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**LABORATORY OF INFORMATION
TECHNOLOGIES**

**REPORT ON RESEARCH ACTIVITIES
IN 2003–2009**

Report to the 107th Session
of the JINR Scientific Council
February 18–19, 2010

Dubna 2010

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Объединенный институт
ядерных исследований
БИБЛИОТЕКА

The main directions of the activity of the Laboratory of Information Technologies (LIT) are aimed at the provision of theoretical and experimental studies conducted at the Joint Institute for Nuclear Research (JINR) and JINR Member States with modern telecommunication, network, informational support and new mathematical and computing methods.

This activity is focused on two directions, namely "Information, Computer, and Network Support of the JINR's Activity" and "Mathematical Support of Experimental and Theoretical Studies Conducted by JINR". These directions are developed in frames of the JINR general topic "Networks, Computing, and Computational Physics".

The Laboratory staff involves high-skilled scientists and engineering personnel, including 25 doctors of science and 60 candidates of science. The LIT staff participated in research work done within 20 topics of the Topical plan for JINR research and international cooperation.

More than 1000 scientific publications in the refereed journals, proceedings of conferences, collaborations reports, electronic publications, and preprints were published in 2003-2009. More than 50 reports were presented to international and national conferences annually. The Scientific report of Laboratory has been published since 2003 and available at the LIT web-site (http://www1.jinr.ru/Reports/2003/english/08a_lit_e.pdf, <http://lit.jinr.ru/Reports/annual-report05/> LITScientificReport_04-05.html, [http://lit.jinr.ru/Reports/ SC_report_06-07/LITSR2006-2007.htm](http://lit.jinr.ru/Reports/SC_report_06-07/LITSR2006-2007.htm), http://lit.jinr.ru/Reports/SC_report_06-07/LITSR2008-2009.htm).

Following a decision of the JINR Committee of the Plenipotentiary Representatives, adopted on March 14-15, 2008 concerning the radical improvement of the computer telecommunication links with major partner organizations in the JINR Member States during the years 2010-2015, the first steps have been undertaken towards the development of a unified Grid-environment of the JINR Member States. Such an infrastructure will allow all the participating sides to effectively join their forces for solving the foreseen fundamental and applied projects in elementary particle physics, nuclear physics, condensed matter physics, computational biophysics, nanotechnologies, etc., the successful realization of which would be impossible without using highly efficient computations, new approaches to distributed and parallel computing, and large amounts of data storage.

The degree of interest towards the LIT activities in the JINR Member States is high. We have a number of collaborators from the JINR Member States: protocols of cooperation with INRNE (Bulgaria), ArmeSfo (Armenia), FZK Karlsruhe GmbH (Germany), IHEPI TSU (Georgia), NC PHEP BSU (Belarus), KFTI NASU (Ukraine), IMIT UAZ (Uzbekistan), WUT (Wroclaw, Poland), IFIN-HH (Romania), etc. LIT have BMBF grant "Development of the Grid-

infrastructure and tools to provide joint investigations performed with participation of JINR and German research centers" and the CERN-JINR Cooperation Agreement on several topics. The project "Development of Grid segment for the LHC experiments" was supported in frames of the JINR-South Africa cooperation agreement in 2006-2008.

Some work was done within participation in common projects: NATO project EAP.NIG 982956 "DREAMS-ASIA" (Development of gRid EnAbling technology in Medicine&Science for Central ASIA), CERN-INTAS projects, Worldwide LHC Computing Grid (WLCG), and Enabling Grids for E-science (EGEEIII) project co-funded by the European Commission (under contract number INFSO-RI-222667) through the Seventh Framework Programme. Grants were afforded by the Russian Foundation for Basic Research and 5 Contracts with Russian Federal Agency of Science and Innovations (FASI). The work under SKIF-GRID project - a programme of the Belarusian-Russian Union State was performed. In cooperation with SINP MSU, RSC "Kurchatov Institute" and PNPI, LIT participates in the Grid National Nanotechnology Network (GridNNN) project performed under the federal target programme of development of the infrastructure of the nanoindustry in the Russian Federation in 2008-2010.

NETWORKING, COMPUTING, INFORMATION SUPPORT

During the years 2003-2009 the Laboratory provided the reliable operation and development of the JINR networking, computing and information infrastructure. The key components of this infrastructure comprise JINR telecommunication data links, local area network (LAN), central information and computing complex (CICC) and basic software for integration of the Institute's information and computing resources in a unified information environment accessible to all users and with using Grid-technologies.

JINR telecommunication data links

The development and upgrade of the JINR telecommunication links include a wide spectrum of activities focused on the growth of the cooperation with the Russian Satellite Communications Company (RSCC), the development of a high-speed network infrastructure in Russia, the improvement of the system of international computer channels for science and education in Russia, the data links with the JINR-participating countries.

Starting from 45 Mbps in 2003 we commissioned in June 2009 a new telecommunication link between JINR and Moscow on the basis of the state-of-the-art technologies DWDM (Dense Wave Division Multiplexing) and 10 Gb Ethernet. Currently 2 optical light-path (*lambda*) are in use gaining 20 Gbps throughput. The throughput can be increased up to 800 Gbps by use of 80 virtual lines through the implementation of additional photonic modules.

Figure 1 shows three places where the devices of the photonic data communication equipment were installed: the central telecommunication node (JINR LIT), settlement Radishevo, and Moscow Internet Exchange (MSK-IX).

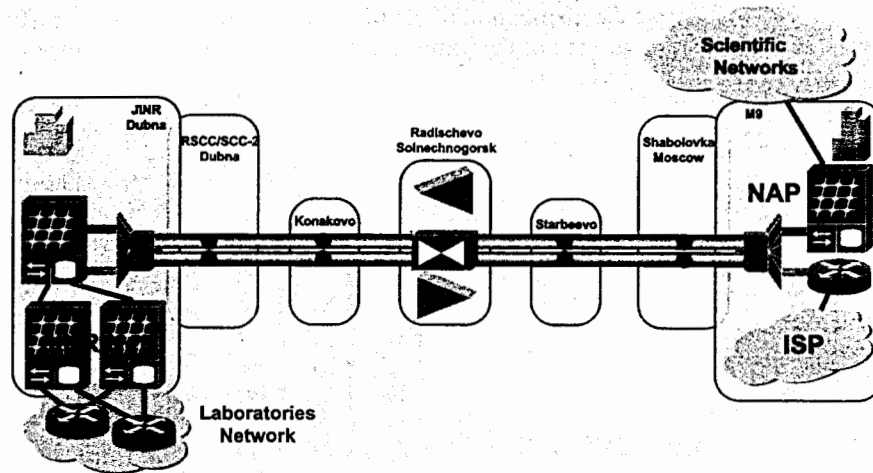


Figure 1: Scheme of the JINR-Moscow telecommunication channel

The development of the JINR telecommunication links on the Dubna-Moscow segment is achieved in cooperation with RSCC, owner of the optical fiber. Other project participants are NORTEL, JET Infosystems, Russian Institute for Public Networks (RIPN), the Computer Networks Interaction Center "MSK-IX".

The main JINR service-provider for access to the Internet is RBNNet (Russian Backbone Network). The parent organization on the support of the RBNNet network, the RIPN, is operating the international channel for science and education and is the trustworthy organization for the Internet Exchange (IX) functioning in Moscow. Important roles in the development of the national scientific infrastructure are also held by the networks RUNNet, RASNet, RUHEP and by several departmental and regional networks. The process of transition of the trunk lines of these networks to the DWDM technology was started. This will allow us to increase substantially the throughput of the channels (from 10 Gbps up to several hundreds Gbps).

The development of the segment of the international channels for science and education joining Russia with the Europe, with a throughput target of 10 Gbps in 2009, and subsequent growth in 2010-2016 is based on the connectivity with GÉANT (pan-European Communications infrastructure serving Europe's research and education community). The JINR-participating countries develop regional and national research and educational networks, many of which are being connected to the GÉANT. As a result of this joint activity, the integration of the Grid-infrastructures of JINR and its Member States will be realized through the high-speed European network GÉANT. This is the overall adopted approach to the integration of the regional networks for science and education in Europe.

Figure 2 shows the distribution of the incoming and outgoing JINR traffic since 2003. The sharp growth of the traffic for the last few years is explained by the activity of LHC experiments.

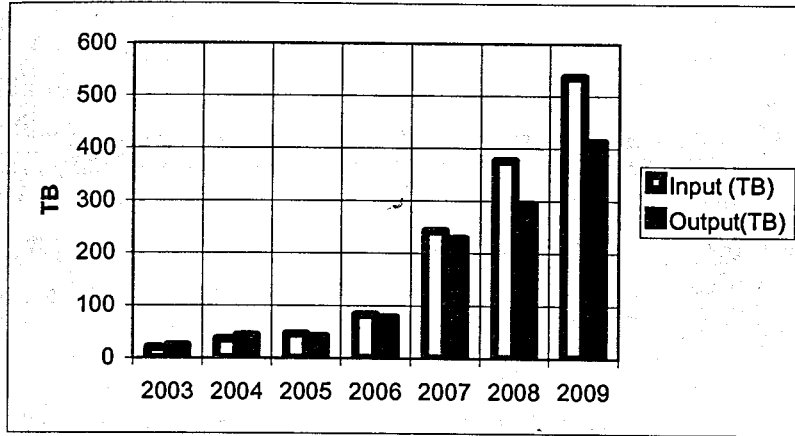


Figure 2: Distribution of the incoming and outgoing JINR traffic since 2003 up to 2009

A point of the local network traffic exchange was organized for JINR and Dubna Internet service providers (ISP) on the base of the JINR network facility. The local traffic of Dubna ISPs goes through this point of traffic exchange without necessity to go through Moscow ISPs. The participants are JINR, LAN-polis, Contact, Telecom-MPK.

For the last few years LIT specialists have performed investigations of information streams in computer networks. The goal of the research is the development of methods and construction of models for the effective control over operation and protection of the networks against overloads and unauthorized access. The research worldwide has shown that the network traffic is a complex dynamic process which cannot be described within existing models. At the same time, the functioning of the computer networks strongly depends upon their hard- and software support, also taking into account the models designed on the basis of the revealed laws and reflecting the peculiar features of the network traffic.

The results of the investigations performed at LIT have shown that in a steady-state mode the distribution of the internet traffic obeys a log-normal law (Fig. 3). The distribution parameters characterize each of such modes. Basing on the artificial neural network (ANN), a dynamic model of the network traffic has been developed with the help of which we managed to reproduce a statistical distribution of its flow as well as to confirm estimation of the embedding dimensionality obtained by the nonlinear dynamics methods. The developed methods of determining the moments of changing the state of the analyzed dynamic proc-

ess provide a way for the effective control over the information traffic. [I. Antoniou, V.V. Ivanov, Valery V. Ivanov, P.V. Zrellov: Nucl. Instr. & Meth. in Physics Research, A 502 (2003) 768-771; I. Antoniou, V.V. Ivanov, Valery V. Ivanov, P.V. Zrellov: Physica A, 324, (2003) 733-753, I. Antoniou, V.V. Ivanov, Valery V. Ivanov, P.V. Zrellov: Particles & Nuclei, Letters, 2004, Vol.1, No.4 (121), pp. 87-100; I. Antoniou, V.V. Ivanov, Valery V. Ivanov, P.V. Zrellov: Particles & Nuclei, 2004, Vol. 35, No.4, pp.984-1019; I. Antoniou, V.V. Ivanov, Valery V. Ivanov, Yu.L. Kalinovsky, P.V. Zrellov: Discrete Dynamics in Nature & Society, 2004, 1(2004) 19-34.]

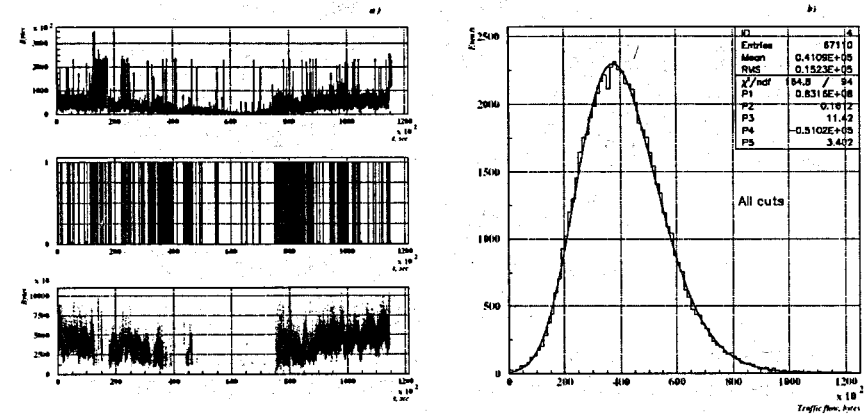


Figure 3: a) top-down: time series of the network traffic aggregated at the level of 1 sec; moments of structural changes; "filtered" traffic corresponding to a day-time, b) statistical distribution for a daytime traffic and its approximation by a log-normal function

JINR local area network

Today the JINR Local Area Network (JINR LAN) comprises 6785 network elements (4506 in the year 2003). The network and computing capacities was continuously growing, what leads to certain difficulties both in the management and in providing the reliable operation of LAN. To overcome these problems, some work on creating a reliable and protected high-speed JINR LAN was done, and the provision of the fail-safe work of the JINR LAN is the primary goal of the network service at LIT.

