CCP2016

Report of Contributions

https://events.saip.org.za/e/ccp2016

Contribution ID: **1** Type: **Poster Presentation**

Effect of viscosity on propagation of MHD waves in astrophysical plasma

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

We determine the general dispersion relation for the propagation of magnetohydrodynamic (MHD) waves in an astrophysical plasma by considering the effect of viscosity with an anisotropic pressure tensor. Basic MHD equations have been derived and linearized by the method of perturbation to develop the general form of the dispersion relation equation. Our result indicates that an astrophysical plasma with an anisotropic pressure tensor is stable in the presence of viscosity and
a strong magnetic field at considerable wavelength

Primary author: Mr ALEMAYEHU, Cherkos (AAU)

Presenter: Mr ALEMAYEHU, Cherkos (AAU)

Session Classification: Poster Session

Track Classification: Astrophysics and Space Physics

Contribution ID: **2** Type: **Oral Presentation**

Dust heating by Alfvén waves using non-Maxwellian distribution function

Wednesday, 13 July 2016 11:15 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Quasilinear theory is employed in order to evaluate the resonant heating rate by Alfven waves, of multiple species dust particles in a hot, collisionless, and magnetized plasma, with the underlying assumption that the dust velocity distribution function can be modeled by a generalized (r, q) distribution function. The kinetic linear dispersion relation for the electromagnetic dust cyclotron Alfven waves is derived, and the dependence of the heating rate on the magnetic field, mass, and density of the dust species is subsequently investigated. The heating rate and its dependence on the spectral indices r and q of the distribution function are also investigated. It is found that the heating is sensitive to negative value of spectral index r.

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Presenter: Dr KIRAN, Zubia (GC University, Lahore, 54000, Pakistan)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Plasma Physics

Contribution ID: **3** Type: **Poster Presentation**

Numerical Study of Microfluidic Transitional Flow Regime Curvature Effects for Compressible Isothermal Gases using Generalized Slip Boundary Conditions

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

In this paper we develop a numerical implementation of a generalized second order boundary condition reported by Guo et al [Physical Review E Vol. 89, 013021 (2014), DOI: 10.1103/PhysRevE.89.013021] for non-equilibrium gas flows and utilize the implementation to investigate microfluidic transitional flow regime curvature effects. The generalized boundary conditions expressed in terms of a nonlinear velocity slip with a wall function are incorporated into a modified nonlinear finite volume discretization incorporating generalized finite differences for the boundary conditions which we develop for an extended Navier-Stokes system of equations. Utilizing the developed computational scheme we then study the influence of transitional flow regime curvature effects in a gas piston-cylinder pressure balance interface gap and report on the observed microfluidic characteristics and behaviour.

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Session Classification: Poster Session

Track Classification: Fluid Dynamics

Contribution ID: **4** Type: **Oral Presentation**

UCLA Particle-in-Cell and Kinetic Simulation Software Center for Plasma Simulation

Wednesday, 13 July 2016 12:35 (20 minutes)

Abstract content
   (Max 300 words)
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Special chars

UCLA has recently established a Particle-in-Cell (PIC) and Kinetic Software Center (PICKSC) for plasma simulation. This center is in the process of providing a variety of open source software resources for the plasma physics community, ranging from codes running on laptops to codes designed to run on millions of cores on emerging computer architectures. The codes provided fall into a number of categories:
1. Skeleton codes (mini-apps). These are small bare bone applications that illustrate algorithms. We have codes that illustrate basic algorithms for beginning students to codes with 1, 2, and 3 levels of parallelization for supercomputer experts. Electrostatic, electromagnetic, and Darwin models are provided, in both Fortran and C, with some Python.
2. UPIC Framework. This provides a collection of tested components for designing new PIC codes, along with reference applications illustrating their use. It currently supports FFT based field solvers. The reference applications can be used for testing ideas and as a base for building new codes. Modest extensions of the reference applications are useful for some Ph.D. level research projects.
3. Educational codes. These codes are designed for teaching important plasma concepts, suitable for interactive classroom use. Both laptops and web based applications are planned.
4. Production codes. These are codes being used by a large number of people for research in many areas of plasma physics. These will include QuickPIC, UPIC-EMMA, OSHUN, and a version of OSIRIS. Some of these codes will heavily utilize the reference applications within UPIC. The goal is to lead a community effort in further developing them.

Design details and current status will be discussed. The center maintains a web site at: http://picksc.idre.ucla.edu/. Contributions to this web site from others are solicited.

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Presenter: Dr DECYK, Viktor (University of California, Los Angeles)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Plasma Physics

Contribution ID: **5** Type: **Oral Presentation**

Coding considerations for standalone molecular dynamics simulations of atomistic structures

Monday, 11 July 2016 15:50 (20 minutes)

**Abstract content
   (Max 300 words)
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While computational materials science has grown substantially, the bulk of research output still remains largely experimental, inevitably leaving the avenue of computation largely unexplored. The laws of Newtonian mechanics allow ab-initio molecular dynamics to model and simulate particle trajectories in material science by defining a differentiable potential function. This paper discusses some considerations for the coding of ab-initio simulation programs for simulation on a standalone computer and illustrates the approach by C language codes in the context of embedded metallic atoms in the face-centred cubic structure. The algorithms use velocity-time integration to determine particle parameter evolution for up to several thousands of particles in a thermodynamical ensemble. Such functions are reusable and can be placed in a redistributable library header file. While there are both commercial and free packages available, their heuristic nature prevents dissection. In addition, developing own codes has the obvious advantage of teaching techniques applicable to new problems. This article is written from the experiential standpoint aimed at developing atomistic and molecular dynamics simulation toolkit development through which initial simulations may be undertaken by interested researchers. The programs codes presented here have been tested successfully on Microsoft C/C++ compiler (Windows 7) and \verb+gcc+ in Ubuntu Linux with little modification for various fcc metal parameters. The outputs compare favorably with published literature sources and confirm the applicability of the software.

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Co-author: Prof. TERBLANS, JJ (Koos) (UFS)

Presenter: OCAYA, Richard (UFS, Department of Physics)

Session Classification: Parallel Track B

Track Classification: Physics Education

Contribution ID: **6** Type: **Oral Presentation**

Protein dynamics as a function of ionic strength, calcium ion concentration and temperature: Calmodulin as a first step

Monday, 11 July 2016 12:20 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Calmodulin protein plays a very crucial role in the calcium signaling inside the eukaryotic cell structure as it can also bind to other proteins/targets and facilitate various activities inside the cell. The response of CaM protein as a function of ionic strength, calcium ion removal and temperature at physiological pH condition is investigated using classical Molecular dynamics simulations. Changing the ionic strength and temperature came out to be two possible routes for observing a conformation change in the protein. As the calcium ions are removed from the protein, it is observed to acquire more flexibility. This flexibility is observed to be more prominent at a higher ionic strength. At a lower ionic strength of 150 mM with all the four calcium ions intact, the N and C-lobes are observed to come close to a distance of 30 Å starting from an initial separation distance of 48 Å. This conformation change is observed to take place around 50 ns in a simulation of 100 ns. As a second parameter, temperature is observed to play a key role in the conformation change of the protein. Earlier these kind of studies have been performed experimentally using fluorescence measurements as in. The calcium bound form of CaM is observed to undergo a reversible conformation change in the range 295-301 K at calcium ion concentration 150 mM. The transition temperature was observed to depend on the calcium ion concentration of the protein. We perform MD simulations of 100 ns each for the temperature range 300-500 K on the apo form of CaM, 3CLN and 1CFD. A remarkable dependence of the temperature is observed on the overall dynamics of the protein as reported in our earlier study. 1CFD shows a much flexible linker as compared to 3CLN whereas the overall dynamics of the lobes mainly N-lobe is observed to be more in later case.

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Presenter: Mr ANEJA, Sahil (University of Delhi)

Session Classification: Parallel Track B

Track Classification: Computational Biology

Contribution ID: **7** Type: **Poster Presentation**

Processes of decollimation of the beam of fullerenes during scattering on it beam of hydrogen.

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
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Special chars

Fullerene with impurities inside (X@C60, where X is N, P, and etc. atoms) can be used as the unit cells for quantum computers (for example, [1]). Based on experimental work [2], and using molecular dynamics method with Brenner interatomic potential [3], we studied a penetration of 8-15 eV hydrogen (H) atoms into fullerenes beam (20 fullerenes, 1eV/molecule). This simulation can be applied to other atoms replacing the Brenner potential by the suitable interatomic potentials. One of our goals was to clarify the mechanism decollimation of beam of fullerene in scattering onto them hydrogen atoms. Process of decollimation of beam of fullerenes may be of some importance in the preparation of nanoelectronic components in this way. The simulation results show that interaction of low-energy beams of fullerenes and hydrogen atoms have pronounced inelastic character.

The transverse velocities, acquired fullerenes as a result of their interaction with hydrogen, are comparable with the velocity of deposition of fullerenes. It can lead to significant spread of fullerenes on the substrate on which they are deposited. When energy of the beam of hydrogen atoms increased, process of decollimation of fullerenes is reduced.

At carrying out of such model calculations should be careful with choice the density of the beam. When the number of atoms in the beam and its energy increase simultaneously, partial or complete destruction of fullerenes can observed.

References

1. W. Harneit Phys. Rev. A65, 032322 (2002)
2. H. Minezaki, et al, Review of scientific instruments, 85, 02A945 (2014)
3. D.W. Brenner et al, J.Phys: Condens. Matter, 14, 783-802 (2002)

Primary author: Mr ALYABEV, Danila (Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan)

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Presenter: Mr ALYABEV, Danila (Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan)

Session Classification: Poster Session

Contribution ID: **8** Type: **Oral Presentation**

Synchronization on Complex Networks

Tuesday, 12 July 2016 11:40 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

The synchronization transition of coupled random frequency oscillators is revisited. The Kuramoto model on a complete graph is known to exhibit a mean-field-type continuous phase transition in both phase and frequency synchronization with a unimodal symmetric distribution of intrinsic frequencies. We consider the Kuramoto model on complex networks such as Erdos-Renyi random networks and scale-free networks, where quenched disorder in connectivity is present in addition to quenched disorder in intrinsic oscillator frequencies. We find that frequency disorder fluctuation induces anomalous finite-size-scaling behaviour near the onset of the synchronization. More interestingly, connectivity disorder fluctuation changes the nature of the synchronization transitions, when the random frequency distribution takes a flat or a bimodal shape.

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Presenter: Prof. PARK, Hyunggyu (Korea Institute for Advanced Study)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **9** Type: **Oral Presentation**

Development of a simulated computer modelling of laser treatment for coronary heart disease

Tuesday, 12 July 2016 11:20 (20 minutes)

Abstract content
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Presently, there is no model that describes the efficacy of lasers in treating coronary artery disease (CAD), which can be used by clinicians with or without minimal side effects. The current conventional CAD treatment with medication or bypass surgery or minimally invasive methods often present serious side effects such as breathing problems, heart attack, and dry cough, amongst others including sudden death (Skiner, 1993: 201-203; Mackinnon et al., 2003: 162).

The objective of this research project is to use a computer modelling approach to develop a model eva

It is demonstrated in Wech (2011: 29) and Karsten (2012: 1 - 2) that the optimal use of lasers as a tr

Mathematical model will be developed using Maxwell's equations and Fresnel's equations to calculate

This research will provide a guideline for a new cost effective and optimal CAD treatment with minimised risk of side effects.

Primary authors: Mr KABEYA, Francois (University of Johannesburg (UJ)); Prof. ABRAHAMSE, Heidi (University of Johannesburg)

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Presenter: Mr KABEYA, Francois (University of Johannesburg (UJ))

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **10** Type: **Poster Presentation**

Plutonium Rock-Like Oxide fuel (ROXf) system , their once-through burning and usage.

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The ROXf is a kind of inert matrix fuel U238-free matrices ,it has a high plutonium transmutation capability. The ROXf consists of chemically stable phases of fluorite 'stabilised ZrO₂ or ThO₂ and spinel MgAl₂O₄' . In this fuel , PuO₂ is solidified in a fluorite phase. With U238-Free matrices , a large part of the plutonium can be burned after irradiation in conventional LWRs. The spent ROXf consists of natural analogous geologically stable phases , and is disposed directly as high level wastes 'HLWs' after about 50 years cooling. From the high plutonium burn up rate and the high stability of the fuel, the ROXf-LWRs system has proliferation resistance and environmental safety. Characteristics of two types of ROXf , Zr-ROX and Th–ROX with weapons-Pu ,in an LWR core arrangement are evaluated by cell burn up calculations and 2-D core calculations using the SRAC code system and JENDL-3 nuclear library. In an LWR of moderator to fuel volume ratio = 1.9 , which corresponds to current PWRs , Pu transmutation rates with the two types of ROXf are large enough and more than 80% and 99% of Pu and Pu239 , respectively, can be burned. The calculated kinetic parameters indicate less moderate characteristics of ROX cores , especially with Zr-ROX .The fertile Th232 in Th-ROX works like U238 in the UO₂ fuel ,making kinetic parameters more moderate and reactivity drop due to burn up smaller than that Zr-ROX. The neutron capture of Th232 to generate U233 , causes the safeguards problem. Thus , the characteristics of Zr-ROX as a typical example , were investigated in this study.

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Presenter: Prof. MOHAMED SALEH, Ashraf Elsayed (BRNO University of Technology)

Session Classification: Poster Session

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **11** Type: **Oral Presentation**

2-Secure and certify studies to work on production of Spiked plutonium.

Tuesday, 12 July 2016 10:20 (20 minutes)

Abstract content
   (Max 300 words)
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In the nuclear weapons sites , work on materials include non nuclear testing of components of weapons that are sitting in the sites that include fundamental physics and engineering experiments on plutonium and investigating technologies for remanufacture of plutonium parts innuclear weapons and work on prodution of spiked plutonium which incorporates more of the isotope plutonium 238 than would normally be found in weapons -grade plutonium, 7.5 % rather than the typical 0.036 % . As plutonium 238 is more radioactive ,the spiking process accelerates the formation of defects that occur within the metal during alpha decay of plutonium ,the new alloy ages more quickly , on the equivalent of 16 years for every year of actual aging, which makes it perfect for experiments on plutonium decay, If typical weapons-grade plutonium , plutonium 239 is spiked with some plutonium 238 , which decay more quickly , the self-irradiation process dramatically picks up speed . If 5% of plutonium 239 is replaced with plutonium 238 , the sample will age 11 times faster than normal plutonium 239 .Aging can be accelerated by a faster of 16 over normal aging processes if 7.5% of the sample is plutonium 238. A useful measure of acceleration aging is defined as the number of years required to reach a radiation dose that results in 10 displacements per atom. Weapons-grade plutonium normally takes 100 years to reach this dose but will need just 6.25 years if it is spiked with 5% plutonium 238. In this paper(oral only), I discuss and present the advanced studies to certify a weapons test that shake , drop, heat and cool sample of fissile materials take place inside the test building.

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Presenter: Prof. MOHAMED SALEH, Ashraf Elsayed (BRNO University of Technology)

Session Classification: Parallel Track B

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **12** Type: **Oral Presentation**

INVITED SPEAKER: Replica Exchange Wang-Landau Simulation of Lattice Protein Folding Funnels

Tuesday, 12 July 2016 14:00 (30 minutes)

Abstract content
   (Max 300 words)
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Understanding protein folding remains a Grand Challenge problem of modern science. The resolution of Levinthal's paradox concerning the ability of proteins to fold rapidly postulates the existence of a rough, "folding funnel" in free energy space that "guides" the protein to its lowest free energy, native state. The funnel is always portrayed schematically as a function of some unknown reaction coordinate and has never actually been observed. We have studied the folding of the protein ribonuclease A by mapping it onto a 124 monomer, coarse-grained lattice HP model [1] and an H0P model [2] that includes "neutral" 0-mers in addition to the hydrophobic H-mers and polar P-mers. (Amino acids are mapped onto one of the three different kinds of monomers, according to hydrophobicity.) Using Replica Exchange Wang-Landau sampling [3], we determined the density of states g(E) to high precision. From g(E) we then calculated the free energy of the protein vs end-to-end distance as a function of temperature. The HP model shows a rather shallow and flat free energy minimum, reflecting the high degeneracy of the ground state. In contrast, the H0P model develops a clear, rough free energy funnel with a relatively low degeneracy ground state. Unlike the common, schematic figures, we find an asymmetric folding funnel that also changes shape substantially as the temperature decreases. Even the location of the free energy minimum shifts as the temperature decreases. To our knowledge, this is the first actual observation of a folding funnel, and its dynamic nature alters our perception of this fundamental concept.

[1] K. A. Dill Biochemistry 24, 1501 (1985).
[2] G. Shi, A. C. K. Farris, T. Wuest and D. P.Landau. J. Phys: Conf. Ser. 686, 012001 (2016)
[3] T. Vogel, Y. W. Li, T. Wuest and D. P. Landau, Phys. Rev. Lett. 110, 210603 (2013)

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Presenter: Prof. LANDAU, David (The University of Georgia)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **13** Type: **Oral Presentation**

Progress toward the discovery of a room-temperature superconductor: theoretical studies of the observed superconductivity above 200K in the sulfur hydride system at high pressure

Wednesday, 13 July 2016 11:35 (20 minutes)

**Abstract content
   (Max 300 words)
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It has been long conjectured (1) that metallic hydrogen or hydrogen-containing compounds offer the possibility of extremely high superconducting temperatures, perhaps at room temperature or above, with some explicit electronic structure studies adding further weight to these ideas (2). The discovery of conventional BCS-like superconductivity in a cubic compound of sulfur and hydrogen by Drozdov, et al. (3) has created great excitement in that the holy grail of a room-temperature superconductor may be possible. The highest Tc reported in the H-S system is 203K for a compound likely in the Im-3m structure under high pressure (3). Theoretical studies of this system have been reported by several groups (4,5). Here we present the advances in the understanding of this and similar systems developed by using ab initio electronic structure calculations to determine their electronic and phononic behavior and the electron-phonon coupling strengths that result from these studies. We show that ab initio computer simulations give a very good understanding of the high Tc that is driven by a combination of strong electron-phonon coupling and high frequency hydrogen optic modes. The role of anharmonicity will be put into perspective and we will discuss the underlying chemical bonding in these systems that can provide a guide to discovering materials with even higher values of Tc.

(1) N.W. Ashcroft, Phys. Rev. Lett. 21, 1748 (1968).
(2) D.A. Papaconstantopoulos and B.M. Klein, Ferroelectrics 16, 307 (1977).
(3) A.P. Drozdov, M.I. Eremets, I.A. Troyen, V. Ksenofontov, and S.I. Shyin, Nature 525, 73-76 (2015).
(4) D. Duan, et al., Sci. Rep. 4, 6968 (2014).
(5) D.A. Papapconstantopoulos, B.M. Klein, M.J. Mehl and W.E. Pickett, Phys. Rev. B 91, 84511 (2015), and references therein.

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Session Classification: Parallel Track B

Contribution ID: **14** Type: **Oral Presentation**

Computational Morphometric Analysis in Astrophysics and Cosmology

Monday, 11 July 2016 12:00 (20 minutes)

Abstract content
   (Max 300 words)
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We discuss the state of the art in morphometric analysis of galactic structures in astrophysical and cosmological scales. From the practical point of view, we present a hybrid many-core Mic60/K40 computational morphometric system to automatically analyze structure and pattern formation in astrophysics (e.g. galaxy classes) and cosmology (e.g. filaments, voids and "Zeldovich-pancakes"). The system includes the original and modified versions of the following coefficients: Concentration, Asymmetry, Euler Characteristic, Smoothness, Entropy and Spirality. Using a sample of spiral and elliptical galaxies from the Galaxy Zoo project as a training set, we employed the Linear Discriminant Analysis technique to classify SDSS Legacy (779,235 galaxies) samples. The cross-validation test shows that we can achieve an accuracy of more than 86\% with our classification scheme. Therefore, a plane in the morphometric parameter space can be defined which separates the elliptical and spiral classes with a mismatch between classes smaller than 10\%. The distance to different space parameters planes as a morphometric index is also useful to characterize structure formation in large-scale structure simulation as from the galactic systems simulated from Millenium and Illustris projects. A selection of quite new methodologies and applications are presented within the context of Data-Intensive Scientific Analysis related to the main data repositories available for extra-galactic astrophysics research. The main challenges in hybrid/heterogeneous computer science for those purposes are addressed.

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Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **15** Type: **Oral Presentation**

ab initio studies of thermoelectric materials for energy conversion applications

Tuesday, 12 July 2016 14:40 (20 minutes)

**Abstract content
   (Max 300 words)
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Special chars**

Energy harvesting requires clean and highly efficient energy conversion technologies. Thermoelectricity is one such technology that achieves thermal-to-electric conversion and vice versa. This is achieved purely by solid state means and has a great potential for applications in waste heat recovery, air conditioning and spot cooling of electronic devices. Attempts have been directed towards exploration of high performance compounds which are yet to be realized. To predict the enhanced electronic structure of Cadmium Oxide (CdO), we doped it with Zn and Mn. The structural properties in terms of volumes and lattice parameters, the band structure and the density of state for both the doped and undoped CdO were determined by the modern ab initio methods based on density functional theory (DFT). We established that indeed doping improved thermoelectric properties of cadmium oxide.

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Presenter: Dr WAFULA, Henry (Physics Department Masinde Muliro university of Science and Technology)

Session Classification: Parallel Track B

Contribution ID: **16** Type: **Oral Presentation**

PLENARY: Kinetic-energy driven superconductivity in cuprate superconductors

Tuesday, 12 July 2016 08:30 (1 hour)

Abstract content
   (Max 300 words)
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Superconductivity in cuprate superconductors occurs upon charge-carrier doping Mott insulators [1], where a central question [2] is what mechanism causes the loss of electrical resistance below the superconducting transition temperature? In this talk, we attempt to summarize the basic idea of the kinetic-energy driven superconducting mechanism in the description of superconductivity in cuprate superconductors [3,4,5]. The mechanism of the kinetic-energy driven superconductivity is purely electronic without phonons, where the interaction between charge carriers and spins directly from the kinetic energy by the exchange of spin excitations induces the superconducting-state in the particle-particle channel and pseudogap state in the particle-hole channel, therefore there is a coexistence of the superconducting gap and pseudogap. This kinetic-energy driven d-wave superconducting-state is controlled by both the superconducting gap and quasiparticle coherence, which leads to that the maximal superconducting transition temperature occurs around the optimal doping, and then decreases in both the underdoped and overdoped regimes. The kinetic-energy driven superconducting mechanism also indicates that the strong electron correlation favors superconductivity, since the main ingredient is identified into a charge-carrier pairing mechanism not from the external degree of freedom such as the phonon but rather solely from the internal spin degree of freedom of the electron.

[1] J. G. Bednorz and K. A. Muller, Z. Phys. B 64, 189 (1986).

[2] P. W. Anderson, Science 235, 1196 (1987); Science 317, 1705 (2007).

