellular networks by using the total transmit power with the constraint on users' data rates, and the total throughput with the constraints on the total transmit power as well as users' data rates, which are jointly integrated into a hybrid-layer design framework to perform radio resource allocation for multiple users, and to effectively decide the optimal system parameter such as modulation and coding scheme (MCS) in order to adapt to the varying channel quality. We propose new heuristic algorithm which balances the accessible data rate, the initial data rates of each user allocated by LTE scheduler, the priority indicator which signals delay- throughput-packet loss awareness of the user, and the buffer fullness by achieving maximization of radio resource allocation for multiple users. It is noted that the overall performance is improved with the increase in the number of users, due to multiuser diversity. Experimental results illustrate and validate the accuracy of the proposed methodology.

View

Comparison of MARTINI and atomistic forcefields for the study of Ceramide Bilayers

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Philip Borbadonakis, University of Crete, Chemistry, Greece
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Abstract: Ceramides bilayers constitute the lipid domain of stratum corneum, the outermost layer of the skin. The biological importance of the specific system arises from the fact that it has major contribution to the barrier function of the skin. The development of modelling approaches for the study of skin permeability is of great importance for the drug and cosmetic industry, as it can reduce but also complement experiments, but demands the molecular study of very large domains of the actual structure. In order to study larger system with molecular dynamics techniques,

functional groups are represented by coarse particles rather than individual atoms. The use of a coarse grained force field relies on less detail than a traditional atomistic (all-atom or united-atom) force field. This enables us to simulate easily yet realiably larger system and study phenomena which evolve at different length scales, such as the diffusion etc. In this work, we attempt to model a typical fully hydrated ceramide bilayer, consisting of 128 molecules of CER NS 24:0, with MARTINI [1], a coarse grain forcefield suitable for molecular dynamics simulations of biomolecular systems. For determining the accurate representation of the ceramide bilayer, we compare the resulting system with the equivalent obtained from atomistic scale simulations [2] on the basis of a series of characteristic structural, thermodynamic, and transport properties, such as: bilayer thickness, density profiles along the bilayer normal, area per lipid, order parameters, radial distribution functions. The system under investigation is a All simulations are carried out at 300 K and 1 bar using four MARTINI parametrizations, considering that presently there are no optimized MARTINI [3,4] input values, specifically parameterized for ceramides. The atomistic forcefields that are used to evaluate the coarse grain process performance are OPLS-UA, GROMOS, BERGER, CHARMM, GAFF. References 1. Marrink, S. J., de Vries, A. H., & Mark, A. E. Coarse Grained Model for Semiquantitative Lipid Simulations. The Journal of Physical Chemistry B, 108(2), 750–760, 2004. 2. Papadimitriou, N. I., Kainourgiakis, M. E., Karozis, S. N., & Charalambopoulou, G. C. Studying the structure of single-component ceramide bilayers with molecular dynamics simulations using different force fields. Molecular Simulation, 1–15, 2014. 3. C.A. Lopez, Z. Sovova, F.J. van Eerden, A.H. de Vries, S.J. Marrink. Martini force field parameters for glycolipids.; J. Chem. Theory Comput., 9, 1694-1708, 2013. 4. Yin Wang, Paraskevi Gkeka, Susanne von Grafenstein, Julian E. Fuchs, Roland G. Huber, Zoe Cournia, Klaus R. Liedl. Parameterization of a Coarse-Grained Model for Ceramides, in preparation, 2013.

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View

The “Demokritos” Cyber-infrastructure for climatic research management

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Abstract: Environmental informatics presently is merely the way to link meteorology and pollution sources to population exposure and determine the impact on human health. More importantly, it is a decision aiding tool for local authorities to predict potential atmospheric pollution problems, optimize actions and policy making activities so as to produce the maximum health benefit. The present work, describes the on-going efforts of NSRD to build a cyber-infrastructure for climatic research management (CCRM) that will essentially contribute to the planning, development, maintenance and coordination of NCSRD systems to help process and disseminate climate related information. The foreseen actions will aid NCSRD to develop and establish a long term sustainable data centre, hosting the data generated in the various R&D activities. CCRM is envisioned as a service-oriented, open-source, web-based network of climate research outcome, pollutant

emissions, data repositories and existing and new data analysis tools. CCRM will focus on the following main areas relevant to climatic research: 1. Air quality modeling, 2. Data analysis, and forecasting; 3. Emissions inventory development and assessment; 4. Use of satellite and ground-based remote sensing information; 5. Scientific visualization; 6. Communication of air quality data to decision-makers and the public; 7. Service-oriented architecture and software development CCRM could additionally provide data hosting and access services to user groups from other relevant infrastructures in the Region, complemented with data from other relevant networks. References 1. Dumitrescu A., Busuioc A., Madalina B., Cheval S., Cazacioc L., “RCM performance in reproducing temperature and precipitation regime in Romania. Application for Banat and Oltenia Plains”, Water Core Meeting Romania, 05 – 07 October 2011 2. Seiler C., Implementation and validation of a Regional Climate Model for Bolivia, Fundacion Amigos de la Naturaleza (FAN-Bolivia), July 2009 3. Stull, R. (2000) “Meteorology for Scientists and Engineers”. Brooks/Cole

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View

Comparison of serial and parallel simulations of a corridor fire using FDS

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Abstract: Current program systems based on the knowledge of CFD (Computational Fluid Dynamics) allow to model the course of fire and its effects on structure and building equipment. This paper deals with comparison of serial and parallel simulation of a corridor fire by the FDS (Fire Dynamics Simulator) system. In parallel realization of the computation, the whole computational domain is divided into computational meshes and computation on each computation mesh is considered as a single MPI (Message Passing Interface) process realised on one computer core. Communication between MPI processes is provided by MPI. Since such procedure causes errors at touches of computational meshes, the aim of this paper is to determine the size of error of simulation results due to parallel computation.

View

CFD MODELING OF LNG SPILL: HUMIDITY EFFECT ON VAPOR DISPERSION

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Abstract: The risks entailed by an accidental spill of Liquefied Natural Gas (LNG) should be indentified and evaluated, in order to design measures for prevention and mitigation in LNG terminals. For this purpose, simulations are considered a useful tool to study LNG spills and to understand the mechanisms that influence the vapor dispersion. In the present study, the ADREA-HF CFD code is employed to simulate the TEEX1 experiment. The experiment was carried out at the Brayton Fire Training Field, which is affiliated with the Texas A&M University system and involves LNG release and dispersion over water surface in open-obstructed environment. In the simulation the source was modeled as a two-phase jet enabling the prediction of both the vapor dispersion and the liquid pool spreading. The conservation equations for the mixture are solved along with the mass fraction for natural gas. Due to the low prevailing temperatures during the spill ambient humidity condenses and this might affect the vapor dispersion. This effect was examined

in this work by solving an additional conservation equation for the water mass fraction. Two different models were tested: the hydrodynamic equilibrium model which assumes kinetic equilibrium between the phases and the non hydrodynamic equilibrium model, in order to assess the effect of slip velocity on the prediction. The slip velocity is defined as the difference between the liquid phase and the vapor phase and is calculated either using the algebraic slip model or by solving the momentum conservation equation for the liquid phase. Different droplet size distributions and a constant diameter model are applied and the results are discussed and compared with the measurements.

View

A parallel approach of COFFEE objective function to multiple sequence alignment

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Abstract: The computational tools to assist genomic analyzes show even more necessary due to fast increasing of data amount available. Thus, the sequence alignment plays an important role in bioinformatics, where obtained results might assist in analyzes and inferences over data achieved. With high computational costs of deterministic algorithms for sequence alignments, many works concentrate their efforts in the development of heuristic approaches to multiple sequence alignments. Heuristics as Progressive Alignment, Ant Colony, Simulated Annealing, Tabu Search and Genetic Algorithms are between the most used ones in multiple sequence alignment tools. However, the selection of an approach which offers solutions with good biological significance and feasible execution time is a great challenge. Thus, this work aims to show the parallelization of the processing steps of MSA-GA tool using multithread paradigm in the execution of COFFEE objective function. The MSA-GA is a tool to perform multiple sequence alignments based on simple genetic algorithm and uses an objective function to check the biological significance of the final alignments. The standard objective function implemented in the tool is the Weighted Sum of Pairs (WSP), which produces some distortions in the final alignments when sequences sets with low similarity are aligned. Then, in studies previously performed we implemented the COFFEE objective function in the tool to smooth these distortions. Although the nature of COFFEE objective function implies in the increasing of execution time, this approach presents points which can be executed in parallel. With the improvements implemented in this work, we can verify the execution time of new approach is 24% faster than the sequential approach with COFFEE. Moreover, the COFFEE multithreaded approach is more efficient than WSP, because besides it is slightly fast, its biological results are better.

View

MaNIAC-UAV - a methodology for automatic pavement defects detection using images obtained by Unmanned Aerial Vehicles

Luiz Henrique Castelo Branco, IFSP, , Brazil
Paulo Segantine, Universidade de São Paulo, Departamento de Transportes - Escola de Engenharia de São Carlos, Brazil

Abstract: Intelligent Transportation Systems - ITS is a set of integrated technologies (Remote Sensing, Image Processing, Communications Systems and others) that aim to offer services and advanced traffic management for the several transportation modes (road, air and rail). Collect data on the characteristics and conditions of the road surface and keep them update is an important and difficult task that needs to be currently managed in order to reduce accidents and vehicle maintenance costs. Nowadays several roads and highways are paved, but usually there is insufficient updated data about current condition and status. There are different types of pavement defects on the roads and to keep them in good condition they should be constantly monitored and maintained according to pavement management strategy. This paper presents a methodology to obtain, automatically, information about the conditions of the highway asphalt pavement. Data collection was done through remote sensing using an UAV (Unmanned Aerial Vehicle) and the image processing and pattern recognition techniques through Geographic Information System.

View

The Emergence of Periodic Behaviours from Randomness

John Pickton, University of Nottingham, Mathematical Sciences, United Kingdom

Abstract: Periodic behaviours can be described with great power and economy using the simple mathematical machinery associated with wave phenomena. However periodic effects can also be ‘observed’ in collections of discrete objects, be they individuals sending emails, fire-flies signalling to attract mates, synapses firing in the brain or photons emerging from a cavity. The identification and origin of what constitutes the wave-like property becomes more difficult to interpret and identify in these instances but can be most simply exemplified by consideration of non-interacting particles moving randomly on a network forming N nodes in a closed loop. Specifically the population dynamics describing the number of particles at a node is a familiar stochastic birth-death process, augmented by particles jumping randomly at rate r to adjacent nodes in either direction. This can result in the emergence of periodic behaviours which occur because of the interaction between the dynamics of the particles and the spatial structure through which they move. For this to happen we show that the network must consist of three or more nodes and the particles must have a preferred direction of jumping. Moreover there are three very different classes of collective behaviour of the populations at the nodes which emerge depending on the value of the birth-rate m. The first occurs when 0<m<r(1-rcos(2pi/N)) in which case the particles become uniformly distributed across all nodes in the network. The second occurs when r(1-cos(2pi/N))<m<2r whereupon the populations become localised and propagate coherently around the network, forming a travelling wave-packet. The last is last regime is m>2r when the all particles collapse into a single node and no longer propagate around the network. Thus distinct coherent structures can emerge purely through random interactions.

View

Computer Simulation of blood perfusion by a contrast in the myocardium using a formulation of single-phase flow in porous media

João Alves, University Federal of Juiz de Fora, Computational Modeling, Brazil
Rodrigo dos Santos, Federal University of Juiz de Fora, Computer Science, Brazil

Rafael de Queiroz, Federal University of Juiz de Fora, Computer Science, Brazil

Abstract: This paper presents a mathematical and computational model that characterizes the spatio-temporal dynamics of blood perfusion in cardiac myocardium. Specifically, we are interested in reproducing qualitative images obtained by contrast-enhanced exams, which are widely used in clinical medicine to evaluate the blood perfusion in the heart. The application of contrast allows the detection of injuries, ischemic regions, fibrosis or tumors. Here we focus on the pathological case associated to subendocardial infarct, which physiological characteristic is a reduced rate of myocardial irrigation by blood (and by implication, lack of oxygen and nutrients for tissue). In our modeling, we will consider the tissue of cardiac myocardium as a porous media, i.e. a solid region with empty spaces. To this end, the modeling was based on differential equations and Darcy's Law, which correlates tissue permeability (low, in the case of a subendicardial infarct), pressure difference and the blood flow in the cardiac tissue. In addition, the work domain is a transversal slice of myocardium.

View

Linearization of an invertible bounded itération in Rd

guy cirier, Université Paris VI, LSTA, France

Abstract: In this paper, we study an iteration f in Rd defined by a diffeomorphism polynomial bounded. So, the image of the invariant curves is relatively compact and we can use the Fourier-Bohr’s representation in the set of almost periodic function (AP). These curves have asymptotically a parameterization with Weierstrass-Mandelbrot’s functions depending on fluctuation’s parameters. So, self-similarity and fractal dimension calculus are justified. We limit the paper to this subject, but we have applied these results to partial differential calculus.

View

A multi-mode cantilever singular point detection using adaptive hypothesis testing

Jakub Dokoupil, CEITEC BUT, , Czech Republic

Abstract: Fundamental analysis of a multi-mode model of the atomic force microscope cantilever shows that at some points; called here singular points, the mode is vanished. Consequently, the order of the input/output behavior is reduced. The singular points can be detected comparing possible candidates on the best model order. The detection is then naturally performed by applying the Bayesian model comparison. Since the exact position of the singular points is not available a priori, an explicit model of updating the probability of tested hypotheses in time is built. More specifically, a mechanism of suppressing absolute information is suggested based on the Bayesian decision problem where the Kullback-Leibler divergence is used.