The JINR Gigabit Ethernet LAN became available for users in March 2004. The gigabit networking structure of JINR integrates the hardware and software facilities providing the basis of the JINR network and information structure, upon which the mentioned infrastructure is built up and developed.

The LIT activity on the creation of the Gigabit Backbone was awarded the first prize of the JINR for 2005.

Major hardware modernization of the JINR LAN central telecommunication node was finally accomplished in 2007. Figure 4 shows the current scheme of the JINR Gigabit Network.

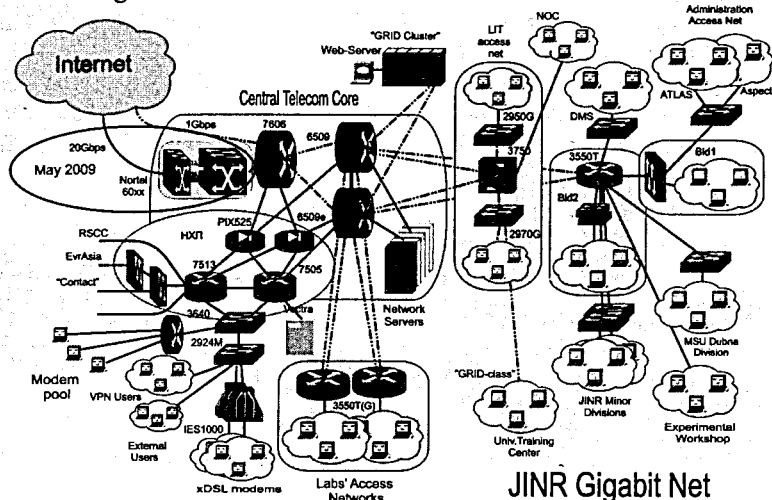


Figure 4: Current scheme of the JINR Gigabit Network

The gigabit networking structure solves the following tasks:

- integration of all JINR computer resources into a unified informational environment;
- organization and provision of remote network access to informational – computational resources for various groups of JINR users, to informational resources of Russian and foreign scientific centres;
- creation of a unified information space for the JINR staff for data exchange between the Institute's subdivisions and between subdivisions and JINR Directorate;
- provision of services of remote access to JINR resources from home PCs of JINR staff members.

In 2009, the JINR LAN included 3645 users, more than 1500 users of mail.jinr.ru service and about 1300 users of remote access VPN. Over 120 network nodes are in round-the-clock monitoring (gateways, servers, basic switchboards, etc.). 15 servers are supported and over 40 user inquiries are served per shift. Introduction of new spam protection systems allowed us to fix about one million spam – messages a day for central mail-servers.

JINR network security is gained with the implementation of hard- and software products in the network infrastructure. To protect the computing and informational servers, users' workstations and active routing and switching network equipment at JINR, the industry-approved AAA approach – Authentication, Authorization, and Accounting was used. During the last two years, the

AAA system has been successfully gradually integrated into LIT-developed product IPDB – a network data base with multiple features of monitoring and control based on IP-addresses. The IPDB became the main tool for the network and system administrators to maintain their current administrative tasks.

JINR information and computing complex

The development of the JINR Central Information and Computing Complex is based on a distributed model of data processing and data storage. Such a model is in agreement with the modern concept of establishing information processing centres for scientific research based on Grid-technologies. The requirements of the LHC experiments stimulate the development of a global Grid-infrastructure, together with the resource centers of all the cooperating organizations. This is of primary concern for such large research centers as the JINR. To reach the objectives in the effective processing and analysis of the experimental data, steep increase in the performance of the CICC cluster and disk space is needed.

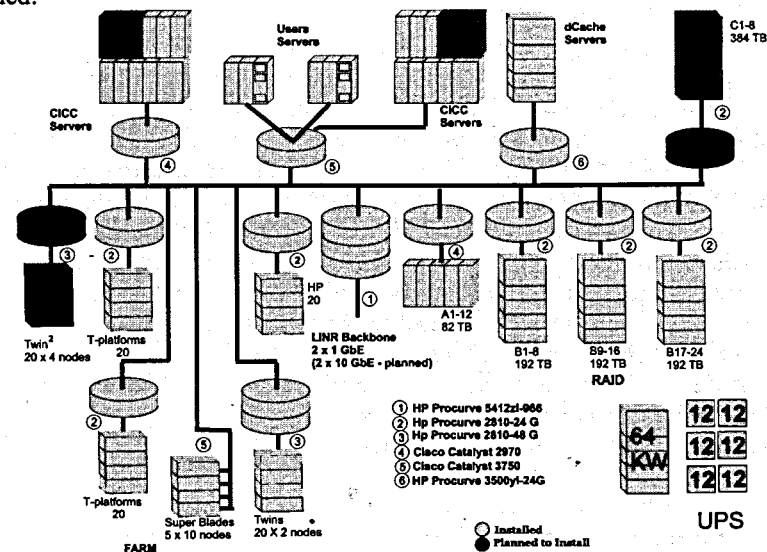


Figure 5: Current structure of the CICC

During the years 2003-2009, the total performance and mass storage resources of the CICC were substantially increased. Starting from 4.3 kSPI95 and disk space 7.7 TB for the time being, the total CICC installed computing power is 2400 kSI2K and the disk storage capacity is 500 TB. Figure 5 shows the current structure of the CICC.

Two essential constraints are to be satisfied by the CICC configuration. First, the floating point computation runs at the CICC cluster have to accommo-

date requests for traditional sequential applications, parallel computing applications, as well as Grid applications launched within various virtual organizations. Second, its upgrade by new acquisitions is always subject to tough financial constraints. As a consequence, new modules are acquired from vendors offering the best price of the day, resulting in heterogeneous computing cluster and disk storage area structures, with home made implementations of the various module interconnects and of the supervising software.

The performance assessment of parallel clusters and its comparison with those of the best computers in the world using the same processor interconnect in the TOP500 list is a good criterion of validation of the quality of the home-made implementations.

The lessons learned from the first results on the measured performance of the JINR-CICC configuration at the end of 2007 [Gh. Adam, S. Adam, A. Ayriyan, E. Dushanov, E. Hayryan, V. Korenkov, A. Lutsenko, V. Mitsyn, T. Sapozhnikova, A. Sapozhnikov, O. Streltsova, F. Buzatu, M. Dulea, I. Vasile, A. Sima, C. Visan, J. Busa, I. Pokorny: *Romanian Journal of Physics*, Vol. 53, No. 5-6, (2008) pp. 665-677; Gh. Adam, S. Adam, A. Ayriyan, V. Korenkov, V. Mitsyn, M. Dulea, I. Vasile: *Romanian Journal of Physics*, Vol. 53, No. 9-10, (2008) pp. 985-991] have been followed by practical home-made optimization of the exchange of information in-between the modules of the extended configuration at the end of 2008 [A. Ayriyan, Gh. Adam, S. Adam, V. Korenkov, A. Lutsenko, V. Mitsyn: *Proceedings of the XII Advanced Computing and Analysis Techniques in Physics Research, PoS(ACAT08)054, 5*]. The results reported in this last paper pointed to relative performance levels at those of the TOP500 computers in the world, with GigaBit Ethernet and InfiniBand interconnects respectively. The learned lessons have been used during the further JINR CICC development in 2009. This contributed to the prominent position of our system within the LHC virtual organizations.

As a result of the implemented optimizations, the system works efficiently for all three abovementioned categories of jobs. Within the Russian Data Intensive Grid (RDIG) consortium, which comprises, besides the CICC JINR, 14 Russian computing centres, our cluster has covered more than 40% of the RDIG share to the LHC projects since 2007.

All the CICC computing and data storage resources can be used both locally and globally (for distributed computations in the WLCG/EGEE grid infrastructure and in the Russian Data Intensive Grid (RDIG) consortium) for all the projects the JINR physicists participate in. The system software has been tuned in an optimal way, providing maximal use of computing resources and the most universal and secure access to the data storage. The *Torque* batch system and the *Maui* scheduler are used for computing resources allocation and accounting.

Basically, access to data is provided by the *dCache* system and partially via NFS. The access to the general-purpose software and user home catalogs is

provided by the *Andrew File System* (AFS). The *Kerberos5* system is used for registration and authentication of local users.

JINR Grid-segment

The task of the development of the JINR Grid-segment and increase of the productivity of the JINR CICC is connected with the requirements of experiments in HEP and relativistic nuclear physics as well as with further applications of Grid-technologies and distributed computing in nuclear physics and nanotechnologies. The LIT has been involved in this process in full since 2003. The LHC project, that is unique on scales of obtained data and from the viewpoint of computer technologies, provides processing and analysis of experimental data using the Grid. The analytical review in the journal "Open Systems" prepared in cooperation with SRINP MSU and SSC RRC "Kurchatov Institute" is devoted to the analysis of work performed in this area at JINR and the Russian centres [Ilyin V., Korenkov V., Soldatov A.: *Open Systems*. 2003. No.1. P.56-66].

One of the LHC projects, the LHC Computing Grid (LCG) foresees design and creation of a distributed information and computing system. The main aim of these project was building a distributed hierarchical architecture of the system of regional centers. The latter provides specific software for each of four LHC experiments (detector response simulation, particle track reconstruction, etc.) as well as general-purpose packages for all experiments, the so-called "general solutions" (programs for automatic installation of applications in the regional centers, hierarchical file systems for data storage in robotized libraries with automatic pumping of demanded files to disk arrays, etc.).

In 2006 the LCG project entered a new phase, i.e. the construction of a global infrastructure of the regional centers intended for processing, storage and analysis of data for a moment of the accelerator start-up. The project is referred to as WLCG (Worldwide LHC Computing Grid). A three-power agreement MoU was signed between CERN, Russia and JINR on participation in this project and obligations on its financing by Russia and JINR in September 2007.

The JINR Grid-segment based on CICC provides for the WLCG environment basic services, special services, PS and testing infrastructure, and software for VOs.

In frames of JINR participation in the WLCG an important work has been done. During all the years JINR participated in Pre-Challenge production for ALICE, ATLAS, and CMS.

In the context of the ATLAS, ALICE and CMS computing requirements for the running phase of the experiment, LIT JINR provides:

- the computing and data storage resources in corpore;
- data replication to the JINR data storage system in the accordance with the JINR physicists' requests (data volumes of TiBs size);
- participation in the Monte-Carlo physical events mass production in accordance with the JINR physicists scientific program.

As a result, all the necessary conditions for data distributed analysis have been provided at the JINR computing center (grid-site JINR-LCG2). It makes possible for the JINR physicists to take a full-fledged part in the experiment at its running phase.

The LIT JINR team has gained a successful experience in the successful development and design of Grid monitoring and accounting systems [<http://rocmon.jinr.ru:8080/>] for Russian Data Intensive Grid (within the EGEE project) and other projects.

The main point is to find scalable, reliable and interoperable solutions for Grid monitoring and accounting, which will be used in real Grid projects. The major part of the results obtained within this work is available as ready-to-use software packages. Tracking the current services' state as well as the history of state changes allows rapid error fixing, planning future massive productions, revealing regularities of Grid operation and many other things. Alongside with monitoring, the accounting is an area which shows how the Grid is utilized by virtual organizations and individual users.

A group of LIT specialists takes an active part in the LHC Dashboard development (grid monitoring system for the LHC experiments) (<http://dashboard.cern.ch/>) [*J. Andreeva, S. Belov, I. Sidorova, E. Tikhonenko et al.: J.Phys.Conf.Ser.119:062008, 2008*]. Quite an interesting option for visualization of monitoring such a distributed system is a mapping Grid infrastructure objects, processes and events on a geographic map. By using geographic information system (GIS) applications like Google Earth, quite an informative and visually attractive representation is achieved. It shows graphically real time animated information covering data flows for both Monte-Carlo Production and Tier0 export, and additional information about running jobs on the ATLAS, CMS, LHCb and Alice (jobs only) grids. [*B. Gaidioz, R. Rocha, S. Mitsyn, M. Devesas Campos: http://dashb-cms-job-devel.cern.ch/dashboard/doc/guides/service-monitor-gearth/html/user/index.html*]

GridCom – the software package for maintenance of automation of access to means of distributed system Grid (for tasks and data) was developed. Work is confirmed by a patent [*Galaktionov V.V.: GridCom, Grid Commander: a graphic environment for work with tasks and data. The certificate on official registration of the computer program №2006614056*].

The LIT participates in the LCG Monte-Carlo Events Data Base (MCDB) creation. MCDB is a special knowledge base designed to keep event samples for the LHC experimental and phenomenological community. It is possible to make an automated Monte-Carlo simulation chain, partially based on usage of HepML [<https://twiki.cern.ch/twiki/bin/view/Main/HepML>] and LCG MCDB [<http://mcdm.cern.ch>]. This way is officially used in the CMS experiment [*S. Belov et al.: Comput. Phys. Commun., Vol. 178, No. 3, 2008, p. 222*].

The LIT home-made events database and repository of generators were also created. Dynamical home-page <http://hepweb.jinr.ru> has been created for

testing Monte Carlo Generators of physical processes. The page also allows one to estimate the main properties of hadron-nucleus and nucleus-nucleus interactions (includes FRITIOF model, HIJING model, and tools for Glauber and Reggeon theories calculation). The server HEPWEB was integrated into the Dubna-Grid environment.

