Poster session
Programme Advisory Committee
for Condensed Matter Physics
(19–20 January, 2017)

Poster abstract	Remarks
1. Software package baYes for Bayesian analysis of the models of superdense nuclear matter EoS **A. Ayriyan, H. Grigoryan, G. Poghosyan** *Laboratory of Information Technologies, JINR; ayriyan@jinr.ru; +74962164875* A software package "baYes" is developed as a tool for Bayesian analysis of the models of superdense nuclear matter using the astrophysical data of compact stars. The package performs the following sequence of calculations: 1. Constucting models of hybrid equations of state (based on investigated models of hadron and quark matter); 2. Calculations of sequence of stable configurations of neutron stars (solving Tolman-Oppenheimer-Volkoff equations); 3. Bayesian analysis using observational data; 4. Creation of demonstrative materials (graphs). The package includes the implementation of parallel computing of stable configurations of neutron stars. A set of realistic hybrid equation of state models allowing first order phase transition from hadronic to quark matter has been investigated by this package. The analysis was based on the data of measured masses of the supermassive pulsars PSR J0348+0432 (Antoniadis at al. Science 340, 6131) and PSR J1614-2230 (Demorest at al. Nature 467, 7319). The results are published in EPJA 52:69 (2016) , http://dx.doi.org/10.1140/epja/i2016-16069-2.	
2. Smart Cloud Scheduler for the JINR cloud **Balashov N., Baranov A., Kadochnikov I., Kutovskiy N., Nechaevskiy A., Pelevanyuk I.** *Laboratory of Information Technologies, JINR* Analysis of the JINR LIT cloud service usage showed that the variety of workloads generated by modern applications leads, in general, to a highly uneven workload distribution and that efficiency of cloud equipment utilization can be potentially increased. In the framework of the cloud service development an intelligent scheduling and adaptive self-organization of virtual computing resources software development is ongoing. The system is aimed at increasing efficiency of cloud resources utilization by the means of using virtual machines consolidation technologies and the method of dynamic resources reallocation that is based on accumulation and analysis of the resources consumption historical records.	

3. Simulation of radiation damage to different neuronal structures with Geant4-DNA toolkit

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Radiation damage to the central nervous system (CNS) has been an on-going challenge for the last decades primarily due to the issues of brain radiotherapy and radiation protection for astronauts during space travel. Although recent findings revealed a number of molecular mechanisms associated with radiation-induced impairments in behaviour and cognition, some uncertainties exist in the initial neuronal cell injury leading to the further development of CNS malfunction. As usual, these initial stages of neuronal injury are hardly accessible to experimental measurements. Many events cannot be investigates experimentally at all. In this regard, development of computation methods for assessing these early stages of radiation damage to CNS is of great interest.

The present study is focused on simulation of physico-chemical effects in synaptic receptors of brain neurons taking into account their complicate structure. With the use of a Geant4-DNA toolkit enabling simulation of particle track traversals to neurons, we investigated direct and indirect effects of radiation damage to a network of individual neurons and to glutamate receptors located in neuron synaptic zones [1–3]. The geometries of neuronal receptors and neuronal network were constructed using experimental data on their molecule and cell morphologies, respectively. The calculations were made for beams of charged particles of different energy within a relatively wide range of linear energy transfer values from a few to hundreds of keV/μm. As the result, mean values were obtained of the stochastic events of energy deposition within small sensitive volumes (359.9 nm^3 and 429.8 nm^3) of the NMDA and AMPA receptors exposed to radiation. The estimation of radiolytic yields in neuronal cells suggests that the observed enhancement in levels of reactive oxygen species may potentially lead to oxidative damage to neuronal components disrupting the normal communication between cells of the neural network.

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3. L. Bayarchimeg, O.V. Belov, M. Batmunkh, O. Lkhagva, Modeling of synaptic receptors under irradiation with charged particles // Mongolian Journal of Physics, 2016. http://mnglps.mn/index.php/en/ (in press)

4. Effects of hypofractionated and standard fractionated irradiation of mice heads with gamma-rays and protons on their pheripheral blood parameters and behavior

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Experiments were performed to study the action of fractionated irradiation of mice heads with γ-rays and protons on their peripheral blood parameters and behavior by the "Open Field" test. Mice were irradiated in two variants of fractionated irradiation:

(1) traditional fractionation (in radiation therapy): 2 Gy once a day, 5 times a week, the total radiation dose 20 Gy;

(2) extreme hypofractionation: 10 Gy once a week, on Mondays, the total radiation dose 20 Gy.