View

Categorification of Quantum Mechanics: Sheaves, Schemes and all that

Michael Zeitlin, IPME RAS, Mathematical Methods in Mechanics Group, Russian Federation
Antonina Fedorova, IPME RAS, Mathematical Methods in Mechanics Group, Russian Federation

Abstract: Sheafification together with microlocalization and the subsequent analysis of quantum dynamics on orbits with special, so-called MRA-filtrations (generating a full tower of the underlying internal hidden scales), considered in the companion paper, are the starting points of our attempt of Categorification Program for Quantum Mechanics and/or General Local Quantum Field Theory. In some sense, we may hope on the same breakthrough as in the golden era of Algebraic Topology and Algebraic Geometry in the 50s and 60s of the 20th Century, which was concluded by Grothendieck's approach and provided the universal description for a variety of long standing

problems. Roughly speaking, in (Quantum) Physics such an approach provides useful, constructive and universal methods to glue the complex local data into the general picture by power machinery taking into account the topological and (algebraical) geometrical data of the underlying hidden internal structures. Definitely, the simple linear algebra of structureless Hilbert spaces cannot describe the whole rich world of quantum phenomena. Our approach introduces (Grothendieck's) Schemes instead of varieties/manifolds as generic quantum objects, naturally encoded the full zoo of phenomenological things discussed in Quantum Mechanics. The key ingredient of such an approach is the bridge between the von Neumann description of measurement together with the Gelfand ideal of the state and GNS (Gelfand-Naimark-Segal)-construction on one side of the river and locally ringed space, structure sheaf and (affine) scheme on the opposite (categorificated) side.

View

Numerical methods for solution of the stochastic differential equations equivalent to the non-stationary Parker's transport equation

Mateusz Kluczek, Siedlce University of Natural Sciences and Humanities in Poland, Faculty of Sciences, Poland
Anna Wawrzynczak, Siedlce University of Natural Sciences and Humanities in Poland, Department of Computer Science, Poland
Renata Modzelewska, Siedlce University of Natural Sciences and Humanities in Poland, Department of Mathematics and Physics, Poland

Abstract: We derive the numerical schemes for the strong order integration of the set of the stochastic differential equations (SDEs) corresponding to the non-stationary Parker transport equation (PTE). PTE is 5-dimensional (3 spatial coordinates, particles energy and time) Fokker-Planck type equation describing the non-stationary the galactic cosmic ray (GCR) particles transport in the heliosphere. We present the formulas for the numerical solution of the obtained set of SDEs driven by a Wiener process in the case of the full three-dimensional diffusion tensor. We introduce the solution applying the strong order Euler–Maruyama, Milstein and stochastic Runge–Kutta methods. We compare the convergence and stability property of the solution for the listed methods. We also discuss the advantages and disadvantages of the presented numerical methods in the context of increasing the accuracy of the solution of the PTE.

View

Hyper fast radiative transfer for the physical retrieval of surface parameters from SEVIRI observations

Giuliano Liuzzi, University of Basilicata, School of Engineering, Italy
Guido Masiello, University of Basilicata, School of Engineering, Italy
Carmine Serio, University of Basilicata, School of Engineering, Italy
Maria Grazia Blasi, Univerity of Study of Basilicata, School of Engeneering, Italy
Sara Venafra, University of Basilicata, School of Engineering, Italy

Abstract: Geostationary platforms, such as the last generation of METEOSAT satellites, have the capability of monitor large portions of our planet with the advantage of having temporal continuity between consecutive observations. Such aspect, although advantageous in terms of the capability to follow the evolution of the geophysical parameters of interest, is very demanding from the computational point of view: an enormous amount of data must be processed in a very reduced time. In this context, we have developed a new, hyperfast radiative transfer code which operates in the framework of the physical simultaneous retrieval of surface emissivity and temperature from SEVIRI (Spinning Enhanced Visible and Infrared Imager) data acquired on the full disk, using a

Kalman Filter (KF) approach to exploit temporal continuity. The code has been adapted from a monochromatic radiative transfer model and speeded up both reducing the number of atmospheric layers, and coarsening the optical depths look-up table used for transmittance, radiance and Jacobians pure analytical calculations. Overall, we have verified that the new code does not affect the accuracy of computed radiances in the three atmospheric window channels of SEVIRI at 12.0, 10.8 and 8.7 microns that we use in the KF algorithm. At the same time, the code is speeded up by a factor of 10 with respect to the previous version, taking a few hundredths of a second for calculating a single spectrum. The code will be exemplified through retrieval exercises of emissivity and surface temperature for a variety of surface features. In particular an application to the massive Greek forest fires in August 2007 will be shown.

View

Mathematical Models for Freeze-Drying Processes

Francesc Font, University of Limerick, , Ireland

Abstract: Freeze-drying or lyophilisation is a dehydration process widely used in the food and pharmaceutical industries mainly for preservation and storage purposes. The process enables materials or slurry products, which have been previously frozen, to be dried under vacuum conditions. From a modelling point of view this is a very complex process; the mathematical models describing freeze-drying include governing equations for the heat and mass transfer of multicomponent mixtures in porous media where phase change and chemical reactions are typically involved. In this talk we will discuss some mathematical models being currently developed in our group describing different steps of the freeze-drying process.

View

Model of transient cooperative phenomena triggered by THz-pulse irradiation

Kunio Ishida, Toshiba Corporation, Corporate Research and Development Center, Japan
Keiichiro Nasu, Institite of Materials Structure Science, KEK, , Japan

Abstract: Recent progress of intense THz-pulse generation technology has made it possible to inject coherent phonons in a macroscopic scale, and the lattice deformation induced by such a process will cause electronic transitions in strongly coupled electron-phonon systems. Based on the analogy to the photoinduced phase transitions observed in various materials, we consider that cooperative interactions between electrons and coherent phonons will lead to the multiplication of excited electrons and/or growth of a transient phase, which is understood by bifurcation of quantum-mechanical wavepackets on adiabatic potential energy surfaces. Taking a model of localized electrons coupled with a quantized optical phonon mode, we discuss the dynamics of the cooperative phenomena by THz-pulse irradiation and, in particular, the role of the number and/or the initial distribution of phonons in the initial creation process of transient phases.

View

Studying the transport properties of a ceramide lipid membrane with Molecular Dynamics simulations

Nikolaos Papadimitriou, National Center for Scientific Research Demokritos, Environmental Research Laboratory, Greece
Stylianos Karozis, National Center for Scientific Research Demokritos, Environmental Research Laboratory, Greece
Michael Kainourgiakis, National Center for Scientific Research Demokritos, Environmental Research Laboratory, Greece

Georgia Charalambopoulou, National Center for Scientific Research Demokritos, Environmental Research Laboratory, Greece

Abstract: The target of this work is to study the transport properties of a lipid membrane whose major component are ceramides. This type of lipid membrane is mostly found in the skin inter-cellular domain. Such membranes present very special transport properties (permeability, diffusivity) so as to determine the entire barrier function of the skin. In this context, we have performed several series of Molecular Dynamics simulations in order to examine the membrane penetration mechanism. The use of computational infrastructure based on GPUs has allowed the simulations to be performed at a fully atomistic level with a time scale in the order of 1 μs. The first substance to be studied is water. In this case, we have studied the diffusion of water under non-equilibrium conditions (e.g. melting of the membrane and channel formation through the membrane) since water can hardly penetrate the membrane under physiological conditions. In a second stage, the work is extended to also cover amphiphile molecules (e.g. aminobenzoate esters) that are more likely to find a penetration pathway through the membrane. Diffusion is studied in both directions: parallel and perpendicular to the bilayer. In the former case the motion of the penetrating molecules in confined between two consecutive lipid bilayers while in the latter, the motion through a channel is actually examined. The major results are the retention time and the diffusion coefficient of the aforementioned substances as well as how the membrane structure is affected by the presence of that molecules.

View

Simulation of adhesion contact on the interface of polymer metal

Maksimov Andrei, Cherepovets State University, Chair of Physics, Russian Federation
Evgeny Proutorov, Cherepovets State University, Chair of Physics, Russian Federation
Olga Maksimova, Cherepovets State University, Ministry of Education and Science of the Russian Federation, Russian Federation

Abstract: In recent years, study of the surface of different polymer structures have been acquired not only theoretical but also practical meaning because their unique engineering characteristics. On the one hand, the solution of the problem concerning the adsorption of macromolecules on different interfaces creates a base for development of the theory of surface properties of polymers [1, 2]. On the other hand, today's society is having the most important technical and economic problems, the corrosion control of metals and other materials. One of the effective methods for protection of metal production from corrosion is the development of polymer coverings of different types (e.g., polyvinylidene fluoride, polyurethane, et al.) depending on their physical-chemical characteristics, the decorative properties and conditions of its using. The quality of polymer coatings is determined, first of all, by its durability, adhesion, resistance to aggressive external environment and also by strength, which as mainly depends on the degree of orientational order of the macromolecules in the layer [3]. These properties of the polymer coating depend on the method of its formation and the chemical modification of the polymer [4]. The high efficiency of the polymer coating is achieved only by the proper choice of thermal and other conditions during the formation of its structure. The aim of this work is to study only the initial stage of physical and chemical processes by the formation of the structure of polymer coating, namely, the creation of a primer adhesive layer after the application of monomer paint solution on the steel sheet before to the polymerization. In this work, by means of a dynamic Monte Carlo method for the modified lattice Langmuir's model of adsorption, the time dependences of the sticking coefficient of monomers on the surface of the steel for the same and different heating rates of the metal sheet and different given values of the interaction constant of the monomers and the energy barrier are calculated. It's shown that there is an optimum temperature regime at which there is the greatest

adhesion monomer coating on the surface of the metal sheet. The simulation results are confirmed by experimental data [4] on study of adhesion strength of the primer layer from the poly-vinyl-butyral on the surface of steel sheet. References [1] Karim A, Kumar S 2000 Polymer Surfaces, Interfaces and Thin Films (Singapore–World Science). [2] Maksimov AV and Pavlov GM 2007 Polymer Science A 49 828 [3] Maksimov AV and Gotlib YuYa Polymer Science A 34 902. [4] Yilgor I 2013 Proc. 12-th Int.Conf. “Polymers in advanced technologies”(Berlin) p 34. [5] Yakovlev AD 2008 Chemistry and technology of paint coatings (St.Petersburg–Chemistry)

View

A Green-Naghdi approach for thermo-electroelasticity

Adriano Montanaro, University of Padua, Department of Mathematics, Italy

Abstract: The constitutive relations of piezoelectric ceramics are essentially nonlinear since the so-called piezoelectric moduli depend on the induced strains. Pioneering papers dealt mainly with the isothermal case. In view of applications, however, thermal effects have to be taken into account in connection with thermo-electric behaviors. The equations of nonlinear thermoelectroelasticity were given in [1] by postulating the Clausius-Duhem inequality. Here we consider an electrically polarizable and finitely deformable heat conducting elastic continuum which interacts with the electric field. Without using the Clausius-Duhem inequality, we exploit nonlinear constitutive equations following a Green-Naghdi approach for thermodynamic theories of type III. In the latter approach a new variable α is involved, which is called {\it thermal displacement} and represents a time primitive of some {\it empirical temperature} T, $$ \dot \alpha(x,t)=T(x,t). $$ Hence the case of transverse isotropy is studied and the constitutive equations for the linearized theory are characterized. [1] H.F. Tiersten, On the nonlinear equations of thermoelectroelasticity, Int. J. Engng Sci., 9, 587–604, 1971.

View

Numerical Simulation of Carbon Dioxide Corrosion GFR

Ju Chunhua, Harbin Institute of Technology, Materials of Technology, China

Abstract: The mechanism of carbon dioxide corrosion GFRP has been considered that belong to chemical corrosion. This paper analysis the supercritical carbon dioxide fluid corrosion GFRP pipe theory at high temperature and high pressure and the destruction of carbon dioxide compressed gas (also known as "gas bomb") to GFRP pipe role. Based on TNT equivalent theory and lamination theory, using large finite ABAQUS software to set up carbon dioxide corrosion GFRP model, then simulate the distribution and propagation of stress wave、the node deflection and the change of model energy.

View

Comparative analysis Taufit and other common software processing lifetime positron spectra

Viacheslav Trukhin, Far Eastern Federal University, Department of theoretical and experimental phisics, Russia

Abstract: In our work, we present a program Taufit that designed for processing of the positron annihilation lifetime spectroscopy (PALS). We produce comparative analysis of the data obtained with other common processing programs PALS-spectra (LT, PALS-fit). Our method is based on the processing of experimental PALS-spectrum by fitting the simulated spectrum of definitely number of exponent to the experimental spectrum by fitting (convolution). As a result, we obtain the important parameters PALS-spectra (intensity, lifetime exponents, annihilation coefficients).

Note that due to that used in the model method, the model spectrum obtained with the experimental spectrum (conformity in ranges 97-99%, which is more accurate among the methods of analysis time spectra). The program was written at the Department of Theoretical and Experimental Physics, School of Natural Sciences, Far Eastern Federal University, Vladivostok.

View

New analytical approach for transition to slow 3-D turbulence

Jaykov Foukzon, Israel Institute of Technology, Haifa, Israel , math, Israel
Elena Menkova, All-Russian Research Institute of Optophysical Measurements, , Russia
A Potapov, Kotel'nikov Institute of Radioengineering and Electronics of the , , Russian Federation

Abstract: Analytical non-perturbative study of the three-dimensional nonlinear stochastic partial differential equation with additive thermal noise, analogous to that proposed by V.N. Nikolaevskii [1]-[5]to describe longitudinal seismic waves, is presented. The equation has a threshold of short-wave instability and symmetry, providing long wave dynamics. New mechanism of quantum chaos generating in nonlinear dynamical systems with infinite number of degrees of freedom is proposed. The hypothesis is said, that physical turbulence could be identified with quantum chaos of considered type. It is shown that the additive thermal noise destabilizes dramatically the ground state of the Nikolaevskii system thus causing it to make a direct transition from a spatially uniform to a turbulent state.