One of the most significant results of the team TDAQ ATLAS at LIT for 2003-2009 was the participation in the development of the project TDAQ ATLAS at CERN and preparation for the startup of ATLAS experiment. The results of the work on creation of the multilevel distributed computing systems of data processing within the TDAQ ATLAS project were reported to international conferences [*M. Abolins et al.: Computing in High Energy and Nuclear Physics 2007, 13:978-0230-63017-8, TRIUMF, Victoria, Canada; A. Corso-Radu et al.: CHEP 2009, 17th International Conference on Computing in High Energy and Nuclear Physics, Prague, Czech Republic; Ciovanna Lehman Miotto et al.: TIPP09 Tsukuba, Japan, KEK, Tsukuba, Japan*]. The concept of the system of remote access in real time (SRART) developed in a context of the analysis and discussion of the opportunities of remote access for monitoring the processes of data acquisition and processing of ATLAS experiment, was repeatedly discussed at the seminars both at CERN and at JINR and reported to the XXII International Symposium on Nuclear Electronic and Computing (NEC ' 2009) in Varna, Bulgaria [*Kotov V.M., Rusakovich N.A.: NEC 2009 - XXII International Symposium on Nuclear Electronics&Computing, JINR, CERN, INRNE BAN (Sofia, Bulgaria), Varna, Bulgaria*]. The SRART system is a component of the general data processing system integrating the computing resources in the unified global distributed Grid-system of processing, storing and transferring data received within LHC experiments at CERN. Research and analysis of the methods and approaches of the remote access developed for LHC experiments and the choice on their basis of a technique of integration of the JINR-developed SRART prototype into the infrastructure of experiments, correspond to world level in the development of large-scale information projects on the creation of geographically distributed Grid-system of data processing and provide required conditions for participation of scientists from the JINR-participating countries in the present-day studies on nuclear physics and particle physics. The work was supported by the Federal Agency on Science and Innovations of Russia, state contract No. 02.514.11.4083 and reported to the resulting conferences [http://www.sci-innov.ru/icatalog_new/entry_68452.htm; http://www.sci-innov.ru/icatalog_new/entry_79275.htm].

The aim of the Laboratory was to develop an educational program on Grid technologies for scientists from JINR and the Member States, students, PhD-students and the teaching staff of Dubna High schools. All over the years reported for the user support to stimulate their active usage of WLCG resources, special courses, lectures, and trainings (<http://www.egee-rdig.ru/rdig/user.php>) were organized. The educational, training and testing grid infrastructure was

built-up and is intensively used for a wide range of tasks related to the training of different groups in grid-technologies as well as research and development activities in this field [V.V. Korenkov, N.A. Kutovskiy: *Open Systems*. 2009. No.10. P.48-51].

The JINR Grid-segment (JINR-LCG2) now is ready for data processing at the LHC start. Now JINR LCG site is the best site in RDIG and our contribution in the year 2009 to ALICE, ATLAS and CMS is shown on Fig.6.

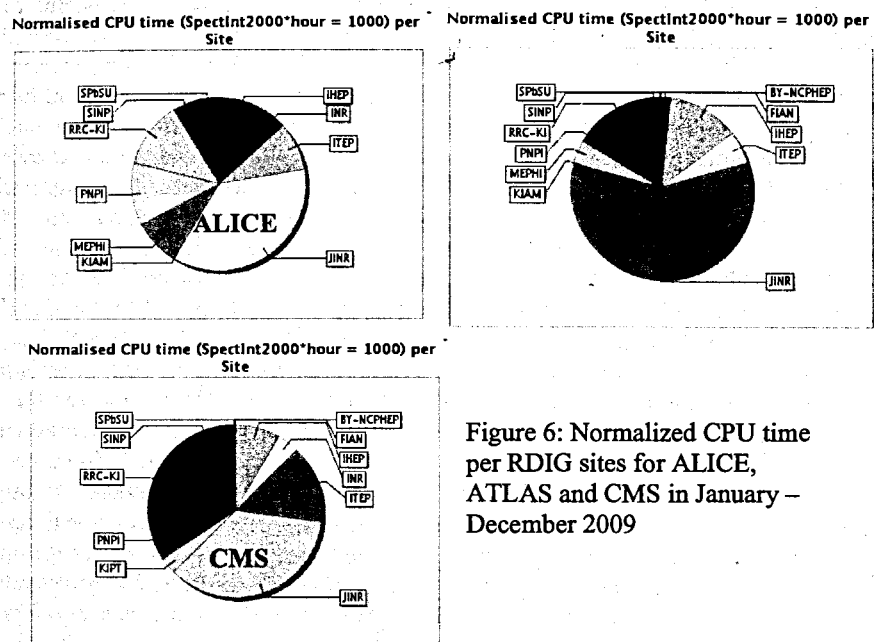


Figure 6: Normalized CPU time per RDIG sites for ALICE, ATLAS and CMS in January – December 2009

Information and software support of the research underway at JINR

The traditional provision of information, algorithmic and software support of the JINR research-and-production activity included a large spectrum of activities both at LIT and JINR levels. This activity traditionally includes development and support of informational WWW/FTP/DBMS-servers of JINR and LIT, creation and storage of electronic documents related to the JINR scientific and administrative activity, development, creation and support of information web-sites of workshops and conferences, administration and support of web-sites of JINR subdivisions and various conferences in a hosting mode as well as support, modernization and maintenance of computer systems of administrative databases (in cooperation with STD AMS JINR). Besides, work should be noted on supporting the automated system of bibliographic data processing for the JINR Library (in cooperation with the JINR Library) and conducting the LIT library

with books and manuals for CICC users as well as support of the retrieval system as to ordering books available in the library, creation and support of electronic editions (web-sites) dedicated to the outstanding scientists of the Institute.

The portal technology is a key performance technology for all modern investigation projects due to the large-scale and world-wide nature of the most scientific and especially experimental collaborations in nuclear and particle physics. This technology is actively used at LIT in the process of development and creation of various information systems with web-interfaces. For instance, for the All-Russia 10th jubilee conference on digital libraries RCDL'2008, a web-portal <http://rcdl2008.jinr.ru> has been created with a possibility of both the participants registration and interactive work with conference materials: sending of thesis and reports via the website, on-line referring, etc. Also, for the portals of journals PEPAN and PEPAN Letters <http://pepan.jinr.ru> to function, a specialized interface has been designed for the authors, editors, referees and administrators providing interconnections with the databases of the journals. Work on the maintenance and modernization of the portal is in progress at present.

Special software for design, development and support of special and general-purpose web-servers based on modern portal service-oriented technologies has been worked out. No special Internet technology knowledge or skills are required to use this software. This software includes a specific database and a set of adjustable web-interfaces (online participant registration, abstract submission and upload of presentation files, keeping news, forming mailing lists, etc.). For example, the following web-sites were developed using this software: <http://www.jinr.ru> – site of the JINR, <http://newuc.jinr.ru/> - site of the JINR University Centre; sites of many conferences under JINR supervision.

Another traditional direction of LIT activity is a consecutive development and support of the library JINRLIB as well as support of program libraries developed by other science centres and organizations and information and technical help to users. The modernization of CICC software and its installation in a 64-bit variant required a full recompilation of programs from JINRLIB library. The full information on the JINR program libraries is available at the specialized WWW-server <http://www.jinr.ru/programs/> and in LIT Information Bulletins.

Work is in progress on the re-engineering technology for distributed computing in a local area network [A.P. Sapozhnikov, A.A. Sapozhnikov, T.F. Sapozhnikova: *Proceedings of the 6th International Conference "Large-Scale Scientific Computing"*, Springer, LNCS, Vol. 4818, pp.700-707].

MATHEMATICAL SUPPORT OF JINR STUDIES

The development of mathematical models of the processes under study and methods for data analysis is an integral part of the research conducted both in experimental and theoretical physics and in other fields of science and technology. The results mainly depend on the adequacy of the mathematical model to the process under study and on the efficiency of applied methods of data analysis.

This trend covers a wide spectrum of investigations under way at JINR according to the JINR Topical Plan for Research and International Cooperation, in high-energy physics, nuclear physics, solid state physics, condensed matter physics, biophysics, information technologies and is fulfilled in close cooperation with all JINR Laboratories.

This activity comprises the following main directions:

- development of new approaches and methods for simulation of physics processes and for experimental data analysis;
- creation of methods and numerical algorithms for simulation of magnetic systems and charged particle beam transport;
- creation of software and computer complexes for experimental data processing and their application in JINR experiments;
- development of numerical schemes and software for simulation of complex physical systems;
- development of methods, algorithms and programs of computer algebra.

Software and computer complexes for experimental data processing

This direction includes creation of large software complexes of general use and program complexes of "local" use (restricted, for instance, by aims of a specific experiment). In particular, this includes programs for simulation of experiments, different frameworks and real-time systems. Some more attractive examples are listed below.

Basing on the work on application of the wavelet analysis to data treatment for small-angle neutron scattering [Soloviev A.G., Litvinenko E.I., Ososkov G.A., Islamov A.H., Kuklin A.I.: *Nuclear Inst. and Methods in Physics Research, A.* 502/2-3 (2003) 498-500] the SAS program aimed to process the spectra measured on YuMO spectrometer was developed and maintained for all those years [<http://www.winfo.jinr.ru/programs/jinrlib/sas/indexe.html>].

Very popular program Gluplot – data plotting package was also included in the JINR Program Library. It was originally intended both as a graphical library and a standalone program, which would allow scientists and students to visualize data. Gluplot handles both curves (2D) and surfaces (3D) [A.G. Soloviev: <http://www.jinr.ru/programs/jinrlib/gluplot/indexe.html>] and was used for visualization of freezeout-surface and applied for visualization of particles distribution in the MPD detector (Fig.7).

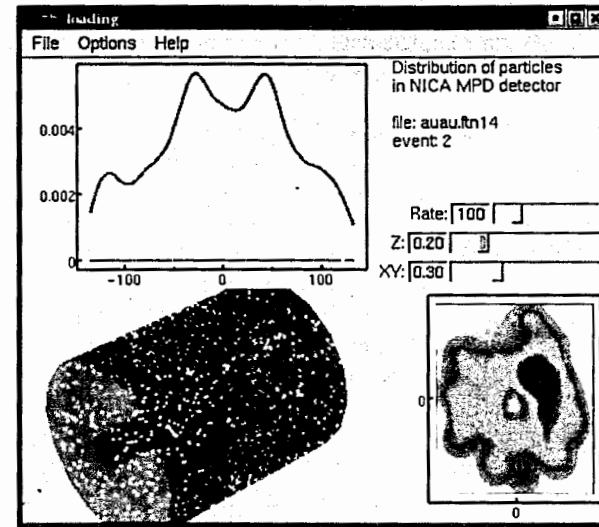


Figure 7: Visualization of particles distribution in the MPD detector by Gluplot

The basic element method (BEM) for decomposition of the algebraic polynomial via one cubic and three quadratic parabolas (basic elements) is developed within the 4-point transformation technique. Representation of the polynomial via basic elements gives a lever at solving various tasks of applied mathematics. So, in the polynomial approximation and smoothing problems the BEM presentation allows one to reduce the computational complexity of algorithms and increase their stability for error by choosing the internal relationship structure between variable and control parameters. This research work based on the autotracking of knots for piecewise cubic approximation was carried out at LIT. An original method and an algorithm for automatic tracking have been developed on the basis of the criterion of uniformity of the third derivative of the cubic model and a recurrent calculation of estimates of this derivative. A real time oriented adaptive algorithm for knot detection has been developed. On the basis of the algorithm, MS Visual C# components and Windows application APCA (Autotracking Piecewise Cubic Approximation) were developed. The efficiency of the algorithm is confirmed by the results of its application to the approximation of complex curves and real data [Dikoussar N.D., Török Cs.: *Mathematical Modelling.* 2006. V. 18, No. 3. P. 23-40; N. Dikoussar, Cs. Török: "Kybernetika", V. 43, No. 4, pp. 533 - 546, 2007; Dikusar N., *JINR Preprint, P11-2009-123, Dubna, 2009. Submitted to the "Mathematical modeling"*].

Instead of the elegant function (Lagrange-Sylvester formula) depending on badly-defined arguments (eigenvalues) suggest was a cumbersome function

(hypergeometrical series) depending on well-defined arguments (matrix invariants). The function of matrix implies the sum of any formal finite or infinite power series with arbitrary coefficients [V.N. Robuk: *Nuclear Instruments and Methods in Physics Research, Section A*, v. 534, pp. 319-323, ISSN:0168-9002, Elsevier, 2004].

Geant4 is a software toolkit for simulation of passage of particles through matter. It is used by a large number of experiments and projects in a variety of application domains, including high energy physics, astrophysics and space science, medical physics and radiation protection. Two string models for the simulation of high energy final states were implemented into Geant4: the Quark Gluon String (QGS) model proposed by N.S. Amelin (JINR) and et al., and the Fritiof (FTF) model essentially improved by V.V. Uzhinsky (LIT, JINR) in the last few years. The Geant4 implementation of the Fritiof model includes a simulation of hadron-hadron interactions with 2-particle final states, a separate simulation of diffraction dissociation, the kinky string production needed for a correct description of inclusive spectra of hadrons in the central region; the reggeon cascade model for simulation of particle cascading into nuclei; accounting the particle formation time; calculation of residual nuclei momenta and excitation energies. The parameters of the components were carefully tuned using the CERN-HERA data base and the HARP collaboration experimental data on hadron-nucleus interactions. All these activities allow a successful modeling of hadron-nucleon and hadron-nucleus interactions starting from 3 GeV projectile energy with a smooth transition to the low energy Geant4 models – the Bertini model, and the binary cascade model (BIC). The implementation is accessible in the last version 4.9.3 of the Geant4 package. It is included in some newly created Physics Lists. The model has no discontinuity in the calorimeter responses in the energy range 8 – 12 GeV. [Geant 4 release 9.3 (2008), <http://geant4.cern.ch/support/ReleaseNotes4.9.3.html>; V. Uzhinsky, J. Apostolakis, G. Folger, V.N. Ivanchenko, M.V. Kossov, D.H. Wright, *Eur. Phys. J.*, C61 (2009) 237.]