The results of the study showed that irradiation of mice heads has no effect on their peripheral blood parameters in both variants of the applied fractionated irradiation and the behavior of mice does not depend on the type of ionizing radiation and the variant of fractionated exposure that we used. On the basis of these results it can be concluded that the option of extreme hypofractionation we have chosen can successfully replace traditional fractionation, which in some cases is applied when carrying out radiotherapy for treating brain tumors. The application of this type of fractionation can lead to shorter terms of radiotherapy and bigger patient capacity of medical centers that conduct radiotherapy.

5. Microstructure and radiation hardening investigation of ODS steels for generation IV nuclear reactors

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Oxide dispersion strengthened (ODS) steels are the most perspective structural materials for fuel cladding of Generation IV nuclear reactors due to their high creep strength and radiation resistance [1]. These properties are caused by the presence of oxide particles dispersed in the ferrite matrix that pin the dislocations and also can act as sinks for radiation defects.

The oxide particles behavior investigation and possible mechanical properties evolution of steels during fission fragment (ff) impact is one of the most interesting and less studied questions by now. Previous investigations have shown the structural instability of oxide particles based on Y-Ti-O compounds during exposure to swift heavy ions simulating ff irradiation.

In the present work, three kinds of ODS steels with different types of oxide particles were irradiated by 167 MeV Xe, 107 MeV Kr and 700 MeV Bi ions at room and elevated temperatures for the fission fragment impact simulation in reactor. The oxide particle and ferrite matrix stability was investigated by transmission electron microscopy (TEM). Mechanical properties of ODS steels were studied by nanoindentation.

TEM observations show the deformed structure of yttrium-titanium oxides of initial and post-irradiated state as well. The role of sample geometry for the structure examination during high temperature irradiation is studied. It was shown that Y-Ti-O oxides are less stable to the swift heavy ions irradiation in comparison with yttrium-aluminium oxides due to the latent track formation. The threshold of electronic stopping power for track formation is defined. It was shown that nanoindentation techniques are relevant methods for studying mechanical properties of irradiated materials. All ODS steels demonstrate the saturation of radiation hardening of 15% for 1 dpa. The observed radiation hardening is well described by the dispersed barrier model.

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6. Main directions of the JINR cloud evolution

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Being running in production for already several years the JINR cloud provides resources used for many activities and tasks. A demand in cloud resources from both individual users and experiments are growing permanently. To cover the resources deficit, work is in progress in three directions: 1) the resources usage optimization with the help of a smart scheduler which consolidates underloaded virtual machines and containers within the hosts; 2) an external clouds integration with the JINR one following the so-called "cloud bursting" approach what a custom driver was developed for; 3) installing more servers. Apart from using the JINR cloud resources among others tasks for so called high throughput computing jobs a research on running high performance computations on virtual machines in cloud environment was carried out. Moreover, an aggregation and visualization of the JINR cloud resources utilization data was re-implemented and moved to external service based on Grafana and InfluxDB. Such shift allowed to avoid an extra step before software update on the JINR cloud front-end node due to eliminating a necessity in validation of compatibility of custom add-ons tightly integrated into OpenNebula graphical user interface called «Sunstone» against its new releases as well as to store a collecting metrics in a database for further analysis against their changes over time and to obtain the dynamics for the selected period.

7. Approach on developing a heterogeneous computing cluster in terms of the HybriLIT cluster

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In 2016 a new component of the heterogeneous cluster HybriLIT – a system of virtual workstations – that is meant for work with applied software installed on the cluster.

The developed polygon includes 8 servers. On the basis of KVM (Kernel-based Virtual Machine), virtual desktops have been installed. Access to COMSOL Multiphysics has been granted as well. A group of users of the cluster was provided with a set of tools for remote access to the virtual desktops.