[3] See, the review, S. Feng et al., Int. J. Mod. Phys. B 29,1530009 (2015).

[4] S. Feng, Phys. Rev. B 68, 184501 (2003); S. Feng et al., Physica C 436, 14 (2006); S. Feng et al., Phys. Rev. B. 85, 054509 (2012).

[5] S. Feng et al., Physica C 517, 5 (2015); Phil. Mag., in press (2016). arXiv:1510.05384.

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Presenter: Prof. FENG, Shiping (Department of Physics, Beijing Normal University, Beijing 100875, China)

Session Classification: Plenary

Contribution ID: **19** Type: **Poster Presentation**

Investigation of the radiation emission influence on properties of liquid water systems

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
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Present work is dedicated to the investigation of the radiation emission influence on those thermodynamic properties of liquid water systems, which are defined by the change of chemical potential of the liquid and its components under the influence of radiation. It was shown, that irradiation of the coexisting phases in stationary state results in the shift of the phase transition points parameters. The shift of temperature and pressure of phase transitions of the first order under the influence of radiation was evaluated taking in count both entropy and interaction factors at the chemical potential of the regarded system. Also we present the first step of a general study on induced radiation damage by 256 water molecules in simulation box at T=(280-315) K at the molecular level by MD. The main goal of this work is to study the water structure, thermodynamics and dynamics changing under induced by the radiation damage from 0.1 keV to 1MeV.
The MD codes used in this study includes all
relevant interactions (cluster formation) and dynamics properties (MSD, VAF and diffusion) to obtain stucture and dynamics properties systems of study under radiation damage.

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Co-author: Dr GAVRUSHENKO, Dmitryi (National Taras Shevchenko University of Kyiv)

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Session Classification: Poster Session

Contribution ID: **20** Type: **Oral Presentation**

Running mean techniques of extracting observed frequencies in Kepler red giant stars

Monday, 11 July 2016 12:20 (20 minutes)

Abstract content
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We have developed a running mean techniques of extracting observed frequencies (individual frequencies) for red giant stars showing solar-like oscillations using data from Kepler space mission. The frequencies are extracted from the periodograms (power spectrum). We use the techniques to study the evolutionary stages (status) of red giant stars by constructing echelle diagrams and measuring the period spacing. Based on the value of the calculated period spacing, we place the red giant stars into red giant branch, red giant clump and secondary red clump. On applying the techniques to stars with well known evolutionary status, we are able to arrive at the same conclusion as other techniques.

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Co-authors: Dr BALONA, Luis A (South African Astronomical Observatory); Prof. MEDUPE, Thebe (North-West University)

Presenter: Mr ABEDIGAMBA, Patrick Oyirwoth (North-West University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **21** Type: **Oral Presentation**

An asymptotic preserving scheme for the Vlasov-Maxwell system in the classical limit

Wednesday, 13 July 2016 11:35 (20 minutes)

Abstract content
   (Max 300 words)
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In order to model non-thermalized plasmas in the fully magnetized and relativistic regime, the relativistic Vlasov-Maxwell (RVM) system is most commonly used. In that context efficient numerical methods have been developed (see, e.g., [1] and [2]). The dimensionless parameter c that determines the relative strength of relativistic effects is the speed of light scaled by the thermal velocity. In some applications, however, the weakly relativistic regime (i.e. where c is large) is of interest. In this case numerical simulations show that the methods that have been developed for the RVM system are extremely inefficient. In addition, many numerical methods are not even able to recover the correct limit behavior (i.e. convergence to the Vlasov-Poisson system).

In this presentation we describe the asymptotic preserving scheme introduced in [3]. This method is robust with respect to the classic limit and imposes no step size restriction. Our approach relies on a time splitting approach for the RVM system and employs an implicit integrator for the linear part of Maxwell's equations. It turns out that the choice of this implicit method is crucial as even L-stable methods can introduce numerical instabilities for large values of c.

To illustrate the efficiency of the numerical scheme in both the relativistic as well as in the classical limit regime we present the results for a number of numerical simulations. We mostly focus on the Weibel instability and on Landau damping. In the relativistic case we compare the asymptotic preserving scheme to the Hamiltonian splitting proposed in [1] and the VALIS method proposed in [2].

References

[1] N. Crouseilles, L. Einkemmer, E. Faou, J. Comput. Phys. 283, pp.224-240 (2015)

[2] N. J. Sircombe, T.D. Arber, J. Comput. Phys. 228, pp. 4773-4788, (2009)

[3] N. Crouseilles, L. Einkemmer, E. Faou, arXiv 1602.09062, (2016)

Primary author: Dr EINKEMMER, Lukas (University of Innsbruck)

Co-authors: Prof. FAOU, Erwan (INRIA-Rennes, Universit\'e de Rennes 1 and IRMAR, Rennes, France); Dr CROUSEILLES, Nicolas (INRIA-Rennes, Universit\'e de Rennes 1 and IRMAR, Rennes, France)

Presenter: Dr EINKEMMER, Lukas (University of Innsbruck)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Plasma Physics

Contribution ID: **22** Type: **Oral Presentation**

Dynamic Modelling on the Crystallization of Mono-sized Cubical Particles under Mechanical Vibrations

Monday, 11 July 2016 11:00 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
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The realization of the densest possible geometrical ordering is one of the most fundamental questions in self-assembly of particles. In this work, the crystallization process of single crystal (disorder-order transition) formed by mono-sized cubical particles under three-dimensional (3D) mechanical vibrations is investigated by the dynamical simulation of discrete element method (DEM). The efficiency of crystallization in various vibration conditions and different shaped containers is analyzed and compared. The evolution of macro property such as packing density and micro properties such as coordination number (CN), radial distribution function (RDF), particle orientation and inter-particle forces during vibrated crystallization are characterized. The results show that the perfect single crystal of mono-sized cubical particles can be reproduced if the 3D vibration conditions are properly controlled. The distribution of particles in the crystallization process is also affected by the container walls, where the crystallization of particles initially emerges. In particular, the disorder-to-order transition is demonstrated as an entropy driven process under the entropic effects of particle shape and geometrical confinement of container walls. These findings can be helpful for our general understanding of self-assembly problems.

Primary author: Mr WU, Yongli (Monash University)

Co-authors: Prof. YU, Aibing (Monash University); Prof. AN, Xizhong (Northeastern University)

Presenter: Prof. AN, Xizhong (Northeastern University)

Session Classification: Parallel Track B

Contribution ID: **23** Type: **Poster Presentation**

Mechanical properties and energy absorption characterization of compressive deformation of Tin-Lead metallic foam with open cells

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
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Abstract — Metallic foams, have a light structure, having particular mechanical characteristics. Many tests have also shown that they have a great capacity for energy absorption, shock absorption, a significant noise reduction and having many applications.
This work is devoted to the development and characterization of metallic foams with open cells based on tin-lead alloy (with 50 % of tin content). The purpose of this paper is threefold. Our first goal will be to the response of the behavior of metallic foams with different relative densities on uniaxial compression tests. Our second goal is dedicated to evaluate the energy absorption capacities during the uniaxial compression tests on metallic foams. Lastly, this paper focuses at the interpretations of the results and findings of our experiments described in this study which will be the subject to predict the mechanical properties of our open metal foams and compare them with the properties of existing metal foams in literature.

Keywords: Metallic foams, Elaboration process, Open cells, Mechanical properties, Energy absorption, Relative density.

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Co-authors: Mrs HASSEIN-BEY, Amel Hind (Student); Prof. ABUDURA, Salam (University)

Presenters: Mr BELHADJ, Abd-Elmouneïm (University); Prof. ABUDURA, Salam (University)

Session Classification: Poster Session

Track Classification: Fluid Dynamics

Contribution ID: **24** Type: **Oral Presentation**

Temperature specification in atomistic molecular dynamics and its impact on simulation efficacy

Tuesday, 12 July 2016 14:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
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The importance of temperature as an energy related state function in physical systems was well established from the earliest days of the physical sciences and was central to the formulation of the laws of thermodynamics. These laws fundamentally state that for an isolated system, knowledge of temperature leads to an assessment of system entropy, which in a sense conveys the stability of the system above absolute zero temperatures. As the development of theoretical and computational methods continues rapidly in diverse branches such as chemistry, condensed matter physics, material science, molecular biology, nanotechnology and others, the effect of temperature on the simulated parameters remains at the heart of all problems. This paper discusses the currently used temperature modelling formalisms in atomistic molecular dynamics simulations. Standalone simulation programs may have variability in the definition of temperature and its evolution in a system. For instance, some specifications of temperature are done indirectly in terms of its effect on the elongation of the lattice parameters, while others employ energy equi-partition and thermostatic approaches. In heuristic simulation programs which are essentially closed off from dissection, this question does not really arise directly but inherently where specification of temperature occurs in the form of a single, external input variable. Simulation as a means of materials research is projected to grow in popularity due to vastly improved computational power and a diversity of research questions for which no commercial programs exist per se. Therefore, standalone programs are also likely to grow in prominence, necessitating clarification of temperature specification. Therefore, we attempt to address the fundamental question of optimal temperature specification in the context of atomistic molecular dynamics simulation context. In particular, we calculate the vacancy formation energies for a number of FCC metals using two separate temperature specification approaches and then discuss the results.

Primary author: OCAYA, Richard (UFS, Department of Physics)

Co-author: Prof. TERBLANS, JJ (Koos) (UFS)

Presenter: OCAYA, Richard (UFS, Department of Physics)

Session Classification: Parallel Track B

Contribution ID: **25** Type: **Oral Presentation**

Phase transition approach to bursting in neuronal cultures : Quorum Percolation models

Tuesday, 12 July 2016 11:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Rather than describing collective behaviors observed in living neuronal networks grown in vitro in terms of oscillator synchronization, the Quorum Percolation model tackles the issue from the point of view of statistical physics and critical phenomena. Under its original form, it is a discrete time dynamics model of information propagation on a directed random graph similar to a cellular automaton and built up according to a simplification of the most relevant biological features : The neurons, located at the nodes, are two state systems whose activation is governed by a fixed threshold (Quorum) rule. A burst is seen as a discontinuity in the activity of the network, interpreted as the occurrence of a giant cluster. We go beyond such a model by introducing several biological relevant developments. The decay, modeled by a discrete time markovian process, accounts for ionic leakage through the membrane of neurons; as a main result, our Monte-Carlo simulations enable to understand how the decay changes the percolation transition, where discontinuities are replaced by steep but finite slopes, or even destroys the transition. Furthermore, while quenched disorder arises from the graph connectivity randomness, a variability in the neuronal excitability can be taken into account with the help of a Gaussian probability distribution of the Quorum. We derive a mean field approach and show its relevance by carrying out explicit Monte Carlo simulations. Such a variability shifts the position of the percolation transition, impacts the size of the giant cluster and can even destroy the transition. Moreover we highlight the occurrence of disorder independent fixed points above the Quorum critical value. A finite-size analysis enables us to show that the order parameter is weakly self-averaging with an exponent independent on the thresholds disorder. At last, we stress that the effects of the threshold variability can be understood by studying a global activation probability.

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Presenter: Dr MONCEAU, Pascal (Laboratoire Matière et Systèmes Complexes UMR CNRS 7057 and Université Paris-Diderot)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **26** Type: **Oral Presentation**

Shear-free Anisotropic Cosmological Models in f(R) Gravity

Wednesday, 13 July 2016 15:20 (20 minutes)

Abstract content
   (Max 300 words)
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A class of shear-free, homogeneous but anisotropic cosmological models in f(R) gravity will be presented. We show that the anisotropic stresses are related to the electric part of the Weyl tensor in such a way that they balance each other. We also show that within the class of orthogonal f(R) models, small perturbations of shear are damped, and that the electric part of the Weyl tensor and the anisotropic stress tensor decay with the expansion as well as the heat flux of the curvature fluid. Specializing in locally rotationally symmetric spacetimes in orthonormal frames, we examine the late-time behaviour of the de Sitter universe in f(R) gravity. For the Starobinsky model of f(R), we study the evolutionary behavior of the Universe by numerically integrating the Friedmann equation, where the initial conditions for the expansion, acceleration and jerk parameters are taken from observational data.

Primary author: Dr ABEBE, Amare (North-West University)

Co-authors: Prof. MOMENI, Davood (Eurasian National University); Prof. MYRZAKULOV, Ratbay (Eurasian National University)

Presenter: Dr ABEBE, Amare (North-West University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Gravitation and Cosmology

Contribution ID: **27** Type: **Oral Presentation**

INVITED SPEAKER: Quantum vs classical optimization: A status update on the arms race

Tuesday, 12 July 2016 09:30 (30 minutes)

**Abstract content
   (Max 300 words)
Formatting &
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Can quantum computers indeed meet the promise of doing complex calculations faster than classical computers based on transistor technologies? While the holy grail of a programmable universal quantum computer will probably still take decades to reach, one can already begin to answer this question by testing programmable quantum annealing machines that are currently being built. These machines, such as the D-Wave 2X, use a non-mainstream method known as adiabatic quantum annealing to perform optimization tasks. In this talk I summarize the most recent benchmarking results on quantum optimization machines.

Primary author: Prof. KATZGRABER, Helmut G. (Texas A&M University)

Co-authors: Dr PERDOMO-ORTIZ, Alejandro (NASA); Mr OCHOA, Andrew J. (Texas A&M University); Dr HAMZE, Firas (D-Wave Systems Inc.); Mr MUNOZ-BAUZA, Humberto (Texas A&M University); Dr MANDRA, Salvatore (Harvard University); Dr SCHNABEL, Stefan (Leipzig University); Dr WANG, Wenlong (Texas A&M University); Dr ZHU, Zheng (Texas A&M University)

Presenter: Prof. KATZGRABER, Helmut G. (Texas A&M University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **28** Type: **Poster Presentation**

Computational Study of Rocket Thrust Vectoring Propulsion Control System Characteristics for Surface Landing Trajectory Paths

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
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In this paper we mathematically formulate the space motion of a rocket in order to investigate different specified surface landing trajectory paths/orientations through an analysis of thrust vectoring forces that are used as control system inputs. The underlying rocket trajectory physical model is formulated in terms of Newton's second law for the translational motion and the corresponding Euler equations for the rotational motion which yield a coupled system of simultaneous non-linear differential equations amenable to numerical solution. Refinements in the rocket's path/orientation are then incorporated through the use of a finite number of control thrusters whose magnitudes are allowed to vary with time with fixed directional orientations relative to the axis of the rocket's main propulsion engine thus introducing known external force and torque loading conditions. Different rocket trajectory paths/orientations are then computationally investigated by incorporating the physical model into an optimization problem to minimize the differences in the predicted and specified paths/orientations through refinements of the control thruster's characteristics subject to spatial and velocity constraints for safe rocket surface landing conditions.

Primary author: Mr RAMNATH, Vishal (University of South Africa)

Presenter: Mr RAMNATH, Vishal (University of South Africa)

Session Classification: Poster Session

Contribution ID: **29** Type: **Oral Presentation**

Canonical and Non-Canonical Ising Spin Glass on Randomly Rewired Regular Lattices

Tuesday, 12 July 2016 12:40 (20 minutes)

Abstract content
   (Max 300 words)
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Spin glass (SG) has been an active research field in theoretical and experimental condensed matter physics in the last four decades It is a random magnetic system mainly characterized by a frozen spin orientation at low temperatures. Frustration and randomness are considered to be the key ingredients for a system to exhibit SG behavior. The so-called non-canonical SG is a new type of SGs[1] where frustration and randomness are different from that of the canonical one where both ferromagnetic (FM) and antiferromagnetic (AF) couplings exist. It is a purely AF system on structures with random connectivity and frustration due to a topological factor. The existence of this new type of SGs on various structures, such as scale free network, rewired lattices and regular graphs for models such as Ising and Heisenberg spins has been reported by several previous studies [2, 3, 4, 5, 6].

Further elaboration of this system is required, in particular for a comparison to the canonical type of each corresponding model such as Ising and Heisenberg model on the same irregular structure. Here we study the Ising models on rewired regular lattices of both canonical and non-canonical SG model. We used Replica Exchange of Monte Carlo method [7] and calculate the SG order parameter to search for SG phase. We estimate the critical temperature and exponents of the SG phase observed.

Primary author: Dr SURUNGAN, Tasrief (Hasanuddin University, Makassar, INDONESIA)

Presenter: Dr SURUNGAN, Tasrief (Hasanuddin University, Makassar, INDONESIA)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **30** Type: **Oral Presentation**

Chaplygin-gas Solutions of f(R) Gravity

Wednesday, 13 July 2016 14:00 (20 minutes)

**Abstract content
   (Max 300 words)
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We explore exact f(R) gravity solutions that mimic Chaplygin-gas inspired Lambda CDM cosmology. Starting with the original, generalized and modified Chaplygin gas equations of state, we reconstruct the forms of f(R) Lagrangians. The resulting solutions are generally quadratic in the Ricci scalar, but have appropriate Lambda CDM solutions in limiting cases. These solutions, given appropriate initial conditions, can be potential candidates for scalar field-driven early universe expansion (inflation) and dark energy-driven late-time cosmic acceleration.

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Co-author: Dr ABEBE, Amare (North-West University)

Presenter: Ms ELMARDI, Maye (UCT)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Gravitation and Cosmology

Contribution ID: **31** Type: **Oral Presentation**

INVITED SPEAKER: Computational Heliospheric Physics; A South African Perspective

Monday, 11 July 2016 11:30 (30 minutes)

Abstract content
   (Max 300 words)
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In heliosheric physics, and space physics in general, we sometimes need to model the transport of charged particles in turbulent plasmas, for example, when simulating cosmic ray propagation in the heliosphere. The resulting equations are Fokker-Planck type partial differential equations that must be solved numerical due to the complexity and multi-dimensionality of the processes involved. Except for using standard finite-difference numerical schemes, we have, in recent years, successfully applied a stochastic differential equation based solver. The latter approach leads to an algorithm that is ideally suited for parallel computation. Recently, a CUDA version of this algorithm was also implemented. In this talk, details and results of various numerical models, all developed in-house and applied to different space physics problems, will be discussed. The wider context of computational physics in South Africa is also discussed: How can we, as South African researchers, contribute to knowledge creation? What is the role of computational physics in human capacity development? What, uniquely South African, obstacles do we face and how can these be overcome?

Primary author: Dr STRAUSS, Du Toit (Centre for Space Research, North-West University)

Presenter: Dr STRAUSS, Du Toit (Centre for Space Research, North-West University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **32** Type: **Oral Presentation**

Ultrahigh-energy neutrino events in current and future neutrino telescopes from nearby Gamma-Ray Bursts

Monday, 11 July 2016 12:40 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

Neutrino Astronomy has gained momentum after discovering cosmic neutrinos by the IceCube Neutrino Observatory at the south pole. A proposed upgrade of IceCube and planned future experiments will increase sensitivity to neutrino fluxes at ultrahigh energies (> PeV). We consider ultrahigh-energy neutrino flux from the Gamma Ray Bursts (GRBs) during the afterglow phase. We calculate this flux by modeling in details the observed afterglow data with standard afterglow theories for nearby long-duration GRBs within redshift 0.5. We also calculate neutrino events from these GRBs in the current and future experiments such as KM3NeT, IceCube Gen-2, Pierre Auger Observatory and JEM EUSO.

Primary author: Mrs K THOMAS, JESSYMOL (Uni. OF JOHANNESBURG)

Co-authors: Dr MOHARANA, Reetanjali (Uni. of Johannesburg); Prof. RAZZAQUE, Soebur (University of Johannesburg)

Presenter: Dr MOHARANA, Reetanjali (Uni. of Johannesburg)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **35** Type: **Oral Presentation**

INVITED SPEAKER: The role of kinetic scales: particle acceleration from shocks and reconnection

Wednesday, 13 July 2016 10:45 (30 minutes)

**Abstract content
   (Max 300 words)
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Non-thermal particles are ubiquitous in astrophysics, but by their very nature can not be described by fluid approximations and require a more detailed description on the kinetic scale. To understand the dynamics it is necessary to study the processes responsible for acceleration and transport of these particles.

The interplay of particle distributions and fields is too complex for an analytic, self-consistent description as they are non-linearly coupled so computer simulations are required. Typically computer models for kinetic plasmas try to solve the Vlasov equation by either representing the distribution function of energetic particles as fields on a grid or via pseudo-particles. This talk focusses on the popular Particle-in-Cell method, where the plasma is represented by pseudo-particles interacting with a grid based electromagnetic field.

While PiC is used for many problems in kinetic plasmas, we focus on the two kinds of acceleration mechanisms, that are most likely responsible for the major fraction of all energetic particles observed in space: Shock fronts and reconnection events. It will be especially highlighted, how to handle the large gap of length scales between the kinetic plasma scales and the outer scales of astrophysical objects.

Primary author: Dr KILIAN, Patrick (North-West University)

Co-authors: Mr SCHREINER, Cedric (North-West University); Prof. SPANIER, Felix (NWU); Prof. BÜCHNER, Jörg (Max-Plank-Insitute for Solar System Science); Dr MUNOZ, Patricio (Max-Plank-Institut for Solar System Science); Dr GANSE, Urs (Helsinki University)

Presenter: Dr KILIAN, Patrick (North-West University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **36** Type: **Oral Presentation**

Computer simulation of the process of defragmentation and ablation of mass during the interaction of shock waves with molecular clouds

Monday, 11 July 2016 14:20 (20 minutes)

**Abstract content
   (Max 300 words)
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In this work the results of numerical simulation of interaction process between strong shock wave generated after supernova explosion and molecular cloud (MC) have been presented in three-dimension gas-dynamical settings. Developed computational code is based on numerical solution of the Euler equations for compressible flow. Gas flow equations were represented conservatively for velocities components and energy. The parallel code using OpenMP for PC hybrid system was developed for modeling. The Intel Vtune Amplifier XE was used to profile the code using GPU. More than a two billion cells mesh (2048x1024x1024) with effective resolution for cloud radius in 128 nodes was implemented. Peculiarities of molecular cloud forming and density fragmentation in time were analyzed during time-consuming simulation. Shock wave strikes the cloud, triggering weak reflected shock waves and transmitted shock that advances in to the cloud. Inner-cloud SW compresses and defragment MC media. Post-processing used allow to find out the circumstances of vortex transfer in MC, ablation and erosion phenomena.

The shock wave interaction with several boundaries of substances with different density complicates the interaction and gives rise of vortex rings. Developing perturbations lead to the formation of vorticity over the surface of the cloud and ablation its matter. Appearing vortexes transfer to the vortex streets and initialize whirlpool studs. The neighboring counter rotating vortexes form the system of primary and secondary vortex structures. These vortex structures are stretched, bended and changing their shape with the time forming secondary, tertiary etc. systems.