Methods and tools for modeling physical processes and experimental data analysis in particle and relativistic nuclear physics

A study of the ME1/1 outer part spatial resolution was made with CRAFT08 and CRAFT09 data of the CMS experiment at CERN. The CSCs operated at the nominal anode-cathode voltage of 3.0 kV. For data processing, only 6-hit tracks were used. At the solenoid field of $B=3.8$ T, the layer spatial resolution is $113 \mu\text{m}$. It has been shown that without the field the spatial resolution degrades to $157 \mu\text{m}$. In addition, a study of the layer spatial resolution across the CSC sensitive area was made. The 6-layer spatial resolution for the CSCs in both endcaps was calculated. From these data the ME1/1 outer part spatial resolution (per CSC) is estimated to be $50 \mu\text{m}$. This is better than the Muon TDR requirement for the ME1/1 spatial resolution ($75 \mu\text{m}$) [CMS Collaboration, *Perform-*

ance of the CMS Cathode Strip Chambers with Cosmic Rays, CMS-CFT-09-011, arXiv:0911.4992, JINST_019T_1109, 2009].

As part of the work on designing a magnetic system for the CBM experiment, series of calculations have been performed for various versions of the superconducting dipole magnet [E.A. Matyushevsky, P.G. Akishin, V.S. Alfeev, A.V. Alfeev, V.V. Ivanov, E.I. Litvinenko, A.I. Malakhov: *CBM-note-2008-00, 2008*]. Figure 8 gives the results of modeling one of the variants of the dipole magnet and calculation of the distribution of the main component of the magnetic field at the median plane of the magnet carried out with the computer code TOSCA.

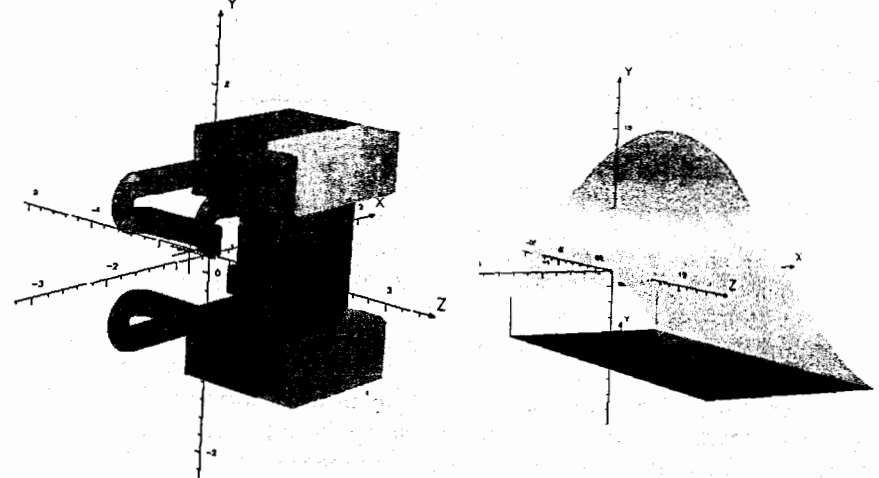


Figure 8: Model of $\frac{1}{2}$ of superconducting dipole magnet for CBM (left) and the magnetic fields (right) calculated with the computer code TOSCA

For solving the problem of the magnetic field optimization of a 4T dipole magnet with circular aperture a mathematical method to minimize sextupole and higher order non-linearities to the tolerable values by variation of angular coil turn position was developed and a numerical simulation for a 2D part magnetic field was performed [P.G. Akishin, A.V. Butenko, A.D. Kovalenko, V.A. Mikhaylov: *Proceedings of EPAC 2004, TUPLT1021390, pp139-1392*; A.G. Akishin, A.V. Butenko, A.D. Kovalenko, V.A. Mikhaylov: *PEPAN Letters, 2006, v.3, n.2(131), pp.105-110*].

A new projection formulation with respect to field vectors for solving the nonlinear magnetostatic problems has been suggested. In contrast to the known projection potential formulations the suggested approach does not require a numerical differentiation to compute a magnetic field. It gives a local classical solution of the problem with the second-order finite elements, permits an effective accuracy control of the approximate solutions and a simple comparison of

computed and measurement results. The unique solvability and the convergence of Galerkin approximations have been proved under standard conditions [Zhidkov E.P., Yuldashev O.I., Yuldasheva M.B.: *Bulletin of Peoples' Friendship University of Russia, Series Applied and Computer Mathematics*, 2003, vol. 2, No. 2, pp. 104-115].

When solving 3D nonlinear magnetostatics problems by the finite element method, generalized approximated solutions are obtained. Within the general theory of the method, the definition of miscalculation is based on the verification of approximation of the exact solution to the problem which is unknown as a rule. The formulas have been derived which link the error of finite-element problems to easily computed local characteristics. These characteristics are residuals for the equations of the problem realized in a classical sense. The developed method was applied to the calculus of a model of the dipole magnet in the PANDA experiment [Zhidkov E.P., Yuldashev O.I., Yuldasheva M.B.: *Bulletin of Peoples' Friendship University of Russia, Series Applied and Computer Mathematics*, 2005, vol. 4, N 1, pp. 93-101].

The LIT team actively participates in the elaboration of the CBM set-up in GSI (Darmstadt). Efficient methods of event reconstruction have been suggested for the experiment prepared as the expected enormous multiplicity of generated particles and the heterogeneous magnetic field make the event reconstruction considerably complicated. In particular, some approaches to track reconstruction in the STS-detector and algorithms of track recognition in the TRD-detector have been developed, algorithms of finding Cherenkov rings in the RICH-detector have been offered, the particle momentum determination methods have been elaborated, various methods for particle identification using the TRD-detector have been developed, etc. Work is in progress on optimization of the geometry of the installation and development of methods of extracting "useful" events. In order to perform an efficient analysis, fast tracking algorithms are essential and a parallel tracking algorithm for the muon detector was developed. A number of very efficient software modules for event reconstruction have been proposed by LIT specialists and included in the CBM framework [A. Airiyan, S. Baginyan, G. Ososkov, C. Hoehne: *Tver Univ.Herald*, No. 17(45), 2007, pp. 15-26; E.P. Akishina, T.P. Akishina, V.V. Ivanov, A.I. Maevskaya, O.Yu. Denisova: *PEPAN Letters*, V.5, No.2(144), 2008, pp. 202-218; T.P. Akishina, O.Yu. Denisova, V.V. Ivanov, S.A. Lebedev: *PEPAN Letters*, V.6, No.2(151), 2009, pp. 245-259; S.A. Lebedev, G.A. Ososkov: *PEPAN Letters*, V.6, No.2(151), 2009, pp. 260-284].

In frames of the hadronic energy reconstruction problem in the ATLAS combined calorimeter a new class of procedures [J. Budagov, J. Khubua, Yu. Kulchitsky, P. Tsiareshka, N. Russakovich, V. Shigaev: *ATL-TILECAL-PUB-2008-006*, CERN, Geneva, Switzerland] based on Artificial Neural Networks (ANN) technique have been developed for reconstruction of energy losses (EDM) in the LAr/Tile dead materials of the ATLAS calorimeter. The ANN pro-

cedures exploit as their input vectors the information content of different sets of variables (parameters) which describe particular features of the hadronic shower of a particular event in the calorimeter. Thorough investigations with MC events for combined test beam 2004 setup (CTB04) have shown that application of these ANN procedures allows one to reach 40% reduction of the EDM reconstruction error compared to the conventional procedure ($EDM_{conv} = C\sqrt{E_{LAr}E_{HCl}}$) used in the ATLAS collaboration.

A hybrid method of pion energy reconstruction in the ATLAS calorimeter was developed and investigated [Yu. Kulchitsky, P. Tsiareshka, J. Khubua, N. Russakovich, V. Shigaev, V. Vinogradov: *ATL-TILECAL-PUB-2008-009*, CERN]. This method uses the modified Local Hadronic Calibration scheme for pion energy reconstruction (developed in DLNP) and the ANN procedure (developed in LIT) for reconstruction of energy losses in the dead material of the calorimeter. The hybrid method was tested on the ATLAS CTB04 data in the range 10 – 350 GeV, $\eta = 0.25$. The test results have shown that an essential improvement of the pion energy resolution is obtained. For example, at 250 and 350 GeV beam energies the pion energy reconstruction error was reduced by 19.7% and 18.8% respectively. As a result, the projected energy resolution for hadrons in the ATLAS calorimeter was increased by the hybrid method. At present, the resolution obtained by the new method is the best one as compared to the results obtained by other methods (more than 2 times better than in the Hadronic Calibration method used by the Oxford-Stockholm group and about 1.5 better than the H1 method results for CTB04 obtained by the Pisa group). The results of the development and investigation were presented at the Hadronic Calibration Meeting (CERN, February 2008).

Particle physics

New experimental data on fluctuations in the multiplicities of negatively charged particles in interactions of light nuclei (p , d , ${}^4\text{He}$, ${}^{12}\text{C}$) with carbon nuclei at a momentum of 4.2 A GeV/c in 4π geometry were analyzed using the Dubna cascade evaporation model, FRITIOF model, and UrQMD 1.3 model. The dependence of the fluctuations on nuclear collision centrality is theoretically described without any exotic assumptions. According to the FRITIOF model, the dependence of the multiplicity fluctuations on the collision centrality is to a large extent governed by fluctuations in the number of "wounded" nucleons that are associated with the experimental observation conditions. The data indicate a behavior similar to that earlier observed by the NA49 Collaboration. The NA49 Collaboration data are also described [A.S. Galoyan, E.N. Kladnitskaya, V.V. Uzhinsky: *JETP Lett.* 86 (2008) 630].

The Monte Carlo event generator of the interactions – DPM generator [Technical Progress Report for PANDA: FAIR-ESAC/Pbar/Technical Progress Report, 2005, GSI, Darmstadt; Physics Performance Report for PANDA: FAIR/PANDA/Physics Book, 2009, GSI, Darmstadt; arXiv:0903.3905 (2009)]

was created. It is grounded on the ideas of the Dual-Parton or Quark-Gluon model. The model combines ideas of the Dual-Topological Unitarization, Regge phenomenology and Quark model. Special efforts were undertaken to calculate cross sections of various reactions – string junction annihilation, one and two quarks annihilation, two string creation as a refraction of the pomeron exchange, and low mass diffraction dissociation. The generator uses Kaidalov's structure functions of baryons and quark/di-quark fragmentation functions. Exact simulation of the elastic antiproton – proton scattering due to coulomb and strong interactions was included too [A. Galoyan, J. Ritman, A. Sokolov, V. Uzhinsky: *arXiv:hep-ph/0809.3804* (2008)]. The generator correctly reproduces multiplicities and compositions of charged particles and inclusive distributions in the energy range of 2 – 20 GeV. Its results are close to the predictions of the UrQMD model, but the code operates much faster than the UrQMD one. The generator has been used for obtaining the results presented in the main PANDA documents. It is applied now for design of various PANDA detectors.

The chiral phase transition at finite temperature T and baryonic chemical potential μ_B within the framework of the SU(3) Nambu-Jona-Lasinio (NJL) model was studied. The QCD critical end point (CEP) and the critical line at finite T and μ_B are investigated: the study of physical quantities, such as the baryon number susceptibility and the specific heat in the vicinity the CEP, will provide relevant information concerning the order of the phase transition. The class of the CEP is determined by calculating the critical exponents of those quantities [Pedro Costa, C.A. de Sousa, M.C. Ruivo, Yu.L. Kalinovsky: *Phys.Rev. D70:116013*, 2004; Pedro Costa, C.A. de Sousa, M.C. Ruivo, Yu.L. Kalinovsky: *Phys. Lett. B647* (2007) p.431-435].

The quarkonium production in a field-theoretical setting was reconsidered and was shown that the lowest-order mechanism for heavy-quarkonium production receives in general contributions from two different cuts. The first one corresponds to the usual colour-singlet mechanism. The second one has not been considered so far. It was treated in a gauge-invariant manner, and new 4-point vertices were introduced, suggestive of the colouroctet mechanism. These new objects enable to go beyond the static approximation. It was shown that the contribution of the new cut can be as large as the usual colour-singlet mechanism at high transverse momentum for J/ψ . In the ψ' case, theoretical uncertainties are shown to be large and agreement with data is possible [J.P. Lansberg, J.R. Cudell, Yu.L. Kalinovsky: *Phys.Lett. B633:301-308*, 2006].

The description of the η - and η' - mesons in the Dyson-Schwinger approach has relied on the Witten-Veneziano relation. The refereed article explores the consequences of using instead its generalization recently proposed by Shore. On the examples of three different model interactions, it was find that irrespective of the concrete model dynamics, the proposed Dyson-Schwinger approach is phenomenologically more successful in conjunction with the standard Witten-Veneziano relation than with the proposed generalization valid in all orders in

the $1/N_c$ expansion [D. Horvatic, D. Blaschke, Yu. Kalinovsky, D. Kekez, D. Klabucar: *Eur.Phys.J. A38:257-264*, 2008].