View

The effect of thermal losses on traveling waves for in-situ combustion in porous medium

Grigori Chapiro, Universidade Federal de Juiz de Fora, Mathematics, Brazil

Abstract: The paper is motivated by a model for the injection of air into a porous medium that contains a solid fuel, taking thermal losses into account [1]. This model was simplified in [2] by disregarding thermal losses and further studied using the singular perturbation technique. In [3] the model was further simplified and all wave sequences for the Riemann problem solution were obtained. Additionally, rigorous proof of the existence of the traveling wave solution was presented. The stability of such solutions was studied in [4]. Taking thermal losses into account is important from a physical point of view because they play an important role in laboratory experiments. In this work the first step in this direction is made. The model investigated in [3,4] is modified by including the thermal losses term, making it more physically realistic. In order to prove the existence of the traveling wave solution, we disregard diffusion effects and the dependence of gas density on temperature. Some numerical examples are presented to illustrate the model. [1] I.Y. Akkutlu and Y.C. Yortsos, The dynamics of in-situ combustion fronts in porous media, J. of Combustion and Flame, 134, pp. 229-247, 2003. [2] G. Chapiro, A. A. Mailybaev, A.J. Souza, D. Marchesin, and J. Bruining, Asymptotic approximation of long-time solution for low-temperature filtration combustion, Comput. Geosciences, 16, pp. 799-808, 2012. [3] G. Chapiro, D. Marchesin and S. Schecter, Combustion waves and Riemann solution in light porous foam, J. of Hyperbolic Differential Equations, v. 11, p. 295-328, 2014. [4] G. Chapiro, L. Furtado, D. Marchesin and S. Schecter, Stability of Interacting Traveling Waves in Reaction-Convection-Diffusion Systems, Accepted in Discrete and Continuous Dynamical Systems, 2015.

View

Simulation of electroseismic effect using Finite Difference Method

Ana Milena Nemocon, University Nacional de Colombia, Física, Colombia

Abstract: In contrast to other geophysical prospecting techniques, electroseismic is able to discriminate between different fluids such as water and hydrocarbons. In this technique, a mechanical wave is produced from an electromagnetic pulse applied on the earth sur- face, when it passes through the material acts differently on the adsorbed layer (Stern layer) and double layer induced in the fluid to saturate the soil (diffused layer). As a consequence, a relative displacement (solid-fluid) is produced and then, a seismic wave response can be detected using geophones. The equations governing the electroseismic effect combine Maxwell's electrodynamics and Biot's wave propagation in porous media, and are known as equations of Pride. In this work, we explore whether a finite differ- ence scheme in the natural domain of the problem, frequency, attain reproduce this phenomenon. The electromagnetic source is given by a Ricker wavelet with a central frequency equal to 20Hz. The numerical method consists in transforming to frequency the input pulse, discretize finite difference equations of Pride to solve with this scheme the answer to input pulse for each frequency, combine and translate the results into the time domain, and apply this to each depth of study. The scheme sheds acceleration data that reproduce the appearance of seismic waves induced by electroseismic effect on the interface of several distinct electrokinetic and poroelastic parameters of the underground, with velocities of the order of those expected for the medium. Meanwhile, the perturbation induced by the vertical propagation of the electromagnetic wave signal is attenuated, as expected, respect to characteristics of the soil. This work is a first step in Colombia in order to find numerical schemes that can reproduce this phenomenon correctly.

View

Fractional travelling wave solutions of the higher order extended KdV equations in a stratified shear flow

Aly Seadawy, Faculty of science, Taibah University, Mathematics, Saudi Arabia

Abstract: Solitary waves solutions are generated by deriving the nonlinear higher order of extended KdV equations for the free surface displacement. The problem formulations of models for internal solitary waves in a stratified shear flow with a free surface are presented. All coefficients of the nonlinear higher order extended KdV equation are expressed in terms of integrals of the modal function for the linear long-wave theory. The electric field potential and the fluid pressure in form traveling wave solutions of the extended KdV equation are obtained. The stability of the obtained solutions and the movement role of the waves by making the graphs of the exact solutions are discussed and analyzed.

View

Stability of capture into autoresonance in nonlinear oscillating systems

Oskar Sultanov, Institute of Mathematics with Computing Center, Department of Differential Equations, Russian Federation

Abstract: Autoresonance is a phenomenon of considerable growth of the energy of forced nonlinear oscillations initiated by a small pumping. The influence of random perturbations on a capture into autoresonance is analyzed. We consider a system of two first-order differential equations describing the initial stage of a capture into autoresonance. Of special interest are solutions with unboundedly growing energy in time at infinity. Such solutions are associated with a resonance phenomenon. In applications, it is assumed that only stable solutions correspond to real physical processes. By the reason of the nonlinearity of the considered mathematical model the explicit formulas for the solutions can not be obtained. However, it is possible to construct an asymptotic expansion for some particular solutions. Stability of such type solutions under white noise is discussed.

View

The Positive Definite Solution to a Nonlinear Matrix Equation

Hyun-Min Kim, Pusan National University, Department of Mathematics, Korea, South

Abstract: The two matrix equations $F(X) = X^{n} + M(B + X^{-1})^{-1}M^{*} - A = 0$ and $G(X) = X^{p} + A^{*}XA - Q = 0$ are studied. Based on the fixed-point theory, the existence and uniqueness of the Hermitian positive definite solution of $F(X)$ are proved. Some elegant estimates of the positive definite solutions of $G(X)$ are obtained. Three iterative methods for computing the positive definite solution of equation $G(X)$ are proposed.

View

On double barrier exit probabilities for the classical risk process with diffusion

Dean Teneng, University of Tartu, Institute of Mathematical Statistics, Estonia

Abstract: We study double barrier exit probabilities for risk processes with spectrally positive Levy perturbations. We derive Pollaczek-Hinchin type formulas using scale functions and obtain analytical results amenable to implementation for the case of exponentially distributed claim size distributions. Approximations for heavy-tailed claim size distributions are analogously obtained.

View

Parameters analysis of a porous medium model for treatment with hyperthermia using OpenMP

Ruy Freitas Reis, Universidade Federal de Juiz de Fora, Modelagem Computacional, Brazil
Felipe Loureiro, Universidade Federal de Sao Joao del-Rei, Department of Thermal and Fluid Sciences, Brazil
Marcelo Lobosco, Universidade Federal de Juiz de Fora, Computer Science , Brazil

Abstract: Cancer is the second biggest cause of death in the world so treatments have been developed trying to work around this world health problem. Hyperthermia is not a new technique, but its use in cancer treatment is at an early stage of development. This treatment is based on overheat the target area to a threshold temperature that causes cell necrosis and apoptosis. To simulate this phenomenon, a three-dimensional porous medium model applied to a under skin cancer treatment using magnetic nanoparticles was adopted. This study presents a sensibility analysis of the model parameters such as the porosity and blood velocity. To ensure a second-order solution approach a 7-points centered finite difference method at space discretization and a predictor-corrector method to time evolution were employed. Due to the massive computations required to find the solution of a three-dimensional model, this paper also presents an attempt to improve performance using OpenMP, a parallel programming API.

View

Simulation of Electroseismics effect in one dimension using finite differences method.

Ana Milena Nemocon, University Nacional de Colombia, Física, Colombia

Abstract: In contrast to other geophysical prospecting techniques, electroseismic is able to discriminate between different fluids such as water and hydrocarbons. In this technique, a mechanical wave is produced from an electromagnetic pulse applied on the earth surface, when it passes through the material acts differently on the adsorbed layer (Stern layer) and double layer induced in the fluid to saturate the soil (diffused layer). As a consequence, a relative displacement (solid-fluid) is produced and then, a seismic wave response can be detected using geophones.

The equations governing the electroseismic effect combine Maxwell's electrodynamics and Biot's wave propagation in porous media, and are known as equations of Pride. In this work, we explore whether a finite difference scheme in the natural domain of the problem, frequency, attain reproduce this phenomenon. The electromagnetic source is given by a Ricker wavelet with a central frequency equal to 20Hz. The numerical method consists in transforming to frequency the input pulse, discretize finite difference equations of Pride to solve with this scheme the answer to input pulse for each frequency, combine and translate the results into the time domain, and apply this to each depth of study. The scheme sheds acceleration data that reproduce the appearance of seismic waves induced by electroseismic effect on the interface of several distinct electrokinetic and poroelastic parameters of the underground, with velocities of the order of those expected for the medium. Meanwhile, the perturbation induced by the vertical propagation of the electromagnetic wave signal is attenuated, as expected, respect to characteristics of the soil. This work is a first step in Colombia in order to find numerical schemes that can reproduce this phenomenon correctly.

View

Analysis of the chaotic maps generating different statistical distributions

Marcin Lawnik, Silesian University of Technology, Faculty of Applied Mathematics, Poland

Abstract: The analysis of the chaotic maps, enabling the derivation of numbers from given statistical distributions was presented . The analyzed chaotic maps are in the form x_{k+1}=F^{-1}(U(F(x_k))), where F is the cumulative distribution function, U is the skew tent map and F^{-1} is the inverse function of F [1]. The analysis was presented on the example of chaotic map with the standard normal distribution in view of his computational efficiency and accuracy. On the grounds of the conducted analysis, it should be indicated that the method not always allows to generate the values from the given distribution. [1] D. Lai, G. Chen: Generating Different Statistical Distributions by the Chaotic Skew Tent Map. International Journal of Bifurcation and Chaos 10(6):1509–1512, 2000.

View

Exact quasi-classical asymptotic beyond Maslov canonical operator

Jaykov Foukzon, Israel Institute of Technology, Haifa, Israel , math, Israel

Abstract: Exact quasi-classical asymptotic beyond WKB-theory and beyond Maslov canonical operator theory of the Colombeau solutions of the -dimensional Schrodinger equation is presented. Quantum jump nature is considered successfully. We pointed out that an explanation of quantum jumps can be found to result from Colombeau solutions of the Schrödinger equation alone without additional postulates.

View

Band structure and density of states in FeAs-based superconductors

Vladimir Kahsurnikov, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Physics of the Solid State and Nanosystems, Russia
Andrey Krasavin, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Physical and Technical Problems of Metrology, Russian Federation

Abstract: The generalized quantum Monte Carlo algorithm was used to obtain one-particle excitation spectrum and electron density of states for two-dimensional FeAs-clusters modeling iron-based superconductors within the limits of the full two-orbital model. The calculations were performed for clusters with sizes up to 10×10 FeAs-cells. The excitation spectra were

reconstructed from Matsubara Green's function. The spectral density of states and the total density of states near the Fermi level were obtained. The data are in accordance with known experimental results. The influence of the cluster size, temperature, and the interaction strength on the density of states was analyzed.

View

INTEGRABLE VARIABLE DISSIPATION DYNAMICAL SYSTEMS: METHODS AND SOME APPLICATIONS

Maxim V. Shamolin, Lomonosov Moscow State University, Institute of Mechanics, Russian Federation

Abstract: This activity is a survey of integrable cases in dynamics of a rigid body under the action of a nonconservative force field. We review both new results and results obtained earlier. Problems examined are described by dynamical systems with so-called variable dissipation with zero mean. The problem of the search for complete sets of transcendental first integrals of systems with dissipation is quite actual; a large number of works are devoted to it. We introduce a new class of dynamical systems that have a periodic coordinate. Due to the existence of a nontrivial symmetry groups of such systems, we can prove that these systems possess variable dissipation with zero mean, which means that on the average for a period with respect to the periodic coordinate, the dissipation in the system is equal to zero, although in various domains of the phase space, either the energy pumping or dissipation can occur. Based on facts obtained, we analyze dynamical systems that appear in dynamics of a rigid body and obtain a series of new cases of complete integrability of the equations of motion in transcendental functions that can be expresses through a finite combination of elementary functions. As exhibits we research dynamical equations of motion arising in studying the plane and spatial dynamics of a rigid body interacting with a medium and also a possible generalization of the obtained methods for studying to general systems arising in qualitative theory of ordinary differential equations, in theory of dynamical systems, and also in oscillation theory.

View

Magnetization of layered high-temperature superconductors with extended ferromagnetic defects

Vladimir Kahsurnikov, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Physics of the Solid State and Nanosystems, Russia
Anastasiia Maksimova, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Physics of the Solid State and Nanosystems, Russian Federation
Igor Rudnev, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Physics of the Solid State and Nanosystems, Russia

Abstract: The magnetization of layered high-temperature superconductors (HTSC) with ferromagnetic nanorods as bulk pinning centers is studied in the 2D model of layered HTSC by using Monte Carlo method. Magnetic part of the interaction energy between a ferromagnetic cylinder of arbitrary radius and fixed magnetization and an Abrikosov vortex was calculated in London approximation. The periodic and nonperiodic lattices of magnetic defects were considered. The vortex configurations arising during magnetization were obtained. The results of calculations were compared with the results for extended nonmagnetic defects.

View

IMPROVEMENT OF ROTATED COMB DECIMATION FILTER MAGNITUDE

CHARACTERISTIC USING SHARPENING TECHNIQUE

gordana Jovanovic Dolecek, Institute INAOE, Electronics, Mexico

Abstract: Decreasing of sampling rate in a digital form is called decimation. This process may introduce aliasing, i.e. non desired replicas of the main spectrum of the decimated signal. That is why we need the filter before decimation. This filter is called the decimation or antialiasing filter. The most popular decimation filter is comb filter which is usually used in the first stage of decimation. However, it has a high passband droop and low attenuations in the folding bands. Different methods have been proposed to improve comb magnitude characteristic. The methods based on simple zero rotations have been proposed recently. In this paper we use the sharpening technique to improve both the passband and the stopband of the comb filter with the rotated zeros. The method is compared with methods based on the rotation of zeros of comb filter.

Acknowledgements: The work is supported by the Conacyt grant 179587.

View

DNA Cyclization Rates versus Sequence Length

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Abstract: Many experiments have demonstrated that DNA exhibits sequence-dependent bending and torsional flexibility which may have biological relevance in the DNA-protein interplay. Such properties have been investigated by several experimental methods including gel electrophoresis, crystallography and, above all, DNA cyclization which permits to test the circularization rates of DNA sequences in the presence of ligase enzymes. From a theoretical viewpoint, cyclization rates can been analyzed via computation of the J-factors which are essentially given by the ratio of the partition functions of circular and linear structures. This program is carried out in the present work by means of the previously developed path integral method for DNA [1-3]. Both homogeneous and heterogeneous molecules are studied to detect the effects of the sequence specificities on the cyclization probabilities. The latter are also evaluated as a function of the sequence length. [1] M. Zoli, Journal of Theoretical Biology Vol. 354, 95-104 (2014). [2] M. Zoli, Soft Matter Vol. 10, 4304-4311 (2014). [3] M. Zoli, The Journal of Chemical Physics Vol. 141, 174112 (2014).

