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LABORATORY OF INFORMATION TECHNOLOGIES

REPORT ON RESEARCH ACTIVITIES IN 2006

Report to the 101st Session
of the JINR Scientific Council
January 18–19, 2007

Dubna 2006

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The main tasks of the Laboratory of Information Technologies (LIT) consist in the provision with both modern telecommunication, network, and information resources and mathematical support of the theoretical and experimental studies conducted by the JINR, Member State institutes at JINR, and other scientific centers.

The LIT activity is focused on two directions, namely "Information, Computer, and Network Support of the JINR's Activity" (topic 09-6-1048-2003/2007, headed by V.V. Ivanov, V.V. Korenkov, and P.V. Zrelov) and "Mathematical Support of Experimental and Theoretical Studies Conducted by JINR" (topic 09-6-1060-2005/2007, headed by V.V. Ivanov, Gh. Adam, and P.V. Zrelov). These directions are developed in frames of the JINR general topic "Networks, Computing, and Computational Physics". The Laboratory staff participated in research work done within 15 topics at the project level and within 21 topics at the cooperation level. Main results of the investigations performed within these topics have been published in well-known journals, proceedings of scientific conferences and preprints.

A number of scientific projects involving LIT staff members have been financed by grants afforded by the Commission of the European Community in frames of the EU-Russia collaboration and INTAS. Ten grants were afforded by the Russian Foundation for Basic Research. Among them, five were directed to the creation and development of the

information, computing and telecommunication infrastructure, while five supported various projects of scientific interest.

During the year 2006, LIT was the main organizer of some workshops and conferences.

On January 17-23, 2006 LIT hosted the XIII interdisciplinary conference "Mathematics. Computer. Education." which is held every January alternately in Dubna and Puschino at the Center of Biological Research of the Russian Academy of Sciences. The Conferences attended annually by more than 300 participants differ from the majority of professional meetings in their scientific - educational orientation. The purpose of the conferences is to get acquainted with new achievements of modern Russian and world science and to find out how matters stand in the "neighboring" areas of knowledge, to meet colleagues - the teachers of schools and higher schools, to discuss their problems and to share experience. The most participants are higher school lecturers simultaneously involved in pedagogical and research work.

10-th Workshop on Computer Algebra was organized on May 23-24, 2006. Attending were more than 30 scientists from Linz (Austria), Turku (Finland), Moscow, St. Petersburg, Belgorod, Samara, Saratov, Tambov, Tver and Dubna, 27 reports were presented.The main goal of the workshops is to provide a forum for researchers on computer algebra methods, algorithms and software and for those who use this tool in theoretical, mathematical and experimental physics. The workshop programme covered the following topics: algebraic methods for nonlinear polynomial and differential equations, symbolic-numeric methods, computer algebra algorithms and software packages; application to theoretical and mathematical physics.

The second international conference "Distributed Computing and Grid Technologies in Science and Education" was held at LIT from 26 - 30 June, 2006. The first conference organized two years ago at JINR, became the first forum in Russia that brought together representatives of Russian centres and JINR Member State institutes working in this field. The second conference was attended by more than 200 specialists from 17 countries (Armenia, Belarus, Bulgaria, Great Britain, Germany, India, Poland, Romania, USA, Czech Republic, Slovakia, Switzerland, Sweden,

Uzbekistan, Ukraine, etc.) and from 46 universities and research centers of Russia. Representatives of commercial enterprises, in particular CISCO and Kraftway, took part at the conference.

The scientific programme of the conference that included 96 reports and presentations covered the following topics: 1) creation and operating experience of Grid-infrastructures in various areas of science and education; 2) methods and technologies of distributed computing; architecture, algorithms; 3) distributed processing and data storage; 4) organization of the network infrastructure for distributed data processing; 5) algorithms and methods of solving applied problems in distributed computing environments; 6) theory, models and methods of distributed data processing; 7) distributed computing within LHC projects; 8) technologies of designing and experience of using distributed information Grid-systems. In frames of the conference organized were two tutorials on Grid: gLite system and NorduGrid.

The international conference "Mathematical Modeling and Computational Physics" (MMCP-2006) devoted to the 50th anniversary of the Joint Institute for Nuclear Research was held in High Tatras Mountains, Slovakia, on 28 August - 1 September, 2006. The Organizers of the Conference were the JINR Laboratory of Information Technologies, the Institute of Experimental Physics of the Slovak Academy of Sciences (Košice) and the Technical University (TU), Košice. The Conference was the fourth one organized by LIT under this name. Under the initiative of our Slovak colleagues, it was for the first time organized outside JINR. The Conference was attended by known specialists in the field of mathematical simulation and computational physics from Austria, Armenia, Belgium, Belarus, Great Britain, Vietnam, Germany, Spain, Italy, Poland, Russia, Romania, Slovakia, USA, Taiwan, Ukraine, Finland, France, and Japan. The Conference included 20 plenary and invited papers and over 40 contributed talks. The Conference highlighted the role of the mathematical modeling and computing methods as an integrating factor in the present-day scientific research in various fields of knowledge: particle physics, physics of solids, hydrodynamics, biology, biochemistry, material studies, quantum computations, economy, computer science, etc.

Networking, computing, information support, and Grid technologies

The network infrastructure must have the quality of controllability as well as high reliability, availability, and serviceability level for the strategically important applications and services of the Institute's activities.

Specific tasks in the area of networking, computing, information support, and Grid are:

1. Provision of JINR and its Member States with high-speed telecommunication data links.
2. Creation of a high-speed, reliable and protected local area network (LAN) of JINR.
3. Creation and maintenance of the distributed high-performance computing infrastructure and mass storage resources.
4. Provision of information, algorithmic and software support of the JINR research-and-production activity.
5. Elaboration of the JINR Grid-segment and its inclusion in European and global Grid-structures.