The 'cusp'-effect in the decay $K^+ \rightarrow \pi^+ \pi^0 \pi^0$ observed in the NA-48/2 experiment was analyzed in frames of the quantum mechanical approach. It was shown how incorporate the electromagnetic effects in the amplitude of this decay (Fig.9) and work out the relevant expressions valid both above and below the two charged pion production threshold $M = 2m$. Comparison of the theoretical results with experiment show that this approach provides quantitative explanation of these effects (Fig.10) [S.R. Gevorkyan, A.V. Tarasov, O.O. Voskresenskaya: *Phys. Lett. B* 2007, V. 649, p. 159].

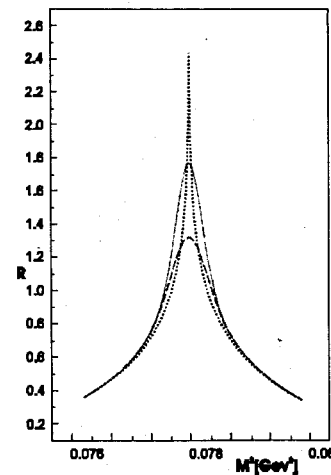


Figure 9: The dependence of the ratio $R(\%) = (|T_c|^2 - |T|^2) / |T|^2$, where the amplitude T_c accounts the various electromagnetic effects, on the square of invariant mass of charged pions

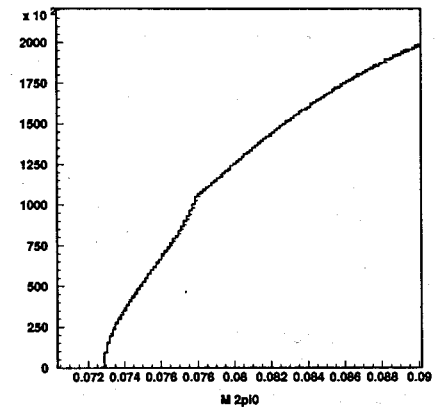


Figure 10: The 'cusp'-effect in the $K \rightarrow 3\pi$ decay. Comparison of the theoretical results (dashed line) with experiment (black line)

A resummation of the perturbative series for the amplitude of lepton pair production in the nucleus-nucleus collisions is performed on the basis of the Watson theorem and hypothesis of the infrared stability. An explicit expression for this amplitude valid up to terms of ninth order in finite structure constant is obtained. [O.O. Voskresenskaya, A.N. Sissakian, A.V. Tarasov, H.T. Torosyan: *Physics of Elementary Particles and Atomic Nuclei, Letters*, 2007, Vol. 4. No. 1(137), pp. 36-41.] The Fermi-Watson theorem is generalized to the case of two coupled channels with different masses. The proposed approach is applied to a final state interaction in K_{e4} decay, but can be easily generalized for the arbitrary two channel task. The impact of the considered effect on the pions phase

shifts is essential in the vicinity of the charged pions production threshold and can be crucial for scattering lengths extraction from experimental data on K_{e4} decay [S.R. Gevorkyan, A.N. Sissakian, A.V. Tarasov, H.T. Torosyan, O.O. Voskresenskaya: arXiv:hep-ph/0704.2675].

Nowadays, a lattice approach to quantum field theory supported by computational possibilities of modern parallel supercomputers made possible an effective and reliable investigation of long-standing nonperturbative problems of high energy physics from the first principles. Joint investigation of gluon and ghost Green functions (propagators) within the frameworks of quantum chromodynamics (QCD) was performed. Gluon and ghost propagators as well as their dressing functions have been computed on very large lattices, thus reaching the deep infrared region of momenta (Fig. 11).

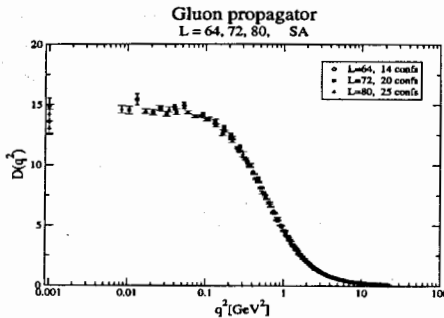


Figure 11: The gluon propagator from different lattices sizes for $\beta=5.7$. The data points drawn at $q^2=0.001$ represent the zero-momentum gluon propagator $D(0)$

The recent results of reported investigations lead to essential modification of existing knowledge on infrared behaviour of gluon and ghost dressing functions and, as a result, of running coupling constant, which were based on the so-called “scaling” solution to the well-known set of Dyson-Schwinger equations. Results of lattice simulations [A. Sternbeck, E.-M. Ilgenfritz, M. Müller-Preussker, A. Schiller, I.L. Bogolubsky: hep-lat/0610053. Journal-ref: PoS (LAT2006) 076; E.-M. Ilgenfritz, M. Müller-Preussker, A. Sternbeck, A. Schiller, I. L. Bogolubsky: hep-lat/0609043, Braz. J. Phys. 37 (2007) 193; I.L. Bogolubsky, E.-M. Ilgenfritz, M. Müller-Preussker, A. Sternbeck: ArXiv:0710.1968, PoS (LATTICE-2007) 290; I.L. Bogolubsky, E.-M. Ilgenfritz, M. Müller-Preussker, A. Sternbeck: Phys.Lett.B 676, 69-73, 2009; arXiv:0901.0736] proved to be in agreement with the so-called “decoupling” solution of Dyson-Schwinger set of equations. Quite recently the nonperturbative analog of the multiplicative renormalisation has been successfully applied for the gluon dressing function in the lattice approach [I.L. Bogolubsky, E.-M. Ilgenfritz, M. Müller-Preussker, A. Sternbeck: PoS (LATTICE 2009) 237, arXiv:0912.2249].

Based on the calculations of A.I. Machavariani, the measurement of the magnetic moments of the Δ^+ resonance with Cristal Ball detector at MAMI in Mainz (Germany) in the reaction $p(e, e') \Delta^+ \rightarrow \gamma \pi^0 p \rightarrow 3\gamma p$ was performed. An ana-

lytical connection between the magnetic moments of the Δ -resonances and the magnetic moments of the nucleons has been found. It has been shown that this formula is the same within the field-theoretical formulations with and without the quark-gluon degrees of freedom [A.I. Machavariani, A. Faessler: Phys. Review C72 (2005) 024002; A.I. Machavariani, A. Faessler: arXiv:0809.1303 and 0804.1322 (submit. in Phys Rev. C and J. Phys. G.)].

Within the scope of Bianchi type-I cosmological model the role of nonlinear spinor field in the evolution of the Universe is investigated. It is shown that depending on the choice of nonlinearity, a spinor field can give rise to a singularity-free Universe [B. Saha, T. Boyadjiev: Phys. Rev. D. v.69, 124010 (2004); B. Saha: Phys. Part. Nuclei. v.37 Suppl. 1, S13 (2006)], accelerate the isotropization process and explain the late time acceleration of the Universe [B. Saha: Phys. Rev. D. v. 74, 124030 (2007); B. Saha: Grav. Cos. v. 12. N. 2-3 (46-47), 215 (2007); B. Saha: Phys. Part. Nuclei. v.40. N. 5, 612 (2009)]. It is shown that in presence of a viscous fluid the model provides an exact solution only for some specific choice of viscosity [B. Saha, Mod. Phys. Lett. A. v. 20, 2127 (2005)] and gives rise to Big Rip singularities [B. Saha, V. Rikhvitsky: Physica D, v.219, 168 (2006); B. Saha: J. Phys. A: Math. Theor. V. 40, 14011 (2007); B. Saha: J. Math. Phys. V. 49, 112502 (2008); B. Saha: Phys. Part. Nuclei. V. 40. N. 5, 656 (2009)]. The role of magneto fluid and cosmic string in the evolution of the Universe is also investigated [B. Saha: Astro. Phys. Space sci. v. 299, 149 (2005); B. Saha, M. Visinescu: Astro. Phys. Space sci., v. 315, 99 (2008); B. Saha, V. Rikhvitsky and M. Visinescu: Central European Journal of Physics v. 8(1), 113 (2010)]. The role of usual dark energy such as cosmological constant, quintessence and Chaplygin gas in the evolution of the Universe is also investigated [B. Saha: Chinese J. Phys. V. 43, 1035 (2005); B. Saha: Astro. Phys. Space sci. v. 302, 83 (2006)]. Quintessence with a modified equation of state was introduced to eliminate the problem of eternal acceleration [B. Saha: Int. J. Theor. Phys. v.45, 983 (2006)].

A program package for computing energy values, reaction matrix and corresponding wave functions in a coupled-channel approximation of the adiabatic approach has been created. From the mathematical point of view, this approach is well known as Kantorovich method. In this approach, a multidimensional Schrödinger equation is reduced to a system of the coupled second order ordinary differential equations on the finite interval with homogeneous boundary conditions of the third type. The resulting system of radial equations which contains the potential matrix elements and first-derivative coupling terms is solved using high-order accuracy approximations of the finite element method. [O. Chuluunbaatar, et al.: Comput.Phys.Commun., 177 (2007), pp. 649–675; O. Chuluunbaatar, et al.: Comput.Phys.Commun., 179 (2008) 685–693; O. Chuluunbaatar, et al.: Comput.Phys.Commun., 178 (2008) 301–330; O. Chuluunbaatar, et al.: Comput.Phys.Commun., 180 (2009) 1358–1375; O. Chuluunbaatar, et al.: Physics of Atomic Nuclei, 71 (2008) 871–878].

Program packages KANTBP, POTHMF, ODPEVP [O. Chuluunbaatar, et al: *Comput.Phys.Commun.*, 177 (2007) 649-675; O. Chuluunbaatar, et al.: *Comput.Phys.Commun.*, 179 (2008) 685-693; O. Chuluunbaatar, et al.: *Comput.Phys.Commun.*, 178 (2008) 301-330; O. Chuluunbaatar, et al.: *Comput.Phys.Commun.*, 180 (2009) 1358-1375] for computing energy values, reaction matrix and corresponding wave functions in a coupled-channel approximation of the adiabatic approach have been created. From the mathematical point of view, this approach is well known as Kantorovich method. In this approach, a multi-dimensional Schrödinger equation is reduced to a system of coupled second-order ordinary differential equations in the finite interval with homogeneous boundary conditions of the third type. The program package is used for the numerical analysis of the mathematical models for the physical processes: photoionization and recombination of a hydrogen atom in a magnetic field (Fig.12) [O. Chuluunbaatar, et al.: *J. Phys. A* 40, (2007) 11485-11524.]; channeling problem for charged particles produced by confining environment [O. Chuluunbaatar, et al.: *Physics of Atomic Nuclei* 72, (2009) 768-778]; adiabatic approach to the problem of a quantum well with a hydrogen-like impurity [A.A. Gusev, et al: *Physics of Atomic Nuclei* 73, (2010) 331-338].

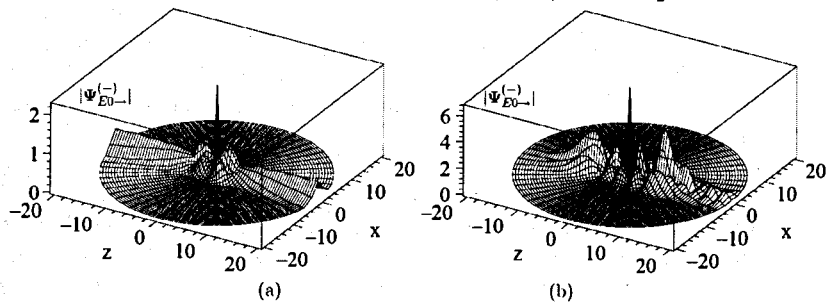


Figure 12: Profiles of total wavefunctions of a hydrogen atom in a magnetic field $|\Psi_{E_{0\rightarrow}}^{(-)}|$ in the xz plane of the continuous spectrum with the states with the energy (a) correspond to the resonance transmission, while those with the energy (b) correspond to the total reflection

Nuclear physics

An approach to calculate the microscopic optical potential (OP) with the real part obtained by a folding (double folding) procedure and with the imaginary part inherent in the high-energy approximation (HEA) has been developed to study numerically a mechanism of elastic and inelastic nucleus-nucleus scattering at energies of tens of MeV/nucleon. A numerical scheme and a computer code have been done. The considered OP does not include free parameters but depends on the nuclear density distributions and nucleon-nucleon scattering amplitude.