View

Compactly supported kernels based method of approximate particular solutions for solving elliptic problems

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Abstract: In this work the method of approximate particular solutions using compactly supported kernels is investigated. In the work of [1] the global RBFs are used in the solution process, and the ill-conditioning of the resultant matrix is observed for solving large-scaled problems. We extended the work of [1] for compactly supported kernels, so that we can solve large-scaled problems in science and engineering. The numerical scheme of the present method of approximate particular solutions is simple to implement and very accurate. Three benchmark problems are solved by the present numerical scheme and the results are compared to other methods in the literature.

.... [1] C. S. Chen, C. M. Fan, P. H. Wen. The Method of Approximate Particular Solutions for Solving Certain Partial Differential Equations, Published online 25 October 2010 in Wiley Online Library (wileyonlinelibrary.com). DOI 10.1002/num.20631.

View

A viscoelastic model to simulate soft tissue materials

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Abstract: Research on modeling the mechanical behavior of soft tissue has growing demand for applications on surgical simulations, pursuing in real time, precise and fast calculations of tissue mechanical deformations. For almost all biological soft tissue, the stress-strain curve exhibit a hysteresis loop showing a nonlinear relationship, meanwhile under different strain rates they are mechanically not very sensitive. Moreover, their hysteresis loop-area does not depend on the strain rate. Hysteresis, relaxation and creep are common features of viscoelastic mechanical behavior. As for most materials, their mechanical properties depend to a large extent on the environmental conditions, mainly the temperature and the type of loading regime applied to the material. The time dependence of a viscoelastic material could be better understood by considering it as composed by an elastic solid and a viscous fluid. Different types of mechanical devices can be constructed provided a particular configuration of elastic springs and dashpots. In this work we explore the possibility to obtain most of the soft tissue mechanical behavior by considering a Kelvin's device coupled to a set of {\it\,in parallel} Maxwell's devices. Then, the resulting model composed of a long series of modified Kelvin bodies must span a broad range of characteristic times resulting in a suitable model for soft tissue simulation. Soft tissue mechanical response under driving static and dynamic deformations on {\it\,2-Dim} system are considered, given the applied stress. We compute the strain deformations as a function of time. We obtain a set of coupled Volterra integral equations, solved via the extended trapezoidal rule scheme, and we use the Newton-Raphson method when solving the remaining coupled equations.

View

From infinitesimal symmetries to deformed symmetries of Lax-type equations

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Abstract: Using the procedure initiated in [J-P. Magnot, International Journal of Geometric Methods in Modern Physics 10(9). articleID 1350043 (2013)], we deform Lax-type equations though a scaling of the time parameter. This gives an equivalent (deformed) equation which is integrable in terms of power series of the scaling parameter. We then describe a regular Frölicher Lie group of symmetries of this deformed equation.

View

Dielectric Relaxation Study of Diethanolamine with Triethanolamine at Melting Points Using Time Domain Reflectometry

Vyankat Pawar, Maharashtra Udayagiri Mahavidyalaya, Physics and Electronics, India

Abstract: The dielectric relaxation study of diethanolamine with triethanolamine binary mixture have been determined over the frequency range of 10 MHz to 20 GHz, at 15, 20, 25, 28, and 30oC using time domain reflectometry (TDR) method for 11 concentrations of the system. The present work reveals molecular interaction between same multi-functional groups [−OH and –NH2] of the alkanolamines (diethanolamine and triethanolamine) using different models (Such as Debye model, Excess model, Kirkwood model and Bruggeman model). The dielectric parameters viz. static dielectric constant (□0), dielectric constant at high frequency (□∞) and relaxation time (□) have been obtained with Debye equation characterized by a single relaxation time without relaxation time distribution by the least squares fit method. The values of static dielectric constant increases up to their melting points and then it decreases with increasing temperatures. This behavior of the static dielectric constant indicates the change of phase from semi-solid to liquid

state of the system. At the melting points, the values of relaxation time suddenly drop down.

View

Magnetization reversal modes in fourfold Co nano-wire systems

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Abstract: Magnetic nano-wire systems are, as well as other patterned magnetic structures, of special interest for novel applications, such as magnetic storage media [1]. In these systems, the coupling between neighboring magnetic units is most important for the magnetization reversal process of the complete system, leading to a variety of magnetization reversal mechanisms. While former simulations concentrated on iron nano-wires with different dimensions [2] and coupling mechanisms [3], this article examines the influence of the magnetic material on hysteresis loop shape, coercive field, and magnetization reversal modes. While nickel (Ni) nano-wire systems do not show special features which have not been found in simulations based on iron (Fe) nano-wires, systems consisting of cobalt (Co) nano-wires show hysteresis loops with several longitudinal steps and transverse peaks, correlated to a rich spectrum of magnetization reversal mechanisms. We show that changing the material parameters while the system geometry stays identical can lead to completely different hysteresis loops and reversal modes. Thus, especially for finding magnetic nano-systems which can be used as quaternary or even higher-order storage devices, it is very sensible to test several materials for the planned systems. Apparently, new materials may lead to novel and unexpected behavior – and can thus result in novel functionalities. [1] T. Blachowicz, A. Ehrmann: Fourfold nanosystems for quaternary storage devices, J. Appl. Phys. 110, 073911 (2011) [2] T. Blachowicz, A. Ehrmann, P. Steblinski, J. Palka: Directional-dependent coercivities and magnetization reversal mechanisms in fourfold ferromagnetic systems of varying sizes, J. Appl. Phys. 113, 013901 (2013) [3] T. Blachowicz and A. Ehrmann: Micromagnetic simulations of anisotropies in coupled and uncoupled ferromagnetic nano-wire systems, Sci World J 2013, 472597 (2013)

View

Reliability of statistic evaluation of microscopic pictures taken from knitted fabrics

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Abstract: One of the techniques which can be used to quantitatively evaluate images statistically is the so-called random-walk approach, resulting in the calculation of the Hurst exponent, which is a measure of the complexity of the picture under examination. Especially long, fine elements in the image, such as fibers, influence the Hurst exponent significantly in comparison to a completely single-color picture. Thus, determination of the Hurst exponent has been suggested as new method to measure the hairiness of yarns [1] or knitted fabrics [2,3]. This is of special importance due to the fact that the existing hairiness measurement instruments are based on different measurement principles which are not necessarily comparable. While the principal usability of this method for hairiness detection has been shown in former projects, the absolute value of the

calculated Hurst exponents is significantly dependent on the technique to take the photographic image of a sample, to transfer it into a monochrome picture, and on possible image processing steps. This article gives an overview of the influence of camera resolutions, edge detection filters, possible definitions of the limit color between black and white for the monochrome image, etc. It shows how these parameters should be chosen in case of typical textile samples and correlates the challenges of this novel method with well-known problems of common techniques to measure yarn and fabric hairiness. [1] T. Blachowicz, S. Aumann, B. Pruß, P. Reiners, A. Ehrmann, M. O. Weber, T. Weide: Optical determination of yarn hairiness using statistical methods, Proceedings of Aachen-Dresden International Textile Conference, Dresden / Germany, November 27-28, 2014 [2] T. Blachowicz, A. Ehrmann, M. Zieliński, M. O. Weber: Quantitative estimation of textile structural complexity using random walking approach, submitted [3] T. Blachowicz, A. Ehrmann, K. Domino, M. O. Weber: Examination of washing relaxation of knitted fabrics by random walking approach, submitted

View

Simulations of a epidemic model with parameters variation analysis for the dengue fever

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Caio Jardim, Universidade Federal dos Vales do Jequitinhonha e Mucuri, ICET, Brazil
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Abstract: Mathematical models can be widely found in the literature for describing and analyzing epidemics. The models that use differential equations to represent mathematically such description are especially sensible to parameters involved in the modelling. In this work, an already developed model, called SIR, is analyzed when applied to a scenario of a dengue fever epidemic. Such choice is powered by the existence of useful tools presented by a variation of this original model, which allow an inclusion of different aspects of the dengue fever disease, as its seasonal characteristics, the presence of more than one strain of the vector and of the biological factor of cross-immunity. The analysis and results interpretation are performed through numerical solutions of the model in question, and a special attention is given to the different solutions generated by the use of different values for the parameters present in this model. Slight variations are performed either dynamically or statically in those parameters, mimicking hypothesized changes in the biological scenario of this simulation and providing a source of evaluation of how those changes would affect the outcomes of the epidemic in a population.

View

Higher order Peregrine breathers solutions to the NLS equation.

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Abstract: The solutions to the one dimensional focusing nonlinear Schrödinger equation (NLS) can be written as a product of an exponential depending on t by a quotient of two polynomials of degree N(N+1) in x and t. These solutions depend on 2N-2 parameters : when all these parameters are equal to 0, we obtain the famous Peregrine breathers which we call P_{N} breathers. Between all quasi-rational solutions of the rank N fixed by the condition that its absolute value tends to 1 at infinity and its highest maximum is located at the point (x=0,t=0), the P_{N}

breather is distinguished by the fact that P_{N}(0,0) = 2N+1. \\ We construct Peregrine breathers of the rank N explicitly for N less than 11. We give figures of these P_{N} breathers in the (x;t) plane; plots of the solutions P_{N}(0;t), P_{N}(x;0), never given for 6

View

Modified planar rotator model for efficient spatial prediction

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Abstract: We introduce a novel spatial prediction method inspired from statistical physics for efficient estimation of missing data with general non-Gaussian distributions on partially sampled Cartesian grids. The prediction model is based on a classical XY (also called planar rotator) spin model, which is modified in order to allow an appropriate one-to-one transformation between the data and spin values and which displays relevant short-range correlations at low temperatures. The spatial correlations present in the data are captured in terms of nearest-neighbor interactions between the spin variables. The only parameter of the present model is the reduced temperature, which is estimated from the sample-based correlations. Having inferred the temperature, conditional Monte Carlo simulations honoring the sample values are performed on the entire lattice to bring the system into thermal equilibrium and subsequently collect prediction statistics. Owing to the fact that the model does not show undesirable critical slowing down, the relaxation process is rather fast and, furthermore, the short-range nature of the interactions allows vectorization of the algorithm. Consequently, the proposed method achieves almost linear scaling with system size, thus being much more efficient than the conventional geostatistical approaches and applicable to huge datasets, such as satellite and radar images.

View

Modifier mass transfer kinetic effect in the performance of solvent gradient simulated moving bed (SG-SMB) process

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Abstract: The solvent-gradient simulated moving bed process (SG-SMB) is the new tendency in the performance improvement if compared to the traditional isocratic solvent conditions. In such SG-SMB separation process the modulation of the solvent strength leads to significant increase in the purities and productivity followed by reduction in the solvent consumption. A stepwise modeling approach was utilized in the representation of the interconnected chromatographic columns of the system combined with lumped mass transfer models between the solid and liquid phase. The influence of the solvent modifier was considered applying the Abel model which takes into account the effect of modifier volume fraction over the partition coefficient. The modeling and simulations were carried out and compared to the experimental SG-SMB separation of the amino acids phenylalanine and tryptophan. A lumped mass transfer kinetic model was applied for both the modifier (ethanol) as well as the solutes. The simulation results showed that such simple and global mass transfer models are enough to represent all the mass transfer effect between the solid adsorbent and the liquid phase. The separation performance can be improved reducing the interaction or the mass transfer kinetic effect between the solid adsorbent phase and the modifier. The simulations showed great agreement fitting the experimental data of the amino acids concentrations both at the extract as well as at the raffinate.

View

MUSIC-type imaging of small perfectly conducting cracks with unknown frequency

Won-Kwang Park, Kookmin University, Mathematics, Korea, Republic of

Abstract: MUltiple SIgnal Classification (MUSIC) is a famous non-iterative detection algorithm in inverse scattering problems. If one knows the applied frequency, very accurate locations of small perfectly conducting cracks can be detected vis MUSIC. Unfortunately, when the applied frequency is unknown, inaccurate locations are identified via MUSIC with wrong frequency data. This fact has been confirmed via various results of numerical simulations; however, the reason behind this inaccurate identification has not been theoretically investigated. Motivated this fact, we identify the structure of MUSIC-type imaging functional with an unknown frequency by establishing a relationship with Bessel functions of order zero of the first kind. Various numerical experiments are performed, to support this analysis of the imaging functional.

View

Aggregate driver model to enable predictable behaviour

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Abstract: The categorization of driving styles, particularly in terms of aggressiveness and skill is an emerging area of interest under the broader theme of intelligent transportation. There are two possible discriminatory techniques that can be applied for such categorization; a micro-scale (event based) model and a macro-scale (aggregate) model. It is believed that an aggregate model will reveal many interesting aspects of human-machine interaction; for example, we may be able to understand the propensities of individuals to carry out a given task over longer periods of time. A useful driver model may include the adaptive capability of the human driver, aggregated as the individual propensity to control speed/ acceleration. Towards that objective, we carried out experiments by deploying smartphone based application used for data collection by a group of drivers. Data is primarily being collected from GPS measurements including position & speed on a second-by-second basis, for a number of trips over a two months period. Analysing the data set, aggregate models for individual drivers were created and their natural aggressiveness were deduced. In this paper, we present the initial results for 12 drivers. It is shown that the higher order moments of the acceleration profile is an important parameter and identifier of journey quality. It is also observed that the Kurtosis of the acceleration profiles stores major information about the driving styles. Such an observation leads to two different ranking systems based on acceleration data. Such driving behaviour models can be integrated with vehicle and road model and used to generate behavioural model for real traffic scenario.

View

An accurate solution of elastodynamic problems by numerical local Green's functions

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Abstract: Green's function based methodologies for elastodynamics in both time and frequency

domains, which can be either numerical or analytical, appear in many branches of physics and engineering. Thus, the development of exact expressions for Green's functions is of great importance. Unfortunately, such expressions are known only for relatively few kinds of geometry, medium and boundary conditions. In this way, due to the difficulty in finding exact Green's functions, specially in the time domain, the present paper presents a solution of the transient elastodynamic equations by a time-stepping technique based on the Explicit Green's Approach method written in terms of the Green's and Step response functions, both being computed numerically by the finite element method. The major feature is the computation of these functions separately by the central difference time integration scheme and locally owing to the principle of causality. More precisely, Green's functions are computed only at $t=\Delta t$ adopting two time substeps while Step response functions are computed directly without substeps. The proposed time-stepping method shows to be quite accurate with distinct numerical properties not presented in the standard central difference scheme as addressed in the numerical example.