JINR telecommunication data links

Development of external JINR computer communications includes:
- a) a high-speed 1 Gbps JINR-Moscow data link,
- b) JINR participation in the new-generation research computer network with Russian and international (GLORIAD, GEANT) segments for provision of JINR's activities,
- c) integration with the educational network of Dubna.

At present, JINR leases 1 Gbps channel to Moscow from the Russian Satellite Communications Company (RSCC «Dubna») 2.5 Gbps channel. JINR has access to the Russian networks and information resources, as well as access to the international channels through shared RBNet+RUNNet in the common 2.5 Gbps data stream (Fig.1). The detailed scheme of design and application of Dubna-Moscow data communication channel was worked-out along with RSCC, Russian Institute for Public Networks, and COMSTAR-United TeleSystems. This assumes JINR PoP at MIX-9 in Moscow.
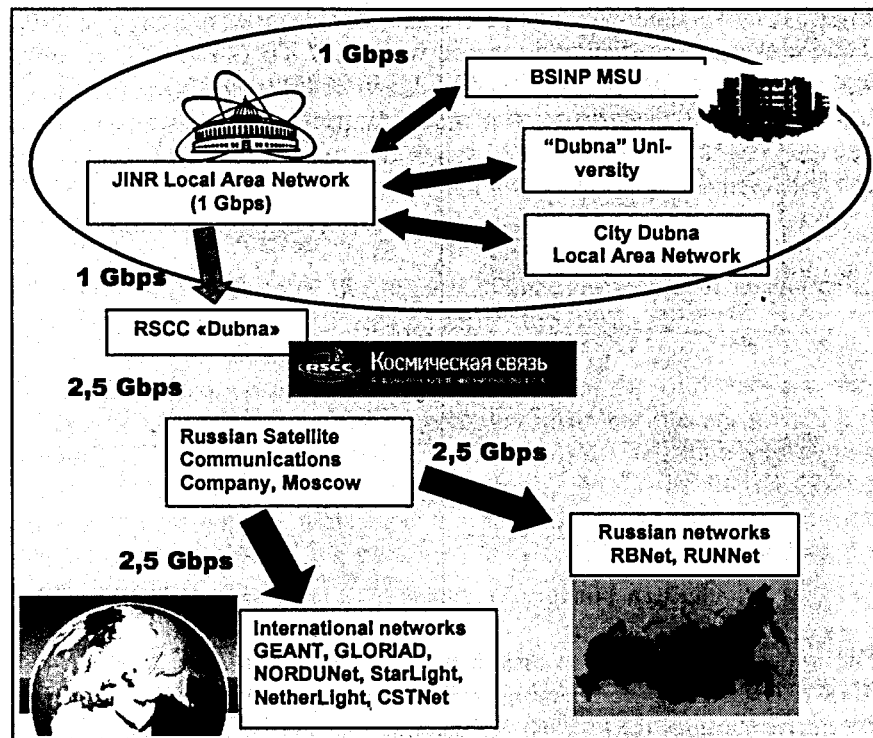

Fig.1. The JINR telecommunication channels

The future development of the external communications is summarized in the following program:
- JINR's participation in the program devoted to the implementation of a new-generation research network;
- development of an international segment within projects GEANT2, GLORIAD, and increasing the throughput of the channels to 10 Gbps in 2007, 40 Gbps in 2010, and 100 Gbps in 2015;
- broadening the Dubna – Moscow channel to 10 Gbps in 2007, 40 Gbps in 2010, and 100 Gbps in 2015;
- integration with the municipal educational network and its development following its transition to new technologies (10 Gb Ethernet);
- development of a corporate network of JINR and its Member States.

Figure 2 shows the incoming and outgoing JINR traffic in 2005 and 2006. Total eleven month incoming traffic was 76.57 TB (43.52 TB in 2005) and outgoing traffic – 68.81 TB (39.4 TB in 2005).
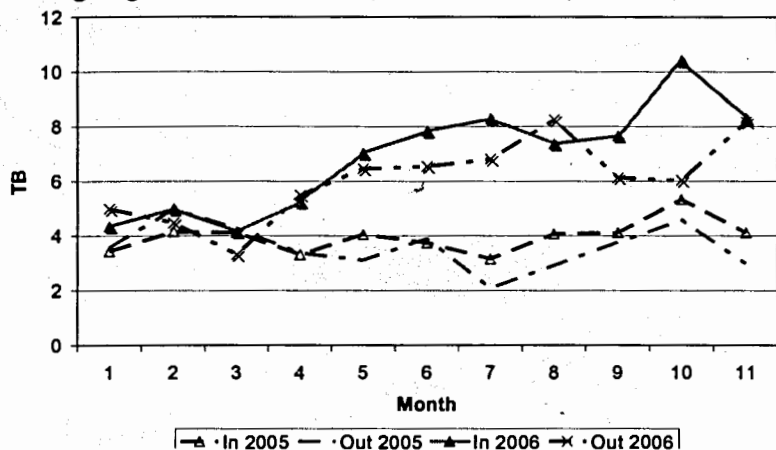

Fig. 2. Incoming and outgoing JINR traffic in 2005 and 2006

The table below shows an eleven month traffic distribution among the JINR divisions whose incoming traffic is greater than 1 TB. LIT incoming traffic includes the total JINR Grid traffic.