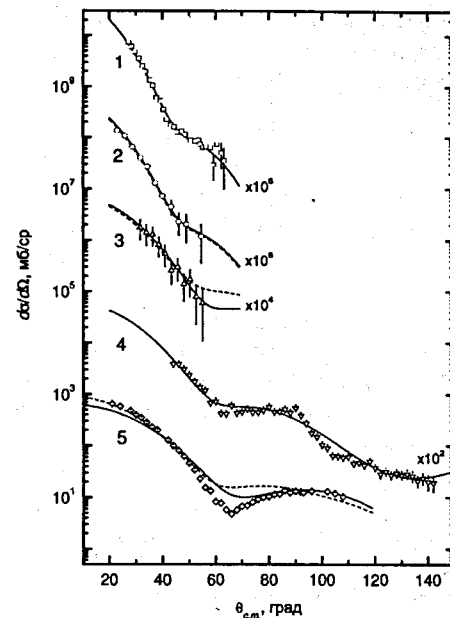


Figure 13: The ${}^8\text{He}+p$ elastic scattering cross sections at different energies calculated using renormalized microscopic optical potential and the LSSM density of ${}^8\text{He}$

The calculated OP is applied to calculate differential and total reaction cross sections in the frame of high-energy approximation as well as on the basis of the standard computer codes (e.g. DWUCK, ECIS) for a numerical solving of a corresponding Schrödinger equation. Calculations of elastic and inelastic scattering were made for ${}^{16}\text{O}+{}^{40}\text{Ca}$, ${}^{90}\text{Zr}$, ${}^{208}\text{Pb}$; a numerical microscopic analysis of the exotic nuclei ${}^{6,8}\text{He}$ structure was performed on the basis of the numerical reproducing of the total cross sections ${}^{6,8}\text{He}+{}^{28}\text{Si}$ and differential cross sections ${}^{6,8}\text{He}+p$ (Fig. 13). The numerical results have a good agreement with experi-

mental data at the energies of 10-100 MeV/nucleon [V.K. Lukyanov, E.V. Zemlyanaya, B. Slowinski: *Bul. Rus. Acad. Sci. Phys.* Vol.68, no.2, 2004, pp.181-186; V.K. Lukyanov, E.V. Zemlyanaya, S.E. Massen, Ch.C. Moustakidis, A.N. Antonov, G.Z. Krumova: *IJMPPE*, V.13, N.3, 2004, pp.573-584; V.K. Lukyanov, E.V. Zemlyanaya, K.V. Lukyanov: *Physics of Atomic Nuclei*, Vol. 69, No. 2, pp.240-254, 2006; V.K. Lukyanov, Z. Metaweï, E.V. Zemlyanaya: *ArXiv: nucl-th/0508015*; *ЯФ*, т.69, вып.8, 2006, pp.1409-1415; K.M. Hanna, K.V. Lukyanov, V.K. Lukyanov, Z. Metaweï, B. Slowinski, E.V. Zemlyanaya: *PEPAN Letters*, 6[135], 2006, pp.105-112; K.B. Лукьянов, Е.В. Земляная, В.К. Лукьянов, И.Н. Кухтина, Ю.Э. Пенионжскевич, Ю.Г. Соболев: *Изв. РАН сер. физ.*, Т.72, вып. 3, 2008, с.382-386; K.V. Lukyanov, V.K. Lukyanov, E.V. Zemlyanaya, A.N. Antonov, M.K. Gaidarov: *Eur. Phys. J. A*, 2007, V.33, p.389-400; K.B. Лукьянов, Е.В. Земляная, В.К. Лукьянов, З. Метавей, Б. Словинский, К.М. Ханна: *Изв.РАН. сер.физ.*, 2008, Т.72, вып.3, с.387-391;

V.K. Lukyanov, E.V. Zemlyanaya, K.V. Lukyanov, D.N. Kadrev, A.N. Antonov, M.K. Gaidarov, S.E. Massen: *Physical Review C*, 2009, V.80, 2, 024609].

The quasiparticle-phonon model approach provides a fairly satisfactory description of the existing properties of the 0^+ states observed in large abundance in many deformed nuclei (^{158}Gd , ^{168}Er , $^{228,230}\text{Th}$, ^{232}U) [N. Lo Iudice, A.V. Sushkov, N.Yu. Shirikova: *Phys. Rev. C* 70, 064316 (2004); N. Lo Iudice, A.V. Sushkov, N.Yu. Shirikova: *Phys. Rev. C* 72, 034303 (2005); D. Bucurescu et al., *Phys. Rev. C* 73, 064309 (2006), *Yad. Fizika*, vol.70, No.8, 2007, 1380-1387; A.I. Levon, G. Graw, Y. Eisermann, R. Hertenberger, J. Jolie, N.Yu. Shirikova, A.E. Stuchbey, A.V. Sushkov, P.G. Thirolf, H.-F. Wirth, N.V. Zamfir: *Phys. Rev. C* 79, 014318 (2009)].

The Cascade Evaporation Model and the Quantum Molecular Dynamic (QMD) model for the description of the spallation reaction have been developed [A. Polanski: *In Progress in High Energy Physics and Nuclear Safety, NATO Science for Peace and Security Series B: Physics and Biophysics*, 2009, p. 319]. The experimental data on energy and multiplicity distributions of protons and momentum spectra of deuterons emitted in the reactions of pions and protons with the energy ranging from 2.5 to 200 GeV with several nuclei are compared to the calculations based on two different model approaches: the CASCADE code and the tube-fireball (TF) model [A. Polanski, B. Slowinski, A. Wojciechowski: *PEPAN Letters*, 4, 3(139), 417-427, 2007].

The design of the accelerator driven subcritical assembly needs a thorough evaluation of build-up of long-lived radioactivity and changes in elemental composition in target materials. A spectrum of particles and residual nuclide mass and charge distributions in reactions of protons and neutrons with heavy targets (^{238}U , ^{208}Pb , ^{207}Pb and ^{206}Pb) has been calculated using the QMD+GEM model [A. Polański, S. Petrochenkov, V. Uzhinsky: *Radiation Protection Dosimetry*, 116(1-4), 582-584, 2005]. The paper [A. Polański, S. Petrochenkov, W. Pohorecki: *Nucl. Instr. Meth. A*, 562, 2, 764-766, 2007] presents the study of polonium production in bismuth foils placed in a lead target. Proton-induced production of residual nuclei ^{206}Po , ^{207}Po , ^{208}Po , ^{209}Po , ^{210}Po in ^{209}Bi foils placed in a lead target irradiated by 660 MeV protons was calculated. A comparison with the calculated spatial distribution of polonium production using CASCADE, MCNPX code and experimental results has been performed.

The paper [Pohorecki W., Horwacik T., Janczyszyn J., Taczanowski S., Bamblevski V.P., Gustov S.A., Mirokhin I.V., Molokanov A.G., Polanski A.: *Radiation Protection Dosimetry*, 115(1-4), 630-633, 2005] presents experimental results of measurement long-lived radioactivity in target materials. Two types of detectors were irradiated inside and/or on the surface of a cylindrical Pb targets irradiated with 660 MeV protons: activation detectors made of typical target materials - Pb, Bi, and track detectors with heavy metal radiators - Bi, Pb, Au, W, Ta. Activities of several radionuclides in Pb and Bi samples were determined. In the track detectors, the density of tracks and their size distributions were meas-

ured. Their spatial distributions were then compared with respective values obtained in the calculations made with the use of CASCADE, FLUKA and MCNPX codes.

The Monte Carlo modeling of the Experimental Accelerator Driven System (ADS), which employs a subcritical assembly and a 660 MeV proton accelerator operating at the DLNP JINR, was performed [A. Polański, S. Petrochenkov, V. Shvetsov, W. Gudowski, P. Selborg: *Nucl. Instr. Meth. A*, 562, 2, 879-882, 2007; W. Gudowski, V. Shvetsov, A. Polanski, C. Broeders: *Nucl. Instr. Meth. A*, 562, 887, 2006] The mix of oxides $\text{PuO}_2 + \text{UO}_2$ MOX fuel designed for the reactor will be adopted for the core of the assembly. The design of the experimental subcritical assembly in Dubna (SAD) is based on the core with a nominal unit capacity of 30 kW (thermal). This corresponds to the multiplication coefficient $K_{\text{eff}} = 0.95$ and the accelerator beam power of 1 kW. The subcritical assembly has been modeled by CASCADE and MCNPX code for different options of the target and fuel elements.

The radiation fields and the effective dose at the Subcritical Assembly (SAD) have been studied with the Monte Carlo code MCNPX [P. Selborg, A. Polanski, S. Petrochenkov, A. Lopatkin, W. Gudowski, V. Shvetsov: *Nuclear Instruments and Methods in Physics Research, Section A*, 550, 313-328, 2005; P. Selborg, A. Lopatkin, W. Gudowski, V. Shvetsov, A. Polański: *Radiation Protection Dosimetry*, 116(1-4), 449-453, 2005]. By separating the radiation fields into a spallation-induced and a fission-induced part, it was shown that the protons and neutrons with energy higher than 10 MeV, originating exclusively from the proton-induced spallation reactions in the target, contribute for the entire part of the radiation fields and the effective dose at the top of the shielding. Consequently, the effective dose above the SAD reactor system is merely dependent on the proton beam properties and not on the reactivity of the core.

The essence of the work [A.A. Polanski, A.N. Sosnin: *Transport Theory and Statistical Physics*, ISSN:0041-1450, eISSN:1532-2424, 37, 5 - 7, 576 - 588, 2008] was to show a comparison of fluxes of secondary particles emitted from the subcritical assemblies being irradiated with proton beams. These assemblies, at present under investigation SAD, with $k_{\text{eff}} = 0.95-0.98$ and the "Energy plus Transmutation" with $k_{\text{eff}} = 0.24$. Monte Carlo modeling are used to forecast production of secondary proton and neutron fluxes in different subcritical assemblies under irradiation with protons in the energy range from 660 MeV up to 2.0 GeV. Neutron and proton spectra emitted from the surface of these assemblies are calculated using a version of the codes CASCADE and MCNPX. The data obtained and the methods developed were used to calculate the parameters of isotope transmutation in various nuclear reactions.

Condensed matter physics, biological research and nanotechnology

A new delay equation is introduced to describe the punctuated evolution of complex nonlinear systems which describe the development of biological species, human societies, growth of organizations, development of technology, and so on. A detailed analytical and numerical investigation provides the classification of all possible types of solutions for the dynamics of the population development. [V.I. Yukalov, E.P. Yukalova, D. Sornette: *Physica D* 238 (2009) 1752-1767.]

Contrary to widespread beliefs, it was shown that no noticeable collective effects, such as superradiance, can appear in molecular magnets, being caused by electromagnetic spin radiation. Spin superradiance can arise in molecular magnets only when these are coupled to a resonant electric circuit. [V.I. Yukalov, E.P. Yukalova: *Laser Phys. Lett.* 2 (2005) 302-308.]

The separated form factor (SFF) method has been developed to study a structure of lipid vesicle populations on the basis of the small angle neutron scattering (SANS). This approach allows one to simulate the neutron scattering length density across the bilayer using various models of internal bilayer structure and hydration. Numerical investigation of the structure and properties of polydispersed populations of unilamellar vesicles has been performed for one-, two- and four-component lipid systems in dependence of temperature. The parameters of the DMPC vesicle population and the internal structure of the lipid bilayer have been investigated in the liquid, ripple and gel phases. A vesicle shape is shown to be changed from a spherical form in the liquid phase to elliptical form in the ripple and gel phases for vesicles prepared via extrusion through pores with the diameter 500 Å. Parameters of the bilayer structure (membrane thickness, thickness of the hydrophobic core, hydration) have been reproduced. A numerical analysis of the SANS data has been performed in the frame of SFF approach to investigate a structure and properties of the ceramide 6 based four-component membrane of unilamellar vesicles at temperatures of 32°C and 60°C. Calculations have shown that the nanostructure of the bilayer of unilamellar highly hydrated vesicular systems is not the same as the nanostructure of the flat bilayer with low hydration. At a small scattering angle region, one observes a deviation of numerical results and experimental data that indicates a strong short-range interaction of vesicles between each other leading to generating cluster structures that confirms the chain-flip transition phenomenon [E.V. Zemlyanaya, M.A. Kiselev, Aswal Vinod: *Crystallography Reports*, V.49, Suppl. 1, 2004, pp.S136-S141; M.A. Kiselev, E.V. Zemlyanaya, V.K. Aswal, R.H.H. Neubert: *European Biophysics Journal*, Vol. 35, No. 6, 2006, pp. 477 - 493; E.V. Zemlyanaya, M.A. Kiselev, J. Zbytovska, L. Almasy, V.K. Aswal, P. Strunz, S. Warteig, R.H.H. Neubert: *Crystallography reports*, 2006, Vol.51 Suppl. 1, pp.S22-S26; M.A. Kiselev, E.V. Zemlyanaya, N.Y. Ryabova, T. Hauss, S. Dante, D. Lombardo: *Chemical Physics*, Vol.345, 2008, pp.185-190; E.V. Земляная, M.A. Киселев, P. Нойберт, И. Кольбрехер, В.Л. Аксенов: *Поверхность: рентгеновские, синхротронные и нейтронные исследования*, №11, 2008, с.14-19].

The Bayesian approach to the automatic adaptive quadrature stemmed from the idea to formulate conditioning diagnostics able to enhance the output reliability of the local quadrature rules [Gh. Adam, S. Adam, N.M. Plakida: *Computer Physics Communications*, Vol. 154, (no. 1), (2003) pp. 49-64]. The derivation of a hopefully complete set of rules, based on the Bayesian inference, was reported [Gh. Adam, S. Adam: *Numerical Methods and Programming: Advanced Computing (RCC MSU) 2009*, Vol.10, pp. 391-397 (<http://num-meth.srcc.msu.ru>)].

The capacity of the effective two-band Hubbard model to predict both the exchange and the spin-fluctuation superconducting pairing mechanisms in cuprates was shown in [N.M. Plakida, L. Anton, S. Adam, Gh. Adam: *JETP Vol. 97 No. 2 (2003) pp. 331-342*] based on an approximate solution of the Dyson equation of the Green function. The rigorous result [Gh. Adam, S. Adam: *J. Phys. A: Math. Theor.*, Vol. 40, (2007) pp. 11205-11219] reported the mean field Green function solution derived using exclusively symmetry properties satisfied by the underlying spin lattice.