View

Inhomogeneous deformation in single crystals of nickel with different hierarchies structural elements

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Abstract: The heterogeneity of plastic deformation of nickel single crystals in view of hierarchy of structural elements is investigated. The dependence of the structural elements forming the domain of deformation, on orientation of an axis of compression of single crystals is established. The deformation in domains and the structural elements is investigated.

View

Oxygen induced effects on avascular tumour growth: a preliminary simulation using an adaptive grid algorithm

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Abstract: Cancer cells oxygenation from surrounding healthy tissue influences the tumour growth in the avascular phase. The effects induced by oxygen on cancer cells dynamics during their interaction with the urokinase plasminogen activator system, are simulated mimicking different biological conditions of the early stage of human tumour proliferation, and under hypoxic conditions, using oxygen supply parameters determined from in vivo experiments. The system of six coupled partial differential equations, arising from the problem modeling, are solved over a one-dimensional domain implementing a moving mesh numerical technique, using the finite element method. Our preliminary computations show that, oxygen concentration at hypoxic conditions cause cancer cells to build inhomogeneous proliferation pattern, similarly to what happens in absence of oxygen, but with a faster invading front.

View

Numerical solution of viscous and viscoelastic fluids flow through the branching channel by finite volume scheme

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David Trdlicka, Czech Technical University in Prague, , Czech Republic

Abstract: This work deals with the numerical modelling of steady flows of incompressible viscous and viscoelastic fluids through the three dimensional channel with T-junction. The fundamental system of equations is the system of generalized Navier-Stokes equations for incompressible

fluids. This system is based on the system of balance laws of mass and momentum for incompressible fluids. Two different mathematical models for the stress tensor are used for simulation of Newtonian and Oldroyd-B fluids flow. Numerical solution of the described models is based on cetral finite volume method using explicit Runge-Kutta time integration.

View

PREDICTION OF THE LIPOPHILICITY OF BILE ACIDS AND THEIR DERIVATIVES BY HIERARCHICAL FUZZY CLUSTERING

Costel Sarbu, Babes-Bolyai University, Cluj-Napoca , Department of Chemistry, Romania

Abstract: Cluster analysis is a large field, both within fuzzy sets and beyond it. Many algorithms have been developed to obtain hard clusters from a given data set. Among those, the c-means algorithms are probably the most widely used. Hard c-means execute a sharp classification, in which each object (compound) is either assigned to a class or not. The membership to a class of objects therefore amounts to either 1 or 0. The application of Fuzzy sets in a classification function causes this class membership to become a relative one and consequently an object can belong to several classes at the same time but with different degrees. The fuzzy c-means algorithms are prototype-based procedures, which minimize the total of the distances between the prototypes and the objects by the construction of a target function. Fuzzy generalized c-means is easy and well improved tool, which have been applied in many fields of chemistry including prediction of biological activity. In this paper, hierarchical fuzzy clustering approach was applied to the study of bile acids lipophilicity using different molecular descriptors available in Alchemy 2000 (17 descriptors) and Alchemy 2000 (11 descriptors). The results obtained indicated a very good performance in terms of classification and prediction for the fuzzy clustering algorithm applied. All the statistical results (the paired t-test, Wilcoxon sign rank-sum test and Friedman ANOVA) confirm the hypothesis that the differences between the experimental and predicted values of lipophilicity for the investigated compounds are not significant and, as a direct consequence, the proposed fuzzy procedure seems to have a strong predictive power.

View

Simple description of shear dynamics of glasses with crystalline local order

Leonid Son, Ural Federal University, , Russian Federation

Abstract: For many glassformers (especially metallic glasses), their structure may be presented as a set of linear topological defects embedded into a media with crystalline local order. Locally, these defects are similar to dislocations and disclinations, so we suggest a description of the shear dynamics in terms of kinks motion along the topological defect lines, as it is adopted in crystalline materials. For the motion of the kink, we write out the Fokker - Plank equation in a self - consistent potential. The glass transition occurs to be described as a localization of the kink.

View

Hierarchical Bayesian approach for estimating physical properties in spiral galaxies: Age Maps for M74

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Abstract: One of the fundamental goals of modern Astronomy is to estimate the physical parameters of galaxies from images in different spectral bands. We present a hierarchical Bayesian model for obtaining age maps from images in the Hα line (taken with Taurus Tunable Filter (TTF)), ultraviolet band (far UV or FUV; from GALEX) and infrared bands (24, 70 and 160

microns (μm); from Spitzer). As shown in Sánchez-Gil et al. 2011 (DOI: 10.1111/j.1365-2966.2011.18759.x), we present the burst ages for young stellar populations in nearby (10 M○, ages α to FUV flux ratio therefore gives a good relative indicator of very recent star formation history (SFH). As a nascent star-forming region evolves, the Hα line emission declines earlier than the UV continuum, leading to a decrease in the Hα/FUV ratio. Through a specific star-forming galaxy model (Starburst 99, SB99), we can obtain the corresponding theoretical ratio Hα / FUV to compare with our observed flux ratios, and thus to estimate the ages of the observed regions. Due to the nature of the problem, it is necessary to propose a model of high complexity to take into account the mean uncertainties, and the interrelationship between parameters when the Hα / FUV flux ratio mentioned above is obtained. To address the complexity of the model, we propose a Bayesian hierarchical model, where a joint probability distribution is defined to determine the parameters (age, metallicity, IMF), from the observed data, in this case the observed flux ratios Hα / FUV. The joint distribution of the parameters is described through an i.i.d. (independent and identically distributed random variables), generated through MCMC (Markov Chain Monte Carlo) techniques.

View

All-phononic Digital Amplification on the Basis of Gap-Soliton Dynamics

Ramaz Khomeriki, Javakhishvili Tbilisi State University, Physics Department, Georgia

Abstract: Conceptual mechanism of amplification of phonons by phonons on the basis of nonlinear band-gap transmission (supratransmission) phenomenon is presented. As an example the system of weakly coupled chains of anharmonic oscillators is considered. One (source) chain is driven harmonically by boundary with a frequency located in the upper band close to the band edge of the ladder system. Amplification happens when a second (gate) chain is driven by a small signal in the counter phase and with the same frequency as first chain. If the total driving of both chains overcomes the band-gap transmission threshold the large amplitude band-gap soliton emerges and amplification scenario is realized. The mechanism is interpreted as nonlinear superposition of evanescent and propagating nonlinear modes manifesting in a single or double soliton generation working in band-gap or band-pass regimes, respectively. The results could be straightforwardly generalized for all-optical or all-magnonic contexts and has all the promises for logic gate operation.

View

Active Flow Control on Laminar flow over a Backward facing step

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Abstract: In the present study, two dimensional flow over a backward-facing step in laminar flow regime with application of active flow control (AFC) technique is analysed. The inspiration for the present work is to gauge the effectiveness of implementing AFC in automobiles to reduce drag, since a considerable amount of the energy needed for a vehicle to move is dissipated at the rear of the vehicle in the form of vortex shedding. In order to analyze the influence of AFC on the boundary layer and the downstream vortex shedding, two different kinds of AFC techniques have been used in this study namely zero net mass flow actuators and fluidic actuators. A parametric non dimensional analysis has been carried out by varying the frequency from 0.025 to 0.1; jet amplitude was modified between 0.05 and 1. Four different positions of the groove were simulated, groove was respectively located at 0.024a, 0.047a, 0.072a and 0.097a, measured

upstream from the right side upper edge. Three different non dimensional groove widths 0.023a, 0.048a and 0.073a were also evaluated, where a is the step height. The idea behind this study was to determine an optimal configuration to reduce the drag on the step and to suppress the vortex dissipation in the wake of the step. It was observed that when using an AFC frequency of ± 10% the vortex shedding frequency, was causing the maximum drag reduction. When comparing the effects of zero net mass flow actuators with the fluidic actuators, it was observed that zero net mass flow actuators were more effective.

View

Medical Imaging Image Quality Assessment with Monte Carlo Methods

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Abstract: The aim of the present study was to assess image quality of PET scanners through a thin layer chromatography (TLC) plane source. The source was simulated using a previously validated Monte Carlo model. The model was developed by using the GATE MC package and reconstructed images obtained with the STIR software for tomographic image reconstruction, with cluster computing. The PET scanner simulated in this study was the GE DiscoveryST. A plane source consisted of a TLC plate, was simulated by a layer of silica gel on aluminum (Al) foil substrates, immersed in 18F-FDG bath solution (1MBq). Image quality was assessed in terms of the Modulation Transfer Function (MTF). MTF curves were estimated from transverse reconstructed images of the plane source. Images were reconstructed by the maximum likelihood estimation (MLE)-OSMAPOSL algorithm. OSMAPOSL reconstruction was assessed by using various subsets (3 to 21) and iterations (1 to 20), as well as by using various beta (hyper) parameter values. MTF values were found to increase up to the 12th iteration whereas remain almost constant thereafter. MTF improves by using lower beta values. The simulated PET evaluation method based on the TLC plane source can be also useful in research for the further development of PET and SPECT scanners though GATE simulations.

View

A theoretical investigation of spectra utilization for a CMOS based indirect detector

for dual energy applications

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Abstract: Dual Energy imaging is a promising method for visualizing masses and microcalcifications in digital mammography. Currently commercially available detectors may be suitable for dual energy mammographic applications. The scope of this work was to theoretically examine the performance of the Radeye CMOS digital indirect detector under three low- and high-energy spectral pairs. The detector was modeled through the linear system theory. The pixel size was equal to 22.5 um and the phosphor material of the detector was a 33.9 mg/cm2 Gd2O2S:Tb phosphor screen. The examined spectral pairs were (i) a 40kV W/Ag (0.01cm) and a 70kV W/Cu (0.1cm) target/filter combinations, (ii) a 40kV W/Cd (0.013cm) and a 70kV W/Cu (0.1cm) target/filter combinations and (iii) a 40kV W/Pd (0.008cm) and a 70kV W/Cu (0.1cm) target/filter combinations. For each combination the Detective Quantum Efficiency (DQE), showing the signal to noise ratio transfer, the detector optical gain (DOG), showing the sensitivity of the detector and the coefficient of variation (CV) of the detector output signal were calculated. The second combination exhibited slightly higher DOG (326 photons per X-ray) and lower CV (0.755%) values. In terms of electron output from the RadEye CMOS, the first two combinations demonstrated comparable DQE values; however the second combination provided an increase of 6.5% in the electron output.

View

Modeling of the Calcium/Phosphorus Mass ratio for Breast Imaging

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Abstract: Breast microcalcifications are mainly composed of calcite (CaCO3), calcium oxalate (CaC2O4) and apatite (a calcium-phosphate mineral form). Any pathologic alteration (carcinogenesis) of the breast may produce apatite. In the present simulation study, an analytical model was implemented in order to distinguish malignant and non-malignant lesions. The Calcium/Phosphorus (Ca/P) mass ratio and the standard deviation (SD) of the calcifications were calculated. The size of the calcifications ranged from 100 to 1000 um, in 50 um increments. The simulation was performed for hydroxyapatite, calcite and calcium oxalate calcifications. The optimum pair of energies for all calcifications was 22keV and 50keV. Hydroxyapatite and calcite calcifications were sufficiently characterized through their distinct confidence interval (99.7%, 3SD) values for calcifications sizes above 500 um, while the corresponding sizes for hydroxyapatite and calcium oxalate characterization were found above 250 um. Initial computer simulation results indicate that the proposed method can be used in breast cancer diagnosis, reducing the need for invasive methods, such as biopsies.

View

Optimum Filter Selection for Dual Energy X-ray Applications through Analytical Modeling

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Abstract: In this simulation study, an analytical model was used in order to determine the optimal

acquisition parameters for a dual energy breast imaging system. The modeled detector system, consisted of a 33.91mg/cm2 Gd2O2S:Tb scintillator screen, placed in direct contact with a high resolution CMOS sensor. Tungsten anode X-ray spectra, filtered with various filter materials and filter thicknesses were examined for both the low- and high-energy beams, resulting in 3.375 combinations. The selection of these filters was based on their K absorption edge (K-edge filtering). The calcification signal-to-noise ratio (SNRtc) and the mean glandular dose (MGD) were calculated. The total mean glandular dose was constrained to be within acceptable levels. Optimization was based on the maximization of the SNRtc/MGD ratio. The results showed that the optimum spectral combination was 40kVp with added beam filtration of 100 um Ag and 70kVp Cu filtered spectrum of 1000 um for the low- and high-energy, respectively. The minimum detectable calcification size was 150 um. Simulations demonstrate that this dual energy X-ray technique could enhance breast calcification detection.

View

Determination of parameters of thin films with rough boundaries

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Abstract: In this contribution the determination of parameters describing the optical properties of thin films using non-linear least squares method is analyzed. It will be shown that the reflectance of rough thin films depends on the rms values of the heights of the irregularities of the boundary roughness of thin films. The measured spectral dependences of reflectance enable us to determine the optical and statistical parameters of thin films through the non-linear least squares fitting algorithm. The possibilities and limitations of this procedure will be demonstrated for thin films on semiconductor substrates.

View

Kinetic model and numerical solution of parameters in the outer region of a multicathode spot vacuum arc

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Abstract: A model of the plasma generated in an arc low-pressure for studying the parameters in this from the kinetic theory is presented. This approach allows for the radial dependence of typical parameters such as electrostatic potential, ion kinetic energy, electron temperature and density, considering a model of spherical symmetry and a fluid in steady state. The behavior of the potential profile in the region around the arc, which causes an extra acceleration of the ions ejected from the cathode spots are studied. The modeled equations were solved numerically using the Runge-Kutta method of fourth order.