JINR Laboratories	Incoming TB	Outgoing TB	Incoming %	Outgoing %
LIT*	30.76	12.99	40.07	18.88
DLNP	12.83	16.76	16.72	24.35
LPP	7.29	9.89	9.5	14.37
FLNR	6.17	2.26	8.04	3.29
VBLHE	5.0	3.71	6.51	5.4
FLNP	4.45	16.38	5.79	23.8
BLTP	3.37	1.98	4.39	2.88
Uni-Dubna	1.73	1.78	2.25	2.58
Adm.	1.35	0.611	1.76	0.87
Servers	1.23	2.0	1.6	2.91
Modem pool	1.17	0.203	1.53	0.29

JINR Local Area Network

Systematic work on the LAN management was performed by the Network Operation Centre (http://noc.jinr.ru/). At present the JINR LAN comprises 5681 computers and nodes (5335 in year 2005). There are 3173 users, 863 modem pool users, and 339 JINR staff members use VPN connection through Lanpolis.

The main goal is to carry out organizational and technical measures to provide the 1 Gbps data transfer rate across the JINR LAN.

During the first six months of 2006 specialists of the LIT Network Service put into operation a software complex intended to scan in the local network the computers infected by Internet worms and their subsequent blocking. This type viruses pose certain problems for the JINR LAN, as each infected computer transferred the parasitic traffic over the network with a high speed (scanning packages) thus appreciably overloading the network equipment.

The software complex functions on the basis of the statistics acquisition server flow.jinr.ru and represents a set of scripts and programs analyzing the internal network traffic as well as the module for the register of the network elements IPDB, allowing to block access to the network for the infected computer.

Since June 2006 (during 4 months) the employers of the network service revealed and investigated almost 230 cases of infecting computers of the JINR network by the Internet worms. Detected were 180 cases of infecting computers of the local network and 50 cases of infecting computers connected through the service of remote access (VPN and the modem pool). As to a percentage ratio, DLNP is a leader - 23 %, and 21 % - the remote access service, FLNR - 17 %, LIT - 10 %.

In each case the infected computer scanned the JINR LAN questioning from 5 up to 40 thousand IP addresses thus creating a peak load breaking the normal functioning of the laboratory connections (for example, the BLTP network access failures in June).

As a result of the work carried out by the Network Service, the intensity of appearing the computers infected with such viruses in the JINR network has been reduced from 15-20 cases per week in early days down to 3-5 cases per month.

Network security is a crucial and permanent problem, asking for steady research. To keep the JINR LAN as a full time working structure, we must perform LAN constant control and protection. From this point of view, the network security issues are considered as processes, not a final product – we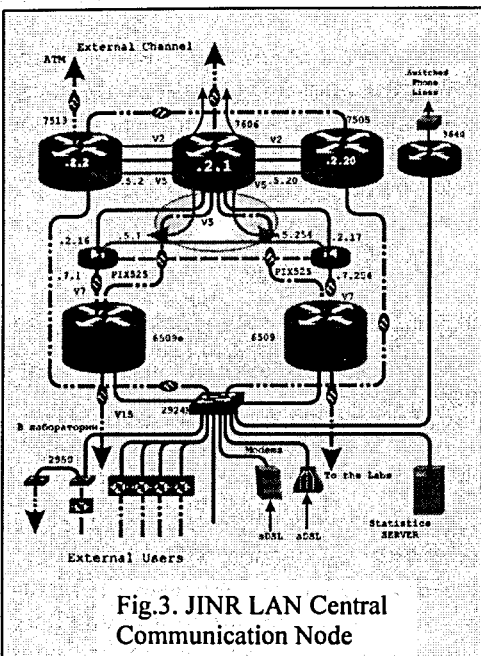 have to continue the process of permanent evaluation of all possible mechanisms to increase the level of security in every element of JINR computer and network infrastructure. The extension of the network services secured remote access to JINR resources from home PC, the Internet access from Dubna hotels – security becomes a parameter of the greatest importance. To be able to deal with security, we have to have an adequate network monitoring tool to accomplish the look-ahead assessment of the entire network environment.

Fig.3. JINR LAN Central Communication Node

In 2006 the Central Communication Node modernization was performed (Fig.3). The goals were to build a fail-proof core of the JINR LAN communication structure, to achieve an appropriate level of the network security, to have good data rate parameters and tools to control maintainability, accessibility, and reliability.

The new powerful switching&routing equipment Internet Cisco 7606 router (processor - Supervisor Engine 720, MSFC3, PFC3B Memory 1 GB, 48-port 10/ 100 /1000, Firewall security system), central switch

Cisco Catalyst 6509E, and VPN router Cisco 7513 were put in operation in 2006.

By the Catalyst 6500 features we can build up the *Evolutionary Infrastructure* using new modules for every Catalyst 6500 Generation (new Supervisor 720, non-blocking 10 GbE, high-density 10 GbE, 16 port GbE, 48 port 10/100/1000 Mbps). Also the *Intelligent Services* – accelerated IP services delivered: IPv6, MPLS, NAT, GRE, enhanced operational management and more will be achieved. *Performance and Application Delivery* – 400 Mpps over a 720 Gbps Switch fabric with higher performance and density 10 GbE and GbE, enables Gigabit everywhere in JINR LAN, and enables new Catalyst 6500 deployments for the next 8 to 10 years.

The future development of the Integrated Datacenter with high performance Supervisor 720 as the Datacenter Core Layer, Datacenter Services Layer with integrated Firewall, content Switching and SSL termination, and Datacenter Access Layer with High Density and Performance 10/100/1000 Mbps will be possible.

This equipment allows us to build up 10 GbE High Performance Computing Datacenter in years 2008-2009 for Grid computing:
- enabling high performance clusters of hundreds of servers per Catalyst 6500;
- cluster of clusters or 'Grid' interconnected by wire-rate 10 GbE;
- long haul DWDM with Cisco ONS products for collaborative environments;
- 256 K route support for iBGP Inter-cluster connections.