Primary author: Prof. RYBAKIN, Boris (MSU M.V. Lomonosov, SRISA RAS)

Presenter: Prof. RYBAKIN, Boris (MSU M.V. Lomonosov, SRISA RAS)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **38** Type: **Oral Presentation**

INVITED SPEAKER: Why and how to calculate momentum dependent self-energy for strongly correlated materials

Wednesday, 13 July 2016 10:45 (30 minutes)

Abstract content
   (Max 300 words)
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Dual nature of electronic spectrum is observed in many correlated electron systems in which 'wave'-like (itinerant) and 'particle'-like (localized) electronic states coexist. This universal behavior is observed in a large class of correlated materials including copper-oxide superconductors, actinides, iron-pnictides, iron-chalcogenides, various complex-oxides, and transition metal di-chalcogenides. Modeling such correlated systems was challenging since both Fermi liquid theory and dynamical mean-field theory become inadequate here. One needs to go beyond and include the full momentum dependence of the self-energy due to non-local density-density correlations. We introduce a momentum-resolved density-fluctuation (MRDF) theory appropriate for this problem.[1-3] Our MRDF model allows us to calculate momentum-dependent self-energy due to various density-density fluctuations. Here, I will present results for several representative correlated materials including cuprate superconductors, actinide compounds, and various complex oxides. The momentum-dependence of self-energy turns out to be crucial to these materials reproducing 'Fermi-arc' feature; universal 'waterfall'-like dispersion as seen in many materials; unique (experimental and theoretical) identification of Mott-gap and antiferromagnetic gap being separated at different energy scale (this is unexpected from the typical Mott physics). We find a generic trend in the dispersion and spectral weight anomaly across all these materials, despite their low-energy properties being very different.

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[2] T. Das, R. S. Markiewicz, A. Bansil, Adv. Phys 63, 151 (2013).
[3] R. S. Dhaka, et al., Phys. Rev. B 92, 035127 (2015).
[4] X. Yin, et al. Phys. Rev. Lett. (in production 2016).

Primary author: Dr DAS, Tanmoy (Indian Institute of Science, Banaglore)

Presenter: Dr DAS, Tanmoy (Indian Institute of Science, Banaglore)

Session Classification: Parallel Track B

Contribution ID: **39** Type: **Oral Presentation**

Dynamical Properties of Granular Materials

Monday, 11 July 2016 11:20 (20 minutes)

**Abstract content
   (Max 300 words)
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We discuss the dynamical properties of granular matter. This system loses energy (cools) continuously because of the inelastic collisions between particles. We focus on freely-evolving granular gases. The gas initially cools in a homogeneous cooling state (HCS), but a clustering instability drives it into an inhomogeneous cooling state (ICS). We present results for the HCS and ICS of granular gases where (a) the restitution coefficient is constant; (b) the restitution coefficient depends on the relative collision velocity. We discuss the analytical and numerical techniques used to study granular gases.

Primary author: Prof. PURI, Sanjay (School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, INDIA.)

Presenter: Prof. PURI, Sanjay (School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, INDIA.)

Session Classification: Parallel Track B

Contribution ID: **40** Type: **Oral Presentation**

Visualizing higher order Brillouin zones with applications

Monday, 11 July 2016 14:50 (20 minutes)

Abstract content
   (Max 300 words)
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It is common for students to use modern electronic structure codes (ESC) as black-boxes with little conceptual understanding of the underlying theoretical and computational details of the main components involved. What are needed are simplified problems that illustrate these concepts and are easily coded by senior undergraduate students.

An important concept in solid state physics is the first Brillouin zone (BZ) which uniquely determines the electronic energies and wavefunctions for electrons in a periodic potential. ESC calculate material properties using integrations over this zone. Higher order zones are also important; the BZ boundaries define Bragg planes and the constant energy Fermi surface for metals sometimes cross these planes. The shape of this surface is important in determining many metal properties and low energy interactions. Students can write a small code, in a language of their choice, that implements a simple algorithm to sort k-points into their respective Brillouin zones for any crystal lattice.

Using this algorithm, we visualize BZ of any order as well as deconstruct the Fermi surface for metals if it extends into higher order zones using the reduced-zone scheme. Visualizations are produced using the freely available plotting programs grace and gnuplot. We present results for 2D and 3D.

Primary author: Dr ANDREW, Richard (University of Pretoria)

Co-authors: Prof. CHETTY, Nithaya (University of Pretoria); Dr SALAGARAM, Trisha (University of Pretoria)

Presenter: Dr ANDREW, Richard (University of Pretoria)

Session Classification: Parallel Track B

Track Classification: Physics Education

Contribution ID: **41** Type: **Oral Presentation**

GPUs in a Computational Physics course

Monday, 11 July 2016 15:30 (20 minutes)

**Abstract content
   (Max 300 words)
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In an introductory Computational physics class of the type that many of us give, time constraints lead to hard choices on topics. Since everyone likes to include their own research in such a class I give fair time to visualiation, but try to also give an overview of many areas. Since about 2007 I have also included 2 lectures on parallel programming algorithms using MPI. Both the principle and the need to break the "fear barrier" of using a large machine with a queuing system via ssh have been sucessfully passed on.

Due to the plateau in chip development and to power
considerations future HPC hardware choices will include heavy use of GPUs. Thus the need to introduce these at the level of an introductory course has arisen. Just as for parallel coding explanation of the benefits and simple examples to guide the hesitant first time user have been selected.

I proposed several student projects using GPUs that include how-to pages, in the style described in [1], so that these examples would provide me with material. I will describe two of the more successful ones: a lattice Boltzman and a Finite Element code, two topics that I previously gave in short overviews, and link to new lecture pages that we developed.

[1] D. Mazvovsky, G. Halioua and Joan Adler, "The role of projects in
(Computational) Physics Education", Physics Procedia, 2012, Vol 34, p 1-5.

Primary author: Dr ADLER, Joan (Technion -IIT)

Co-author: Mr NISSIM, Gal (Technion - IIT)

Presenter: Dr ADLER, Joan (Technion -IIT)

Session Classification: Parallel Track B

Track Classification: Physics Education

Contribution ID: **42** Type: **Oral Presentation**

INVITED SPEAKER: Paradigms for Electronic Structure Codes

Monday, 11 July 2016 14:20 (30 minutes)

Abstract content
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In most solid state physics research groups today powerful desktop computers and sophisticated, user-friendly electronic structure codes (ESC) based
on density functional theory (DFT) enable students to study complex physical systems with ease. During the course of their study these students learn
about DFT and how to use ESC, but seldom get an opportunity to understand the algorithms that make these codes accurate and efficient. As a result
they do not develop the necessary computational skills that make
them transferable to other scientific working environments. In an attempt to
address this, we have developed paradigms to the electronic structure problem
that involve self-contained mini computational problems that enhance students' understanding of particular key aspects of ESC.
In this talk we give an overview of the mini projects developed thus far as
well as those we will work on in future.

Primary author: Prof. CHETTY, Nithaya (University of Pretoria)

Co-authors: Dr ANDREW, Richard (University of Pretoria); Dr SALAGARAM, Trisha (University of Pretoria)

Presenter: Dr SALAGARAM, Trisha (University of Pretoria)

Session Classification: Parallel Track B

Track Classification: Physics Education

Contribution ID: **43** Type: **Oral Presentation**

The effect of a warm electron beam on fast electron-acoustic nonlinear potential structures in multi-electron species plasmas

Wednesday, 13 July 2016 15:00 (20 minutes)

**Abstract content
   (Max 300 words)
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Arbitrary amplitude fast electron-acoustic solitons are studied in a multi-electron component plasma with cool, warm and hot electrons and cool ions treated as inertial (adiabatic) fluids. The warm electrons are treated as drifting relative to other plasma species. Effects of the beam drift speed on the existence regions of fast electron-acoustic solitons and their coexistence are examined. We also investigate the effect of warm electron beam drift speed on the existence of supersolitons. The relevance of our results in connection to the generation mechanism of various electrostatic turbulences such electrostatic hiss, magnetic burst noise, auroral kilometric radiation(AKR), broadband electrostatic noise(BEN) and other nonlinear wave phenomenon is also discussed.

Primary author: Mr MBULI, Lifa Nicholas (University of the Western Cape/SANSA)

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Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Plasma Physics

Contribution ID: **44** Type: **Poster Presentation**

Sustainable numerical scheme for molecular dynamics simulation of the dusty plasmas in an external magnetic field

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The method, which allows one to carry out computer simulation of system of the charged particles in a strong external homogeneous magnetic field with the time step that is independent on the Larmor oscillation time, was generalized for the case of the presence of the surrounding background for the moving particles. An example of such a system is complex dusty plasma. In this type of complex plasma charged microparticles of solid state move in the background plasma of ions, electrons and atoms (molecules). Under the influence of the magnetic field B particle with specific charge q / m performs the rotation at the Larmor frequency. It is also influenced by the friction force that occurs when it moves in the external environment. In work [1] on the basis of the Taylor expansion of the position and velocity vectors the numerical scheme, which is resistant to a change in time step at a large external magnetic fields, was obtained. The time step in this scheme is independent on the Larmor period of oscillation. In our work we have put the frictional force in the Velocity Verlet scheme, performing all these steps, described in [1], for obtaining of the sustainable scheme. We deduced the new stable second-order numerical scheme for solving the equations of motion of particles in an external homogeneous stationary magnetic field and the background environment.
In this scheme a choice of the time step is not limited by the relation between time step and Larmor frequency. So, correctly taking into account a strong magnetic field and friction force, which both depend on the particles velocities, we obtained solution resistant to a change in the time step within the second-order Velocity Verlet propagation scheme.

References

1. Q. Spreiter and M. Walter, J. Comput. Phys. 152, 102 (1999).

Primary author: Prof. DZHUMAGULOVA, Karlygash (IETP, al Farabi KazNU)

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Presenter: Prof. DZHUMAGULOVA, Karlygash (IETP, al Farabi KazNU)

Session Classification: Poster Session

Track Classification: Plasma Physics

Contribution ID: **45** Type: **Poster Presentation**

The capture cross sections at the electron collisions with hydrogen atom and proton in the dense semiclassical plasma

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Investigation of the interaction between particles and plasma properties is of great interest in many areas of physics such as atomic and plasma physics. It is important for the development of the plasma technologies. One of the elementary processes in plasma is the electron capture process. In this work the electron capture processes by the hydrogen atom and proton were investigated. The motion of the electron in the field of the the motionless atom or proton was considered on the basis of the perturbation theory and the solving of the equation of motion. The interaction potentials between the electron and the hydrogen atom and also proton were presented in works [1,2]. These effective potentials, taking into account the quantum-mechanical effects of diffraction of particles and plasma screening effects, have finite values at the distances close to zero.
In this work the electron capture radius, which was determined by equating the kinetic energy of impacting electron and the interaction energy between the electron and the hydrogen atom or proton, was presented. The trajectories of the electron in the field of the atom and proton were simulated. Obtained results of the electron capture by the atom and proton were compared. Using the electron capture probability, the electron capture cross section was calculated.

References

[1] T.S. Ramazanov, K.N. Dzhumagulova, Effective screened potentials of strongly coupled semi-classical plasma, Phys.Plasm. 9 (2002) 3758-3761
[2] T.S. Ramazanov, K.N. Dzhumagulova, Y.A. Omarbakiyeva, Effective polarization interaction potential “charge-atom” for partially ionized dense plasma, Phys. Plasm. 12 (2005) 092702

Primary author: Ms SEISEMBAYEVA, Madina (IETP, al Farabi KazNU)

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Presenter: Prof. DZHUMAGULOVA, Karlygash (IETP, al Farabi Kazakh National University)

Session Classification: Poster Session

Track Classification: Plasma Physics

Contribution ID: **46** Type: **Poster Presentation**

Multiscale simulations of structure and thermomechanical properties of phthalonitrile heat-resistance resins

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Phtalonitrile-based matrixes are thermostable resins used for durable reinforcement materials. The resins are typically produced by two-stage curing of phthalonitrile monomers in presence of initiator. During the first low temperature stage (˜200deg;C), nitrile groups transform into intermonomer bonds between isoindoline groups, which is the typical polymerization path. The second curing stage is aimed to reach higher conversion rate and produced at elevated temperatures (300 – 350deg;C), at which triazine can be formed by three monomers. Effectively, triazine is a triple link between monomers, making the topology of the polymer network even more complex. The effect of triazine crosslinks in the structure and physical properties of the material is important but unclear up to now.

We have developed a multiscale simulations scheme of phthalonitrile thermosetting resins. The scheme contains a set of consecutive phases from dissipative particle dynamics (DPD) level to molecular dynamics. On the first step, we simulate two-stage curing process with DPD technique. The length of low-temperature and high-temperature stages is controlled by the aim conversion rates known from experimental study. On the next step, a reverse mapping procedure is used to convert coarse-grained structures onto atomistic ones. The obtained atomistic structures are then refined by a Monte Carlo procedure with soft repulsive potentials to avoid insufficient structural motifs such as the short cycle spearing. Then we run short relaxation within molecular dynamics (MD). The prepared material samples are used for the following MD simulations to estimate thermophysical and mechanical properties of the material.

In this report, we present and discuss thermophysical and mechanical properties for the phthalonitrile matrixes obtained with using different comonomers and polymerization protocols.

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Presenter: Dr RUDYAK, Vladimir (Lomonosov Moscow State University, Faculty of Physics)

Session Classification: Poster Session

Contribution ID: **47** Type: **Oral Presentation**

INVITED SPEAKER: From 2D to 3D and 1D: Manipulating charge and spin at oxide heterointerfaces

Wednesday, 13 July 2016 10:15 (30 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

Advances in thin film growth techniques, which allow for the precise layer-by-layer growth of epitaxial materials, have opened the door to numerous discoveries which were not previously achievable through bulk synthesis techniques. Pertinent examples include emergent phenomena at perovskite oxide heterointerfaces such as two-dimensional electron gases, interfacial superconductivity and novel magnetic properties. In this presentation, I will discuss the use of first principles calculations to explore how chemical identity, interface density and overlayer nanostructuring can be used to modulate the density, dimensionality and mobility of charge carriers as well as magnetism at oxide heterostructure interfaces. For example, using first principles simulations, we demonstrate that in La δ-doped SrTiO₃ (STO) superlattices with relatively thin STO layers, three-dimensional conductivity can be achieved in a transparent oxide material. This 3D transparent conductivity is a direct result of the appreciable overlap of the quantum mechanical wavefunctions between neighboring δ-doped layers with negligible changes to the STO electronic band structure. Furthermore, I will discuss our efforts to understand how nanostructured patterning of the LaAlO₃ overlayer can be used to create a 1 dimensional electron gas. Finally, I will discuss how the injection of charge at the interface between two antiferromagnetic oxides fosters the emergence of interfacial ferromagnetism. Together, these results demonstrate an unprecedented control over charge and spin at an interface thus opening the door for the use of these materials in a wide range of applications. This work was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division through the Office of Science Early Career Research Program.

Primary author: Dr COOPER, Valentino (Oak Ridge National Laboratory)

Presenter: Dr COOPER, Valentino (Oak Ridge National Laboratory)

Session Classification: Parallel Track B

Contribution ID: **48** Type: **Oral Presentation**

PIC simulation of scattering and absorption of an ultraintense short-pulse laser in a finite-size plasma

Wednesday, 13 July 2016 12:15 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

The scattering and absorption of an intense, short-pulse laser in a relativistic under-dense plasma is investigated applying a fully kinetic 1D-3V particle-in-cell simulation code. The nonlinear phenomena related to the propagation of laser pulse in a finite-size under-dense plasma such as absorption and scattering have been studied in details. The results show that the laser pulse is depleted by the wake excitation at low plasma densities and the maximum laser absorption occurs at the phase-mixing time. We have expressed the explicit reasons for the anomalous behavior of the laser absorption rate in both magnetized and un-magnetized finite-size plasma. Studying the kinetic results associated with the distribution function of plasma electrons shows that in a special range of the plasma and laser parameters a large amount of laser energy is transferred to electrons to produce energetic electrons with bulk velocity in the laser direction. The obtained results in this paper have direct relevance to recent experiments on the intense laser–plasma interactions with applications to the particle acceleration, high energy particle production as well as the fast ignition concept.

Primary author: Dr KARGARIAN, Ameneh (Kharazmi University)

Co-authors: Dr HASANBEIGI, Ali (Kharazmi University); Prof. MEHDIAN, Hassan (Kharazmi University); Dr HAJISHARIFI, Kamal (Kharazmi University)

Presenter: Dr KARGARIAN, Ameneh (Kharazmi University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Plasma Physics

Contribution ID: **49** Type: **Poster Presentation**

Deposition of C, C₂, CH, CH₂ and CH₃ onto graphene: structures and structural changes of graphene

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Using energy minimization method the more stable structures of C₂, CH, CH₂ and CH₃ molecules and of defect-free graphene were found. For description of the interatomic potential we used Brenner interatomic potential [1], which is specifically parameterized for the carbon and hydrogencarbon systems. Then by the molecular dynamics method and using the same Brenner potential, computer modeling of deposition of C, C₂, CH, CH₂ and CH₃ particles onto defect-free graphene was carried out.
The results of computer simulations, the structures and the various structural changes of graphene caused by the deposition of carbon atoms and C₂, CH, CH₂ and CH₃ molecules are presented and discussed.

1. D.W. Brenner, O.A. Shenderova, J.A. Harrison, S.J. Stuart, B. Ni, S.B. Sinnot, J. Phys: Condens. Matter 14, 783 (2002).

Primary author: Mr STELMAKH, Vasiliy (Institute of Ion-Plasma and Laser Technologies)

Co-authors: Dr DZHURAKHALOV, Abdiravuf (Department of Mathematics and Computer Science, University of Antwerp); Dr YADGAROV, Ishmumin (Institute of Ion-Plasma and Laser Technologies)

Presenter: Mr STELMAKH, Vasiliy (Institute of Ion-Plasma and Laser Technologies)

Session Classification: Poster Session

Contribution ID: **50** Type: **Oral Presentation**

INVITED SPEAKER: Computational modeling of cosmic rays in the neighbourhood of the Sun

Monday, 11 July 2016 11:00 (30 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The heliosphere is defined as the plasmatic influence sphere of the Sun and may stretch far beyond the solar system. Cosmic rays, as charged particles with energy between 1 MeV and thousands of GeV, arriving from our own Galaxy and beyond, penetrate the heliosphere and encounter the solar wind and imbedded magnetic field so that when observed they contain useful information about the basic features of the heliosphere. In order to interpret these observations, measured on and close to the Earth and farther away by several space missions, and to gain understanding of the underlying physics, we need to simulate the heliosphere and the acceleration, propagation and transport of these cosmic rays with numerical models. These types of models vary from magnetohydrodynamic (MHD) based approaches for simulating the heliospheric geometry to using standard finite-difference numerical schemes to solve transport-type partial differential equations with a varying complexity. How these models have been developed locally to do internationally competitive research and as a major training tool for human capacity development will be discussed. How they are applied to various astrophysics, cosmic ray and heliospheric space physics issues with interesting examples will be illustrated.

Primary author: Prof. POTGIETER, Marius (North-West University)

Presenter: Prof. POTGIETER, Marius (North-West University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **51** Type: **Oral Presentation**

MORTICIA, A software package for determining optical surveillance system effectiveness.

Thursday, 14 July 2016 09:00 (20 minutes)

Abstract content
   (Max 300 words)
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Surveillance modelling in terms of the standard Detect, Recognise and Identify (DRI) thresholds remains a key requirement for determining the effectiveness of surveillance sensors. With readily available computational resources it has become feasible to perform statistically representative evaluations of the effectiveness of these sensors.A new capability for performing this Monte-Carlo type analysis is demonstrated in the MORTICIA (Monte-Carlo Optical Rendering for Theatre Investigations of Capability under the Influence of the Atmosphere) software package developed at the CSIR. This first generation open-source integrated software package is developed primarily in the Python programming language and aims to provide all the functionality required to perform statistical investigations of the effectiveness of optical surveillance systems in specific or generic deployment theatres. This includes modelling of the mathematical and physical processes that govern amongst other components of a surveillance system; a sensor's detector and optical components, a target and its background as well as the intervening atmospheric influences. In this paper we discuss integral aspects of the bespoke framework that are critical to the longevity of all subsequent modelling efforts. Additionally, some preliminary results in the form of target image simulations and sensor quality metrics are presented.

Primary author: Mr RAMKILOWAN, Ari (CSIR)

Co-author: Mr GRIFFITH, Derek (CSIR)

Presenter: Mr RAMKILOWAN, Ari (CSIR)

Session Classification: Parallel Track B

Contribution ID: **52** Type: **Oral Presentation**

First principles study of layered xLi₂MnO₃•(1-x)LiMO₂ (M = Mn, Ni, Co, etc.) cathode materials

Wednesday, 13 July 2016 15:40 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The demand for higher energy density lithium ion batteries makes Li-rich layered xLi₂MnO₃•(1-x)LiMO₂ (M = Mn, Ni, Co, etc.) among the most attractive candidates for future cathode materials. It drawn much attention recently as alternative cathode materials because of its high specific capacities > 280 mAh/g [1] when charged to over 4.6V. Unfortunately, xLi₂MnO₃•(1-x)LiMO₂ suffers some practical problems for commercial application, including 1) first cycle irreversible capacity loss associated with the elimination of oxide ion vacancies from the layered lattice, 2) limited performance at high rates associated with the insulating Li₂MnO₃ component and thick solid electrolyte interfacial (SEI) layer, 3) capacity fade after moderate cycling caused by interfacial stability, electrolyte oxidation, surface film formation and transition metal dissolution and 4) voltage fade during long cycling caused by structural instability and phase changes. To overcome these limitations, efforts, such as surface modification [2] and elemental doping [3] have been investigated by experimental and theoretical approaches. First principles density functional theory calculations have been used on Li-rich layered cathode materials [4] to elucidate and exemplify the relationship between structures, electronic, phase stability and electrochemical properties and play an important role in developing and optimizing new energy storage and conversion materials. In this study we are going to investigate structural, electrical and thermal properties of xLi₂MnO₃•(1-x)LiMO₂ using density functional theory (DFT) in the first principles calculations. Based on atomic scale understanding of those mechanisms, we will reveal some helpful methods to overcome the performance degradation problems in these cathode materials.