View

On the exit probability of the extended Sznajd model and the Kirkwood approximation

André Timpanaro, University of São Paulo, Physics, Brazil
Serge Galam, SciencesPo, CEVIPOF, France

Abstract: Kondrat's extension of the Sznajd model is a sociophysics model where agents can have 2 different opinion states (-1 and +1) and that allows for more flexible interactions among the agents than in other models, like the traditional Sznajd model or the two components model. The time evolution of this model is given by choosing at each time step an agent i and 2 of its neighbours j and k. The agent i will then change its opinion with probability $P(s_is_j, s_is_k)$. We use the Kirkwood approximation to investigate the exit probability E(p) (the probability that the

system ends up in the state where all the agents have opinion +1, given that the initial condition is drawn with no correlations and with a probability p for an agent to have opinion +1) of this model in one dimension. The Kirkwood approximation has recently been used to succesfuly calculate this probability in the usual Sznajd model, despite doubts about the soundness of the approximation it implies. Comparing our analytical results with simulations shows that there are more cases beyond the Sznajd model where the approximation is acurate, while there are also cases where it gives the wrong answers. We also extend the investigation to cases where the exit probability doesn't exist and test the predictions numerically in these cases.

View

Basic model for traffic interweave

Ding-wei Huang, Chung Yuan Christian University, Physics, Taiwan

Abstract: We propose a three-parameter traffic model, which summarizes our previous study of a twenty-four-parameter cellular automaton model for traffic dynamics at roundabout. The system consists of a loop with two junctions. The three parameters control the in-flow, the out-flow (from the junctions,) and the interweave (in the loop.) The dynamics is deterministic and governed by the Asymmetric Simple Exclusion Process (ASEP) with parallel update. The boundary conditions are stochastic, which include in-flow, out-flow, and interweave. We present preliminary results for a complete phase diagram and all possible phase transitions. Both numerical simulations and analytical results are discussed. On a simple roadway without traffic interweave, traffic dynamics is a competition between in-flow and out-flow which results in two phases: free flow and conventional congestion. On the complex roadway with traffic interweave, there are two more types of congestion: bottleneck and gridlock. The proposed model is able to present economically a clear perspective to these four distinct phases. There are six possible transitions among these four phases. The three transitions among free flow, conventional congestion, and bottleneck (i.e., without involving gridlock) are the typical first-order transitions with an abrupt change of density. Transition between gridlock and free flow is also abrupt. Transition between gridlock and bottleneck is smooth and continuous. Transition between gridlock and conventional congestion is absent. We observe only five transitions among the four phases. Instead of directly related to conventional congestion, gridlock can be taken as an extreme limit of bottleneck. Both bottleneck and gridlock are caused by the traffic interweave. This model can be useful to clarify the characteristics of traffic phases. This model can also be extended for practical applications.

View

Study of stochastic dependence between antirecessionary monetary support of enterprises with weak dynamic and their net operating loss

Ekaterina Khnyreva, Samara State Aerospace University, Department of Mathematics, Russian Federation

Abstract: This paper deals with the study of presence of one-factorial stochastic dependence between distribution law of fixed volume of antirecessionary monetary support of enterprise with weak dynamic and size of its net operating loss during time of crisis. There is shown this stochastic dependence by the example of an enterprise from subsection AA of All-Russian classifier of economic activity “Farming, hunting and forestry”.

View

A new approach for modelling lattice energy in finite crystal domains

Yevgen Bilotsky, Aalto University, Department of Material Science and Engineering, Finland

Abstract: Yevgen Bilotsky, Aalto University Foundation School of Chemical Technology, Department of Material Science and Engineering, Finland Michael Gasik, Aalto University Foundation School of Chemical Technology, Department of Material Science and Engineering, Finland Evaluation of internal energy in a crystal lattice requires precise calculation of lattice sums. Such evaluation is a problem in the case of small (nano) particles because the traditional methods are usually effective only for infinite lattices and are adapted to certain specific potentials. In this work, a new method has been developed for calculation of lattice energy. The method is a generalisation of conventional geometric probability techniques for arbitrary fixed lattices in a finite crystal domain. In our model, the lattice energy for wide range of two-body central interaction potentials (including long-range Coulomb potential) has been constructed by using the absolutely convergent sums. No artificial cut-off potential or periodical extension of the domain (which usually involved for such calculations) have been made for calculation of the crystal energy under this approach. As an example of the applications of this techniques, the energy of Coulomb potential has been plotted as the function of the domain size. Evaluation of internal energy in a crystal lattice requires precise calculation of lattice sums. Such evaluation is a problem in the case of small (nano) particles because the traditional methods are usually effective only for infinite lattices and are adapted to certain specific potentials. In this work, a new method has been developed for calculation of lattice energy. The method is a generalisation of conventional geometric probability techniques for arbitrary fixed lattices in a finite crystal domain. In our model, the lattice energy for wide range of two-body central interaction potentials (including long-range Coulomb potential) has been constructed by using the absolutely convergent sums. No artificial cut-off potential or periodical extension of the domain (which usually involved for such calculations) have been made for calculation of the crystal energy under this approach. As an example of the applications of this techniques, the energy of Coulomb potential has been plotted as the function of the domain size.

View

Stability of de Sitter solution in mimetic f(R) gravity

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Abstract: The mimetic f(R) gravity is revisited from the stability of de Sitter point of view. We show that how de Sitter evolves stable in the cosmological era. Our investigation can be used as a potentially interesting idea for early inflation as well as late time acceleration expansion.

View

Estimation of bone Calcium-to-Phosphorous mass ratio using dual-energy nonlinear polynomial functions

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Abstract: In this study an analytical approximation of dual-energy inverse functions is presented for the estimation of the calcium-to-phosphorous (Ca/P) mass ratio, which is a crucial parameter in bone health. Bone quality could be examined by the X-ray dual-energy method (XDEM), in terms of bone tissue material properties. Low- and high-energy, log-intensity measurements were combined by using a nonlinear function, to cancel out the soft tissue structures and generate the dual energy bone Ca/P mass ratio. The dual-energy simulated data were obtained using variable Ca and PO4 thicknesses on a fixed total tissue thickness. The XDEM simulations were based on a bone phantom. Inverse fitting functions with least-squares estimation were used to obtain the fitting coefficients and to calculate the thickness of each material. The examined inverse mapping functions were linear, quadratic, and cubic. For every thickness, the nonlinear quadratic function provided the optimal fitting accuracy while requiring relative few terms. The dual-energy method, simulated in this work could be used to quantify bone Ca/P mass ratio with photon-counting detectors.

View

AVALON: definition and modeling of a vertical takeoff and landing UAV

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Abstract: Unmanned Aerial Vehicles (UAVs) have been used in numerous applications, like remote sensing, precision agriculture and atmospheric data monitoring. Vertical takeoff and landing (VTOL) is a modality of these aircrafts, which are capable of taking off and landing vertically, like a helicopter. This paper presents the definition and modeling of a fixed-wing VTOL, named AVALON (Autonomous VerticAL takeOff and laNding), which has the advantages of traditional aircrafts with improved performance taking off and landing in small areas. The principles of small UAVs development were followed to achieve a better design and to increase the range of applications for this VTOL. Therefore, we present the design model of AVALON validated in a flight simulator and the results show its validity as a physical option for an UAV platform.

View

Electromagnetic Coherent Effects in Metamaterials with Randomly Rough Surfaces

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Abstract: Metamaterials are composite structures made of small metallic or dielectric particles. These particles play the same role as atoms or molecules in ordinary materials, which makes metamaterials considered as « artificial materials ». In this paper, we consider a three-dimensional disordered medium with randomly rough interfaces. For classical waves, the most interesting case is that of three-dimensional disorder. The quantity that obeys the disordered wave equation – the electric field – is a vector and not a scalar as in the Schrödinger equation. If many theoretical and numerical approaches have been developed to model transport of scalar light in random media, few or even no method at all nowadays can deal with ensembles of complex nanoparticles in

interaction between themselves and randomly rough boundaries. This aspect of the problem was never considered in detail up to now. In mesoscopic physics, multiple light scattering in disordered potentials gives rise to complex wave interference phenomena, like speckle correlations or Anderson localization of light, and to applications like imaging through opaque biological tissues or photovoltaics. We present a theory of transport based on an equation for second statistical moment, i.e. the Bethe-Salpeter equation in which the vectorial character of electromagnetic wave is taken into account. We can derive the radiative transfer equation from the Maxwell equations. The procedure is to write the Maxwell equations in an integral form with the help of Green tensors and to apply the Wigner transform to the equation obtained. The main advantage to starting from wave equations is that we are able to take into account new contributions to the scattered intensity such as the enhanced backscattering and the correlations between the scatterers that cannot be obtained from phenomenological radiometric considerations. This paper deals with the coherent backscatter enhancement effect, called the weak localization effect, which occurs when the electromagnetic intensity is scattered back to the source, it is coherent effect experienced by waves when propagating through a disordered system despite the randomness of the system. The Bethe-Salpeter equation is constructed in order that the medium and the boundaries are treated on the same footing. With this unified Bethe-Salpeter equation, a general expression is obtained, whatever the choice of the scattering operators used at the boundaries. Mathematically, the way to study the solution of the generalized Bethe-Salpeter equation is based on the use of diagrammatic perturbation theory. The description of the backscattering enhancement reduces to augmenting the diagrammatic expansions of the transfer equation by the contribution of the so-called most-crossed diagrams. In our approach, we use scattering operators which are a unified way to describe how electromagnetic waves interact with scatterers and boundaries. To use these operators, we have introduced two kinds of Green tensors. The first one describes the field scattered by the volume, which contains the scatterers, and by the randomly rough boundaries. The second type of Green tensors gives the field scattered by a slab with rough boundaries where the scatterers have been replaced by a homogeneous medium described by an effective permittivity. With these Green tensors, we can separate the contributions of the surfaces and the volume. The Quasi-Crystalline Coherent Potential Approximation (QC-CPA) is taken into account for the contribution of the random medium, which is made of spherical nanoparticles of given permittivity in a homogeneous dielectric background medium. For 3-dimensional slabs with nanoscale roughness and nano-particles, the enhanced backscattering is produced by different mechanisms, wave scattering by the same boundary, wave coupling by the two boundaries or wave scattering by the randomly distributed nano-particles. We give some numerical examples of scattering properties of random structures in thin films. Up to this point we have considered linear radiative transfer theory. In a region of high disorder, wave packet do not spread out, they are standing waves exponentially vanishing at infinity, we are in a localization regime while traveling quasi-plane waves are considered in transfer theory. As the strong localization predicted by Anderson is a non-perturbative theory, the development of computational schemes based on perturbation theory is a challenging problem. The different developed methods extrapolate the estimates from the region of weak disorder to the region of high disorder. Berginc, G. and Maradudin, A.A., "Scattering properties of random structures in thin films," in [Optical thin films and coatings], A Piegari and F. Flory (Ed.), Woodhead Publishing Limited, Oxford, 177-289 (2013).

View

Nonergodicity in Binary Alloys.

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Abstract: For binary liquids with limited miscibility of the components, we provide the corrections to the equation of state which arise from the nonergogic diffusivity. It is shown that these corrections result in lowering of critical miscibility point. In some cases, it may result in a bifurcation of miscibility curve: the mixtures near 50% concentration which are homogeneous at the microscopic level, occur to be too stable to provide a quasi - eutectic triple point. These features provide a new look on the phase diagrams of some binary systems. In present work, we discuss Ga-Pb, Fe-Cu, and Cu-Zr alloys. Our investigation connects their complex behavior in liquid state with the shapes of their phase diagrams.

View

THE SINGULARITY OF THE ANHARMONIC OSCILLATOR

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Abstract: The general solution of the equation anharmonic oscillation of a physical pendulum is considered as a function of the nonlinearity parameter and has a singularity at zero. This means that the application of different methods of regular decompositions in this parameter is impossible. Perturbation theory in the transformed canonical variables, using the new parameter of smallness was developed.

View

Automatic trace extraction and pattern identification for vertical ionograms

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Abstract: Ionograms represent the observation data of ionosonde that transmits radio waves toward the ionosphere while sweeping frequencies and measures the delay time of reflected signals. The result diagram expresses signal strength as a contour with the apparent altitude being taken on the axis of ordinate, and frequency on the axis of abscissa. The scaling and interpretation of ionograms attract continuous interest in both the scientific and practical context. Unfortunately, it is a time-consuming task to manually scale ionograms and evaluate the related ionospheric parameters. In this paper, we propose a method of two-step automatic ionogram recognition. The first stage is the data pre-processing that includes different filtering technique to eliminate artifacts and distortion due to other users of the high-frequency channel and the ionosphere. The second stage is automatic pattern identification based on the Canny method and correlation analysis. This technique were tested using ionograms of the ionosonde “Cyclon-GPS” that was developed in Kazan federal university. “Cyclon-GPS” is a vertical sounding ionosonde with a working frequency range from 1 to 32 Mhz and “minute by minute” regime of ionograms recording. The proposed technique was successfully applied for stable trace extraction (like F-, E-, D-layers). Additionally it allowed us to detect automatically sporadic effects like Es-layer and traveling ionospheric disturbance (TID).