Central Information and Computer Complex

The creation of the distributed high-performance computing infrastructure and mass storage resources is centered around the JINR Central Information and Computer Complex (CICC) as a core of the distributed infrastructure.

More than 500 staff members of JINR and other research centres are using the JINR Central Information and Computing Center. The JINR

CICC is part of the Russian Grid Segment used for LHC and other applications. Nowadays the JINR CICC comprises: an interactive cluster of common access; a common access computing farm for carrying out simulation and data processing for a number of physics experiments in which the JINR participates, and for carrying out parallel calculations on the basis of the modern network technologies (Myrinet, SCI, etc.); LHC Computing Grid (LCG) farm for the tasks of the LHC experiments included into a worldwide Grid infrastructure.

With the last acquisitions, the JINR CICC comprises 160 CPUs, 17 TB RAID-5, and 39 TB Certon100 disk memory. Total performance of computer centre is now 100 kSI2K. JINR CICC facilities were used by experiments E391A (KEK), KLOD, COMPASS, D0, DIRAC, HARP, CMS, ALICE, ATLAS, HERAb, H1, NEMO, OPERA, HERMES, CBM, PANDA, etc., for mass event production, data simulation and analysis.

The JINR CICC users distributed over JINR divisions are tabulated as follows:

LIT	DLNP	LPP	VBLHE	Non JINR Grid users	FLNR	BLTP	FLNP	Adm.
182	120	60	48	33	28	15	12	9

The table below shows the percentage of CPU time using by JINR Laboratories at CICC:

VBLHE	DLNP	LIT	BLTP	FLNR	LPP	FLNP
40%	36%	13%	8%	2%	0.2%	0.1%

The future plans include the development of JINR Central Information and Computing Complex as a core of the distributed Grid infrastructure:
- development of the CICC infrastructure meeting the needs of collaborations, JINR users, and JINR Member States;
- development of JINR's Grid segment with a fully functional set of services;
- participation in international, national, and regional projects of developing Grid technologies (LCG, EGEE, OSG, NorduGrid, Dubna-Grid, etc.);

- participation in developing the technologies of application gridification that will allow applied software packages to be adapted to the Grid environment;
- research into, and modeling of the open networks behavior during their use in distributed systems of processing super-large data volumes (several terabytes) in the few-to-few mode of virtual connections, including the hierarchical and domain architecture of the network infrastructure.

Grid-technologies and LCG project

The work on creation of computing services and Grid-technology deployment in data processing was in progress. Number of work on this direction have been performed in frames of JINR participation in LCG/EGEE projects:
- support and development of the JINR LCG-segment in frames of the global LCG infrastructure (the last gLite version (302), VOboxes for ALICE and CMS, SE with dCache usage 31 TB, Xrootd door in dCache and XROOTD for ALICE were installed);
- LCG middleware testing/evaluation (gLite testing and deployment);
- grid-monitoring of the LCG-infrastructure at JINR and others sites of the Russian Tier2 cluster (a total renewal of monitoring system: monitoring server, operating system, web-server, Java version); new features such as information on resources usage in the more detailed form; information on users with access via Grid certificate; channel bandwidth monitoring were implemented);
- evaluation of new Grid technologies in context of their usage in LCG (Globus Toolkit 4 testing&evaluation);
- re-design of JINR LCG web-portal and initial filling with information;
- MCDB development (data base structure; basic modules and interfaces for direct files download from Castor in CERN or via gridFTP; adopting the system to demands of physics collaborations; automatic DB backup to AFS at CERN);
- maintenance of PYTHIA and HERWIG validation home-pages; integration of HEPWEB in GENSHER environment (more than 4000 references are collected and processing now in HEPWEB, evaluation

of possible integration HEPWEB into LCG environment has been performed using project Dubna-Grid);

- participation in ARDA activities in coordination with experiments (testing of AtCom/LEXOR usage for ATLAS; testing of gLite-AMGA metadata service replication functionality and performance; two test-suites – for gLite-AMGA metadata service and for AMGA replication performance studies – have been created and used). AMGA is a superstructure above DBMS (MySQL, PostgreSQL, Oracle or SQLite) with an independent of a particular DBMS interface aimed at the operation in a metadata catalog mode and in a file catalog mode. AMGA supports creation of mirror copies of any tree of subdirectories with access only for reading, only a master copy possessing access for recording. Such mechanism of distributing access to metadata is claimed by many applications within the Grid-environment. The designed set of tools for testing the functionality checks up correctness of replication of changing the data of the catalog for the most commands of record AMGA (i.e. those commands which can change the catalog contents);

- participation in Service Challenges in coordination with LHC experiments and Tier1 at Karlsruhe (a successful participation during a year in Service Challenges for CMS, ATLAS and ALICE);

- user's support to stimulate their active usage of LCG resources (courses for LCG administrators and ALICE users from Ukraine institutes on February 28-March 3, 2006; LCG training for ATLAS users at on May 15-19, 2006; courses on Grid-technologies for participants of the second international conference "Distributed computing and Grid technologies in science and education").

At present the JINR LCG infrastructure comprises:

Basic services:
- Berkely DB Information Index (BDII);
- Proxy Server (PX);
- Resource Broker (RB).

Specific services:
- 2 VOboxes (for ALICE and CMS);
- ROCMON;
- MON-box.