Under the occurrence of *isolated local integrand irregularities* (singular or turning points, finite jumps), the discretization of the initial integration domain within a binary subrange tree scheme placing the offending null-measure points at the subrange boundaries yield the right numerical solution provided accurate boundary locations and precise integrand lateral limits are derived. To this aim, associated thin boundary layer problems are formulated. These are correctly solved [Gh. Adam, S. Adam, A. Tifrea, A. Neacsu: *Romanian Reports in Physics*, Vol. 58, no. 2, (2006) pp. 107-122; Gh. Adam, S. Adam: *Physics of Particles and Nuclei Letters*, Vol. 5, No. 3, (2008) pp. 269-273] provided the involved computations over neighbouring machine number distances *preserve the ordering relationships* valid within the field of the real numbers.

The reduction of the order of both the normal and anomalous correlation functions involving the singlet hopping pointed to an accurate mean field description in terms of pairs of fermionic operators. This study allowed the proof [Gh. Adam, S. Adam: *Journal of Optoelectronics and Advanced Materials*, Vol.10, No. 7, July 2008, pp. 1666-1670] of the *spin-charge separation* both for normal (charge-spin) and anomalous (singlet-spin) correlations. Correction factors coming from three-site terms produced by the order reduction procedure have been explicated [S. Adam, Gh. Adam: *Romanian Journal of Physics*, Vol. 53, No. 9-10 (2008) pp. 993-999].

The scrutiny of the evidence coming from experimental data as well as the mathematical reformulation of the mean field eigenvalue problem in normal form pointed [Gh. Adam, S. Adam: *Romanian Journal of Physics*, Vol.54, No.9-10 (2009)] to the need to renormalize the hopping part of the Hamiltonian of the model with a factor proportional with the doping concentration in the low-doping limit.

In cooperation with the University of Cape Town, the particle-like excitations of nonlinear dispersion matter have been studied in the frame of models of condensed matter theory and nonlinear optics based on the nonlinear Schrödinger equation (NLS). A numerical technique and a corresponding computer code were developed for numerical continuation of bright and dark solitons of the damped-driven NLS equation at the plane of parameters of damping and driving. New classes of localized solutions have been found (bound states of stationary solitons; time-periodic two-soliton complexes), bifurcations and stability of them were classified in the both cases of focusing and defocusing nonlinearity [I.V. Barashenkov, S.R. Woodford, E.V. Zemlyanaya: *Phys. Rev. Lett.* Vol.90, No. 5 (2003) 054103; I.V. Barashenkov, S.R. Woodford, E.V. Zemlyanaya: *Progress of Theoretical Physics Supplement*, No.150, 2003, pp.317-320; I.V. Barashenkov, E.V. Zemlyanaya: *SIAM Journal of Applied Mathematics*, V.64, N.3, p.800, 2004; E.V. Zemlyanaya, I.V. Barashenkov, S.R. Woodford: *Lecture Notes in Computer Sciences*, Vol.3401 (2005) Springer, p.590; I.V. Barashenkov, S.R. Woodford, E.V. Zemlyanaya: *Phys. Rev. E*, Vol.75 (2007) 026603; E.V. Zemlyanaya, I.V. Barashenkov, N.V. Alexeeva: *Lecture Notes in Computer Sciences*, Vol. 5434 (2009) pp.139-150; E.V. Zemlyanaya, A.N. Alexeeva: *TMP*, V.159, No.3, 2009, pp.536-544].

For the first time the existence of exotic breather-type asymptotics was proved for solutions of non-standard linear differential equations $U_{tt} = U_{xx} + U_{ttt}$, $U_{tt} = U_{xx} + ibU_{xxx} + U_{ttt}$, $U_{tt} = U_{xx} + ibU_{ttt} + U_{ttt}$, $U_{tt} = U_{xx} - U_{xxxx}$ with discontinuity initial data. The problem had been stated by Academician N.S. Bakhvalov, coauthor of the book N.S. Bakhvalov, G.P. Panasenko "Averaging processes in periodic media". These equations arise in studying wave motion in periodic stratified media. These solutions have very oscillating behaviour and therefore couldn't be obtained by standard numerical computations. Asymptotic solutions when $t \rightarrow \infty$ are proved. The results obtained are very important for the fundamental research as well as for numerous applications especially in the mechanics of composite materials [S.I. Serdyukova: *Dokl. Ross. Akad. Nauk*, 2003, vol.389, no.3, pp.305-309; S.I. Serdyukova: *Dokl. Ross. Akad. Nauk*, 2007, vol.415, no.3, pp.310-314; S.I. Serdyukova: *Dokl. Ross. Akad. Nauk*, 2009, vol.427, no.1, pp.17-23].

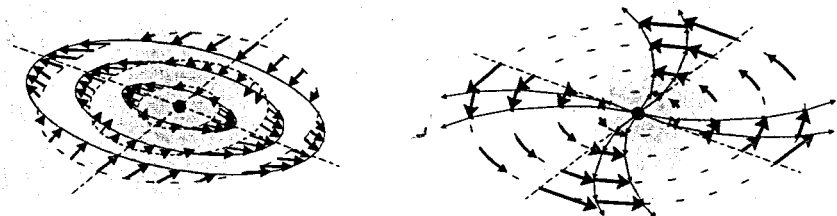
In frames of cooperation with FLNR with the purpose of description of the evolution of thermoelastic waves arising in materials exposed to a pulse beam of accelerated ions, a system of three equations in partial derivatives has been proposed for the first time within a mathematical thermal spike model. A comparative analysis of numerical solutions to the obtained system of equations and a system of two classical equations of thermoelasticity has been performed. For the first time, a modified mathematical model of thermal spike has been suggested that takes into account the motion of a projectile ion inside the material at its irradiation and the mathematical thermal spike model is applied to research of thermal processes in the double-layered structure Ni (2 micron)/W

exposed to bismuth ions. For the first time a 3D thermal spike model is applied to research of thermal processes in anisotropic materials exposed to high-energy heavy ions [I.V. Amirkhanov, A.Yu. Didyk, E.V. Zemlyanaya, I.V. Puzynin, T.P. Puzynina, N.R. Sarker, I. Sarhadov, V.K. Semina, Z.A. Sharipov, A. Hofman: *PEPAN Letters*, 2006, V.3, No.1(130), pp.63-75; I.V. Amirkhanov, A.Yu. Didyk, N.R. Sarker, I. Sarhadov, V.K. Semina, Z.A. Sharipov, A. Hofman: *PEPAN Letters*, 2006, V.3, No.5(134), pp.80-91; I.V. Amirkhanov, A.Yu. Didyk, I.V. Puzynin, V.K. Semina, Z.A. Sharipov, A. Hofman, Yu.N. Cheblukov: *PEPAN*, 2006, V.37, No.6, pp.1592-1644; И.В. Амирханов, А.Ю. Дидык, Д.З. Музафаров, И.В. Пузынин, Т.П. Пузынина, Н.Р. Саркар, И. Сархадов, З.А. Шарипов: *Поверхность*, 2008, №5, с.1-10; И.В.Амирханов, И.В.Пузынин, Т.П.Пузынина, З.А.Шарипов: *Вестник ТвГУ. Серия: Прикладная математика*, 2009, (12), с. 17-27].

Local electronic and magnetic properties of transition metal oxides $Ba_2V_3O_9$, $RBaCo_2O_{5.5}$ ($R = Ho, Gd$) and $LaCoO_3$ were calculated with the use of ab initio methods of quantum-chemical cluster computations [B. Schmidt, V. Yushankhai, L. Siurakshina, P. Thalmeier: *Eur. Phys. J. B* 2003, V. 32, P. 43-47; *Journal of Magnetism and Magnetic Materials* 2004, V. 272-276, P.673-675; L. Siurakshina, B. Paulus, V. Yushankhai: *Eur. Phys. J. B* 2008, V.63, P. 445-450, 2008]. Quantitative descriptions for low-temperature magnetic behaviour of $Ba_2V_3O_9$, and experimentally observed magnetic phase transitions in $RBaCo_2O_{5.5}$ ($R = Ho, Gd$) and $LaCoO_3$ were given. The complex oxides under consideration as well as their chemically related compounds are used as materials for micro-electronic devices of new generation and basic elements for solid oxides fuel cells (SOFC) in hydrogen energetics.

Based on the principles of classical hydrodynamics and Newtonian gravity, the theory of hydrogravity, formulated in the manner of hydromagnetic theory, is developed to account for the gravitational effect of global pulsations of a star on the motions of the ambient gas-dust interstellar medium. The main feature of the proposed theory consists in introduction of a new equation, $-\dot{\mathbf{g}} = 4\pi G\mathbf{J} + \mathbf{rot}[\mathbf{g} \times \mathbf{J}] / \rho = 0$, which discovers coupling between Newtonian gravitational field intensity, \mathbf{g} , and material current $\mathbf{J} = \rho\mathbf{v}$, where ρ is density of gas-dust interstellar medium and \mathbf{v} is a velocity of displacements in this medium. The analytic derivation of the dispersion relation for canonical gravity waves at the free surface of an incompressible in viscid liquid is presented, illustrating practical usefulness of the proposed approach, heavily relying on the concept of classical gravitational stress introduced long ago by Fock and Chandrasekhar, and accentuating the shear character of this mode. Computed in the long-wavelength approximation, the periods of these gravity-driven shear modes, referred to as quasistatic modes of hydrogravity, are found to be proportional to periods of the gravity modes in the neutron star bulk. Given that collective oscillations of cosmic plasma in the wave under consideration should be accompanied by electromagnetic radiation and taking into account that only the radio waves of

this radiation can freely travel through the galactic gas-dust clouds, it is conjectured that the considered effect of gravitational coupling between seismic vibrations of a neutron star and fluctuations of the galactic interstellar medium should manifest itself in the radio range of pulsar spectra [Bastrukov S., Molodtsova I., Podgany D., Papoyan V., Yang J., Murray D.: *JETP* 99 (2004) 449-459].



These pictures give us a geometrical illustration of material displacements in circumstellar hydrogravity waves generated by a spheroidally (left picture) and torsionally (right picture) oscillating neutron star.

A new approach, based on the cellular automata, for modeling the structure dynamics of UO_2 at different cross-section average burns-up is suggested. Micrographs of the surface with magnification of 1250X were used in the study. It is shown that the approach provides efficient means for modeling the surface structure dynamics both at local and global levels and the pores formation. Fractal analysis shows that the fractal properties of the surface strongly depend on the radiation damage of the material. Some evidences for existence of self-organization process in UO_2 at high average burn-ups were obtained [I. Antoniou, E.P. Akishina, V.V. Ivanov, B.F. Kostenko, A.D. Stalios: *Chaos, Solitons and Fractals*. 2003. V.18; I. Antoniou, V.V. Ivanov, B.F. Kostenko, J. Spino, A.D. Stalios: *Chaos, Solitons and Fractals*. 2004. V.19. PP.731-737].

When calculating the thermodynamic properties and three-dimensional structures of macromolecules, such as proteins, one should have an efficient algorithm for computing the solvent-accessible surface area and its gradient of macromolecules. A new analytical method has been proposed for this purpose. In the proposed algorithm the transformation is considered that maps the spherical circles formed by intersection of the atomic surfaces in three-dimensional space onto the circles on a two-dimensional plane, and the problem of computing the solvent-accessible surface area is reduced to the problem of computing the corresponding curve integrals on the plane. The algorithm is suitable for parallelization. Testing on many proteins as well as a comparison to the other analogous algorithms have shown that our method is accurate and efficient [Sh. Hayryan, Ch.-K. Hu, J. Skrivanek, E. Hayryan, I. Pokorny: *Journal of Computational Chemistry*, 26 (2005), 4, 334-343].

If calculating the solvation energy of proteins, the hydration effects, drug binding, molecular docking, etc., it is important to have an efficient and exact algorithms for computing the solvent accessible surface area and the ex-

cluded volume of macromolecules. A Fortran package based on the new exact analytical methods for computing volume and surface area of overlapping spheres has been presented. In the considered procedure the surface area and the volume are expressed as surface integrals of the second kind over the closed region. Using the stereographic projection the surface integrals are transformed to a sum of double integrals which are reduced to the curve integrals. MPI Fortran version is described as well. The package is also useful for computing the percolation probability of continuum percolation models [J. Busa, J. Dzurina, E. Hayryan, Sh. Hayryan, Ch.-K. Hu, J. Plavka, I. Pokorny, J. Skrivanek, M.-Ch. Wu: *Computer Physics Communications* 165 (2005) 59-96].

During 2007-2009 in cooperation with colleagues from the Institute of Protein, RAS, Institute of Biophysics of Cell RAS and Institute of Theoretical and Experimental Biophysics RAS, LIT researchers implemented a project named «Molecular cartography of DNA, RNA and proteins in the distributed computing environment». New algorithms have been developed and a software complex has been designed to construct molecular surfaces of spiral molecules of double-chained DNA (B-form), RNA (A-form) as well as spiral molecules of extended proteins or else their fragments (for example, the widespread alpha-spiral form). Such a unified method of mapping the extended structures of nucleic acids and proteins was realized for the first time. It essentially supplements the known methods of 3D computer simulations of molecular structures. The designed software complex allows one to perform computations, construction and analysis of the maps of relief and functional color of the molecular surfaces on the basis of corresponding spatial structures of high atomic resolution. Besides, it provides a way for massive computations of the maps of molecular surfaces within the high-performance distributed computing environment of CICC JINR. This approach reduces more than 10-20 times the time required for research on the structures of proteins and nucleic acids as compared to the manual routine work with the use of ordinary graphic interfaces.