View

Euclidean Complex Relativistic Mechanics: A New Special Relativity Theory

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Abstract: Relativity Theory was fundamental for the development of Quantum Physics. These parts of Physics are applied to sections, such as Chemistry, Biology, Pharmacology and Medicine. As a result, a significant change on Relativity will lead to changes on the above scientific sections. Special Relativity, as is applied until now, cancels the transitive attribute in parallelism, when three observers are related, because Lorentz Boost is not closed transformation. In this presentation, considering Linear Space-time Transformation, we demand the maintenance of Minkowski Space-time distance S2. In addition, we demand this Transformation to be closed, so there is no need for axis rotation. The solution is a matrix (Vossos Matrix) containing complex numbers. As a result, space becomes complex, but time remains real. Thus, the transitive attribute in parallelism, which is equivalent to the Euclidean Request, is also valid for moving observers. Choosing real space-time for the unmoved observer (O), all the natural sizes are real, too. Using Vossos Transformation for moving observers, the four-vectors' zero component (such as energy) is real, in contrast with space-components that are complex, but their norm is real. It is proved that moving relative to (O) human (O΄) meter length, according to Lorentz Transformation. In addition, we find rotation Matrix Vossos-Lorentz that turns natural sizes' complex components to real. We also prove that speed of light is invariant, when complex components are used and Vossos Transformation is closed for three sequential observers. After, we find out the connection between two moving relative to (O) observers: X΄΄= ΛLO΄΄(O) ΛLO(O΄) X΄. We applied this theory, finding relations between natural sizes, that are the same as these extracted by classic relativity, when two observers are related (i.e. relativistic Doppler shift is the same). But, the results are different, when more than two observers are related. Vossos Transformation of electromagnetic tensor Fμv, leads to complex electromagnetic fields for a moving observer. When the unmoved observer (O) and a moving observer (O΄) are related, the unmoved observer (O) measure the same real electromagnetic fields as those are given, using Lorentz Transformation, but moving observer (O΄) measure complex electromagnetic fields with the same form. Complex electromagnetic tensor turn to real using the form F΄ = ΛBLO΄(O) F΄BΛBLO(O΄) . When there are two moving, relative to (O) observers (O΄) and (O΄΄), their real electromagnetic tensors are related, using the form F΄΄= ΛLO΄΄ (O) ΛL O(O΄) F΄ [ΛLO΄΄ (O) ΛL O(O΄)]T . In addition, we prove that the relation between two moving, relative to (O) observers, when they use real coordinates, causes a real rotation between their frames. The turn is opposite to the turn of Thomas and has a little different measure, when the velocities are small. We apply these to the Uniform Circular Motion and to the hydrogen atom, considering that the proton is the unmoved observer (O) and the laboratory observer (O΄) has infinitesimal velocity. Using Perturbation Theory we calculate the position of the fine structure peaks of the atomic spectrum. The result is better not only than this extracted using P. Dirac Theory, but also than that extracted using L. H. Thomas Method.

View

Coexistence of pure and mixed states in nonlinear maps

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Abstract: Coherence and interaction are important concepts in physics. While interaction describes a relations between individual objects such as forces acting between distinguishable particles, coherent objects exists only in purpose to describe a single object. For example each component of a vector provides us with only partial information. The whole picture is reviled only when the components are coherently related to their generating vector. Another example is singlet of two spin $\frac{1}{2}$- particles. The true nature of these two coherent particles is described by a spin-less single particle. Apparently it seems that objects can be either coherent or non-coherent but they cannot be both simultaneously. This is almost true. We show that a system can be coherent

and non-coherent simultaneously but an observer can distinguish only one concept at a time.

View

Modeling of strain in magnetic media by method movable cellular automata

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Leonid Afremov, Far Eastern Federal University, Departament of Theoretical and Experimental Physics, Russian Federation
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Abstract: This paper represents ideas of the application of the method Movable Cellular Automata for modeling the distribution of magnetic particles in an elastic non magnetic matrix. The basic principles of mathematical model and algorithms is shown below. The model is represented as an ensemble of N discrete elements (automata), which identified the characteristic physical properties, rules of interaction and the possible states. Nearby automata capable of forming bonds with each other. Each machine can have 4 neighbors in a square package or 6 neighbors in the dense packing in the 2D model. Bound pair belong the same piece of material, and pair of unrelated automata belong to different fragments. The criterion for the formation of link and the link gap is the distance between the automata. The part of automata uniformly magnetized and interact with each other like magnetic dipoles. The special conditions can be given for certain groups of automata, for example, the lower layer can be fixed, and the upper layer can be influenced by an external force. Critical integration time step dt affects the accuracy of the calculations. Speed of sound in the medium venv possible to use for evaluate dt: dt = 0.25(d/venv), venv = √ (K/ρ + 4G/3ρ), ρ - density, K - bulk compression modulus, G - shear modulus. In the case of different types of automata the smallest of their respective times is accepted. Offset the automaton from its position at the previous step is calculated according to the Werle's scheme. At each step of integration the forces, acting on the automaton by the system is calculated, after a new speed and new coordinates of automata is calculated. The resultant force is the sum of the elastic and viscous forces, as well as force of the magnetic interaction automata.

View

Spin transport of the frustrated quasi-two-dimensional Heisenberg antiferromagnet

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Abstract: We use the Self Consistent Harmonic Approximation together with the Kubo formalism of the Linear Response Theory to study the spin transport in the quasi-two-dimensional frustrated Heisenberg antiferromagnet in a square lattice with easy-plane ion single anisotropy at zero temperature. The regular part of the spin conductivity $\sigma^{reg}(\omega)$ is determined for several values of the critical ion single parameter D_{c}, that separates the low D region from the large D quantum paramagnetic phase. We have obtained an abrupt change in the spin conductivity in the point of phase transition indicating a strong influence of frustration on the spin transport properties.

View

Modeling study of magnetic phase transition in amorphous ultrathin films

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Abstract: There is magnetic ordering process to model in the approximation of the “average spin” in amorphous ultrathin films. The formalism of the model is based on the assumption that the interaction field of the spin magnetic moment with the nearest magnetic moments is distributed in a random manner. By replacing instantaneous values of the magnetic moments with the ensemble average values of the magnetic moments and using distribution function of the interaction fields, it is easy to derive equations determining the relative average magnetic moments in each film monolayer. It has been shown as a result of modeling study that the average magnetic moment, the critical temperature of the magnetic phase transition and critical concentration of percolation depends on the film thickness. As expected, the critical temperature of the magnetic phase transition increases with the number of monolayers and the critical concentration of the transition from an ordered state to a disordered decreases.

View

Modeling of the size effect on the hysteresis characteristics of core/shell (Co/Au) nanoparticles

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Abstract: Study of nanoparticles led to the emergence of new structures, so-called core/shell nanoparticles. Notable among these are the Co/Au nanoparticles, which are due to the unique properties widely used in biomedicine . Feature of the magnetic properties of Co/Au nanoparticles is determined by the exchange interaction at the core/shell boundary. For investigation of hysteresis characteristics of Co/Au nanoparticles a model of two-phase nanoparticles was used: Ellipsoid-shaped Co/Au nanoparticle contains uniformly magnetized ellipsoidal cobalt core with long axis coincides with the long axis of the core/shell nanoparticle oriented along an axis Oz; It's considered that the cristalography anisotropy axis of cobalt parallel to the axis Oz, and spontaneous magnetization vectors of both phases Is(Au) and Is(Co) are located in one plane yOz which contain long axes of phases; External magnetic field H is applied along axis Oz. Modeling of the magnetization process of Co/Au nanoparticles revealed that coercive field and spontaneous magnetization is reduced with size, due to the increased role of thermal fluctuations in the system. Obtained results are in good agreement with an experiment.

View

A necessary condition for applying the MUSIC algorithm in limited-view inverse scattering problems

Won-Kwang Park, Kookmin University, Mathematics, Korea, Republic of

Abstract: It has been confirmed through the results of various numerical simulations that the MUltiple SIgnal Classification (MUSIC) algorithm can be applied to limited-view inverse scattering problems. However, the application of this algorithm is somewhat heuristic. In this study, we identify a necessary condition for applying MUSIC to the imaging of a collection of small, perfectly conducting cracks. This is based on the fact that the MUSIC imaging functional can be represented as an infinite series of Bessel functions of integer order of the first kind. We perform some numerical experiments on noisy synthetic data to support our findings.

View

Effect of β^- — charged eradiation and its calculation in the nuclear electrodynamics

theory

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Abstract: The study of own fields and charged particles motion and also charged fission splinters of a heavy nucleuses into nonrelativistic approximation is the subject of this paper research. The main efforts are concentrated in quest of charged share components by the radioactive β^- — disintegration. The corresponding field equations and equations of motion in the nuclear electrodynamics processes are obtained and their solutions are found. Analysis of the microscopic equations is generalized to the level of the macroscopic description of continuous medium electrodynamics and is accompanied by quantumomechanical additions.

View

Thermodynamic properties of the quantum wells with arbitrary combination of Dirichlet and Neumann boundary conditions in electric field

Oleg Olendski, King Saud University, King Abdullah Institute for Nanotechnology, Saudi Arabia

Abstract: Thermodynamic properties of the one-dimensional quantum well (QW) with miscellaneous permutations of the Dirichlet (D) and Neumann (N) boundary conditions (BCs) at its surfaces in the perpendicular to the surfaces electric field $\mathscr{E}$ are calculated in the framework of canonical and two grand canonical ensembles. A pronounced maximum accompanied by the adjacent minimum of the canonical specific heat c_V dependence on the temperature T for the flat pure Neumann QW and their absence for other BCs are predicted and explained by the structure of the corresponding energy spectrum. Applied field leads to the formation of the new or modification of the existing extrema what is qualitatively explained by the influence of the associated electric potential. A salient maximum of c_V is observed on the T axis for one fermion and its absence for any other number N of corpuscles. Qualitative and quantitative understanding of this phenomenon employs the analysis of the chemical potential and its temperature dependence for different N. It is proved that critical temperature T_{cr} of the Bose-Einstein (BE) condensation increases with the applied voltage for any number of particles and for any BC permutation except the ND case at small intensities $\mathscr{E}$ what is explained again by the modification by the field of the interrelated energies. It is shown that even for the temperatures smaller than T_{cr} the total dipole moment $\langle P\rangle$ may become negative for the quite moderate $\mathscr{E}$. For either Fermi or BE system, the influence of the electric field on the heat capacity is shown to be suppressed with N growing. Different asymptotic cases of, e.g., the small and large temperatures and low and high voltages are derived analytically and explained physically.

View

Lightlike relaxed elastic lines on oriented surface in Minkowski space

gülşah aydın şekerci, süleyman demirel university, science and arts faculty, Turkey

Abstract: The optimality for a lot of discipline is an important. The search for extremes is the subject of research for mountaineers, scientists, mathematicians, physicists, biologists. So, the calculus of variation was developed with its e§ects. One of these e§ects is relaxed elastic line. Because, a curve which minimizes the value of energy density is called relaxed elastic line. In this study, we analyzed relaxed elastic line in Minkowski space which is the mathematical modeling of Einsteinís relativity theory. For this space, when oriented surface is lightlike and the curve is lightlike, we calculated necessary boundary conditions to be extremal of the curve. So, we examined all of situations and we obtained the results by taking advantage from the relationship

between the curve and the surface

View

Why does a nonextensive model fit experimental radiobiology data even for large doses?

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Abstract: The effects of radiation on a tissue (being it healthy or cancerous) are well described by current linear-quadratic (LQ) radiobiological model for low absorbed doses around the 2 Gy often used in clinical fractionation. However, experimental data show a disagreement between the predicted and the observed effect of large doses. The Sotolongo et al. (2011) radiobiological (SRB) model, derived from Tsallis nonextensive entropy, has shown a good agreement with experiments for high absorbed doses, where LQ overestimates the dose required for a required effect. Other studies have reported a crossover in LQ model where its effects are underestimated for large doses. In this paper we develop a mechanistic version of the SRB model and show that it can reproduce both behaviors with a minimum set of assumptions. We compare the results of our simulations with some data reported in the literature. We also trivially adapt this model to fractionated radiotherapy and, in particular, to hypofractionation for which we draw some conclusions.

View

Graph model of intradisciplinary connections in example of general physics course

Tatyana Gnitetskaya, Far Eastern Federal University, School of Natural Sciences, Russian Federation

Abstract: The model of an intradisciplinary connections was elaborated on the base of the theory of graphs. Every connection which appears in training content may be presented as oriented marked graphs. Each graph is a tree. In this paper we presented definition and model of intradisciplinary connections for example of physics course. The quantitative parameters of model are described in this paper. Quantitative method based on this model could be help to optimize a content of physics course. Furthermore using this model we can distinguish fundamental notions, laws and other elements of knowledge to separate group. This group is very important during the process of creating training course.

View

Effects of molecular complexity and reservoir conditions on the discharge coefficient of adapted gas-dynamic nozzles

Alberto Guardone, Politecnico di Milano, Department of Aerospace Science and Technology, Italy

Abstract: The transonic flow at the throat section of a gas-dynamic nozzle is studied in adapted conditions to assess the influence of the fluid molecular complexity and total thermodynamic state on the discharge coefficient. The Sauer method is applied to solve the transonic perturbation potential equation in the vicinity of the nozzle throat for a general, non-ideal thermodynamic fluid model. For the first time, an analytical expression is derived that allows one to compute the discharge coefficient in terms of the nozzle curvature at the throat section and of the value of the fundamental derivative at sonic conditions, which depends on the fluid molecular complexity and on the thermodynamic state in the reservoir. The analytical model exposes a linear dependence of

the discharge coefficient on the value of the fundamental derivative of gasdynamics in sonic conditions. Computational Fluid Dynamics simulations are presented to verify of the theoretical findings and to assess the limits of the small perturbation hypothesis. The present findings are relevant to non-ideal fluid flows in gas-dynamics nozzles, including Organic Rankine Cycle engines for renewable energy applications, super-critical CO2 nozzle flows, valves operating with compressible fluids and space propulsion applications.

View

Thermal stress analysis for laser cutting corner with a fluctuant cutting speed in steel plate

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Hong Shen, Shanghai Jiao Tong University, School of Mechanical Engineering, China
Zhengchun Du, Shanghai Jiao Tong University, School of Mechanical Engineering, China

Abstract: The temperature and thermal stress field are important factors for controlling laser cutting quality. In the present study, thermal stress field analysis for laser cutting corner with a fluctuant cutting speed is carried out. Firstly, a three-dimensional (3-D) finite element model is established to simulate the temperature and thermal stress field. Then the factors of influencing the cutting speed fluctuation such as corner angle and cutting speed are studied in laser cutting corner. It is found that the constrained cutting speed at the corner introduces the phenomenon of corner burning and uneven residual stress distribution. The predicted temperature, thermal stress results agree well with the experiment data through the laser cutting corner experiment of 3 mm steel plate.