PPS and testing infrastructure (for testing and evaluations Grid middleware):

- the last gLite version (302);
- SE with dCache usage (16 TB) and 15 TB are in a progress of connection;
- XROOTD and XROOTD door in dCache for ALICE;
- last versions of atlas-releases, atlas-offline, atlas-production packages for ATLAS;
- CMKIN, CMSSW, OSCAR, ORCA, COBRA packages for CMS and DaVinci, Gauss packages for LHCb.

The investigation of a problem «Calibration of forward calorimeters with the help of a radioactive source» was performed in frames of research on RDMS CMS. On the basis of the analysis of this subject domain, a logic model of the system has been constructed that subsequently became a basis of the physical realization. The database is intended for storing information on a radioactive source, detectors, sectors, towers, tubes, values of their geometrical coefficients as well as the obtained values of the tower calibration coefficients. As a result of this work, a database has been constructed, a data input procedure has been completely implemented, and the information system with a viewing Web-interface (http://lib.jinr.ru/fia/cms/hf/titul.html) was realized. The system allows one to take information on source tubes (Source Tubes), used calibration methods (Methods), primary initial data (RunsDatabases), calibration coefficients of the towers (Tower Coeffs).

A package GridCom (Grid Commander) has been developed that represents a client part (GridCom) as a graphic shell for work of the user with problems and data in LCG and a program – the Lexor inquiries executor.

Fulfilled were JINR's obligations on participation in the on-line SW TDAQ development: components of on-line SW Resource Manager and Event Dump are included in the structure of the on-line SW TDAQ release, prepared by TDAQ cooperation to start-up in 2007 at a Dress Rehearsal stage.

The TDAQ ATLAS JINR team participates in engineering the Data Quality (DQ) Monitoring system. According to the ATLAS Operation Model, the DQ Monitoring will be included in all phases of data processing, beginning from on-line up to off-line and including calibration, alignment and monitoring of the reconstruction quality on Tier 0-2 . To participate

in this work, a test-bed has been assembled in LIT for installation of Data Quality Monitoring Framework Software.

The Dubna-Grid project was elaborated in 2004 in the Laboratory of Information Technologies in collaboration with other partners from the universities of Dubna, Chicago and Lund. The main aim of the project is the creation of a multi-purpose town scale network of distributed meta-computing on the basis of vacant computing resources of "office" computers. The project foresees creation of a common pool of accessible nodes of more than 1500 units.

The current status of the project:
- A test-bed of the distributed meta-computing environment of Dubna city has been created. More than 200 virtual nodes have been configured in computer classes of Dubna university, LIT Grid Laboratory, MIREA computer classes and Dubna secondary schools.
- Mass installation technologies and spreading software to all accessible nodes of the meta-cluster have been developed.
- Monitoring system of the meta-cluster has been developed.
- The meta-cluster has been integrated with JINR batch system.
- First real tasks have been performed (including real tasks for the ATLAS experiment).
- Integration of HEPWEB server in Dubna-Grid environment is realized.

The Grid Laboratory "GridLab" is created in LIT. The aim of the Laboratory is 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. Technically, "GridLab" is a specialized segment of the "Dubna-Grid" project, consisting of a module of six working nodes and one server.

Information and software support

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. Hard work was undertaken towards systematic development and maintenance of databases and information systems taking into account the user needs. The work was also in noticeable progress on the development of the WWW tools at the JINR and LIT main information servers: www.jinr.ru and lit.jinr.ru. Members of the LIT staff provided necessary work for the JINR's STD AMS on the software and centralized support of the administrative databases.

The consecutive development of the program library JINRLIB was in progress. The library is replenished with new programs created by JINR specialists. Six software packages were added in 2006. The Library programs are converted to double precision, the results of the work are checked-up on computer platforms Unix and Windows.

The maintenance of the program libraries developed by other research centres and organizations (CPCLIB, CERNLIB) and provision of the information and technical help to users continue.

The full information on the JINR program libraries is available at the specialized WWW-server http://www.jinr.ru/programs/ and in LIT News Bulletins.

A regular actualization of the content of the central servers, their technical support and modernization of the software environment are performed in frames of supporting the JINR unified information environment on the basis of the central JINR site and LIT site. A new version of the LIT site, devoted to the 40th anniversary of LIT, has been developed and started-up.

One of directions in this area is participation in the development, creation and support of information Web-sites of various conferences, workshops, symposia organized by LIT and other JINR Laboratories (at their requests, on the central information servers). For example, a www-site of the XXXIII International Conference on High Energy Physics (ICHEP' 06) was designed in 2006.

The maintenance and modernization of administrative databases (in co-operation with STD AMS of JINR) was in progress. In view of transition to the 1C platform, a number of functions have been added to maintain

data exchange between the outdated platform and the new one, between the participants of drawing up documents and accountants. The drawing up of documents of the JINR tangible assets accounting base has been realized by completion, development and modernization of documents on tangible assets accounting in 1C according to the JINR requirements, etc.

In progress was the maintenance and development of the interactive information environment for operative access to scientific and technical information in the Internet that allows efficient work of the Institute's scientific staff with bibliographic and factual data. It includes references to encyclopedias, directories, databases on particle and nuclear physics, Internet book-shops, provides access to text-through journals of Russian and foreign publishing houses, etc. It is available at http://dbserv.jinr.ru/~genis/Infpublish.htm. The work was done in cooperation with the specialists of the JINR Library.