As a result, an effective method has been obtained, and it was applied for study of recognition, analysis and classification of binding regions of functionally important protein-DNA complexes. The proposed method allows introducing the novel data bank of the molecular-surfaces and electrostatic potentials for all transcription factors of homeodomains from wide class of species. On these bases very fast analysis of recognition areas and types of their classification became possible for the large set of protein-DNA complexes presented in international protein data bank PDB (Protein Data Bank) and nucleic acid data bank NDB (Nucleic Acid Database). The project was implemented under support of the Russian Foundation for Basic Research [Yu.N. Chirgadze, V.V. Ivanov, R.V. Polozov, V.S. Sivozhelezov, V.A. Stepanenko, P.V. Zrellov: *Proceedings of the 3rd Intern. Conf. Distributed Computing and Grid-Technologies in Science and Education, JINR, Dubna, D11—2008-176, 2008, pp. 233-237; T.P. Akishina, P.V. Zrellov, V.V. Ivanov, R.V. Polozov, V.S. Sivozhelezov: Proceedings of the 3rd Intern.*

Conf. Distributed Computing and Grid-Technologies in Science and Education, JINR, Dubna, D11—2008-176, 2008, pp. 221-224; Иванов В.В., Зрелов П.В., Полозов Р.В., Катаев А.А., Сивозжезов В.С.: В сб. Ядерная физика и нанотехнологии. Дубна: ОИЯИ, 2008, стр. 293-311; Chirgadze Y.N., Zheltukhin E.I., Polozov R.V., Sivozhelezov V.S., Ivanov V.V.: J. Biomol. Struct. Dyn. 2009 26(6) pp.687-700; Chirgadze Y.N., Larionova E.A., Ivanov V.V.: J. Biomol. Struct. Dyn. 2009 27(1), pp.83-96].

Computer algebra and applications

In collaboration with R. Kragler, University of Applied Sciences, Weingarten, Germany and A.N. Prokopenya, Brest Technical University, Belarus, the first version of the Mathematica-based simulator of quantum computation has been created. The simulator has a more friendly user interface, higher computational performance and better facilities for implementation and testing quantum algorithms than all other known Mathematica simulators of quantum computers. Computational efficiency of the simulator is illustrated in Fig. 14.

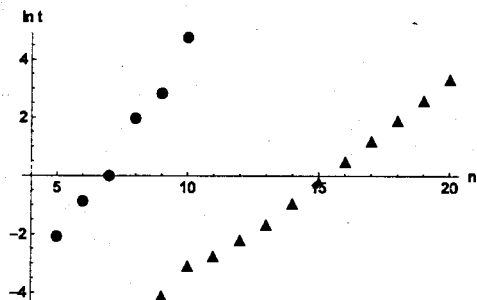


Figure 14: CPU time for computing circuit matrix for tensor product of n Hadamard (left data) and Pauli (right data) gates

[V.P. Gerdt, R. Kragler, A.N. Prokopenya: In: "Computer Algebra Systems in Teaching and Research / CASCR 2007", University of Podlasie, Scieldce, Poland, 2007, pp.135-144; V.P. Gerdt, R. Kragler, A.N. Prokopenya: Proceedings of the DST-UNISA-JINR symposium, University of South Africa, Pretoria, 2007, pp.219-232; V.P. Gerdt, R. Kragler, A. Prokopenya: Acta Academiae Aboensis, Ser. B, Vol. 67, No. 2, 2007, pp.28-38; V.P. Gerdt, R. Kragler, A.N. Prokopenya: Physics of Particles and Nuclei Letters, Vol.6, No.7, 2009, 526-529; V.P. Gerdt, R. Kragler, A.N. Prokopenya: Lect. Notes Comp. Sci., 5743, 2009, 106-117].

Since 2005 the investigation of discrete dynamical systems has been in progress. Discrete systems deserve study by both application (nanostructures, for example, by their nature are discrete, not continuous, formations) and fundamental reasons. The concept of a system of discrete relations on the abstract sim-

plicial complex — natural generalization of cellular automata or systems of polynomial equations over finite fields — and developed algorithms for analysing compatibility and constructing canonical decompositions of such systems. Application of these techniques to some cellular automata allowed one to obtain a number of new results [V.V. Kornyak: Lect. Notes Comp. Sci., 3718, Springer 2005, pp. 272-284; V.V. Kornyak: Programming and Computer Software, 32, No. 2, 2006, pp. 84-89]. The main aim is the development of new methods, algorithms and software for investigation and simulation of discrete dynamical systems with symmetries. Such systems include, for example, such important carbon nanostructures as graphemes, fullerenes and many others. These structures and their symmetry groups are shown in Fig.15.

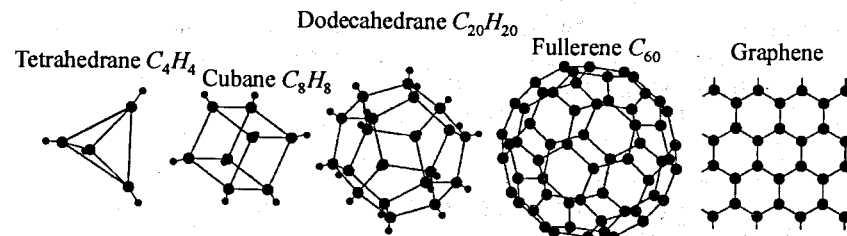


Figure 15: Symmetries of 3-valent (hydro)carbon nanostructures

In the case of deterministic systems important relations between symmetries and dynamics were revealed and investigated by means of computer experiments. For quantum discrete systems a new approach to their quantizing was suggested based on introduction of gauge connection with its values in multidimensional unitary representation of some group [V.V. Kornyak: Lect. Notes Comp. Sci., 4194, Springer 2006, pp. 240-250; V.V. Kornyak: Programming and Computer Software, 33, No. 2, 2007, pp. 87-93; V.V. Kornyak: Lect. Notes Comp. Sci., 4770, Springer 2007, pp. 236-251; V.V. Kornyak: Programming and Computer Software, 34, No. 2, 2008, pp. 84-94; V.V. Kornyak: Lect. Notes Comp. Sci., 5743, Springer 2009, pp. 180-194].

New heuristically good selection strategies were discovered for nonmultiplicative prolongations that is important to speed-up computation of Groebner bases by involutive methods. The computational efficiency of the new strategies was investigated. Due to their implementation into the specialized computer algebra system GINV this system became the fastest open source software in the world with respect to the speed of computation of Groebner bases [V.P. Gerdt, Yu.A. Blinkov: Programming and Computer Software, 33, No.3, 2007, p.147].

The study of solving the inverse problem for a discrete two-dimensional Schrödinger equation describing wave motion on lattice was performed. An original algorithm for reconstructing the discrete potential together with eigenfunctions of given spectrum and prescribed symmetry conditions providing "smooth" prolongation of the eigenfunctions from rectangular to the whole plain

was developed by using CAS REDUCE [S.I. Serdyukova: *Nuclear Instruments and Methods in Physics Research A*, 534 (2004), p.304-308].

The intense coherent radiation interaction with a charged spinning particle has been studied within the Newtonian mechanics beyond the conventional electric-dipole approximation and taking into account complete treatment of the magnetic part of the Lorentz force of a laser field. With the aim to analyze the dependence of bipartite entanglement on a laser's intensity a simple model has been formulated. As the analysis shows, the entanglement characteristics of spin degrees of freedom strongly depend on the intensity of a laser radiation. It was shown that corrections due to the intensity lead to a new effects changing the non-dipole pattern very drastically. In particular, the maximally entangled two qubit Werner state, that is stable under the weak laser radiation, can be transformed into a separable state for a sufficiently strong laser. The predicted nonlinear effects in a strong laser-matter interaction can be used to manipulate the entanglement when the control parameter is the laser intensity instead of its frequency [P. Jameson, A. Khvedelidze: *Phys. Rev. A* 77, 053403 (2008); M. Eliashvili, V. Gerdt, A. Khvedelidze: *Phys. of Atomic Nuclei*, 72, No. 5, 786 (2009)].

An algorithmic research of cohomology, one of the main tools for investigation of topological peculiarities in different mathematical and physical structures, was performed. A new efficient algorithm in C for computing cohomology of Lie algebras and superalgebras was developed and implemented [V.V. Kornyak: *Programming and Computer Software*, 29, No.2, 2003, pp.94-99; V.V. Kornyak: *Nuclear Inst. and Methods in Physics Research*, A, 502, 2003, pp. 627-629; V.V. Kornyak: *Programming and Computer Software*, 30, No.3, 2004, pp. 157-163]. The algorithm allows one to solve several difficult problems. In particular, the full cohomologies of some restricted Lie algebras of Hamiltonian vector fields (cochain complex of one of them has a dimension of 8388608) were computed for the first time [V.V. Kornyak: *Computer Analysis, Programming and Computer Software*, 31, No. 2, 2005, pp. 8790].

An original method is suggested for regulating entanglement production in a system of multitrap and multimode Bose-Einstein condensates coupled through a common resonant modulating field. The proposed method can be used in processing information and quantum computing [V.I. Yukalov, E.P. Yukalova: *Phys. Rev. A* 73 (2006) 022335-10].

Recent achievements in microfabrication technology afford opportunities of constructing quantum wells, superlattices, quantum wires and dots with properties of particle confinement. As it was shown by Paul and Raether, Gaponov and Miller, under definite conditions a particle can be localized in a nonuniform high frequency electromagnetic field. The technique of constructing a periodic time-dependent Hamiltonian admitting exact solutions with the use of exactly soluble time-independent Hamiltonian, unitary time-dependent transformations and a proper choice of initial states was elaborated [A.A. Suzko: *Phys.Lett.*, 2003, vol. A 308, 267-279]. In particular, the periodic time-dependent Hamilto-

nians are generated whose expectation values for cyclic solutions, spin-expectation values and probability density in a given point of space-time do not depend on time. It means that quantum particles can be confined by time-dependent potentials. This result is a quantum-mechanical analog of the classical Gaponov, Miller, Paul effect.

The time evolution matrices are obtained in an explicit form and used to construct logic gates for computation [A.A. Suzko, G. Giorgadze: *Phys. Part. Nucl.*, (2008) Vol. 39, No.4. p.578-596; A.A. Suzko, G. Giorgadze: *Physics of particles and Nuclear Letters*, (2008) Vol.5, No.3, pp 157-160; A.A. Suzko, G. Giorgadze: *Contemporary Mathematics and Its Applications*, Vol. 44, *Quantum Computing*, (2007) pp 141-151]. A way of obtaining entanglement operator is discussed, too.

The study of the generalized Schrödinger equation with a position-dependent (effective) mass has recently attracted interest in condensed matter physics as well as related fields of physics. In particular, the effective mass Schrödinger equation is used for the description of electronic properties of semiconductor heterostructures and quantum dots. One of the most important problems of quantum engineering is the construction of multi-quantum well structures possessing desirable spectral properties. The method of Darboux transformation operators allows one to solve the problem of reconstruction of quantum well potentials with a predetermined energy spectrum. The Darboux transformations for generalized time-dependent and time-independent Schrödinger equations [A.A. Suzko, G. Giorgadze: *Physics of Atomic Nuclei*, Vol.70 (2007), 604-607; A.A. Suzko, I. Tralle: *Acta Physica Polonica*, B 39, (2008), P.545-567; A.A. Suzko, A. Schulze-Halberg, *Phys.Lett. Vol. A* 372 (2008) 5865-5871; A.A. Suzko, A. Schulze-Halberg, E.P. Velicheva: *Physics of Atomic Nuclei*, Vol.72 (2009), 858-865; A.A. Suzko, A. Schulze-Halberg: *J.Phys.*, Vol. A 42 (2009) 295203-295217] was constructed. The intertwining relations, supersymmetry and Darboux transformations was studied. The intertwiners in an explicit form were obtained, by means of which the arbitrary-order Darboux transformations for our class of equations can be constructed. A corresponding supersymmetric formulation was developed and proved equivalence of the Darboux transformations with the supersymmetry formalism. This generalized Darboux transformations comprises a position-dependent effective mass case and a case of linearly energy-dependent potentials, as well as a conventional case of Schrödinger equation. On concrete examples it was shown how to apply the Darboux transformations technique for modeling quantum well potentials with the given spectrum for investigation of low-dimensional structures in nanoelectronics.

Conferences

During the period 2003-2009, LIT organized the workshops and conferences:

- International workshop "Quantum Physics and Communication", 2003, 2005, 2007;
- International Symposium on Nuclear Electronics & Computing, 2003, 2005, 2007, 2009;
- International Conference "Mathematics. Computer. Education", 2004, 2006, 2008;
- International Conference "Distributed Computing and Grid-technologies in Science and Education", 2004, 2006, 2008;
- Workshop on Computer Algebra, 2005, 2006, 2007, 2008;
- Tenth Anniversary All - Russian Scientific Conference RCDL'2008 "Digital Libraries: Advanced Methods And Technologies, Digital Collections";
- International conference "Mathematical Modeling and Computational Physics", 2006, 2009.