View

Evaluation of connectedness between the university Physics and Chemistry courses basing on the graph model of inter-subject links

Tatyana Gnitetskaya, Far Eastern Federal University, School of Natural Sciences, Russian Federation
Elena Ivanova, Far Eastern Federal University, School of Natural Sciences, Russia

Abstract: An application of the graph model of inter-subject links to University Physics and Chemistry courses is presented in this paper. A part of inter-subject space with directions of inter-subject links from Physics to Chemistry in the group of physical concepts has been shown. The graph model of inter-subject links includes quantitative indicators. Its numerical values are given in the article. The degree of connectedness between the data of Physics and Chemistry courses is discussed for the courses considered. The effect of the courses placement within a curriculum on the value of their connectedness is shown. The placement of courses within a curriculum can provide the study of the courses at the same time or consecutive study, when one course precedes another.

View

Semiclassical corrections to black hole entropy and the generalized uncertainty principle

Elias Vagenas, Kuwait University, Physics, Kuwait

Abstract: In this paper, employing the path integral method in the framework of a canonical description of a Schwarzschild black hole, we obtain the corrected inverse temperature and entropy of the black hole. The corrections are those coming from the quantum effects as well as

from the Generalized Uncertainty Principle effects. Furthermore, an equivalence between the polymer quantization and the Generalized Uncertainty Principle description is shown provided the parameters characterizing these two descriptions are proportional.

View

Large deviation estimates for a non-markovian Levy generator of big order

Rémi Léandre, Université de Franche-Comté, Laboratoire de Mathématiques, France

Abstract: There are much more semi-groups than semi-groups which are represented by stochastic processes. On the other hand, there are a lot of formulas in stochastic analysis which are natural. The theory of pseudodifferential operators allow to understand a lot of partial differential equations, including parabolic equations. On the other hand we have imported in the theory of non-markovian semi-groups a lot of tools of stochastic analysis. Stochastic analysis formulas are valid for the whole process. Their interpretation for non-markovian semi-groups work only for the semi-group.

View

Theoretical and explanation of the regio and stereoselectivity mechanism of Diels Alder reaction of the lactones derivatives

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Abstract: The Diels–Alder (DA) reaction is a powerful tool in organic synthesis and in the chemical industry. They allow, as private individuals, the formation (by bimolecular or intramolecular reaction) of a cycle with six atoms in a regioselective manner, while authorizing the presence of many functional groups. The lactonic cycle corresponds to a structural part is very frequently met in the natural products, in particular in sesquiterpenes which have for some of them, a multiple biological activity. In this work we studied, the Diels-Alder reaction involved a lactone derivative as a diene and a dienophile activated by a sulfoxyde groups both experimentally and theoretically. This type of sulfoxyde presents high stereo- and regioselectivity. our experimental finding schows that, the application of the reaction of Diels-Alder between a lactonic diene (standard B) and a dienophile (standard (A)) sufficiently reactive gives the product (C). In order to explain this experimental finding, theoretical investigation of the mechanism of the regio and stereoselectivity of this DA reaction has been carried out. The calculations have been performed in gas phase, in water solvent. The reaction mechanism corresponding to the formation of major isomers is elucidated by the analysis of the relevant stationary points of the potential energy surface and intrinsic reaction coordinate calculations. The obtained results put in evidence the importance of hydrogen bonding formed between the solvent molecules and the dienophile fragment in the acceleration of this DA reaction. The calculations are carried out with the Gaussian 09 suite of programs using the B3PW91 exchange-correlation functionals together with the 6–31G (d, p) basis set and the obtained results are in good agreement with experimental outcomes.

View

THEORETICAL STUDY FOR THE INTERACTION ACETYLCHOLINESTERASE-POSIPHEN DRUGS: ALZHEIMER DISEASE CASE

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Abstract: The senile insanities are defined like the regression of mental faculties of the old subject. The Alzheimer's disease [1] in fact part, its fundamental characteristic is the deterioration of cognition, in particular the dysmnesy. A major pathological hallmark of Alzheimer disease (AD) is the appearance in the brain of senile plaques that are primarily composed of aggregated forms of β-amyloid peptide (Aβ) that derive from amyloid precursor protein (APP). Posiphen (1) tartrate is an experimental AD drug that reduces Aβ levels without toxicity and it lacks acetylcholinesterase inhibitory activity [2]. The deterioration of the system of transmission of the nerve impulse via acetylcholine plays a central role in the cognitive decline. It corresponds to a reduction amongst specific receivers nicotinic of the neuro-transmitter acetylcholine. The degeneration of the cholinergic system evolves to the death of the neurons. Three therapeutic approaches were employed in an attempt at improvement of the nicotinic neurotransmission: increase in the acetylcholine synthesis, the activation of the receivers nicotinic and the inhibition of the acetylcholinesterase [3-4], enzyme responsible for the degradation of the neuro-transmitter (I). The current therapeutic choice is directed towards the inhibitors of the acetylcholinesterase, from where the objective of this work which consists in studying the interaction posiphen - acetylcholinesterase by molecular modeling methods.

View

Neutrinos in an Expanding Universe

Richard Wigmans, Texas Tech University, Physics, United States

Abstract: The Universe contains several billion neutrinos for each nucleon. In this talk, we follow the history of these relic neutrinos as the Universe expanded. At present, their typical velocity is a few hundred km/s and, therefore, their spectra are affected by gravitational forces. This may have led to a phenomenon that could explain two of today’s great mysteries: The large-scale structure of the Universe and the increasing rate at which it expands.

View

Low frequency wave modes of liquid-filled flexible tubes

Yuan-Fang Chou, National Taiwan University, Department of Mechanical Engineering, Taiwan

Abstract: Many canals in the human body are liquid-filled thin wall flexible tubes. In general the P-wave and S-wave velocities of tube material are much slower than the sound velocity of the liquid. It is interested to study the dynamic deformation of the wall caused by pressure fluctuation of liquid. In the low frequency range, the liquid pressure is essentially axial symmetric. Therefore, axial symmetric wave propagation modes are investigated. The calculated spectrum shows there are two modes with zero frequency limit. Phase velocities of these two modes are much smaller than the sound velocity of the liquid. They are also slower than the P-wave velocity of the tube material. At very low wave number, radial displacements of both liquid particles and tube are very small compared to their axial counter parts. As the frequency goes higher, boundary waves can be observed. The energy are mainly propagating in the neighborhood of liquid-solid interface.

View

Photocatalytic Degradation of TOC by Fe2O3/TiO2 Coated on Light Ceramic

Ju Chunhua, Harbin Institute of Technology, Materials of Technology, China

Abstract: Anatase titanium oxide (TiO2) films were prepared by a conventional sol-gel method on ceramic substrates as an inexpensive photocatalyst for degradation of hydroquinone in water. Investigation of the crystallinity and crack of the Fe2O3/TiO2 Coated on Light Ceramic by XRD and SEM showed that the proper heat-treatment temperature was 400 oC, and the as-obtained film displayed best photocatalytic activity among the prepared samples from different calcination temperatures. The prepared inexpensive photocatalyst also displayed good reproducibility, with the photocatalytic activity being maintained at about 54% after 4 cycles. A pseudo-first order reaction model was discovered for the photocatalytic mechanism of the Fe2O3/TiO2 Coated on Light Ceramic.

View

Application of Qiang-Dong Proper Quantization Rule to pseudoharmonic potential and its thermodynamics properties

Babatunde FALAYE, Federal University Lafia, , Nigeria

Abstract: Motivated by the recent works [J. Math. Chem. 50 (2012) 881, Chem. Phys. 421 (2013) 84], we attempt to study the thermodynamics properties of some diatomic molecules interacting via pseudoharmonic molecular model. The recently proposed Qian-Dong proper quantization rule have been employed in our calculations. The results also include rotational-vibrational energy spectrum for some diatomic molecules.

View

ASSESSMENT OF THE OPTICAL AND SOLID STATE PROPERTIES OF MANGANESE SULPHIDE (MnS) THIN FILM; THEORETICAL APPROACH.

Emmanuel Ugwu, Ebonyi State University, Dept. of Indutrial Physics,, Nigeria

Abstract: Assessment of the optical and Solid State properties of MgS thin film using theoretical approach of beam propagation technique in which a scalar wave is propagated through the material thin film deposited on a substrate with the assumption that the dielectric medium has homogenous reference dielectric constant term, and a perturbed dielectric term, representing the deposited thin film medium is presented in this work. These two terms, constituted arbitrary complex dielectric function that describes dielectric perturbation imposed by the medium of for the system. This is substituted into a defined scalar wave equation in which the appropriate Green's Function was defined on it and solved using series solution technique in conjunction with Born approximation method in order to obtain a model equation of wave propagating through the thin film. This was used in computing the propagated field for different input regions of field wavelength such as ultraviolet, visible and infrared region respectively during which the influence of the dielectric constants of the thin film on the propagating field were considered. The results obtained from the computed field were used in turn to compute the band gaps, solid state and optical properties of the thin film such as reflectance, Transmittance and reflectance. The electrical and optical conductance was also computed

View

Mathematical modeling a "Farady cage" new electronic structure for atoms

petru popovici, High school C-tin Bursan Hunedoara, enineering, Romania

Abstract: Mathematical modeling explaining the behavior of the elements from Mendeleev's Periodic Table, suggesting a new model of the distribution of electrons, completely different from the distribution suggested by Bohr and later by Somerfield, as well as from the subsequent

developments of these models. This distribution is a ‘Faraday cage’- type, based on the geometrical interpretations of curves in space-time continuum created by vibrations of particles. Here are some of the aspects explained by the model that I suggest: the behavior of rare gases, the electrical conductivity of metals, the variations of the electron affinity in the entire periodic table, and even the specific behaviors of a number of elements from the point of view of their electron affinity. The above-mentioned elements are N, Mg, Mn, Zn, Cd, Hg, Hf, which are elements with zero electronic affinity, similar to that of rare gases, although they are in the middle of series and of active periods from the point of view of the electron affinity. I finally developed the model up to the level of actinides, the geometric interactions of the type of coherent waves at such complexity of the ‘Faraday Cage’ being excessively complex for me to simulate. The key with which I verified the model was the natural course in the occurrence of more chemical reactions that is invariably, according to the model that I suggested, the course of growth of the system’s entropy. In the case of reversible reactions, according to the calculations resulting from the model that I suggested, the system’s entropy before the occurrence of a chemical reaction is approximately equal to the system’s entropy after the occurrence of the chemical reaction.

View

Goldbach problem for matrices over Principal Ideal Rings

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S. Katre, Savitribai Phule Pune University, , India

Abstract: Goldbach conjectured that every even integer > 2 is a sum of 2 primes. Analogous problem was considered for integral matrices by researchers such as Vaserstein, Bloy Greg, H. Qin and J. Wang. We solve this problem for matrices over Principal Ideal Rings and consider it more generally for matrices over commutative rings with unity.

View

Multi-scale modelling for hadrontherapy

Michaël Beuve, University Lyon1 , Institute for Nuclear Physics , France

Abstract: Hadrontherapy is an innovative external radiotherapy based on tumour irradiations with light ions, like swift protons or carbon ions. The efficiency of this therapy is based on a very accurate and advantageous ballistic, and, on the biological efficiency of light ions in tumour. Biological effects induced by ionizing radiations is a complex function of many parameters. Some are related to the biological endpoint in consideration, the type of irradiated cells, and the cell environment. Some others are related to the irradiation characteristics. While considering the specific case of swift ions, not only the dose of irradiation but also the ion charge, the ion energy, the irradiation temporal and spatial substructures need to be considered. We develop multiscale models, from atomic to patient scale, with the aim of understanding and improving treatments with hadrontherapy. In particular, we developed a new model: nanoxTM (NAdosimetry and Oxidative stress). The nanoxTM model takes as input, dosimetric quantities at various scales (starting from nanoscale), but also the production of radicals induced radiolysis.

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View

Forecasting systemic transitions in high dimensional stochastic complex systems

Henrik Jeldtoft Jensen, Imperial College London, Mathematics, United Kingdom

Abstract: Forecasting systemic transitions in high dimensional stochastic complex systems

View

Loop quantum gravity: overview and recent developments

Jorge Pullin, Louisiana State University, Department of Physics & Astronomy, United States

Abstract: Loop quantum gravity: overview and recent developments

View

Gravitational Wave Astrophysics

Gabriela Gonzalez, Louisiana State University, Department of Physics and Astronomy, United States

Abstract: Gravitational Wave Astrophysics

View

Cluster Formation in Granular Dynamics, Bird Flocking and Chimera States

Tassos Bountis, University of Patras, Department of Mathematics, Greece

Abstract: Cluster Formation in Granular Dynamics, Bird Flocking and Chimera States

View

Novel computational approaches in electronic structure calculations

Kalman Varga, Vanderbilt, Physics, United States

Abstract: Novel computational approaches in electronic structure calculations

View

Network of Collaborations in European Research Programs: Accepted vs. Rejected Proposals

Panos Argyrakis, University of Thessaloniki, Department of Physics, Greece

Abstract: Network of Collaborations in European Research Programs: Accepted vs. Rejected Proposals

View

Dynamics of irradiation: from molecules to nano-objects and from material science to biology

Eric SURAUD, Universite Paul Sabatier, Laboratory of Theoretical Physics, France

Abstract: We discuss microscopic mechanisms of irradiation in clusters and molecules. We consider the case of isolated molecules/clusters [1] and/or in contact with an environment [2]. We use Time Dependent Density Functional Theory (for electrons) coupled to Molecular Dynamics (for ions) and follow explicitly in time both irradiation and response of the system. Examples are taken from free metal clusters, from fullerenes, from molecules of biological interest and from clusters deposited on a surface or embedded in a matrix [2,3]. We analyse in particular the properties of emitted electrons (photo electron spectra, angular distributions...) which constitute a key tool of analysis of the properties of irradiated clusters and molecules [4,5]. We also discuss the possibility of pump and probe scenarios (opening the road to manipulation at the molecular scale) with help of dedicated laser pulses, exploring in particular very short times scales down towards

the attosecond domain. References [1] F. Calvayrac et al, Phys. Reports 337(2000)493 [2] P. M. Dinh et al, Phys. Reports 485 (2009) 43 [3] Z.P. Wang et al, Int. J. Mass Spect. 285 (2009) 1430 [4] Th. Fennel et al, Rev. Mod. Phys. 82 (2010) 1793 [5] P. Wopperer et al, Phys. Rep. 562(2015)1

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