Software and computer complexes for experimental data processing

The problem of optimization of the 2D magnetic field of a 4 T dipole magnet with the aperture diameter of 100-110 mm for a fast cycling synchrotron is considered. A single layer coil is made of hollow superconducting NbTi cable designed at operating current of 30 kA. The description of mathematical method developed for minimization of higher harmonic of the magnetic field by variation of the coil current loops angular

Fig.4

position is given. The numerical simulation results for 2D magnetic fields are presented. *[Akishin P. G., Butenko A. V., Kovalenko A. D., Mikhailov V. A. The Magnetic Field Design of 4 T Fast Cycling Superconducting Dipole Magnet PEPAN Letters, 2006, v.3,n.2(131),pp.105-110].*

A study of the equation-of-state of high compressed nuclear matter is the aim of the CBM collaboration. It is assumed to carry out t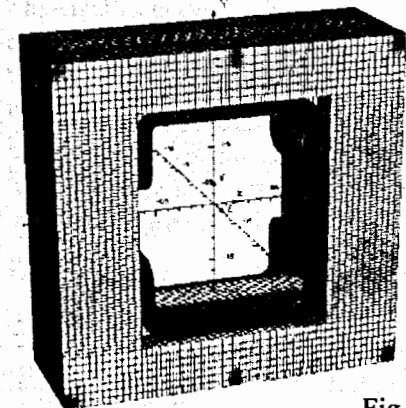he investigation at the future GSI accelera-tor on the event-by-event analysis base. In 2006, the computer modeling of various variants of a super-conducting dipole magnet for CBM experiment was carried out. On the basis of a multivariate spline approximation, differentiated approximations of the magnetic field in the working area of the magnet have been constructed (Fig.4). The modeling of the magnetic systems of the accelerator complex GSI SIS100 was performed, too.

Though expected non-homogeneous magnetic field and large multiplicity of produced particles make the reconstruction of events extremely complicated. For solving of the problem it is needed a finding and fitting of particle tracks in various parts of the setup (STS, TRD, RICH, TOF, ECAL), recognition of rings in RICH, reconstruction of primary and secondary vertices and so on. The CBM group of JINR LIT has proposed a set of effective methods for event reconstruction and has created corresponding computer codes which either are implemented in the CBM computational system, or are tested and trialed now. In particular, two algorithms of track reconstruction in the region of STS detector have been presented, two approaches for Cherenkov ring finding in RICH have been proposed, methods for charged particle momentum determination have been developed and so on. This interesting and useful work is continued now. *[P.G. Akishin, E.P. Akishina, S.A. Baginyan, Victor V. Ivanov, Valery V. Ivanov, I.V. Kisel, B.F. Kostenko, E.I. Litvinenko, G.A. Ososkov, A.M. Raportirenko, A.A. Soloviev, P.V. Zrelov, V.V. Uzhinsky. Methods for event reconstruction in the CBM experiment, JINR Communication, E10-2006-48, Dubna, Russia, 2006, pp. 25].*

Method of internal alignment of HERA-B OTR PC chambers is discussed. The method is based on simultaneous fit of the track and alignment parameters using Millepede matrix reduction and singular value decomposition. Software which implements this idea has been developed, the method has been studied on Monte Carlo models with different levels of simulation. A method generalization for the case of track nonlinear model has been proposed. *[I. Belotelov, A. Lanyov, G. Ososkov. A Study of Millepede Alignment Algorithm on Monte Carlo Model of HERA-B Outer Tracker. PEPAN Letters, 2006, v. 3, n.4(133), pp. 66-83].*

The results of applying a method of internal alignment of HERA-B OTR PC chambers are discussed. The method is based on simultaneous fit of the track and alignment parameters using Millepede matrix reduction and

singular value decomposition. After extensive tests of the method on different Monte-Carlo models, a number of studies have been done using real data taken by HERA-B in a 2002-2003 run period. Misalignment influence on reconstruction of individual tracks and physics signals, decays of J/ψ and K^0_s, has been studied. *[I. Belotelov, A. Lanyov, G. Ososkov Data-Driven Alignment of HERA-B Outer Tracker. PEPAN Letters, 2006, v. 3, n.5(134), pp. 105-110].*

A review of methods of computational physics that were developed at JINR to investigate various theoretical physics models of complex physical processes has been prepared. A general mathematical formulation of equations for the models under study is given. Numerical methods used are described. Information on the developed computer codes is presented. The following physical processes models are discussed: evolution of quasi-bound states in the bound states mesic molecules depending on the effective mass and application to a mesic atom scattering problem; non-adiabatic connection of helium antiproton ion channels for obtaining bilateral estimations of the transition energy levels; ionization of a ground state helium atom by fast electrons. Effective two-particle models of complex quantum-mechanic systems for nuclear interactions in high-energy approximation were investigated. Research was carried out on wave processes in nonlinear media and particle-like excitations in the models of condensed matter, nonlinear optics, astrophysics, and Josephson junctions in superconductors. The results of the numerical analysis are demonstrated. *[И.В.Пузынин, Т.Л.Бояджиев, С.И.Виницкий, Е.В.Земляная, Т.П.Пузынина, О.Чулуунбаатар. О методах вычислительной физики для исследования моделей сложных физических процессов. ЭЧАЯ, Т.38, вып.1, 2007].*

The research work on the autotracking of knots for piecewise cubic approximation carried out at LIT gives an algorithmic solution to the segment approximation problem that is important for applications and very difficult from a theoretical viewpoint. The main goal is to find an optimal subdivision so that the errors over the subintervals are as small as possible. This problem is closely related to the optimum choice of knots in approximation by cubic spline. An original method and an algorithm for automatic tracking of a cubic segment of a curve have been developed on the basis of the criterion of uniformity of the third derivative of the cubic model and a recurrent calculation of estimations of this derivative. A real time - oriented adaptive algorithm for knot detection has been developed.