Such an approach allowed users work with specialized software and accelerate their computations.

Organization of managing and service components transferred to the environment of virtual machines has been changed.

The chosen method of developing the heterogeneous computing cluster allows meet the requirements of scalability and reliability of the cluster.

The developed hardware-software environment of the HybriLIT cluster provides users with wide possibilities for development of applications by means of parallel programming technologies.

8. Simulation of Cloud Computation MPI Applications

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The use of long Josephson junctions (LJJ) in superconducting high precision nanodevices is one of the most advanced areas of modern electronics. Theoretical JJ studies are performed at the JINR. The calculations of the designed parallel algorithms have been performed on Cloud (cloud.jinr.ru) and Heterogeneous Infrastructures (hybrilit.jinr.ru) of Multi-Functional Information and Computing Complex (miccom.jinr.ru) hosted at the Laboratory of Information Technologies of Joint Institute for Nuclear Research (Dubna, Russia).

It is necessary to test the parallel algorithm for various combinations of parameters (processor speed, network throughput, buffer size etc.) to optimize the parallel computation scheme. This problem could be solved by simulating of the calculation process at the LIT heterogeneous infrastructure. The originality of the authors approach consists in applying discrete event simulation to describe the MPI software as multiple cores in a single server as well as VM interconnected in a cloud. The simulation program SyMSim developed at LIT (symsim.jinr.ru) is used for modeling MPI computational processes.

9. Assymetric track-etched single nanopores for use in the sensor technology

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During the past few years, artificial single nanopores, i.e. those in track membranes, have attracted much interest due to their potential applications in nanofluidics, sensor technology and information processing [1-4].

In this work we determined the reproducibility of properties of asymmetric single nanopores prepared in Hostaphan polyester films by chemical etching of tracks of accelerated heavy ions [5]. These nanoscale objects exhibit high ion current rectification. The influence of variations in geometry of pores on their electrical conductance properties was studied. The current-voltage characteristics of nanometer-sized pores were registered in KCl solutions. The sample surfaces were observed using Field Emission Scanning Electron Microscopy. The correlation between the ionic conductance properties and the nanopore morphology is discussed.

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10. Studies of Iron and Copper Exposed to Heavy Iron Implantation Using Positron Annihilation Spectroscopy

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Variable energy positron beam and conventional positron lifetime spectroscopy were used to study pure iron and copper exposed to irradiation with 167 MeV Xe^{26+} heavy ions with different doses of 10^{12}, 10^{13}, 5×10^{13}, 10^{14} ions/cm^2. The presence of vacancy-type defects and dislocations induced by implantation was confirmed in Doppler spectroscopy characteristics. For iron the positron lifetime spectroscopy revealed the presence of large cluster of about 15-27 vacancies and dislocations. The dislocations are distributed at the depth of about 18 μm i.e. almost twice deeper than the ion implantation range from the surface exposed to the heavy ions implantation. Possible explanation is the long-range effect attributed to the ion implantation into materials. For copper decreasing of the positron diffusion length from 135 nm for unirradiated sample, to 82 nm for the lowest and to 46 nm for the highest applied dose was noted. It points out increasing defect concentration with the increase of the fluence. However, the defected zone covered with the implanted range for copper and the so called "long range effect" wasn't observed in this case.

11. Development of Positron Annihilation Spectroscopy at the LEPTA Facility

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The report presents the status of the upgrading the LEPTA facility for further development of the positron annihilation spectroscopy (PAS) method application at the LEPTA facility. The research in solid state physics performed currently at the LEPTA is based on slow monochromatic positron flux from the injector. And the PAS method is sensitive to microdefects in solids. A pair of gamma quanta, born as a result of a positron-electron annihilation, carries information about the density of the defects that have the size less than 10 nm and are located at certain depth from the surface of the sample being studied. The depth depends on the positron energy that can be varied at the Lepta from 50 eV to 36 kV.

The new positron transfer channel at the LEPTA was designed, fabricated and mounted during the second half of 2016 and positron beam was transferred through the channel. This channel allows us to develop more advanced PAS method – so called "Positron Annihilation life-time spectroscopy". New monochromatic positron source supplied with the autonomous LHe cooling system with emitter-source of the activity of 30 mCi was mounted as well.