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[2] S-T. Myung etal., J. Phys. Chem. C, 2007, 111, 4061-4067

[3] M. Iftekhar, etal., J. Electrochem. Soc., 2014, 161(14), A2109-A2116

[4] T. Tamura etal., Modelling and Simulation in MSE, 2012, 20(4), 045006-1-045006-9

Primary author: Mr GELETO, Seid Mohammed (Jimma University, Jimma Institute of Technology, Ethiopia)

Co-author: Dr KEBEDE, Mesfin Abayneh (Council for Scientific and Industrial Research (CSIR), Pretoria, South Africa)

Presenters: Dr KEBEDE, Mesfin Abayneh (Council for Scientific and Industrial Research (CSIR), Pretoria, South Africa); Mr GELETO, Seid Mohammed (Jimma University, Jimma Institute of Technology, Ethiopia)

Session Classification: Parallel Track B

Contribution ID: **53** Type: **Oral Presentation**

INVITED SPEAKER: Modelling the progenitors and environments of stellar explosions

Wednesday, 13 July 2016 10:15 (30 minutes)

Abstract content
   (Max 300 words)
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Smoothed Particle Hydrodynamics (SPH) is a Lagrangian technique particularly suited to simulating hydrodynamical flows with arbitrary geometries. We briefly highlight the physics behind the method and its application to a wide range of problems in astrophysics. We then focus on 3D SPH models of the progenitors and environments of stellar explosions, with RS Ophiuchi, a symbiotic nova system consisting of a red giant and an accreting white dwarf which undergoes thermonuclear outbursts every 10-20 years, as the primary example. Our results show that the circumstellar outflow is highly asymmetric with evidence for a dense, equatorial component and bipolar ejecta morphology. The white dwarf is thought to be close to the Chandrasekhar mass making the system a likely Type Ia supernova progenitor. We discuss the origin and formation of the circumstellar structures in detail, and the observable spectroscopic and photometric signatures we expect from their collision with the explosive supernova ejecta.

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Co-authors: Prof. PODSIADLOWSKI, Philipp (Oxford University); Dr BOOTH, Richard (Oxford University)

Presenter: Dr MOHAMED, Shazrene (SAAO)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **54** Type: **Oral Presentation**

Device Simulation using Symmetric Smoothed Particle Hydrodynamics

Wednesday, 13 July 2016 11:15 (20 minutes)

Abstract content
   (Max 300 words)
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The real-space approach is widely used for electronic structure calculations. In particular, it is used for large systems, because a real-space mesh is suitable for large-scale parallel computing. The real-space approach also allows the capture of a clear physical image. For the simplest real-space implementation, the higher-order finite-difference method is used as a discretization technique. Besides, there are also meshfree methods as real-space implementations. These methods have an advantage in their non-uniform distribution of computation points, which also reduces computational costs.

As one of the meshfree technique, we have been studied Smoothed Particle Hydrodynamics (SPH) which is applied to the electronic structure calculation. SPH was originally developed for hydrodynamic problems, which deal with complex shapes, large deformations and free surfaces. It is a typical meshfree particle method, in which the system is represented by a finite set of arbitrarily distributed particles without using any mesh. However, SPH is known for its low accuracy. As one of alternatives, Symmetric Smoothed Particle Hydrodynamics (SSPH) is proposed. In this study, we have applied SSPH to the HEMT device simulation. In layered structures such as FET, the current density is mainly dependent on the electron mobility and the electronic field in the vicinity of the gate part, where both of them are recognized as a constant. With this approximation, the relation between the channel current and the gate applied voltage can be obtained by one dimensional calculation. Then, it is easier to confirm the device properties in the SSPH technique. This study evaluates the accuracy of SSPH for this typical electronic structure calculation. The results are then easily compared to the finite-difference method. In this paper, we will demonstrate some of practical electronic structure calculations using non-uniformly distributed particles.

Primary author: Prof. ZEMPO, Yasunari (Hosei University)

Co-authors: Mr KITAYAMA, Kiyoaki (Simulatio Corporation); Mr TOOGOSHI, Mitsuki (Hosei University)

Presenter: Prof. ZEMPO, Yasunari (Hosei University)

Session Classification: Parallel Track B

Contribution ID: **55** Type: **Poster Presentation**

Computational and theoretical study of Cd doped ZnO phase separation

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Cd and Zn are isoelectronic transition metals, and hence CdO alloying with ZnO could manifest interesting features infused CdO-ZnO structures. Importantly, Cd doping reduces the energy bandgap and results in a red-shift of absorption edge hence, one can envision varying the Cd doping concentration to tailor the electronic gaps to produce materials of interest for UV sensors, UV LEDs, UV protecting layers. Incorporation of Cd into ZnO produces a material with increased conductivity and increased carrier concentration versus the parent ZnO. In the present study, a direct correlation of structural and optical properties of Zn_{1-X}Cd_XO (0.55 ≤ X ≤ 0.85) has been developed both theoretically and computationally. Zn_{1-X}Cd_XO nanopowders synthesized via sol-gel route are used to compare the optical properties with computational calculations done using COMSOL MultiPhysics 5.2. The Zn_{1-X}Cd_XO nanopowder exhibits the coexistence of hexagonal ZnO and cubic CdO phase. The narrow energy gaps indicate that both hexagonal and cubic Zn_{1-X}Cd_XO systems have potential as material for solar energy applications. We give direct evidence for a chemical phase separation using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR).

Primary author: Mr JULE, LETA (UNIVERSITY OF THE FREE STATE)

Co-authors: Prof. DEJENE, Francis (University of the Free State); Dr RORO, Kittessa (CSIR-Energy center)

Presenter: Mr JULE, LETA (UNIVERSITY OF THE FREE STATE)

Session Classification: Poster Session

Contribution ID: **56** Type: **Oral Presentation**

Confining Boundary Conditions For Simulation of Electron-Ion Plasma by Antisymmetrized Wave Packet Molecular Dynamics

Wednesday, 13 July 2016 15:20 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

The method of Wave Packet Molecular dynamics is an approximate quantum method for numerical simulation of many-particle dynamics. In this method single electron wave functions are expanded in a set of floating Gaussian wave packets (WP). A trial many-body wave function is constructed depending on the quantum statistical properties of the simulated ensemble, for example for fermions (electrons) a single Slater determinant antisymmetrized product is usually used for each spin projection. The resulting equations of motion follow from the variational principle. In this work we study a system of electrons in a 3D confinement potential constructed from harmonic walls and a flat floor in each spatial direction.

The unlimited broadening of the Gaussian wave packets and underestimation of the electron-electron and electron-ion collision frequencies is known to be the major problems of the WPMD method [4] when applied to many-particle systems with homogeneous density, for example plasma systems. We show however that the method is able to excellently describe the thermodynamics of a confined fermionic system. The infinite WP broadening is directly related to the infinite statistical sum in an unconstrained system and does not appear in the confined system. For example, the nearest image boundary conditions guarantee the periodicity of expectation values but do not limit the number of allowed states in the simulated system.
We show that for the confined electron-ion system the AWPMD model does not suffer from the unlimited wave packet broadening problem and the electron wave packet parameters perform finite ergodic motion in the available system phase space. The implementation of the proposed model to simulation of the extended warm dense matter is presented.

Primary author: Dr VALUEV, Ilya (Kintech Lab Ltd.)

Co-author: Mr LAVRINENKO, Yaroslav (JIHT RAS)

Presenter: Dr VALUEV, Ilya (Kintech Lab Ltd.)

Session Classification: Parallel Track B

Track Classification: Quantum Many Body and Strongly Correlated Systems

Contribution ID: **57** Type: **Oral Presentation**

INVITED SPEAKER: The yielding transition in amorphous solids

Tuesday, 12 July 2016 14:30 (30 minutes)

**Abstract content
   (Max 300 words)
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Amorphous solids are ubiquitous in nature and among man made materials. Glasses, gels, and granular matter offer broad classes of examples. Many other soft materials, such as foams, emulsions, pastes, dense colloidal suspensions, biological assemblies such as the cytoskeleton in cells, and geophysical bodies such as the earth's crust, indicate the range and variety of matter in amorphous solid forms. Since many types of glasses, e. g. polymer glasses and metallic glasses, are used as structural materials, the mechanical behavior of glasses under application of external stresses is a very important characteristic to understand. In the context of both crystalline and amorphous solids, mechanical response is sought to be understood in terms of reversible, elastic response to applied stress, and irreversible, plastic deformations. In the context of crystalline solids, plasticity has been analyzed and understood as arising from the presence of dislocation defects in the crystal structure. In the case of amorphous solids, since the microscopic structure is disordered, there is no meaningful way in which defects analogous to dislocations can be identified. An aspect of the mechanical response that is of particular significance is yielding. From a theoretical point of view, much interest has also focused on whether one may understand yielding in amorphous solids as a non-equilibrium phase transition in a driven system. Many investigations have addressed plasticity, and the nature of yielding, in amorphous solids through atomistic computer simulations. A particular approach has been to consider amorphous solids subjected to large amplitude oscillatory strain in the limit of zero temperature and strain rates. Results from extensive simulations exploring the dependence of system size and amplitude of the cyclic deformation on the steady state of the deformed amorphous solids, and what the reveal about the nature of the yielding transition, will be discussed.

Primary author: Prof. SASTRY, Srikanth (Jawaharlal Nehru Centre for Advanced Scientific Research)

Co-authors: Mr PARMAR, Anshul Deep Singh (Jawaharlal Nehru Centre for Advanced Scientific Research); Dr LEISHANGTHEM, Premkumar (Jawaharlal Nehru Centre for Advanced Scientific Research)

Presenter: Prof. SASTRY, Srikanth (Jawaharlal Nehru Centre for Advanced Scientific Research)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **58** Type: **Oral Presentation**

A study on Quark-Gluon plasma equation of state using with finite quark mass

Tuesday, 12 July 2016 12:40 (20 minutes)

**Abstract content
   (Max 300 words)
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Special chars**

We study the QGP equation of state using finite quark mass with the finite size effect by taking into account of Multiple Reflection Expansion (MRE). The quark mass improves the calculation of free energy in the formation of QGP droplet. Finally, the model results provide QGP equation of state that matches well with the lattice results.

Primary author: Dr KUMAR, Yogesh (University of Delhi)

Co-author: Mr SETHY, P. K. (University of Delhi)

Presenter: Dr KUMAR, Yogesh (University of Delhi)

Session Classification: Parallel Track B

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **59** Type: **Oral Presentation**

Random Field Ising Models: Fractal Morphologies and their Implications

Tuesday, 12 July 2016 12:20 (20 minutes)

Abstract content
   (Max 300 words)
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We use a computationally efficient graph cut method to obtain ground state ($T = 0$) morphologies of the random field Ising model (RFIM) on (i) simple cubic (SC), (ii) body-centered cubic (BCC) and (iii) face-centered cubic (FCC) lattices. We determine the critical disorder strength Δ_c with high accuracy. For the SC, BCC and FCC lattices, $\Delta_c = 2.278 \pm 0.002, 3.316 \pm 0.002$ and 5.160 ± 0.002 respectively and are the most accurate estimates in the literature so far. The ground states states consist of correlated "domains" of up and down spins, analogous to those in phase ordering systems. The small-r behaviour of the correlation function exhibits a {\it cusp regime} characterized by a cusp exponent α signifying rough fractal interfaces. It is distinct for the three lattice types in the ferromagnetic phase, but identical in the paramagnetic phase. Our computations indicate that the activation energy for growth of a domain of size L obeys a power law $E_B(L) \sim L^{2-\alpha}$, and is consistent with theoretical predictions. Consequently, the barrier energy for a domain of size L is significantly different for the three lattice types. This observation emphasizes the crucial role played by the lattice structure on domain growth and relaxation in complex systems. The implications of ground state morphologies in diverse experimental systems, well represented by the RFIM, are also examined.

Related Papers:

1. Arunkumar Bupathy, Varsha Banerjee and Sanjay Puri, Physical Review E, 93, 012104 (2016).

2. Gaurav P. Shrivastav, Manoj Kumar, Varsha Banerjee and Sanjay Puri, Physical Review E, 90, 032140 (2014).

3. Gaurav P. Shrivastav, Siddharth Krishnamoorthy, Varsha Banerjee and Sanjay Puri, Europhysics Letters, 96, 36003 (2011).

Primary author: Prof. BANERJEE, Varsha (Indian Institute of Technology, New Delhi 110016, India)

Presenter: Prof. BANERJEE, Varsha (Indian Institute of Technology, New Delhi 110016, India)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **60** Type: **Poster Presentation**

The SAPBC method on local, non-cluster updates algorithms of Monte Carlo simulation: A study on more convergence of spin correlation at critical temperature

Monday, 11 July 2016 16:30 (1 hour)

**Abstract content
   (Max 300 words)
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Here, we work out the computational technique of Screw-Antisymmetric PeriodicBoundary condition (SAPBC Method) on local, non-cluster update algorithms of Isotropic nn square lattice Ising model of Monte Carlo Simulations as well. The SAPBC Method, actually, is an extended mixed method of Screw (helical) and Antisymmetric periodic boundary conditions beyond connection from of nearest neighbor spin of the main lattice to even far away block of the outer (foreign) neighbor spin arrays.In the project,Meanwhile of description of geometry exact details of method and way of spin interaction, have applied to critical slowing down in order to achieve more convergence of spin correlation at critical temperature. Actually, in general, at critical temperature algorithms performed by using SAPBC Method have faster correlation and much shorter autocorrelation time than algorithms performed by using PBC Method. We will also see that Autocorrelation function for the typewriter Metropolis algorithm was found to be zero at high temperatures. For low temperatures it fell to zero and stayed there. The SAPBC Method also confirms and consists with the law of the spatial correlation length with its dynamical critical exponent. Therefore, it can be used as a trenchant method applied to boundary conditions of Monte Carlo simulation problems extending on a variety of other models such as XY-Pots-Heisenberg model and also cluster algorithms such as Wolf, Swendsen-Wangas, Hoshen-Koppelman as well.

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Session Classification: Poster Session

Contribution ID: **61** Type: **Poster Presentation**

Development of software package for the computer simulation of the dynamic properties of dense ICF plasmas

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

At the present time the study of the dense ICF plasma properties is not only of fundamental interest, but it also has various important technological applications [1-2]. During design engineering of such plasma systems it is necessary to image complicated processes in dense plasma. In this connection the role of computer simulations equipped with visualization methods for analysis of processes in dense ICF plasma is increasingly important.
Scientific visualization is becoming a key ingredient of research, development, and discoveries in numerous fields of science and technology. Scientific visualization systems help not only to represent the results of calculations, but also to integrate and analyze the results of calculations and experiments accumulated earlier [3].
In this work we present a software package based on modern information technologies that allows rapid analysis and visualization of the properties of dense plasmas. We calculate dynamic properties (stopping power, relaxation time, penetration depth) of plasma by using the Coulomb Logarithm on the basis of the effective potentials taking into account quantum diffraction and screening effects at short and large distances, respectively. The system for visualization is constructed on the basis of the OPEN-GL and 3D MaxStudio, C# platforms.

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Session Classification: Poster Session

Track Classification: Plasma Physics

Contribution ID: **62** Type: **Oral Presentation**

Efficient parallelization of scientific computer codes: Two case studies using the PGAS programming model

Thursday, 14 July 2016 09:30 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Efficient implementation of numerical methods is one of the most important aspects of computational physics. Especially simulations that are computationally expensive or run for a long time benefit from the use of modern HPC systems. To fully exploit the potential of these systems, parallelization of the code is necessary. Developing a parallel code, however, is usually a difficult task for the developer.
The partitioned global address space (PGAS) approach is a programming model that promises to simplify the process of parallel programming as compared to the widely used MPI model.
In this study we have used unified parallel C (UPC), an extension to the C programming language that implements the PGAS paradigm, to evaluate the ease of development as well as the efficiency of this programming model for two different case studies representative for a wide variety of problems commonly found in computational physics applications:
On the one hand, we implemented a Godunov solver for the two dimensional Euler equations of gas dynamics. This case is a compute bound problem due to the Riemann solver needed to compute the flux at the cell interfaces but employs a fairly straight forward data structure.
On the other hand, we have investigated a sparse matrix vector multiplication (SPMV) problem resulting from solving the diffusion equation using cell-centered finite volumes. This problem uses a highly irregular mesh in order to allow for the simulation of complicated structures (e.g., the human heart). This case is memory bound and uses a non-trivial data structure.

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Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Fluid Dynamics

Contribution ID: **63** Type: **Poster Presentation**

Entanglement entropy of the Q ≥ 4 quantum Potts chain

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
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Special chars

The entanglement entropy, S, is an indicator of quantum correlations in the ground state of a many body quantum system. At a second-order quantum phase-transition point in one dimension S generally has a logarithmic singularity.
Here we investigate the Q-state quantum Potts chain for Q ≥ 4 and calculate S across the transition point. The density matrix renormalization group (DMRG) method was applied and a logarithmic divergence was found for the Q=4 at the second-order phase transition and finite jump of S for Q=6 & 8 at the first-order quantum phase transition. The jump of the entanglement entropy S is analytically calculated in leading order of Q and was found in good agreement with the DMRG results. Furthermore, the DMRG data are considered from several aspects in order to demonstrate that the DMRG method can be an appropriate technique for calculating the entanglement entropy at or around the phase transition.

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Session Classification: Poster Session

Contribution ID: **64** Type: **Oral Presentation**

Monte Carlo Computation of the Effective Sherman Function

Tuesday, 12 July 2016 10:00 (20 minutes)

Abstract content
   (Max 300 words)
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Mott polarimetry is used to determine the spin-polarization of electron beams in wide energy range (up to several MeV).

Azimuthal asymmetry (related to the Sherman function) in Mott scattering of a polarized electron beam is measured. As the measurement is performed on targets of finite thicknesses, the effective Sherman function has to be used, in which multiple interactions of the electron are accounted for. These effects cannot be calculated analytically and simulation tools must be used; experimental data covering wide range of scattering angles exist for a few energies only.

PEBSI Monte Carlo simulation was upgraded towards usefulness to compute the effective Sherman function. Description of Mott scattering was improved and polarization transfer in Møller scattering was included in the code.

Reliability of the simulation was proved by comparison with experimental data for a 100 keV polarized electron beam incident on 10 - 500 nm Au targets in the scattering angle range from 20 to 160 degrees; a good agreement was found.

The angular and energy distributions of scattered electrons were studied, both for all particles and based on interaction types which took place in the target. Electrons originating from Møller scattering were found to have important impact on the effective Sherman function if low energy particles are taken into account, leading to significant decrease of the analyzing power of the polarimeter. This effect can be avoided by imposing proper detector cuts on electron energy.

Optimizing the measurement comes down to choosing the optimal scattering angle and target thickness for electrons of a given energy. The angular dependence of the Sherman function was analyzed from this perspective. Simulation allows to exclude regions less suitable for measurement (e.g., where the Sherman function undergoes rapid changes with scattering angle). Dependence of the Sherman function on target thickness (for a given scattering angle) was also analyzed and compared to commonly used parameterizations.

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Session Classification: Parallel Track B

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **65** Type: **Oral Presentation**

Computation of ion potential for simulation of nonequilibrium warm dense matter

Wednesday, 13 July 2016 14:20 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

In this work we consider stationary nonequilibrium warm dense states where electrons move relative to the ions. A situation that is ubiquitous in dense plasmas including electron or ion beams, laser accelerated electrons, or ions penetrating a dense quantum plasma or a metal (ion stopping). For the computer simulation of ions in such system the ion-ion potential is starting point. To compute the effective dynamically screened ion potential a linear response description of the electrons via the Mermin dielectric function is utilized with electron-electron collisions taken into account in the relaxation time approximation [1, 2]. The ion potential strongly deviates from the static Yukawa potential [3] exhibiting the familiar oscillatory structure with attractive minima between ions. The results of the investigation show the importance of finite temperature effects even when the electron thermal energy is lower than the Fermi energy. Finally, we obtain the minimal electron streaming velocity for which attraction between ions occurs. The observed effects should be of high relevance for transport under warm dense matter conditions, in particular for laser-matter interaction, electron-ion temperature equilibration and for stopping power. The dynamically screened effective potential can be directly used for MD simulations of classical ions on the background of streaming quantum electrons as discussed in Ref. [4]. This allows to obtain first principle static and dynamic results for the ion component, including the range of strong ion coupling.

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Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Plasma Physics

Contribution ID: **66** Type: **Oral Presentation**

Screened interaction potentials between compound particles for simulation of complex plasmas

Wednesday, 13 July 2016 14:40 (20 minutes)

Abstract content
   (Max 300 words)
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Effective interaction potentials are widely used in computer modeling in such areas as plasma physics, condensed matter physics, physics of colloidal systems, as well as nanotechnology. Usually, one of the plasma components is ideal or weakly coupled, whereas the other component (consisting of relatively inert particles) creates a strongly coupled subsystem on the background of mobile weakly coupled particles. In this case strongly correlated relatively inert particles can be investigated via effective interparticle interaction potentials, where initially screening provided by mobile weakly coupled particles (electrons), whereas many-body effects due to strongly coupled species included naturally in simulations such as molecular dynamics or Monte-Carlo. In this work it is shown that the method of multipole expansion allows to easily find interaction potentials between compound particles screened by weakly coupled component of plasma even without spherical symmetry, if we know the effect of the medium on the potential of individual particles comprising compound particles [1]. Obtained screened potential was used for molecular dynamics simulation of a 2D charged dust system taking into account the effect of the induced dipole moment of a dust particle [2, 3]. As it is known, in gas discharge the dust particle and ions focused by the dust grain can be considered as a one compound particle with non-zero dipole moment. Elongated dust particles can also have an induced dipole moment due to charge separation in the external electric field.

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Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Plasma Physics

Contribution ID: **67** Type: **Poster Presentation**

The Introduction of Heterogeneous Computing Platforms into the ATLAS Trigger at CERN

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
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The ATLAS detector at CERN is undergoing upgrades with a view to running at maximum design luminosity in 2022. The increase in luminosity implies either an increased data production rate, or decreased signal-to-noise ratio, or both concurrently. The luminosity increase therefore necessitates an upgrade of existing computing platforms, specifically in the ATLAS Trigger system. To address this problem, the GPU Demonstrator team at CERN is conducting research regarding the integration of Graphics Processing Units (GPU) into the ATLAS Trigger server farm. The ATLAS dectector and its associated processing server farms, like the other detectors in the Large Hadron Collider (LHC), were conceived and implemented before general-purpose processing with GPU (GPGPU) was a viable option. As a result, the detector infrastructure (instrumentation, front-end hardware, software analysis packages) must be adapted, where possible, for parallelism in order to gain from the move into heterogeneous computing platforms. This paper describes some of the problems associated with this adaptation and their potential solutions.

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Session Classification: Poster Session

Contribution ID: **68** Type: **Oral Presentation**

Entropic Multi-Relaxation Time Lattice Boltzmann Model for Complex Flows

Thursday, 14 July 2016 09:50 (20 minutes)

Abstract content
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Entropic lattice Boltzmann methods (ELBM) were introduced to overcome the stability issues of lattice Boltzmann models for high Reynolds number turbulent flows. However, to date their validity has been investigated for only simple flows due to the lack of appropriate boundary conditions. We present an extension of entropic multi-relaxation time lattice Boltzmann models to complex flows in three dimensions. We study in detail the setup of a simplified internal combustion engine with a valve/piston arrangement. This arrangement allows us to probe the non-trivial interactions between various flow features such as jet break-up, jet-wall interaction, formation and break-up of large vortical structures among others in a comparison to high-order spectral element DNS simulations and experimental data. Moreover, we show that the implicit subgrid features of the entropic lattice Boltzmann method can be utilized to further reduce the grid sizes and the computational costs, providing an alternative to modern modeling approaches such as Large-Eddy Simulations (LES) for complex flows.