The algorithm is simple in computing and stable to errors. 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 approximation of complex curves and real data. *[Dikoussar N.D. and Török Cs. "Mathematical Modelling", Vol.18, No.3, P.23-40, 2006].*

The results of Monte-Carlo modeling of the experimental accelerator-driven electronuclear system composed of the sub-critical assembly and DLNP JINR Phasotron have been presented. The expected thermal power of the Sub-critical Assembly in Dubna (SAD) is about 30 kW. A possibility of assembly power increase without changes in design and basic elements is considered. The proposed assembly upgrade gives power increase up to 100 kW. It is of importance that the proposed upgrade operations can be performed both before and after the run with nominal power and partial fulfillment of a basic experimental program.*[Petrochenkov S.A., Polanski A., Shvetsov V.N. Submitted to "Particles and Nuclei, Letters"].*
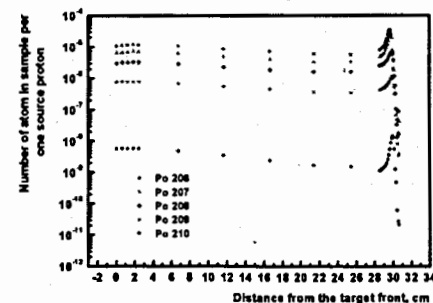
Fig.5. Spatial distribution of speeds of producing polonium in the target

Computations have been done on studying speeds of forming polonium isotopes in bismuth foils placed into a massive lead target exposed to a 660 MeV proton beam. The calculation was performed by two methods: first, the isotope yield was computed with the help of the MCNPX program. Then the MCNPX code was used only to calculate a proton spectrum in various points of the target, and then the calculated spectrum was turned off with experimental data on the cross-sections of obtaining polonium in reaction Bi (p, xN+g) Po (Fig.5). Thus, a spatial distribution of speeds of producing polonium has been received. *[A.Polanski, S. Petrochenkov , W. Pohorecki. Proton-Induced Polonium Production in Mas-*

sive Lead-Bismuth Target Irradiated by 660 MeV Protons. Nuclear Instruments and Methods in Physics Research A. 562 (2006) pp 764-766].

Nuclear physics

A phenomenological optical potential is generalized to include the Coulomb and nuclear interactions caused by the dynamical deformation of its surface. In the high-energy approach, analytical expressions for elastic and inelastic scattering amplitudes are obtained where all the orders in the deformation parameters are included. The multistep effect of the 2^+ rotational state excitation on elastic scattering is analyzed. Calculations of inelastic cross sections for the ^{17}O ions scattered on different nuclei at about hundred MeV/nucleon are compared with experimental data (Fig.6) and an important role of the Coulomb excitation is established.
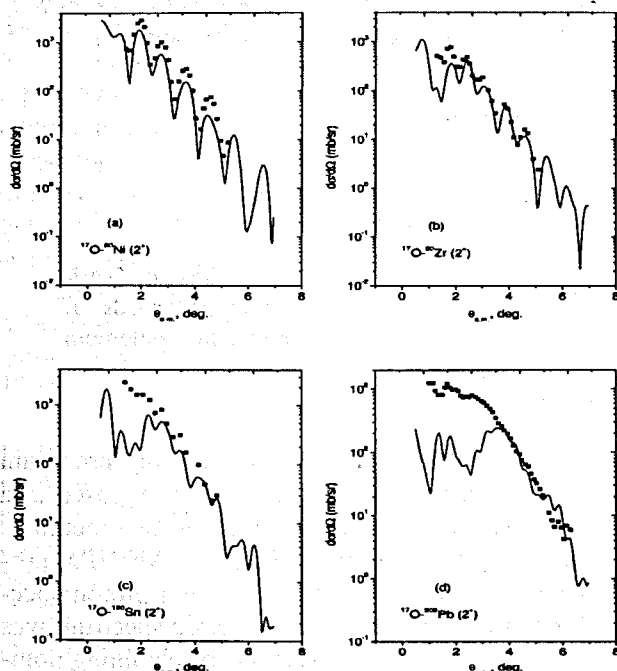
Fig.6. Comparison of the calculated inelastic scattering differential cross sections with the experimental data

[V.K.Lukyanov, Z.Metawei, E.V.Zemlyanaya. High-Energy Approach for Heavy-Ion Scattering with Excitations of Nuclear Collective States. ЯФ m.69, вып.8, 2006, pp.1409-1415].

For the nucleus-nucleus scattering, the complex potential is obtained which corresponds to the eikonal phase of an optical limit of the Glauber-Sitenko high-energy approximation. The potential does not include free parameters, its real and imaginary parts depend on energy and are determined by the reported data on the nuclear density distributions and nucleon-nucleon scattering amplitude. Alternatively, for the real part, the folding potential can be utilized which includes effective NN-forces and an exchange term as well. The efficiency of the approach is confirmed by agreements of calculations with experimental data on elastic scattering cross-sections. *[E.V.Zemlyanaya, M.A.Kiselev, J.Zbytovska, L.Almasy, V.K.Aswal, P.Strunz, S.Wartevig, R.H.H.Neubert. Structure of unilamellar vesicles:numerical analysis nased on small-angle neutron scattering data. Crystallography reports, 2006, Vol.51 Suppl. I, pp.S22-S26].*

The (semi-)microscopic double-folding nucleus-nucleus optical potentials are suggested for consideration of inelastic scattering with excitation of collective nuclear states by using the adiabatic approach and the elastic scattering amplitude in the high-energy approximation. The analytical expression for inelastic scattering amplitude is obtained keeping the first order terms in the deformation parameter of a potential. Calculations of inelastic cross sections for the ^{17}O heavy ions scattered on different nuclei at about hundred Mev/nucleon are made, and the acceptable qualitative agreement with the experimental data is obtained without introducing free parameters. *[K.M.Hanna, K.V.Lukyanov, V.K.Lukyanov, Z.Metawei, B.Slowinski, E.V.Zemlyanaya. Excitation of Nuclear Collective States by Heavy Ions within the Model of Semi-Microscopic Optical Potential. Письма в ЭЧАЯ, 6[135], 2006, pp.105-112].*