First results of operation of new cryogenic source and the new positron transfer channel are presented in the report.

12. Structural parameters of silver hydrosols: electron microscopy and small angle X-ray scattering

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Silver nanoparticles are widely used in electronic, optical and sensor devices including special substrates for surface-enhanced Raman spectroscopy (SERS). Modification of track-etched membranes with silver nanoparticle is a promising application aimed at fabrication of flow-throw SERS substrates with high sensitivity to different analytes including biologically important molecules. Reproducible fabrication of SERS substrates requires detailed knowledge of nanoparticles' properties such as size distribution, surface charge, content of agglomerates, and others.

In this work we studied silver hydrosols, i.e. silver water suspensions, prepared using electric discharge technology [1]. The silver particles are formed due to the dispersion of the electrode metal in a high-current discharge between closely spaced silver electrodes and further transfer of dispersed silver particles in water. Solutions were investigated on Rigaku [2] (MIPT, Dolgoprudny, Russia) and BM29 [3] (ESRF, Grenoble, France) instruments by small angle X-ray scattering method. SAXS curves were treated by the Fitter [4] and SasView programs [5], where triaxial ellipsoids and chain of spheres models were shown to be the best fits. For the chain of spheres model we obtained fit parameters 8.6, 7.1 and 5.0 nm as radii, with 20%, 30% and 50% polydispersity, respectively, for three different samples of suspension. Polyethylene terephthalate track-etched membranes were modified by polyethyleneimine and then coated with Ag nanoparticles. Electron microscopy assay was performed with a Hitachi SU8020 instrument. Histograms of particle size distributions were obtained upon electron microscope images of membrane surface. In summary, structural parameters of silver particles were obtained and polydispersity was estimated using two different analytical methods.

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[4] http://yumo.jinr.ru/software/fitter
[5] http://www.sasview.org/index.html

13. Structure and formation threshold of latent tracks in Al_2O_3 irradiated with swift heavy ions

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A combined numerical approach including original Monte-Carlo (MC) code TREKIS and classical molecular dynamics (MD) is applied to investigate the structure and formation threshold of swift heavy ion tracks in Al_2O_3. MC code describes the excitation of the electronic subsystem and energy transfer to the lattice, while MD is used to study the relaxation kinetics of the ion subsystem. The passage of Xe 167 MeV results in formation of a cylinder-like discontinuous disordered region of about 2 nm in diameter due to relaxation of the excess lattice energy. The size and structure of ion track is consistent with the recent transmission electron microscopy observations. The estimation of formation threshold of SHI tracks in Al_2O_3 gives the value of ~7 keV/nm. The result of simulation of the x-ray diffraction patterns of irradiated material demonstrates that Al atoms sublattice damaged stronger than the oxygen sublattice. The study of the relaxation kinetics of the lattice revealed the propagation of elastic waves out of the ion track.

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14. Heterogeneous cluster HybriLIT: IT-ecosystem

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In order to increase the efficiency of work on the heterogeneous cluster HybriLIT, there appears a need to develop and support an information-computing environment for work with parallel programming technologies used in the process of developing high performance applications and carrying out computations by means of resources of the heterogeneous cluster.

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15. Cloud platform for data management of the environmental monitoring network: UNECE ICP VEGETATION case

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The aim of the UNECE ICP Vegetation program is to identify the main polluted areas, produce regional maps and further develop the understanding of the long-range transboundary pollution. Since January 2014, the coordination of moss surveys in 36 European and Asian countries has been conducted from the JINR in Russia. To manage monitoring data a cloud platform is proposed. It consists of a set of inter-connected services and tools deployed and hosted in the JINR cloud. Motivation, basic principles and architecture of the platform are presented.

16. Analysis of the new possibilities of using Intel Xeon Phi processors for solving application programs

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The main objective of the testing was to compare the performance of two generations of Intel processors: Intel Xeon processors, which are present in the structure of the heterogeneous cluster HybriLIT, and Intel Xeon Phi 72XX processors, the access to which was provided by ZAO RSC Technologies. Testing included both these of specialized packages for testing (Linpack Benchmark) and various program packages.