Further, exploiting the stability properties of ELBM, those models are employed in combination with a novel multi-domain, grid refinement algorithm allowing for an increased accuracy. The numerical scheme is validated using standard benchmarks such as the turbulent channel flow for Re=180,...,590 (based on the friction velocity) and the flow past a sphere at Re=10000. After validation it is applied to full two-way coupled fluid-structure interaction simulations of self-propelled swimmers in three dimensions, yielding insight into the fundamental mechanisms of propulsion occurring in nature.

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Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Fluid Dynamics

Contribution ID: **69** Type: **Oral Presentation**

Textured superhydrophobic surfaces: Reducing contact time of an impinging drop

Thursday, 14 July 2016 10:30 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
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Discovery and understanding of novel mechanisms of drop repellence from hydrophobic and superhydrophobic surfaces is of profound interest in many applications including self-cleaning, water resistance, anti-icing etc. The recent surge of interest on this topic [Bird et al., Nature 2013, Liu et al., Nature Physics 2014, Nature communications 2015, Schutzius et al., Nature 2015] has been predominantly experimental in nature. Apart from the demanding process of surface fabrication and coating, these investigations provide little insights into the associated flow phenomena (especially inside the droplet) mainly due to the hierarchy of scales involved in surface texture - from millimeter to sub-micron scale.

We present here an entropic lattice Boltzmann model for multiphase flows that is capable of qualitatively and quantitatively capturing the flow physics involved in such droplet wall interactions, especially in presence of complex surface texturing. Apart from thorough validation and analysis (including contact time, droplet shapes and energy budget analysis) of droplet wall interactions, we propose novel surface textures that are capable of reducing the contact time of the droplet with the surface. These novel surface structures are then validated with experiments thus demonstrating the predictive capabilities of the underlying simulation technique.

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Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Fluid Dynamics

Contribution ID: **70** Type: **Oral Presentation**

Finite element model of a calibration chamber

Tuesday, 12 July 2016 12:20 (20 minutes)

**Abstract content
   (Max 300 words)
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A calibration chamber is a test tool in which the dc electric field strength and the air ion density created by Corona wires are both controlled. Positive Corona effect is modeled using Kaptzov's assumption and the driven equations are the coupled Poisson-Continuity equations. The FEM of the wire-to-plane configuration is validated using experimental and numerical results found in literature. Then the actual geometry of the calibration chamber, with both Corona and isolating grids is modeled and found in perfect agreement with the theory used for Multi Wire Proportional Chambers developed for Nuclear Physics.

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Session Classification: Parallel Track B

Contribution ID: **71** Type: **Oral Presentation**

On formation of bubble structure near the island of inversion

Tuesday, 12 July 2016 11:40 (20 minutes)

Abstract content
   (Max 300 words)
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Depletion of the central density or formation of a hollow structure (Bubble) drew a lot of interest both from the theorists [1-3] as well as from the experimentalists [4,5] due to its conflicting nature vis-a-vis the property of saturation of the nuclear force. One can expect gross deviation from density saturation for finite Fermi systems in which single particle spectrum is discrete instead of a continuum. The formation of shells changes drastically for exotic nuclei having large isospins. As a result new properties of nuclei manifest in this region.

`It is generally believed that non-occupation of s-states of exotic nuclei leads to central depressio`

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Session Classification: Parallel Track B

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **72** Type: **Oral Presentation**

High Performance Memory Efficient Finite Difference Time Domain Algorithms for Large Meshes

Thursday, 14 July 2016 09:20 (20 minutes)

Abstract content
   (Max 300 words)
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The Finite Difference Time Domain (FDTD) method is widely used in modern computational electrodynamics. Its traditional implementation is a Yee scheme assuming second order explicit synchronous mesh update and its performance is memory-bound. To overcome this limit thre appear memory efficient approaches, for example, new classes of Locally Recursive Nonlocally Asyncronous (LRnLA) algorithms for explicit stencils of different orders are regularily proposed.

LRnLA is based on a representation of the problem by a space-time dependency graph and its recursive decomposition into subgraphs.
Depending on computer architecture, the decompositions are organized in space-time shapes maximally preserving data locality, i.e. being conformal to the memory hierarchy of the computer.
The LRnLA algorithms are suitable for processing large spatial meshes, since, unlike in the traditional synchronous mesh update, their efficiency (number of processed mesh cells per unit time) does not drastically drop with growing total mesh size.

The main difference between the algorithms of LRnLA family is the focus on various types of parallelism and memory subsystem hierarchy. This way, all current classes may be advantageous in different conditions.
We are testing various approaches to implement LRnLA algorithms for FDTD code on CPU architectures, including many-core clusters. The aim is to efficiently utilize CPU hierarchy and types of parallelism with the use of LRnLA algorithms of different classes. In this work the results of several current implementations are presented. We show tests of performance dependency on problem size on different computer archtectures. We demonstrate that it is possible to drastically increase operational intensity of the FDTD code implementation and to shift finite-difference simulation closer to compute-bound domain.

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Session Classification: Parallel Track B

Contribution ID: **73** Type: **Oral Presentation**

Computational study of nonlinear spectroscopy including saturated absorption and four wave mixing in two and multi-level atoms

Tuesday, 12 July 2016 15:40 (20 minutes)

Abstract content
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We report on the study of two and multi-level atoms interacting with multiple laser beams. The semi-classical approach is used to describe the system in which the atoms are treated quantum mechanically via the density matrix operator, while the laser beams are treated classically using Maxwell's equations.
We present results of a two level atom interacting with single and multiple laser beams and demonstrate Rabi oscillations between the levels. The effects of laser modulation on the dynamics of the atom (atomic populations and coherence) are examined by solving the optical Bloch equations. Plots of the density matrix elements as a function of time are presented for various parameters such as laser intensity, detuning, modulation etc. In addition phase-space plots and Fourier analysis of the density matrix elements are provided.
The atomic polarization, estimated from the coherence terms of the density matrix elements, is used in the numerical solution of Maxwell's equations to determine the behavior of the laser beams as they propagate through the atomic ensemble. The effects, of saturation and hole-burning, are demonstrated in the case of two counter propagating beams with one strong beam and the other being very weak.
The above work is extended to include four-wave-mixing in four level atoms in a diamond configuration. Two counter propagating beams of different wavelengths drive the atoms from a ground state|1> to an excited state |3> via an intermediate state |2>. The atoms then decay back to the ground state via another intermediate state |4> resulting in the generation of two additional correlated photon beams. The intermediate state |4> has a substructure allowing for an uncertainty in the precise decay path. The characteristics of these additional photons are studied.

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Session Classification: Parallel Track B

Contribution ID: **74** Type: **Oral Presentation**

Effect of Mo alloying elements on Ni silicides formation

Wednesday, 13 July 2016 12:35 (20 minutes)

Abstract content
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Abstract
A small amount of Mo as alloying element with Ni thin film on Si(100) substrate can greatly enhanced the thermal stability of nickel monosilicide formed by rapid thermal annealing (RTA). The study was carried out using X-ray diffraction (XRD), Raman spectroscopy, Rutherford backscattering spectrometry (RBS), Scanning Electronic Microscopy (SEM), Energy Dispersive X-ray (EDX) and four probe sheet Resistance (Rs). One possible reason for the enhanced NiSi thermal stability is attributed to the presence of Mo alloying element at the grain boundaries and interfaces of NiSi film, leading to the increase in the interfacial energy change. The increase of the activation energy for the NiSi2 nucleation and the thermal stability of NiSi compound are studied.

Keywords: alloying elements, NiSi stability, XRD, Raman spectroscopy, RBS, SEM, EDX, Rs.

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Session Classification: Parallel Track B

Contribution ID: **75** Type: **Oral Presentation**

Improved Maximum Entropy Method applied to Real-time Time-Dependent Density Functional Theory

Tuesday, 12 July 2016 16:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Time-dependent density functional theory (TDDFT) is a powerful tool for analyzing optical properties of medium-to-large sized molecule. We employ a real-time and real-space technique to solve the time-dependent Kohn-Sham equations. In our procedure to calculate optical properties, we use the time-series data, namely the dynamic dipole moment, from whose Fourier transform (FT) optical properties are calculated in a usual technique. The spectral resolution depends on the length of the dipole moment. To obtain the good resolution, the computational cost is quite expensive.

To solve this difficulty, we apply Maximum entropy method (MEM) to the spectral analysis of time-dependent dipole moments of molecules. As a new improved MEM, we proposed to use the concatenated data set made from several-times repeated raw data together with the phase to avoid the side effect of the artificial periodicity. With this improvement, we have successively obtained the much better spectral resolution of the target peak. In the analysis of optical properties, we are interested in the lower energy peak, corresponding to the band gap area. Basically, to obtain the high resolution of spectrum, MEM requires less number of time steps compared to that of FT, and it is widely used for the analysis of the natural phenomenon of the long period such as seismic waves and solar cycles, obtaining a fairly good resolution and accuracy even with a short time series data. Thus, this improvement will make a further advantage of MEM.

We applied this technique to the spectral analysis of the TDDFT dipole moment of typical some molecules such as oligo-fluorene, benzene and other materials. The results show the higher resolution and the emphasized peak near the band gap without being affected by the artificial periodicity. The characteristic features of this technique will be presented including the further possibilities of improvements.

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Presenter: Mr TOOGOSHI, Mitsuki (Hosei University)

Session Classification: Parallel Track B

Contribution ID: **76** Type: **Oral Presentation**

Simulating the synchrotron emission from Active Galactic Nuclei jets with grid based relativistic hydrodynamic code

Monday, 11 July 2016 14:00 (20 minutes)

**Abstract content
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Grid based numerical hydrodynamic codes have been used to simulate the evolution of a variety of astrophysical environments, ranging from stellar winds to accretion disks in binary systems. These simulations can be used as valuable tools in the correlation between theoretical models and observational data. In this study a grid based relativistic hydrodynamic simulation is created, using the freely available numerical code PLUTO ver 4.2, to study possible causes of variability in AGN. The code uses shock-capturing Godunov-type methods to solve the fluid dynamic conservation equations on a structured mesh grid. To simulate the production of a jet similar to those observed in AGN a three dimensional static grid was created containing 512x512x512 computational cells. A uniform background medium was assigned to this grid, while a nozzle was defined on the z=0 boundary to inject a pressure matched relativistic jet, with Γ=10 (v=0.995c), into the medium. The simulation showed the formation of a central collimated relativistic beam along with a surrounding cocoon region. In addition, a post-processing emission modelling code is being developed, in order to determine the emission produced by such a relativistic jet. The emission model utilizes the data produced by the hydrodynamic code in order to calculate intensity maps based of the synchrotron self absorption model, which has been previously applied in analytical models. The emission code specifically takes into account the effects produced by the relativistic motion of the emitting regions which can lead to effects such as the Doppler boosting observed in blazars. Synchrotron based emission models can be applied to other astrophysical objects such as X-ray binary systems which means that the application of the emission code can be adapted to other studies.

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Presenter: Mr VAN DER WESTHUIZEN, Izak (University of the Free State)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **77** Type: **Oral Presentation**

INVITED SPEAKER: Massively parallel Monte Carlo simulations with population annealing

Tuesday, 12 July 2016 10:00 (30 minutes)

Abstract content
   (Max 300 words)
Formatting &
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While Moore's law of semiconductors has ensured for over forty years that the next generation of processors works significantly faster than the current one, for the last ten years or so serial code has not seen any speed-up from new hardware which, instead, achieves performance improvements only from packing more and more cores onto a single die. As a consequence, scientists working with computer simulations need to move away from intrinsically serial algorithms to find new approaches that can make good use of potentially millions of computational cores. Population annealing, that was initially suggested by Hukushima and Iba [1] and more recently was studied systematically by Machta [2], is a sequential Monte Carlo scheme that is potentially able to make use of such highly parallel computational resources. Additionally, it promises to allow for the accelerated simulation of systems with complex free-energy landscapes, much alike to the much more well known replica-exchange or parallel tempering approach. The relative performance with respect to such more traditional techniques, the appropriate choice of population sizes temperature protocols and other parameters, the estimation of statistical and systematic errors and many other features, however, are essentially uncharted territory. Here, we use a systematic comparison of population annealing to Metropolis as well as parallel tempering simulations for the Ising model to gauge the potential of this new approach, and we suggest a range of heuristics for its application in more general circumstances.

[1] K. Hukushima and Y. Iba, in The Monte Carlo Method in the Physical Sciences, Vol. 690 of American Institute of Physics Conference Series, edited by J. E. Gubernatis (2003), pp. 200–206.

[2] J. Machta, Phys. Rev. E 82, 026704 (2010).

Primary author: Dr WEIGEL, Martin (Coventry University)

Presenter: Dr WEIGEL, Martin (Coventry University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **78** Type: **Oral Presentation**

Simulating cosmic ray modulation over a solar cycle

Monday, 11 July 2016 15:00 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

This work studies modulation of galactic cosmic rays in the heliosphere by using a state-of-the-art, time dependent numerical modulation model to calculate cosmic ray transport inside the heliosphere. Results will be compared to different spacecraft observations, in particular observations from Voyager 1 and 2. It will be shown that when incorporating the most recent theoretical advances of the transport coefficients in such a model, which solve the Parker transport equation, that the model result in compatibility with spacecraft observations on a global scale.

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Co-authors: Prof. POTGIETER, Marius (NWU); Prof. FERREIRA, Stefan (NWU)

Presenter: Mr MOHLOLO, Timothy (North West University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **80** Type: **Poster Presentation**

Plasmon excitation in OLED with the DTMaxwell code

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Verification of DTmaxwell code by simulation of OLED with corrugated cathode.

We have developed a Finite Difference Time Domain (FDTD) code DTMaxwell for General Purpose Graphical Processing Units (GPGPU) architecture with the use of Locally Recursive non-Locally Asynchronous (LRnLA) algorithms DiamondTorre [1].
Its performance was tested and good results were achieved on a desktop computer, as well as on many-GPU supercomputer.
This time, as a practical illustration of the advantages of our approach, we solve a large-scale problem of Surface Plasmon Polaritons (SPPs) excitation. SPP is excited by a point source placed in a close proximity (less than 100 nm) to a two-dimensional periodically corrugated metallic (silver) surface with a pitch of 400 nm. This problem is essential for simulation of SPP losses in both Organic and inorganic Light Emitting Diodes (OLEDs and LEDs) and design of OLEDs/LEDs with improved outcoupling efficiency. The simulation in question requires large meshes (>100GB of data) because of the large spatial decay lengths of SPPs (up to several tens of microns), whereas the mesh step should be kept sufficiently small (less than 5 nm) in order to account for strong field gradients at the dielectric-metal interfaces. Using this problem as a test case, we evaluate our code on different computers and compare to the previous solutions of such problem.

[1] Perepelkina A.Yu., Levchenko V. D., DiamondTorre Algorithm for High-Performance Wave Modeling // Keldysh Institute Preprints (2015) No. 18. 20 p.
[2] Sergei Belousov et al, Outcoupling efficiency of OLEDs with 2D periodical corrugation at the cathode, 2016 J. Phys. D: Appl. Phys. 49 085102

Primary author: PEREPELKINA, Anastasia (Keldysh Institute of Applied Mathematics)

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Presenter: PEREPELKINA, Anastasia (Keldysh Institute of Applied Mathematics)

Session Classification: Poster Session

Contribution ID: **81** Type: **Poster Presentation**

Ab initio studies of isolated boron substitutional defects in graphane

Monday, 11 July 2016 16:30 (1 hour)

**Abstract content
   (Max 300 words)
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Special chars**

We have systematically studied the energetics, electronic and structural properties of various configurations of B substituting CH pair located on a single hexagonal ring of graphane using first-principles calculations. The number of substitutional defects considered ranges from one to six B dopants and isomers are formed by choosing different doping sites for the same number of dopants. Based on the formation energy analysis, we found that isomers differ significantly in relative stability. For instance, meta and para isomers (B defects surrounded by C atoms) are energetically favourable, whereas the formation of B - B bond (ortho) is unstable. The density of states show a transition from semiconductor to metallic with increasing number of B dopants. This modulation of band gap, to a great extent, is an indication that B-doped graphane systems can be exploited for band gap-related applications.

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Co-author: Prof. CHETTY, Nithaya (University of Pretoria)

Presenter: Dr MAPASHA, Edwin (University of Pretoria)

Session Classification: Poster Session

Contribution ID: **82** Type: **Poster Presentation**

Development of Plasma Fluid Model in Microwave Rocket Supported by Magnetic Field

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Discrete plasma were obtained at atmospheric pressure in the discharge experiments for a microwave rocket. However, the microwave plasma transitioned from discrete to diffusive patterns with decrease in an ambient gas pressure, while increasing the propagation speed of the ionization front. Thrust performance of a microwave rocket was degenerated at low pressures because of the high-speed propagation of the ionization front and the smaller energy-absorption rate of the plasma. An external magnetic field is applied to the breakdown volume to suppress the propagation speed of the plasma and increase the energy-absorption rate due to an electron cyclotron resonance heating. The one-dimensional particle-in-cell with Monte Carlo Collision simulation (PIC-MCC) is conducted to trace motions of the electron and ion under the magnetic field. The shock wave driven by gas heating is enhanced inside the rocket nozzle by applying the magnetic field, which results in improvement of the thrust performance at low pressures. However, the multi-dimensional breakdown dynamics is not discussed under the magnetic field using the fully kinetic model because of a huge computational load. The fluid model of the plasma transport under the magnetic field is constructed to reduce the computational load for the multi-dimensional simulation. The transport coefficients of the charged particles are evaluated based on swarm simulations using the PIC-MCC code, which are introduced into the fluid model to keep consistency between the fluid and particle models. The plasma pattern of the fluid model is in good agreement with that of the PIC-MCC model at 0.5 atm. Multi-dimensionality of the breakdown plasma is examined using the fluid simulation, and the discrete plasma structure is induced by reflections of the incident microwave from the overcritical plasma.

Primary author: Dr TAKAHASHI, Masayuki (The University of Tokyo)

Presenter: Dr TAKAHASHI, Masayuki (The University of Tokyo)

Session Classification: Poster Session

Track Classification: Plasma Physics

Contribution ID: **83** Type: **Poster Presentation**

Structure-dynamic approach of nanoionics. Theory and computer exploration.

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
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Special chars

We have put forward structure-dynamic approach (SDA) [1,2] for computer modeling of the dynamic behavior of solide electrolyte (SE) nanosystems with fast ionic transport (FIT) and for the further development of nanoionics [3]. Theoretical system of SDA includes a structural layered 1D-hopping atomic model of the region with a non-uniform potential landscape, a method of "hidden" variables (excess concentrations of mobile ions induced by external influence on crystallographic planes), a physico-mathematical formalism (based on the principle of a detailed balance and the kinetic equation in the form of the particle conservation law), and a method of uniform effective field. A new notion - the Maxwell displacement current on a potential barrier and the essential definition of effective electrostatic field (corrected uniform Gauss field) [2,4] are given. The computer exploration (in the "Wolfram Mathematica" package) of the ion-transport and dielectric-polarization processes of model SE nanosystems are analyzed, and such modes of solid state ionics as "near constant loss" and Johnsher's universal dynamic response (the power law of the real part of frequency dependent conductivity) are explained. The results of this work will help to overcome certain problems, which hinder development of the perspective matrix devices with FIT at the nanoscale level, such as memory cells with SE-programmed metallization, supercapacitors of micron sizes with a record high density of energy and charge, field effect transistors with SE gates, sensors and memristors.

[1] A.L. Despotuli, A.V. Andreeva. Nano and Microsystem Technique. 9 (2012) 16.
[2] A.L. Despotuli, A.V. Andreeva. Ionics 21 (2015) 459.
[3] A.L. Despotuli, V.I. Nikolaichik. Solid State Ionics. 60 (1993) 275.
[4] A.L. Despotuli, A.V. Andreeva. Ionics 22 (2016) DOI 10.1007/s11581-016-1668-3

Primary author: Dr DESPOTULI, Alexandr (Institute of Microelectronics Technology and High Purity Materials RAS)

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Presenters: Dr DESPOTULI, Alexandr (Institute of Microelectronics Technology and High Purity Materials RAS); Prof. ANDREEVA, Alexandra (Institute of Microelectronics Technology and High Purity Materials RAS)

Session Classification: Poster Session

Contribution ID: **84** Type: **Poster Presentation**

Density function theory study of TiO₂ Brookite (100), (101) and (210) surfaces doped with ruthenium (Ru) and Calcium (Ca) for application in dye sensitized solar cell

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
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Special chars

Since the discovery of water photolysis on a TiO₂ electrode by Fujishima and Honda in 1972, TiO₂ has attracted extensive attention as an ideal photocatalytic material because of its excellent properties such as high activity, good stability, nontoxicity and low cost. Thus, it has been widely used in the fields of renewable energy and ecological environmental protection. However, as a wide band gap oxide semiconductor (Eg = 3.14 eV), brookite TiO₂ can only show photocatalytic activity under UV light irradiation (lambda; < 387.5 nm) that accounts for only a small portion of solar energy (approximately 5%), in contrast to visible light for a major part of solar energy (approximately 45%). Therefore, how to effectively utilize sunlight is the most challenging subject for the extensive application of TiO₂ as a photocatalyst. Because of the unique d electronic configuration and spectral characteristics of transition metals, transition metal doping is one of the most effective approaches to extend the absorption edge of TiO₂ to visible light region, which either inserts a new band into the original band gap or modifies the conduction band (CB) or valence band (VB), improving the photocatalytic activity of TiO₂ to some degree. In this work, the structural optimizations, band structure, and electronic density of states of doped and un-doped TiO₂ (100), (101) and (210) surfaces were performed by using the first principles calculations based on DFT using a plane-wave pseudopotential method. The generalized gradient approximation (GGA) was used in the scheme of Perdew-Burke-Ernzerhof (PBE) to describe the exchange-correlation functional. All calculations were carried out with CASTEP (Cambridge Sequential Total Energy Package) code in Materials Studio of Accelrys Inc.

Primary author: Mr DIMA, Ratshilumela Steve (University of venda)

Co-authors: Dr MALUTA, Nnditshedzeni Eric (University of Venda); Dr MAPHANGA, Rapela (University of Limpopo); Prof. SANKARAN, V (University of Venda)

Presenter: Mr DIMA, Ratshilumela Steve (University of venda)

Session Classification: Poster Session

Contribution ID: **85** Type: **Oral Presentation**

A fast - Monte Carlo toolkit on GPU for treatment plan dose recalculation in proton therapy

Tuesday, 12 July 2016 11:20 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

An innovative cancer treatment technique called particle therapy is emerging. It consists of irradiating solid tumors with beams of protons or ions. Thanks to the peaked shape, called Bragg Peak, of charged particles energy deposition in matter it is possible to concentrate the dose on the tumor and to reduce the damage to healthy tissues. This selectivity in energy release involves the necessity of an high level of accuracy in the calculation and optimization of the beams to be sent to the patient. This computation is performed by Treatment Planning System (TPS).
Nowadays one of the major issues related to the TPS in particle therapy is the large CPU time needed. We developed a software toolkit (FRED) for reducing dose recalculation time by exploiting Graphics Processing Units (GPU) hardware. Thanks to their high parallelization capability, GPUs significantly reduce the computation time, up to factor ˜100 respect to a standard CPU running software. The transport of proton beams in the patient is accurately described through Monte Carlo methods. Physical processes reproduced are: Multiple Coulomb Scattering (double and triple Gaussian models), energy straggling and nuclear interactions of protons with the main nuclei composing the biological tissues. FRED toolkit does not rely on the water equivalent translation of tissues, but exploits the Computed Tomography anatomical information by reconstructing and simulating the atomic composition of each crossed tissue. FRED can be used as an efficient tool for dose recalculation, on the day of the treatment. In fact it can provide in about one minute on standard hardware the dose map obtained combining the treatment plan, earlier computed by the TPS, and the current patient anatomic arrangement.
Assessment results of FRED performance in terms of accuracy and calculation time in comparison to commercial TPS and the full MC approach (Fluka) will be presented.

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Session Classification: Parallel Track B

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **86** Type: **Oral Presentation**

Solar cell performance of AgInS₂ materials from DFT and GW/BSE calculations

Tuesday, 12 July 2016 15:40 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Ternary compounds chalcogenides are among the potential semiconductor materials for solar photovoltaic cell applications. We present first principle calculations of the electronic and the optical properties of the chalcopyrite and orthorhombic phase of AgInS₂ , using the GW many body perturbation theory built on top of the hybrid functional HSE06 orbitals. For an accurate description of the absorption spectra, we account for the quasihole-quasielectron interaction by solving the Bethe Selpeter equation (BSE). Based on the bandgaps and absorption coefficient from these calculations, we predicted the solar cell efficiency of these compounds. It is found that these compounds have GW bandgaps in the range of the experimental values and their solar cell efficiency is estimated at more than 20%.

Primary author: Dr DONGHO NGUIMDO, G.M. (University of the Witwatersrand)

Co-author: Prof. JOUBERT, Daniel (University of the Witwatersrand)

Presenter: Dr DONGHO NGUIMDO, G.M. (University of the Witwatersrand)

Session Classification: Parallel Track B

Contribution ID: **87** Type: **Poster Presentation**

Systematic study of the anomolous feature of actinide region

Tuesday, 12 July 2016 16:30 (1 hour)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

We work on systematic study of the anomolous feature of actinide regions. In this study, we analyze the experimental data for actinide nuclei. The calculation is agreed well with the expected results from the theoretical model.

Primary author: Mrs JAIN, Poonam (Amity University, noida)

Co-author: Dr GOEL, Alpana (Amity University)

Presenter: Mrs JAIN, Poonam (Amity University, noida)

Session Classification: Poster Session

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **88** Type: **Oral Presentation**

Computational Studies of Ru and Sr-doped anatase TiO₂ on three low index surfaces for application on DSSCs

Tuesday, 12 July 2016 15:00 (20 minutes)

Abstract content
   (Max 300 words)
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Titanium dioxide (TiO₂) is considered very close to an ideal semiconductor for photocatalysis because of its high stability, low cost and safety toward both humans and the environment. Therefore doping TiO₂ with different element has attracted researchers as the most important way of improving the width of the band structure and the adsorption on different wavelength region in order to improve the efficiency of catalytic activity and conversion. In this work we are focusing on how to enhance the efficiency of DSSCs using the density function theory (DFT) technique. We firstly vary the distance between the anatase TiO₂ surface and the added atom Ru. Each Ru-doped anatase TiO₂ (100) and (110) surfaces were optimized in order to get the total energies and structure to see the effect of the separation between the defect and the surface of TiO₂. Secondly we take the system that gives the least energy and calculate their properties, i.e. density of state (DOS), Band gaps and optical. Our results shows that the band gaps of pure anatase TiO₂ (100) and (110) surfaces are greater than the band gaps of Ru-doped anatase TiO₂ (100) and (110) surfaces. Which means that the Ru-doped anatase TiO₂ (100) and (110) surfaces have the high photocatalytic activity than pure TiO₂, because the larger the band gap, the greater the difficulty for the valence electrons to jump to the conduction band, thus explains poor electricity conductivity of non-metals.

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Presenter: Mr NEMUDZIVHADI, Hulisani (University of venda)

Session Classification: Parallel Track B

Track Classification: Computational Physics

Contribution ID: **89** Type: **Poster Presentation**

Asymmetric Shock Wave Generation in Microwave Rocket Using Magnetic Field

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

A beamed-energy propulsion is a novel launching system to reduce the launch cost of small satellites. The flight demonstrations of a beamed-energy vehicle were performed, which indicated that the beam-riding flight became unstable and deviated from the incident beam line, because the enough feedback forces for bringing the vehicle position closer to center of the beam line cannot be maintained during the repetitive-pulses flight. The flight simulations revealed that decoupling between the angular moment and the centering-feedback force is important on maintaining the beam-riding flight; however, such decoupling method was not proposed in past studies. It is necessary to induce the asymmetric shock wave inside the microwave-rocket nozzle for obtaining the lateral- and angular-feedback forces. The asymmetric shock wave can be generated inside the nozzle if spatial distribution of the gas heating by beam irradiations is not uniform. Hence, an external magnetic field is applied to the rocket nozzle in order to obtain non-uniformity of the gas heating. The gas heating is locally enhanced by the electron cyclotron resonance (ECR) heating under the magnetic field. The energy-absorption rate is evaluated under the magnetic field using a fully kinetic model of the plasma transports coupled with an electromagnetic wave propagation. The shock wave propagation inside the nozzle is reproduced using the computational fluid dynamics code based on databases of the energy-absorption rate obtained by the particle simulation. The asymmetric shock wave is obtained by controlling the ECR region inside the nozzle, and the lateral- and angular-feedback forces are induced because of interactions between the shock wave and the nozzle wall. A spatial distribution of the external magnetic field is designed to decouple the lateral-feedback force from the angular moment for keeping the beam-riding flight.

Primary author: Dr TAKAHASHI, Masayuki (The University of Tokyo)

Presenter: Dr TAKAHASHI, Masayuki (The University of Tokyo)

Session Classification: Poster Session

Track Classification: Plasma Physics

Contribution ID: **90** Type: **Oral Presentation**

Bound states and decays in Relativistic Quantum Mechanics.

Tuesday, 12 July 2016 12:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
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The numerical aspects of the solution of a bound state problem in relativistic quantum mechanics are considered and the completely covariant formulation of the problem is first presented. The systems with a general central potential are quantized and the wave equation for the eigenstates given by 16-components spinor, is deduced in a spherical basis. Because of the symmetries the spectral problem reduces to the solution of a singular boundary value problem of the fourth order. It is shown how Padé approximants can help or directly substitute the integration of the system. It is also shown how to deal with the addition of a perturbation term representing the spin-spin interaction.
The calculation of the hyperfine levels and decays of hydrogenic atoms, the determination of the meson masses and the widths of radiative decays of bottomonium states are finally described showing the excellent agreement with experimental data. (Refs: J. Phys. A 38 (2005) 1345–1370; J. Phys. A 39 (2006) 15207–15223; Phys. Rev. D 87, 034021 (2013); J. Phys. B 48 (2015) 085002 (9pp); arXiv:1604.08043 (2016)).

Primary author: GIACHETTI, Riccardo (Physics Department, University of Florence, Italy)

Presenter: GIACHETTI, Riccardo (Physics Department, University of Florence, Italy)

Session Classification: Parallel Track B

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **91** Type: **Poster Presentation**

Fractal - Scaling approaches in Radar and Radio Physics

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
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Currently the inadequacy of conventional physical models is clearly felt. Revolutionary steps which consist in transfer of integer measure signals obtained by a system to the fractional measure space and following calling of scaling ratios allow to bring absolutely new ideas and methods into conventional areas of classical radio physics and radio electronics and to get results rather unexpected for practice which are however physically valid. Fundamental issues concerning the application of fractal theory, fractional operators and scaling effects in radio location, radio engineering and radio physics are considered in this report. Multiple examples of such approach utilization in different directions of science and engineering are presented. Essential discrepancies of this fundamental direction and classical ways of development are shown basing on the problems of radio location, antenna systems, detectors and processing of multidimensional signals. Mathematical and physical problems arising from using the global fractal-scaling method proposed by the author and existing method of fractional operators are considered. The author develops and strengthens his ideas that the new “fractal” dimension must be firmly introduced into science and engineering at that not to an auxiliary role but as the fundamental clarifying factor. The fractal radio physics, fractal radio engineering and fractal radio location which are peculiar radio sciences inspired with the spirit and ideas of classical radio physics and radio engineering are fundamentally new directions. Here one need to combine physics, mathematics, engineering and see a new physic-mathematical problem in a technical issue and do practical conclusions for engineering from solving such a problem. Introduction of fractals, scaling effects and fractional operators may imply the radio electronics future since all the previous and present radio electronics is based exceptionally (and only!) on the theory of integral-valued functions and does not take into account the fractional measure in the informational theory.

Primary author: Prof. POTAPOV, Alexander (V.A.Kotel’nikov Institute of Radio Engineering and Electronics, Russian Academy of Sciences)

Presenter: Prof. POTAPOV, Alexander (V.A.Kotel’nikov Institute of Radio Engineering and Electronics, Russian Academy of Sciences)

Session Classification: Poster Session

Contribution ID: **92** Type: **Oral Presentation**

Large Scale Fully Kinetic 3D PIC Simulation for the Awake Collaboration

Wednesday, 13 July 2016 11:55 (20 minutes)

Abstract content
   (Max 300 words)
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The AWAKE collaboration proposes to use the beam generated by CERN's SPS to drive plasma wakefield acceleration and generate electrons in the TeV regime.
There have been extensive numerical investigations into the proposed setups using a lot of different methods and techniques. Nonetheless, a fully kinetic 3D simulation of the whole process has not yet been implemented, mainly due to the immense computational resources required for it. There are, however, several processes and instabilities which are not present in, e.g. cylindrically symmetrical simulations. Carefully chosen parameter ranges and setup parameters made sure that these processes will not affect the validity of the results. In order to verify these assumptions and to do a direct comparison between different theoretical models we prepared the current experimental setup using the particle-in-cell (PIC) code PSC.
We secured the necessary resources on the SuperMUC petascale system in Munich. The setup consists of a 30cm long ion beam traversing a 10m long plasma channel. The plasma wakefield will trigger a longitudinal instability, called self-modulation-instability (SMI), seeded by a large density gradient at the front of the beam. The SMI will then result in micro-bunching of the ion beam which will in turn lead too non-linear growth of the wakefield. An electron witness beam enters the wakefield via side-injection and is accelerated. A resolution of 130 points per plasma wavelength is necessary. The full simulation uses a moving window approach and consists of about 22 billion cells containing more than 66 billion quasi-particles running for about 2 million timesteps. Using a large fraction of the SuperMUC system, this simulation still takes several weeks to complete and produces about 300TB of data.
We describe the necessary software modifications needed to achieve a reasonable well scaling PIC solution to this problem as well as technical details and pitfalls we encountered.

Primary author: Mr MOSCHUERING, Nils (LMU Munich)

Co-authors: Prof. RUHL, Hartmut (LMU Munich); Dr LOTOV, Konstantin (Budker Institute of Nuclear Physics Novosibirsk)

Presenter: Mr MOSCHUERING, Nils (LMU Munich)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Plasma Physics

Contribution ID: **93** Type: **Oral Presentation**

Electric field effects on the ionization cluster size distribution (ICSD) using the GEANT4 Monte Carlo toolkit.

Monday, 11 July 2016 11:40 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

In nanodosimetry, Monte Carlo procedures are used to study the physical characteristics of charged particles used in the irradiation of cancerous tumors (in particular the DNA) by conducting simulations in condensed matter. A property of relevance in this investigation is the so called "track structure" of ionising particle tracks which is characterized by nanodosimetric parameters related to the initial chemical/biological effects of radiation to DNA. To benchmark these calculations, ionisation experiments in low density gases (e.g. propane) with similar ionisation characteristics to those of water or DNA are used to measure the nanodosimetric parameters (e.g. ICSD). The gas is introduced in a low pressure chamber with an extraction aperture and an electric field is applied to aid in the extraction of the resulting ions. The ions are produced by the interaction of the particle under investigation with the chamber gas. The ions are extracted and guided to an ion counting detector. The amount of ions counted is related to the type and energy of the particle and also the physical characteristics of the chamber gas.

Simulations of protons (0.1 – 10.0 MeV) in water vapor have shown increases of up to 17% in the ICSD in an electric field of 60 V/cm which is not expected and this presents challenges in the measurement of ICSD. Results on further investigations of this effect using alpha particles and carbon ions also show this increase and will be presented.

Electric field effects on the measurement of nanodosimetric parameters should be accounted for in order to compensate for the increase in ICSD, in order to correctly predict the initial damage to DNA.

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Presenter: Mr NGCEZU, Sonwabile (University of the Witwatersrand)

Session Classification: Parallel Track B

Contribution ID: **94** Type: **Oral Presentation**

Finding motifs in DNA and protein sequences using set match

Monday, 11 July 2016 12:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Background: Gene selection affects many biological traits that influence diseases. Accurately finding genes that influence traits of interest is very important as isolating such genes is useful in diagnosis and drug development. An important process in gene identification is isolation of motifs or short sequences of amino acids. These motifs lead to finding relationships among genes.

Results: This paper proposes using both exact match and expectation maximization string searches to find motifs in genes. String matching techniques are useful in finding motifs. A new string matching approach that combines Boyer-Moore and Expectation-Maximization is recommended after implementing and analysis of some of the classical methods. Motifs components were placed in sets rather than exact strings. The method improved motif identification of MBD found in human hemoglobin that are preserved but have some differences.

Conclusions: The problem of string matching with application to Bioinformatics and Genomics was studied. Implementation of the simple match, Knuth-Morris-Pratt, and Boyer-Moore methods shows that the Boyer-Moore method is the most efficient. To enable this efficient method be more applicable to genomic motif finding, a preprocessing phase that uses expectation-maximization and creates sets of equally likely residues is recommended.

Primary author: Mr CHIRWA, Robert (University of Louisville)

Presenter: Mr CHIRWA, Robert (University of Louisville)

Session Classification: Parallel Track B

Track Classification: Computational Biology

Contribution ID: **95** Type: **Oral Presentation**

Understanding the role of the subtstrate in off-lattice simulations of graphene growth on copper

Monday, 11 July 2016 12:40 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Chemical vapour deposition (CVD) growth of graphene on copper has been identified as the most promising route for scalable synthesis of graphene. It is important to understand the fundamental surface growth mechanisms in order to optimise material quality, but detailed in situ imaging of growth in CVD is extremely difficult. Comparison of post-growth experimental data with dynamic simulations of growth can overcome this problem.

Experimental observations of partial-coverage graphene grown on copper foils with well-defined crystallographic microstructure [e.g. (111), (100) and (210) grains] indicate clearly that the surface orientation affects the growth rate, island size distribution (ISD) and orientation of graphene islands [NR Wilson, Nano Research 6.2 (2013): 99-112]. Ab inito simulation cannot reach length scales relevant to these phenomena, and it would be challenging to use such methods even to address interaction of growing graphene with the local symmetry of the crystalline substrate.

In this work we introduce a minimal off-lattice model which captures variations in growth rate, island orientation and ISD between different low index copper faces. We compare our simulation data to available experimental results, in particular finding similar graphene orientations for the different low index Cu faces. Our model is also capable of exploring the effect of mismatch, thermal expansion and surface disorder.

Primary author: Mr ENSTONE, Gwilym (University of Warwick)

Presenter: Mr ENSTONE, Gwilym (University of Warwick)

Session Classification: Parallel Track B

Contribution ID: **96** Type: **Oral Presentation**

Structural determination and electronic properties of one-dimensional Te crystals encapsulated inside carbon nanotubes

Wednesday, 13 July 2016 11:55 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

We use the ab initio random structure searching (AIRSS) method to determine the geometries of one-dimensional (1D) nanowires formed by encapsulating Te atoms inside single-walled carbon nanotubes (SWCNT). Particular attention is given to narrow SWCNTs (NSWCNTs) with diameters between 5 and 11 Aring;, since chemical interactions between such NSWCNTs and the encapsulated Te atoms are, in principle, more likely to occur than in SWCNTs with larger diameters. We show that there is a clear preference for the confined Te atoms to form 1D nanowires with helical symmetry. Also, despite the small diameters of the NSWCNTs studied, we show that chemical interactions between the encapsulated nanowires and the NSWCNTs do not play a crucial role in determining the geometries of the most energetically favourable structures. The calculated structural parameters of the encapsulated nanowires are in excellent agreement with the structures synthesised in our experiments. A comparison between our theoretically predicted and experimentally measured electronic and spectroscopic properties shows that our combined theoretical-experimental approach allows for a very precise characterisation of such systems.

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Session Classification: Parallel Track B

Contribution ID: **97** Type: **Oral Presentation**

Particle simulations on the GPU using the Blaze-DEM code

Thursday, 14 July 2016 09:40 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Numerical simulation of particulate materials is required in many industrial processes with applications ranging from ball mills in mining to powder mixers in pharmaceuticals. While the discrete element method (DEM) has become the defacto standard for numerical simulation of particulate materials , the large computational cost associated with the method limits the number of particles that can be simulated in a realistic time frame on a typical computer to less than a million. Simulations of millions of particles are only possible on expensive clusters which are typically not accessible to the majority of users. However, the computational architecture plays a significant role on the performance that can be realized. In the last few years the trend of increasing Central Processing Unit (CPU) clock speed resulting in more computations being performed in the same time period has stopped due to the physical limits on the materials used in the manufacturing of computer hardware. While computational power still scales with Moore's Law, this scaling is now achieved through increasing the number of computing cores on a single chip as opposed to make a single core faster. Leading this evolution from multi core to many core processing chips is the Graphical Processor Unit (GPU) that can perform billions arithmetic operations in parallel (7.52 TFLOPS). In this paper we present the GPU based code Blaze-DEM that allows for tens of millions of particles to be simulated on a single pc. We will look at the GPU specific algorithms for DEM as well some experimental and simulation results for industrial processes such as silos , ball mills and pulp lifters.

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Co-author: Dr WILKE, Daniel (UP)

Presenter: Dr GOVENDER, Nicolin (CSIR/UJ)

Session Classification: Parallel Track B

Contribution ID: **98** Type: **Oral Presentation**

Molecular dynamics studies of Schottky and Frenkel defects in cubic boron nitride

Tuesday, 12 July 2016 16:00 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

Schottky and Frenkel defect energies in boron nitride are studied using the classical molecular dynamics. Tersoff potentials are used to enlighten the boron-nitrogen, boron-boron and nitrogen-nitrogen interactions in the bulk and defect structures. The formulation uses the NVT Evans ensemble to obtain the various defect energies. Boron and nitrogen vacancy defect energies relative to bulk boron nitride total energies are used to get more insight on cubic boron nitride as a strong material. The nature of Schottky and Frenkel defects in this material are discussed.

Primary author: Dr MOSUANG, Thuto (University of Limpopo)

Presenter: Dr MOSUANG, Thuto (University of Limpopo)

Session Classification: Parallel Track B

Contribution ID: **99** Type: **Poster Presentation**

Analysis of temperature dependent thermopower of iron chalcogenide superconductors

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The newly discovered class of Fe-based chalcogenide superconductors is attracting worldwide attention due to their applicative potential with transition temperatures above 50 K and very high upper critical fields as well as for fundamental studies of superconducting mechanisms. In present study, thermopower (S) of FeSe_{0.5}Te_{0.5} bulk sample was investigated. Anomalous behavior was observed in thermopower with the absolute value of S reaches as high as 11 mu;V/K (at 300 K). The complicated temperature dependence of thermopower is an indication of change in majority charge carriers in the low temperature regime. Our theoretical results indicate that the variation of thermopower with temperature can be explained by conventional electron diffusion and phonon drag mechanisms.

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Session Classification: Poster Session

Contribution ID: **100** Type: **Poster Presentation**

Pressure-induced structural phase transition of zinc oxide

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
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The high-pressure technique is useful to understand physical properties because the technique can directly control bond length and phase transition. As a general trend, the pressure-induced phase transition causes an increase of coordination number with a drastic change of their physical properties. Here, we attempt to explore the pressure-induced phase transition from the sixfold-coordinated NaCl structure (B1) to the eightfold-coordinated CsCl structure (B2) in CdO by applying an effective interionic interaction potential, which includes the long range Coulomb, van der Waals (vdW) interaction and the short-range repulsive interaction upto second-neighbor ions within the Hafemeister and Flygare approach. Assuming that both the ions are polarizable, the Slater-Kirkwood variational method is employed to estimate the vdW coefficients for CdO. The estimated value of the phase transition pressure (Pt) and vast volume discontinuity in pressure volume phase diagram identifies the structural phase transition from B1 to B2 structure.

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Session Classification: Poster Session

Contribution ID: **101** Type: **Oral Presentation**

Computational modelling of sulfides minerals

Tuesday, 12 July 2016 14:20 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

Sulfides minerals are an important group of minerals. They are many found in nature and of industrial significant because they serve as a source of various metal pyrites. We used Dmol, Vienna Ab-initio Simulation Package (VASP) and Density Functional Tight-Binding (DFTB+) modules to study electronic and structural properties of pyrite, marcasite, as well as phases and surface of cobalt binary sulfides structures. We parameterized cobalt sulfide (CoS) using DFTB+ and calculated different structures of cobalt sulfides and showed good structural properties with other calculations. We used DFTB+ method to calculate both ab-initio and molecular dynamic simulations for large structures of FeS₂ at high temperatures of 1500 K. The structural properties such as lattice parameters, bulk modulus and elastic constants in FeS₂ were in good agreement with previous other calculations and experimental results. The DFTB+ molecular dynamics calculation of FeS₂ showed the Radial Distribution Function (RDF), Density of States (DOS) and decreased the band gap at high temperature. Using DFTB+ we alloyed iron sulfide with oxygen and showed the band gap increased.

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Co-author: Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Dr LETSOALO, Thabo (University of Limpopo)

Session Classification: Parallel Track B

Contribution ID: **102** Type: **Oral Presentation**

Discontinuous transition in a suppressed random cluster growth model

Tuesday, 12 July 2016 15:20 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
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Percolation is known to be a second order continuous phase transition and applied in a variety of problems ranging from physical sciences, mathematics as well as to computer science and social problems. However, recently Achlioptas demonstrated a discontinuous percolation transition by adopting a stochastic rule for cluster growth on a fully connected graph. An enormous attention has been generated to relook into the problem in recent time. A suppressed cluster growth model on the 2D square lattice is developed and its critical properties are studied. The lattice is initially populated with certain concentration &rho and all finite clusters are identified. These finite clusters are then allowed to grow with a time dependent probability which depend on the ratio of the mass of a cluster to the mass of the largest cluster present at that time. The growth process follows all the criteria of the original percolation model and cluster statistics is collected at the end of the growth process. As the initial seed concentration is varied continuously, say from 0.50 to 0.01, the model displays a crossover from continuous phase transition at high &rho value to a discontinuous transition at low &rho value without passing through a sharp tricritical point. The discontinuous transition is identified as a first order percolation transition.

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Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **103** Type: **Poster Presentation**

Radiative Molecular Dynamics: First concept

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
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Radiative molecular dynamics is capable of modeling the details of N interacting radiating relativistic charged particles. As is well-known, molecular dynamics simulations have a computational load that scales as N*N. We present a new concept, for which the computational load scales linearly with N. The linear scaling with N is achieved by subdividing the computational domain of each particle into near and far-field domains. In the near fields domain of each particle an M*(M-1) problem with M«N is solved, where M is the number of particles in the near field domain of the particle under consideration. With the help of the BBGKY hierarchy of reduced probability functions it is explained under which conditions our radiative molecular dynamics model promises to be accurate.

Primary author: Mr HERZING, Christian (LMU)

Co-author: Prof. RUHL, Hartmut (LMU)

Presenters: Mr HERZING, Christian (LMU); Prof. RUHL, Hartmut (LMU)

Session Classification: Poster Session

Track Classification: Plasma Physics

Contribution ID: **104** Type: **Poster Presentation**

First-principles study of Fe impurities in MgO

Tuesday, 12 July 2016 16:30 (1 hour)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

Transition metal doped dilute magnetic semiconductors offer a number of interesting possibilities in the pursuit of spinelectronic materials which exploit career spin and its associated magnetic moment in addition to its charge, for novel solid-state device applications. We performed a first-principles investigation on the electronic and magnetic properties of Fe as an isolated substitutional impurity defect in MgO, considering the effects of charge state, spin state and Fermi level position. The calculations were carried out within density functional theory, using the plane-wave pseudopotential method and the generalized gradient approximation plus the effective Hubbard U approach. Our results indicate that there is a metastable intermediate spin state for the impurity in the doubly positive charge state, in addition to the high and low spin states. Further, we predict that the positively charged impurity orders ferromagnetically in p-type MgO, with a significantly high magnetic stabilization energy of 21 meV and a large magnetic moment desirable for novel spintronic applications.

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Co-author: Prof. LOMBARDI, Enrico (UNISA)

Presenter: Dr MOLEPO, Mahlaga (University of South Africa)

Session Classification: Poster Session

Contribution ID: **105** Type: **Oral Presentation**

Investigation of Two-dimensional lattice thermal transport in graphene using phonon scattering mechanism

Wednesday, 13 July 2016 15:00 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

The extremely high thermal conductivity observed in graphene and its applications as thermal management material in future nanoelectronic circuits have rattracted significant attention and motivated for theoretical investigations on thermal conductivity. Two-dimensional lattice thermal transport in graphene is investigated using phonon scattering mechanism. The in-plane lattice thermal conductivity is demonstrated by incorporating the scattering of phonons with defects, grain boundaries, electrons, and Umklapp phonon scatterings in the model Hamiltonian. The lattice thermal conductivity dominates in graphene is an artifact of Umklapp phonon scattering mechanism around room temperatures. A very high phonon mean free path of the order of few hundred nanometers is estimated which seems to be responsible for observed high thermal conductivity. It is experienced that heat transport by phonons and scattering rates are substantially different in a quasi-two-dimensional system such as graphene compared to the three-dimensional bulk crystals. The obtained results are in good agreement with the available experimental data and reflect the two-dimensional nature of phonon transport in grapheme which is dominated by phonon scatterings.

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Presenter: Prof. CHOUDHARY, Kamal Kumar (Indian Military Academy, Dehradun - 248007 (UK), India)

Session Classification: Parallel Track B

Contribution ID: **106** Type: **Oral Presentation**

Stability and magnetic interaction of embedded Fe clusters in diamond

Tuesday, 12 July 2016 15:20 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
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The origin of high Curie temperature ferromagnetism in dilute magnetic semiconductors and oxides has often been attributed to clustering and crystallographic phase separation of magnetic atoms, which has a detrimental impact on the properties of the host material for target applications. To determine the effect of clustering on the magnetic properties of transition metal doped diamond, we present Density Functional Theory calculations on the stability and magnetic interactions of embedded Fe atoms by considering various possible cluster configurations. We find that Fe atoms have a strong tendency to form clusters in diamond, with Fe-C-Fe cluster configurations being energetically more favourable than simple Fe-Fe pair formation. Similarly, the cluster binding energy and ferromagnetic stabilization energy is dependent on the arrangement of Fe atoms within the cluster, with the ferromagnetic state being favoured for smaller clusters containing up to three Fe atoms. Since studies of magnetic interactions of transition metal atoms in semiconductors has mostly focused on single doping assuming homogenous distribution, these results present important implications to the understanding of magnetic ordering of dopants in diamond and other dilute magnetic semiconductors.

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Co-author: Prof. LOMBARDI, Enrico (University of South Africa)

Presenter: Dr BENECHA, Evans (University of South Africa)

Session Classification: Parallel Track B

Contribution ID: **107** Type: **Oral Presentation**

Particle Remapping with Deformation Tracking for Collisionless Fluid Flow

Monday, 11 July 2016 14:40 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

Particle-in-Cell methods are a popular approach to numerically modelling collisionless fluids for plasma physics and cosmology applications. However, these methods are known to suffer from particle noise that reduces the accuracy of the obtained solutions for long time evolutions. Phase-space remapping can reduce these errors, but is computationally expensive when applied globally. We will discuss a local remapping strategy that tracks the deformation of the particles from their initial coordinates and only remaps in regions of the flow where the particle stretching has become too large.

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Co-authors: PHIL, Colella (LBNL); BRIAN, Van Straalen (LBNL)

Presenter: ANDREW, Myers (LBNL)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **108** Type: **Oral Presentation**

PLENARY: Recurrent flows: The clockwork behind turbulence

Thursday, 14 July 2016 08:00 (1 hour)

Abstract content
   (Max 300 words)
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Turbulence is THE unsolved problem of classical physics. For almost two centuries we have had the equations that describe the motion of fluids, but partial differential equations are in principle infinite-dimensional dynamical systems, numerical simulations track millions of computational degrees of freedom - what are we to make out of all this data? Well, in the world of moderate Reynolds numbers, everyday turbulence of fluids flowing across planes and down pipes a velvet revolution is taking place. Experiments are almost as detailed as the numerical simulations, DNS is yielding exact numerical solutions that one dared not dream about a decade ago, and dynamical systems visualization of turbulent fluid's state space geometry is unexpectedly elegant. What emerges is a picture of low-Reynolds turbulence as a walk among a set of unstable invariant solutions.

We shall take you on a tour of this newly breached, hitherto inaccessible territory. The talk is aimed at anyone who had ever wondered why - if no cloud is ever seen twice - we know a cloud when we see one? And how do we turn that into computation? Now, once you get home, you can do it yourself: all results and numerical software are available through our group's collaborative e-book ChaosBook.org and open-source Computational Fluid Dynamics codes available on Channelflow.org and Openpipeflow.org.

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Presenter: Prof. CVITANOVIC, Predrag (Georgia Tech)

Session Classification: Plenary

Track Classification: Fluid Dynamics

Contribution ID: **109** Type: **Oral Presentation**

Networks of Spiking Neurons for the Control of Movement

Monday, 11 July 2016 14:00 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

The human brain has about 85 billion neurons, of which about 15 billion are in the cortex. These cortical neurons fire action potentials (spikes) at a rate of about 10 Hz – about 150 billion spikes per second. This activity underlies our sensory perceptions, thoughts, decisions, and actions. One of the central problems of systems neuroscience is that of decoding these spatial and temporal patterns of neural activity, to interpret them and assign meaning to them. In recent years much progress has been made in decoding activity of neurons in the motor cortex, an output area of the brain that controls movement through its projection to muscles via the spinal cord. Recent and continuing increases in the experimental ability to simultaneously track the dynamics of many constituent elements within these networks present a challenge to theorists: to provide conceptual frameworks and develop mathematical and numerical tools for the analysis of such vast data. The subject poses great challenges, as the systems are noisy and the available information is incomplete.

Theoretical efforts to construct models that capture the underlying relationship between neural activity and movement have exploited Generalized Linear Models based on the exponential family of probability distributions; the Bernoulli and Poisson distributions are relevant to the case of networks of elements that communicate via pulses, such as neurons. From a theoretical point of view, we continue to make progress in our understanding of the neural code. From a practical point of view, our increasing ability to extract motor information from these signals has allowed us to translate neural activity into commands to control computer cursors and robotic manipulators. The potential of this approach to restore motor behavior in severely handicapped patients motivates pioneering interdisciplinary research in Brain Machine Interfaces (BMIs), an area at the frontier of systems neuroscience.

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Presenter: Prof. SOLLA, Sara A. (Northwestern University)

Session Classification: Parallel Track B

Track Classification: Computational Biology

Contribution ID: **110** Type: **Poster Presentation**

Computing radiation parameters for atoms and multicharged ions within relativistic energy approach: Advanced code

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

We present the results of computing radiation (transitions probabilities, oscillator strengths etc) parameters of atoms and ions on the basis of advanced computer code within relativistic approach to calculation of the in spectra of multicharged ions, based on energy approach and relativistic many-body perturbation theory [1]. The key feature of the presented basis theory is an implementation of the optimized one-particle representation [3] into the frames of the S-matrix energy formalism. It provides a consistent approach to minimize gauge-non-invariant contributions to gf values and thus it make our approach significantly more advantagable in comparison with standard Hartree-Fock (HF), Dirac-Fock (DF) methods. We have carried out calculating energies, radiation and Auger transition probabilities for Li- and Zn-like ions (Z=10-70). It is checked that all gf values, obtained within our approach in different photon propagator gauges (Coulomb, Babushkin, Landau) are practically equal. As example in table below we list our results (REA) on gf of the 4s2(1S0)- 4s4p (1P01) transition in some Ne-Zn-like ions. For comparison the HF, DF, DF (with fitting to experiment) and model potential (MP) calculation data are presented too (look [1] and refs. therein).
[1] A.V.Glushkov, L.N.Ivanov, E.P.Ivanova, in Autoionization Phenomena in Atoms (Moscow State Univ.) 55 (1986); L.N.Ivanov, E.P.Ivanova, E.V.Aglitsky, Phys.Rep. 166, 315 (1988); A.V. Glushkov, L.N. Ivanov, Phys.Lett.A 170, 33 (1992); O.Yu. Khetselius, Int.J.Quant.Chem.109, 3330 (2009).

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Co-authors: Mrs ANTOSHKINA, Olga (Odessa State University-OSENU); Prof. KHETSELIUS, Olga (Odessa State University-OSENU); Mr ZAICHKO, Pavel (Odessa State University-Odessa); Ms KULAKLI, Tatyana (Odessa State University-OSENU); Mr BUYADZHI, Vasily (Odessa State University-OSENU)

Presenter: Mr BUYADZHI, Vasily (Odessa State University-OSENU)

Session Classification: Poster Session

Contribution ID: **111** Type: **Poster Presentation**

Non-linear dynamics of quantum and laser systems with elements of a chaos: Advanced computational code

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The work is devoted to chaos-geometric modelling, analysis, prediction of a chaotic dynamics of quantum-generator and laser systems. The computing code includes a set of a analysis methods such as correlation integral, fractal analysis, average mutual information, surrogate data, false nearest neighbours algorithms, the Lyapunov's exponents, Kolmogorov entropy scheme, spectral methods, new prediction (predicted trajectories, neural network etc) ones s [1]. We present the results of studying chaos generation in the low- and high-attractor time dynamics of semiconductor GaAs/GaAlAs laser system with delayed feedback. It has been numerically shown that firstly arising periodic states of the system transform into individual chaotic states and then global chaotic attractor with a chaos generation scenario through period-doubling bifurcation, which is significantly modified. There are computed original data on the Lyapunov's exponents (+, +), correlation (chaos – 2.2; hyperchaos – 7.4), embedding (correspondingly 4 and 8), Kaplan-York (correspondingly 1.8 and 7.1) dimensions, the Kolmogorov entropy (0.15-0.71). We present the results of the complete numerical investigation of a chaos generation in the low- and high-attractor time dynamics of the erbium one-ring fibre laser (EDFL, 20.9mV strength, lambda;= 1550.190nm) with the control parameters: the modulation frequency f and dc bias voltage of the electro-optical modulator. It has been numerically shown that there are realized the one-period (f = 75MHz, V = 10V; f = 60MHz, V = 4V), two-period (f = 68 MHz, V = 10V; f = 60MHz, V = 6V) and chaotic (f = 64MHz, V = 10 V and f=60MHz, V=10V) regimes in dependence on f, V values. All invariants have been computed too.
[1] A.V.Glushkov et al, in: Adv. in Neural Networks, Fuzzy Systems and Artificial Intelligence, Ser.: Recent Adv. in Computer Engineering, Ed. J.Balicki.(Gdansk, WSEAS Pub.). 21, 143 (2014); Sensor Electr. and Microsyst.Techn. 11(4), 43 (2014).

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Presenter: Mr BUYADZHI, Vasily (Odessa State University-OSENU)

Session Classification: Poster Session

Contribution ID: **112** Type: **Poster Presentation**

Chaos-dynamical computational method of forecasting evolutionary dynamics of environmental systems: Atmospheric pollutants dynamics

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The aim of our present study is (1) to present new computational complex approach to studying and forecasting dynamics of environmental systems, based on using non-linear analysis and chaos theory methods such as wavelet and fractal formalism, mutual information, correlation integral, false nearest neighbour algorithm, Lyapunov exponent's analysis, surrogate data, stochastic propagators method, memory, Green's functions approach; (2) to identify the concentration space-temporary evolution dynamics for CO₂, CO, NO₂, SO₂ in the atmosphere of industrial cities (Amsterdam, Gdansk and Odessa) during the 2003-2009 (3) to present new prediction computational model to forecasting the atmospheric pollutants evolutionary dynamics (new "Geomath" technology). The simple way to identify the chaos in time series is as follows:
(1) To determine time delays, the concept of mutual information is used;
(2) To determine attractor dimensions, it is used the correlation integral method and false nearest neighbours algorithm;
(3) To refine the data, we use surrogate data sets;
(4) we evaluate the Lyapunov's exponents.
All dynamical and topological invariants have been computed. We develop a new non-linear prediction method and compare the predicted values with both last one hundred data and nine hundred random data in the series. As an example, the real and predicted concentrations of CO₂, CO, NO₂, SO₂ etc in Gdansk, Amsterdam and Odessa regions are presented. Our results can be considered as first examples of quite satisfactory short-range forecasts for the air pollutants.

1. Glushkov A.V., Methods of a chaos theory to complex systems, 2012, Odessa, Astroprint ;
2. Glushkov A., Khokhlov V., Loboda N.,Bunyakova Y., 2008. Atm. Env. 42: 7284.
3. Glushkov A.V., Khetselius O., BunyakovaY., 2009. Proc.of 8th Int. Carbon Dioxide Conference.-Jena (Germany) T2; Lanfredi, M., Machhiato, M., 1997. Europhys. Lett. 40: 589. Chelani, A.B., 2005. Int. J. Environ. Stud. 62: 181

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Presenter: Mr BUYADZHI, Vasily (Odessa State University-OSENU)

Session Classification: Poster Session

Contribution ID: **113** Type: **Poster Presentation**

Computational Code in Atomic and Nuclear quantum optics: computing multiphoton and autoionization resonances in a strong external electromagnetic field

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

We present an advanced combined relativistic operator perturbation theory (PT) and energy approach [1,2] computational approach to dynamics of finite Fermi systems (heavy atoms, nuclei, molecules) in an intense laser field. Numerical results of computing multi-photon resonance and ionization profile in Na, Cs, Ba atoms are listed [2]. New data on the DC, AC strong field Stark resonances, multi-photon and autoionization resonances, ionization profiles for a few heavy atoms (Eu, Tm, Gd, U) are presented. The direct interaction of super intense laser fields in the optical frequency domain with nuclei is studied within the operator PT and the relativistic mean-field (plus Dirac-Woods-Saxon) model [2,3]. T A nuclear dynamic (AC) Stark shift of low-lying nuclear states due to off-resonant excitation by laser field (Γ˜1025-1035 W/cm²) is studied and is described within the operator perturbation theory and the relativistic mean-field (RMF) model for the nucleus [2]. We list results of AC Stark shifts of single proton states in nuclei ¹⁶O, ¹⁶⁸Er, ¹⁷¹Yb and compared these data with known results [3]. Shifts of several keV are reached at intensities of roughly 10³⁴ for ¹⁶O, ⁵⁷Fe and 10³² W/cm² for heavier nuclei.
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Presenters: Prof. GLUSHKOV, Alexander (Odessa State University-OSENU); Ms GURSKAYA, Marina (Odessa State University-OSENU)

Session Classification: Poster Session

Track Classification: Atomic, Molecular and Optical Physics

Contribution ID: **114** Type: **Poster Presentation**

Computational modelling of electroweak interaction effects in atomic and molecular systems within Nuclear-QED perturbation theory

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Nowdays the atomic parity on-conservation (PNC) in finite Fermi systems has a potential to probe a new physics beyond the Standard model. In our paper we systematically apply computational code based on the QED many-body perturbation theory (PT) [1,2] to precise numerical calculation of the PNC effect in heavy atoms with taking into account the relativistic, nuclear, radiative corrections. The key element is in an accurate taking into account the correlation corrections of the PT second and higher orders (dominating classes: Coulomb interaction screening; interaction «particle-hole» ; mass operator iterations), which is based on using the Feynman diagrammatic technique and Green function (GF) method. There are presented the results of the calculating PNC amplitudes for a number of heavy atomic systems (¹³³Cs, ¹⁷³Yb, ²⁰⁵Tl, etc) with account of the exchange- correlation, Breit, weak e-e interactions, radiative, nuclear (magnetic moment distribution, finite size, neutron “skin”) corrections. The nuclear spin-dependent PNC interactions due to nuclear anapole moment (ka contribution), Z-exchange interaction from nucleon axial-vector (AnVe) currents (k2), the combined hf and spin-independent Z exchange interaction from nucleon vector (VnAe) currents (khf) are considered too.
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Presenters: Prof. GLUSHKOV, Alexander (Odessa State University-OSENU); Ms GURSKAYA, Marina (Odessa State University-OSENU)

Session Classification: Poster Session

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **115** Type: **Poster Presentation**

New computational dynamical approach to Earth system modelling: energy and angle momentum balance, teleconnection, atmospheric radiowaveguides

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The satellite data and data of observing the radio-waveguide parameters (especially in the low troposphere layers) is the informative basis of the modern atmosphere long-term forecasts. As any water quantities in atmosphere are formed on the basis of the cycle- and front-genesis (or in the convective non-stability lines) one can introduce the corresponding model on the basis of the computational thermodynamics and hydro-mechanics of the corresponding processes. We present principally new non-linear computational statistical and dynamical methods of monitoring and modelling the Earth system low-frequency scale processes on the basis of observing some summated contributions of low frequency oscillations for geophysical factors. They base on the energy and angle moment balance relations with stochastic elements and new scheme for calculation of the macro-turbulence regime in typical atmospheric processes, which are known as atmospheric circulation forms [1]. The balance analysis allows to predict the large-scaled atmospheric transformations and teleconnection phenomena and to give their quantitative description. We carried out a series of the PC experiments at the Pacific ocean region in order to study global mechanisms in the atmospheric models and check the seasonal sequences of the conservation (or disbalance) of the Earth atmosphere angle momentum and to provide new predictors for the long-termed and super long-termed forecasts of the low frequency atmospheric processes. The current function (complex velocity) fields are calculated for typical atmospheric circulation's forms. Besides, we have adapted the modified numerical theory of the macro-turbulence for possible using the atmosphere radio-waveguides as a special effective predictors in the long-termed plan.
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Presenters: Prof. GLUSHKOV, Alexander (Odessa State University-OSENU); Ms GURSKAYA, Marina (Odessa State University-OSENU)

Session Classification: Poster Session

Contribution ID: **116** Type: **Oral Presentation**

The Schrödinger equation on a Lagrange mesh

Tuesday, 12 July 2016 15:00 (20 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

Atomic, molecular and nuclear systems are quantum mechanical systems that are accurately described by the Schrödinger equation. Theoretical studies of these systems require the solution of the many-body Schrödinger equation that involves realistic interactions in the systems. It is common knowledge that the Schrödinger equation can be solve exactly only for a few types of interaction potentials. Therefore, only numerical solutions of the equation are possible even for systems with few constituents. Although variational methods have been shown to generate accurate numerical solutions to the Schrödinger equation, such methods are computationally demanding. The Lagrange-mesh method is a semi-variational method that combines the Lagrange basis expansion with Gauss quadrature approximation. This combination leads to a set of simple algebraic equations that can be solved fast and accurately. In this work the Lagrange-mesh method is used to solve the two- and three-dimensional Schrödinger equation in polar coordinates. General matrix elements for the Hamiltonian depending only on the grid points and can be used with any system are presented for the first time. Results with selected Hamiltonian related to some few-body systems are within machine accuracy.

Primary author: Prof. RAMPHO, Gaotsiwe Joel (University of South Africa)

Presenter: Prof. RAMPHO, Gaotsiwe Joel (University of South Africa)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Contribution ID: **117** Type: **Oral Presentation**

Learning problem-solving skills in a distance education physics course

Monday, 11 July 2016 15:10 (20 minutes)

Abstract content
   (Max 300 words)
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Special chars

Instructional material for computational physics courses can be presented through face-to-face, online or just print technology. The effectiveness of each of these presentation modes in learning computational physics need to be investigated. In this paper we present the results of a study on the effectiveness of combinations of delivery modes of distance education in teaching problem-solving skills in a first-level distance education physics course. A problem-solving instruction with explicit teaching of a problem-solving strategy and worked-out examples was implemented in the course. The course was presented through correspondence, online using a learning management system, as well as two face-to-face discussion classes. The study used the ex post facto research design with stratified sampling to investigate the effect of the learning of the problem-solving strategy on the problem-solving performance. The number of problems attempted and the mean frequency of using strategy in problem solving in the three strata were compared. Inferential statistics were used to compare the means for the three strata. The finding of the study indicated that the blended-learning approach had no statistically significant effect in the learning of problem-solving skills in a distance education module.

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Co-author: Prof. RAMOROLA, Mmankoko (University of South Africa)

Presenter: Prof. RAMPHO, Gaotsiwe Joel (University of South Africa)

Session Classification: Parallel Track B

Track Classification: Physics Education

Contribution ID: **118** Type: **Oral Presentation**

Study of Effective atomic numbers of Bioactive Glasses for Photon Interaction

Tuesday, 12 July 2016 11:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Bioactive glasses are a group of synthetic silica-based bioactive materials with unique bone bonding properties. Bioactive glasses are widely used in joint replacements, bone plates, etc. As a consequence, various human organs and bioactive material are exposed to X-rays and gamma rays. Once some parts of the human body is replaced by bioactive material, it is very important to know that how these material can be affected by exposing with X-or gamma radiation. This work was carried out to study the nature of mass attenuation and effective atomic numbers of bioactive glasses for gamma or X-rays. In the present study, we have calculated the effective atomic number, electron density for photon interaction in the energy range 1 keV to 100 MeV of selected of bioactive glasses SiO₂-Na₂O-CaO-P₂O₅, SiO₂-CaO-P₂O₅ and SiO₂-CaO. We have also computed the single valued effective atomic number by using XMuDat programme. It is observed that variation in effective atomic number (ZPI, eff) depends also upon the weight fractions of selected bioactive glasses and range of atomic numbers of the elements. The XMuDat calculates Zeff, XMuDat by assuming photoelectric absorption as the main interaction process where as Nel, XMuDat assuming Compton scattering as the main interaction process.

Primary author: Dr MALIPATIL, Anil Shantappa (Department of Physics, Veerappa Nisty Engineering College, Shorapur-585220, KARNATAKA, INDIA)

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Presenter: Dr MALIPATIL, Anil Shantappa (Department of Physics, Veerappa Nisty Engineering College, Shorapur-585220, KARNATAKA, INDIA)

Session Classification: Parallel Track B

Contribution ID: **119** Type: **Poster Presentation**

Domain Wall Structure and Electric Polarization in BiFeO₃

Tuesday, 12 July 2016 16:30 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

BiFeO₃ is a well-studied multiferroic material with distorted perovskite structure where electric polarization P parallel to [111] and cycloidal spin order with the propagation vector Q perpendicular to [111] directions (3-fold degenerate). Recently, an additional electric polarization P' acommpanied by Q has been observed, which is proposed to be applied to a 3-state memory devices. We study a model which includes spin interactions and anisotropies to represent the magnetism of BiFeO₃, and analyzed the model using Monte Carlo as well as LLG methods. The model reproduces magnetization curves as well as electric polarizations as a function of magnetic fields (cross-correlation curves). Spurious polarizations created by domain wall structures are also observed, which explains exotic featrues of the cross-correlation curves observed in BiFeO₃.

Primary author: Prof. FURUKAWA, Nobuo (Dept. of Physics, Aoyama Gakuin Univ.)

Presenter: Prof. FURUKAWA, Nobuo (Dept. of Physics, Aoyama Gakuin Univ.)

Session Classification: Poster Session

Contribution ID: **120** Type: **Oral Presentation**

INVITED SPEAKER: From carbon speciation to transport properties of carbon rich liquids of the upper mantle from molecular dynamics simulations

Thursday, 14 July 2016 09:00 (30 minutes)

**Abstract content
   (Max 300 words)
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Special chars**

Although the carbon content of the mantle is very low it plays an important role in the mantle dynamics. In the upper mantle, carbon has mainly the form of carbonates and at the onset of fusion the molten fraction of the mantle are carbonate rich liquids or even molten carbonates. Upon reaching shallower depths, the liquid formed gets richer in silicate content. These carbonate rich liquids have a very low viscosity and low density and thus impact the mantle dynamics. They are also characterized by high ionic conductivity, about four order of magnitude larger than that of molten silicates. This property led to evidence of the presence of these liquids at a few hundred kilometers depth through magnetotelluric experiments.

These properties are directly linked to the microscopic structure of these liquids. Here, we employ two levels of molecular dynamics simulations, first-principle molecular dynamics and classical molecular dynamics, to identify the microscopic structures of carbonate rich fluids and predict their density and transport properties. Some consequences on the mantle geophysics will then be discussed.

Furthermore, we show that molten carbonates can solvate CO₂ and we found a new mechanism for CO₂ transport through fast O²⁻ exchange. This may have implication for CO₂ capture and storage.

Primary author: Prof. VUILLEUMIER, Rodolphe (Ecole Normale Supérieure - UPMC)

Presenter: Prof. VUILLEUMIER, Rodolphe (Ecole Normale Supérieure - UPMC)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Fluid Dynamics

Contribution ID: **121** Type: **Oral Presentation**

PLENARY: Development of particle-in-cell code KLAPS and its applications in laser plasma physics

Thursday, 14 July 2016 11:30 (45 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

In this talk, I will introduce the development of our particle-in-cell (PIC) code KLAPS[1] for laser-plasma physics studies and its applications in fast ignition for inertial confined fusion[2] and MV/cm terahertz (THz) radiation generation[3-5] etc. With the help of PIC simulation, the co-operation with experiments of femtosecond X-ray generation and complete absorption of intense laser pulses will be briefly introduced.

Fast ignition scheme was proposed in 1994 to rapidly heat a compressed fusion fuel by a short-duration (10ps=10-11s), high-power (PW=1015watt) ignition laser and then gain huge energy by nuclear fusion. It requires that fast electrons of MeV produced by the ignition laser are transported over 100mm distance to heat a high-density core region. The key is how to achieve a coupling above 10% from the laser to the core. Coupling of 20% was demonstrated experimentally in 2001 [Nature 412, 798] with a cone-inserted target. However, recent experiments reported much lower coupling of only a few percent. The very different results could be related to different preplasmas formed by the ignition laser prepulses in the cones. To clarify this point, we firstly developed an integrated PIC simulation approach [1] (named two-system PIC) to self-consistently include the whole heating physics of fast ignition. Our simulation showed that different presplasm levels caused significantly difference in the coupling. To reduce the preplasma effect, we propose a magnetically assisted (MA) fast ignition scheme [2] using a cone-free target supplemented by an external 20-megagauss magnetic field to confine the fast electron motion. Such a target also does not suffer from asymmetry in target compression, as is the case for a cone-inserted target. The MA scheme was demonstrated by our integrated PIC simulation[1]. With this PIC approach we directly obtained the laser-to-core coupling of 14%. Quantitative comparison among the MA scheme, the cone-inserted scheme, and the original scheme was performed, for the first time via integrated simulations. It is shown that the coupling can be enhanced by 7-fold with the magnetic field, which can even exceed that obtained with the cone-inserted scheme.

THz radiation sources with tunable polarization and frequencies are in high demand for diverse THz technologies such as THz spectroscopy and coherent control. Currently the widely studied two-color laser scheme can provide a powerful THz source. Such a source basically has linear polarization and a broad bandwidth[3,4]. Here, we propose an approach[5] to generate circularly polarized, narrow-band THz radiation with continuously tunable frequency. In this approach, a 100-tesla magnetic field is imposed along the propagation direction of the two-color linearly polarized laser driver. Stable magnetic fields of this order are already experimentally available. In the proposed approach, the radiation frequency is linearly proportional to the magnetic strength. The rotation direction of the new radiation can be controlled by the magnetic field sign. This radiation has a many-cycle waveform rather than the usual single-cycle waveform as in the case without the magnetic field. This approach is demonstrated by PIC simulations (with KLAPS code) and further explained by theoretic analysis.

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Presenter: Dr WANG, Wei-Min (Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China)

Session Classification: CCP2015 Winner Plenary

Contribution ID: **122** Type: **Oral Presentation**

INVITED SPEAKER: Impacts of interlayer and substrate interactions on low dimensional crystals

Wednesday, 13 July 2016 14:00 (30 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

One- and two-dimensional crystals experience strong perturbations from their nearby environments exhibiting unique realization of new electronic structures and interaction driven states. In this talk, I will review my recent computational studies exploring possible alternations of fundamental electronic structures of low dimensional crystals under influences of stacking, external mechanical forces, and substrate screenings, etc.

Primary author: Prof. SON, Young-Woo (Korea Institute for Advanced Study)

Presenter: Prof. SON, Young-Woo (Korea Institute for Advanced Study)

Session Classification: Parallel Track B

Track Classification: Material and Nano Sciences

Contribution ID: **123** Type: **not specified**

Welcome Reception

Contribution ID: **124** Type: **Oral Presentation**

PLENARY: Simulated synthesis, characterisation and performance of nano-architectured energy storage materials.

Wednesday, 13 July 2016 09:00 (1 hour)

Abstract content
   (Max 300 words)
Formatting &
Special chars

An increasing demand for energy and a shifting to renewable energy resources, has accelerated development of energy generation and storage for use in solar energy harvesting, electric vehicles, electricity grid backups. Enhanced performances of lithium ion rechargeable batteries, such as higher capacity, improved rate capability and sustained capacity retention for longer cycles are now achieved with various nano-architectures and were studied with a wide range of experimental techniques [1].

Electronic structure and atomistic simulations are capable of elucidating structural, transport and predicting performance of battery electrodes [2]. A major challenge associated with generating atomistic models is to capture the wealth of microstructural features observed experimentally and to follow evolvement of lithiated phases obtained after intercalation, associated with charging and discharging of batteries. One technique that is capable of spontaneously generating various nanostructures and introducing complex microstructures is the atomistic simulated amorphisation and crystallization method [3].

In this presentation such technique, which is based on molecular dynamics, used in conjunction with classical force fields, is employed to illustrate simulated synthesis and characterisation of different nano-architectures, i.e. nano- spheres, sheets, rods, porous and bulk of binary metal oxides such as MnO₂ and TiO₂. Furthermore, the nano-architectures are lithiated, to imitate charging and discharging, and their structural aspects and performance are characterized by simulated X-ray diffraction patterns and voltage profiles respectively. In particular, the relationship between mechanical properties, microstructural features and electrochemical activity in nanoporous and bulk structures is highlighted. Such connection is extended to why the ternary nano Li₂MnO₃, an end member of high voltage composite cathodes, is electrochemically active whilst its bulk form is inactive [4]. Lastly, nano-architectures, associated with the Li-Mn-O ternary were synthesised from amorphous spinel nanosphere. The resulting crystallised nano-architectures are characterised and the presence of a composite consisting of the layered Li₂MnO₃ and spinel LiMn₂O₄ together with a variety of defects, including grain boundaries and ion vacancies are observed, from XRDs and microstructural features. This is a step towards addressing the challenge of voltage fade in the composite layered spinel cathodes, which have high capacity and energy density [5]. Preliminary work beyond Li-ion batteries, particularly related to Li-S, will be introduced.

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Presenter: Prof. NGOEPE, Phuti (University of Limpopo)

Session Classification: Plenary

Track Classification: Material and Nano Sciences

Contribution ID: **125** Type: **Oral Presentation**

INVITED SPEAKER: Thomas Dietel (University of Cape Town) for the ALICE Experiment at the LHC

Tuesday, 12 July 2016 09:30 (30 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The ALICE Collaboration studies the Quark-Gluon Plasma, a new state of nuclear matter at extreme temperatures and densities which is created in high-energy collisions of heavy nuclei at CERN's Large Hadron Collider (LHC).

The LHC is one of the largest producers of scientific data, and the ALICE Experiment alone has collected more than 10 petabytes of data since 2010. The processing and analysis of this data requires online processing in the High-Level Trigger as well as offline processing using the Worldwide Large Computing Grid (WLCG). We will discuss the current computing strategy of ALICE and outline selected tools and methods used in the processing of this data volume.

Upgrades to the LHC and the ALICE apparatus scheduled for a long shutdown in 2019/20 will enable ALICE to inspect 100 times more collisions, requiring a rethinking and redesign of the ALICE computing model, including a tighter integration of online and offline computing and new software algorithms, communication protocols and
system architecture.

Primary author: Dr DIETEL, Thomas (University of Cape Town)

Presenter: Dr DIETEL, Thomas (University of Cape Town)

Session Classification: Parallel Track B

Track Classification: High Energy, Nuclear and Particle physics

Contribution ID: **126** Type: **Oral Presentation**

INVITED SPEAKER: Simulating the formation of the first galaxies and black holes in the Universe

Thursday, 14 July 2016 10:50 (20 minutes)

**Abstract content
   (Max 300 words)
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Special chars**

I will discuss recent progress in cosmological hydrodynamic simulations of galaxy formation at unprecedented volumes and resolution. I will focus on predictions for the first quasars and their host galaxies and their contribution to reionization from the BlueTides simulation. BlueTides is a uniquely large volume and high resolution simulation of the high redshift universe: with 0.7 trillion particles in a volume half a gigaparsec on a side. This is the first simulation large enough to resolve the relevant scales relevant to the formation of the first large galaxies and quasars. These massive objects at high redshifts will be investigated with the next generation telescopes (Euclid, JWST and WFIRST).

Primary author: Prof. DI MATTEO, Tiziana (Carnegie Mellon University)

Presenter: Prof. DI MATTEO, Tiziana (Carnegie Mellon University)

Session Classification: Parallel Track A: Astrophysics and Space Physics, Plasma, Gravitation and Cosmology

Track Classification: Astrophysics and Space Physics

Contribution ID: **127** Type: **Oral Presentation**

PLENARY: The Square Kilometre Array: Big Telescope, Big Science, Big Data.

Monday, 11 July 2016 09:30 (1 hour)

Abstract content
   (Max 300 words)
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The Square Kilometre Array (SKA) is a next generation global radio telescope currently undergoing final design by a collaboration of institutions in 11 countries. The SKA will be one of the largest scientific projects ever undertaken, designed to answer some of the big questions of our time: What is Dark Energy? Was Einstein right about gravity? What is the nature of dark matter? Can we detect gravitational waves? When and how did the first stars and galaxies form? What was the origin of cosmic magnetic fields? How do Earth-like planets form? Is there life, intelligent or otherwise, elsewhere in the Universe?

The SKA radio telescope dish array is coming to South Africa toward the end of this decade. When completed it will consist of thousands of radio antennas spread out over an area of thousands of kilometres in Southern Africa. The SKA will create 3D maps of the universe 10,000 times faster than any imaging radio telescope array ever built. Precursor telescopes based on SKA technologies are under construction here in South African and in Western Australia and will begin scientific investigations in late 2016. These developments foreshadow one of the most significant big data challenges of the coming decade and the beginning a new era of big data in radio astronomy, in which researchers working at the forefront of data science will be a critical part of astronomical discovery. An integral part of the SKA design is the systems and infrastructure to enable collaborative research on big data sets by globally distributed research teams.

Primary author: Prof. TAYLOR, Russ (University of Cape Town (SKA))

Presenter: Prof. TAYLOR, Russ (University of Cape Town (SKA))

Session Classification: Plenary

Track Classification: Astrophysics and Space Physics

Contribution ID: **128** Type: **Oral Presentation**

Computational study of dye adsorption in nano TIO₂ film for the applications in dye sensitized solar cells using different computational techniques

Wednesday, 13 July 2016 12:15 (20 minutes)

**Abstract content
   (Max 300 words)
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Special chars**

The theoretical and computational studies of dye sensitized solar cells (DSSCs) can contribute to a deeper understanding of these types of solar cells. In the current study the density functional theory and the finite element methods are used to understand the factor affecting the dye adsorption and electronic properties of the TIO₂ semiconductor as the main element of DSSCs. The light adsorption occurs in dye molecules adsorbed on a highly porous structure of TIO₂ film. The processes followed experimentally for dye uptake is by dipping the TIO₂ semiconductor electrode into the dye solution for periods of several hours to several days. To understand the process of dye adsorption on the surface of TIO₂, the DFT calculations was carried out to study the electronic structure of the ruthenium doped brookite TIO₂ surface. The factors controlling the dye uptake process are also investigated, using a simple model based on the Langmuir isotherms. Our computational modelling results show that the adsorption of dye into the TIO₂ nanotubes film is controlled by the diffusion coefficient, the adsorption-desorption ratio and the initial dye concentration.
Keywords: Solar Cells, Dye Sensitized, Dye, Surface Coverage, Langmuir

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Presenter: Dr MALUTA, Nnditshedzeni Eric (University of Venda)

Session Classification: Parallel Track B

Track Classification: Material and Nano Sciences

Contribution ID: **129** Type: **Oral Presentation**

PLENARY: Understanding and designing novel nanomaterials from first principles

Wednesday, 13 July 2016 08:00 (1 hour)

Abstract content
   (Max 300 words)
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Special chars

Advances in theoretical methods for calculating the properties of materials from first principles, aided by the ever-continuing development of faster computers, now enable us to gain insight into why materials possess the properties they do. Such insights can then be leveraged so as to enable us to "rationally" design new materials that are tailored for specific applications.

After a brief general survey of recent advances in such methods, with special emphasis on ab initio density functional theory, I will cite some examples from work in my group. For example, in the field of nanoscale alloys, we have shown that Fe and Au, though bulk-immiscible, form a two-dimensional surface alloy that is stabilized by magnetic interactions; this prediction was confirmed by experiments in the group of Sylvie Rousset. Another prediction, that conceivably has applications for nanocatalysis, was our prediction that depositing gold nanoparticles on an oxide substrate that has been doped with an electron donor would change the morphology of the particles from three-dimensional to two-dimensional; this idea was subsequently shown to work by experiments in the group of Hajo Freund. We have also shown that there is reason to believe that the change in morphology is accompanied by an improvement in catalytic properties. We have also recently shown how the oxidation state of nanomaterials can be tuned by varying their size and environment; as a part of this study, we have suggested a novel yet simple way to interpret experimental data from XANES.

In the field of computational design of materials, one is increasingly placing greater emphasis on the development of 'descriptors', which can then be utilized to screen a large number of candidate materials quickly. I will describe some efforts in our group to develop such descriptors.

I will conclude my talk with some brief remarks about the relevance of carrying out programs of computational physics in a developing country, and the possibility of carrying out interesting research even with modest computational resources.

Primary author: Prof. NARASIMHAN, Shobhana (JNCASR)

Presenter: Prof. NARASIMHAN, Shobhana (JNCASR)

Session Classification: Plenary

Track Classification: Material and Nano Sciences

Contribution ID: **130** Type: **Oral Presentation**

INVITED SPEAKER: Challenges for Parallel Programming Models and Languages of post-petascale and exascale computing

Thursday, 14 July 2016 10:30 (30 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

Europe, the US, Japan and China are racing to develop the next generation of supercomputer – exascale machines - capable of a million trillion calculations a second by around 2020. To realize exascale systems, there are many challenges and issues including architectures and programming models to exploit billions of parallelism and the limitation of power consumption. Toward a post-petascale system as the next of Japan's petascale facility, the K computer, the project, FLAGSHIP2020, has been launched to develop and deploy the post-K computer the last year. While there are two major different approaches for exascale, manycore-based and accelerator-based, we take manycore-based approach for our Post-K computer. OpenMP is a key to make use of manycore efficiently, and is to be evolved for exploiting large parallelisms and integration with communication layers. In this talk, projects for post-petascale and exascale computing in Japan will be described, and challenges for parallel programming models and languages in these projects will be addressed.

Primary author: Prof. SATO, Mitsuhisa (AICS, RIKEN)

Presenter: Prof. SATO, Mitsuhisa (AICS, RIKEN)

Session Classification: Parallel Track B

Track Classification: Software and Hardware Development

Contribution ID: **131** Type: **Oral Presentation**

INVITED SPEAKER: Quantum critical behavior of a superfluid-insulator transition

Wednesday, 13 July 2016 14:30 (30 minutes)

**Abstract content
   (Max 300 words)
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Special chars**

We investigate the quantum phase transitions as well as the phase diagram of a two-dimensional quantum rotor model with off-diagonal disorder by means of large-scale Monte-Carlo simulations. In contrast to the exotic critical behavior found in other random quantum systems, this Hamiltonian features a conventional (finite-disorder) critical point with power-law scaling but with critical exponents that differ from the clean ones. We also address the percolation quantum phase transition across the lattice percolation threshold, and we relate our findings to a general classification of phase transitions with quenched disorder. Moreover, we discuss technical aspects of our computational approach that permit the efficient simulation of random quantum systems including anisotropic finite-size scaling and improved Monte-Carlo estimators.

Primary author: Prof. VOJTA, Thomas (Missouri University of Science and Technology)

Presenter: Prof. VOJTA, Thomas (Missouri University of Science and Technology)

Session Classification: Parallel Track B

Track Classification: Quantum Many Body and Strongly Correlated Systems

Contribution ID: **132** Type: **Oral Presentation**

INVITED SPEAKER: High Performance Computing Developments in South Africa and the Continent in support of increasing demands of Research

Thursday, 14 July 2016 11:00 (30 minutes)

**Abstract content
   (Max 300 words)
Formatting &
Special chars**

South Africa has a growing demand of computational resources to enable research in various domains of science and engineering. The research areas aim at addressing challenges and opportunities ranging from climate change, energy security, manufacturing, health and geographical advantages. As a response to these demands, the Department of Science and Technology has invested in National Cyber-Infrastructure, to accelerate progress in these fields. In this paper, success in deploying high-end computing resources in South Africa and the region, will be discussed. Furthermore, the paper will also address the steps taken in building the necessary human capital to support these developments. The recently completed petascale HPC system will also be presented.

Primary author: Dr SITHOLE, Happy (Chpc)

Presenter: Dr SITHOLE, Happy (Chpc)

Session Classification: Parallel Track B

Track Classification: Software and Hardware Development

Contribution ID: **134** Type: **Oral Presentation**

PLENARY: Efficient and accurate first-principles predictions of structures and energies for Materials Science, Chemistry and Biology

Thursday, 14 July 2016 12:15 (45 minutes)

Abstract content
   (Max 300 words)
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Special chars

In materials science, chemistry, and biology, it is of critical importance to know if one atom or molecule can bind to another and with how much energy. The strengths of different types of bonds between atoms and molecules can vary from several meV to several eV. Although some first-principles methods can provide accurate descriptions of all bond types, those methods are not efficient enough for studies of complex systems (e.g., large systems, ab initio molecular dynamics, and high-throughput searches for functional materials). We show here that the recently developed non-empirical strongly constrained and appropriately normed (SCAN) meta-generalized gradient approximation (meta-GGA) within the density functional theory framework predicts accurate geometries and energies of diversely-bonded molecules and materials (including covalent, metallic, ionic, hydrogen, and van der Waals bonds), significantly improving over its predecessors, at comparable efficiency, the GGAs that dominate materials computation. Often SCAN matches or improves upon the accuracy of a computationally expensive hybrid functional, at almost-GGA cost. SCAN captures the intermediate-range van der Waals (vdW) interaction, which is largely missed by the conventional GGAs and hybrid functionals. The addition of the long-range vdW correction to SCAN results in a versatile vdW functional that is accurate and outperforms its competitors for a variety of vdW-dominated systems, including layered materials and organic molecules adsorbed on metal surfaces.

Primary author: Prof. SUN, Jianwei (University of Texas at El Paso)

Presenter: Prof. SUN, Jianwei (University of Texas at El Paso)

Session Classification: CCP2016 Winner Plenary

Track Classification: Material and Nano Sciences