The double-folding model and the high-energy approximation (HEA) of the microscopic theory of scattering are involved to construct the nucleus-nucleus optical potentials. Calculations of differential elastic and total reaction cross sections are compared with experimental data. Data on reactions of exotic nuclei ^{6}He and ^{6,7}Li with ^{28}Si are analyzed in the framework of microscopic optical potential with the real and imaginary parts obtained with a help of the double-folding procedure and by using the current models of densities of the projectile nuclei (Fig.7). The microscopic double-folding Coulomb potential is calculated and its effect on cross sections is compared with that when one applies the traditional Coulomb potential for the uniform charge distribution. The semi-microscopic potentials are constructed from the renormalized micro-

scopic potentials and their derivatives to take into account collective motion effects and to get the fairly well agreements with experimental data. *[E.V.Zemlyanaya, K.V.Lukyanov, V.K.Lukyanov, I.N.Kukhtina, A.N.Antonov, K.M.Hanna, B.Slowinski. Calculations of nucleus-nucleus microscopic optical potentials and the respective elastic differential and total reaction cross sections. In: "Nuclear Theory'25", proceedings of 25th International Workshop on Nuclear Theory (June 26 - July 1, 2006, Rila Mountains, Bulgaria) ed. S. Dimitrova, Heron Press Ltd., Sofia, 2006 (in press)].*
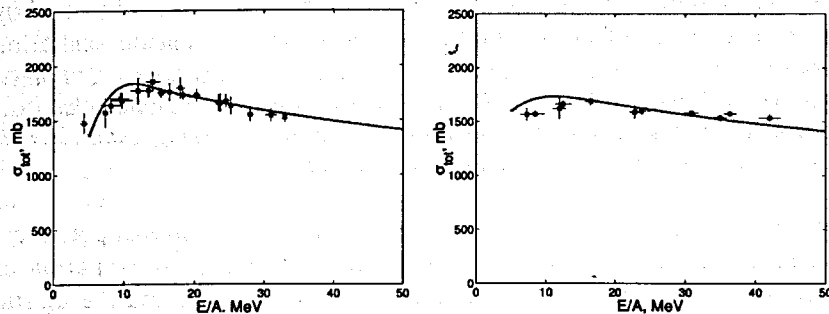

Fig.7. Energy dependence of total reaction cross sections of ^{6}He+^{28}Si (left panel) and ^{6}Li+^{28}Si (right panel). *From the talks given on the International Symposium on Exotic Nuclei EXON-2006 (July 17-22, 2006, Khanty-Mansiysk, Russia) and LVI International Conference "Nuclei-2006" (September 4-9, 2006, Sarov, Russia); will be published in proceedings of these conferences; authors:K.V.Lukyanov, I.N.Kukhtina, V.K.Lukyanov, Yu.E.Penionzhkevich, Yu.G.Sobolev, E.V.Zemlyanaya*

A mathematical model of a gravitating, rapidly rotating, superdense configuration has been constructed using Bethe-Johnson, Oppenheimer-Volkov and Raid equations for a nuclear matter state. An existence of critical solutions of the equation for hydrostatic equilibrium of the stationary rotating, gravitating, superdense configuration is demonstrated by analytical and numerical calculations. In the bifurcation points with respect to the model parameters, a derivation takes place of the solutions for the dense distributions that are asymmetric with respect to rotation axis. The investigation of these solutions has been performed. *[Е.В.Беспалько, С.А.Михеев, И.В.Пузынин, В.П.Цветков. Гравитирующая быстровращающаяся сверхплотная конфигурация с реалистическими уравнениями состояния. Матем. моделир., 2006, Т.18, вып.3, с.103-119].*

Particle physics

The quarkonium production in a field-theoretical setting was reconsidered. It is 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, introduced were new 4-point vertices, suggestive of the colour-octet mechanism. These new objects enable one 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. New contributions to heavy-quarkonium production. Phys. Lett. B 633 (2006) 301-308].*
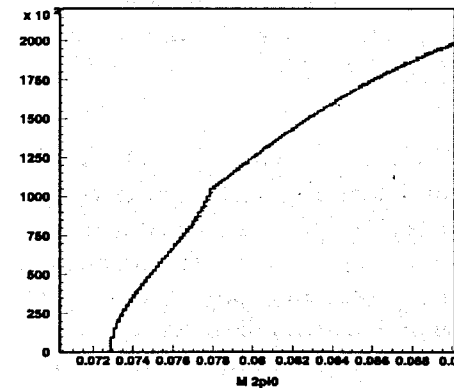

Fig.8. The "cusp"-effect in the $K^+ \to \pi^+\pi^0\pi^0$ decay. Comparison of the theoretical results (red line) with experiment (black line). *From the paper of S.R.Gevorkyan, A.V.Tarasov, O.O.Voskresenskaya "The quantum mechanical treatment of the "cusp"-effect in the $K^+ \to \pi^+\pi^0\pi^0$ decay" To be published in J. Phys. B.*

The "cusp"-effect in the $K^+ \to \pi^+\pi^0\pi^0$ decay observed in the NA-48 experiment was analysed in the frame of the quantum mechanical approach. Comparison of the calculated cross sections show that this approach provides the satisfactory explanation of this effect (Fig.8). An expression for the amplitude of lepton pair production in the nucleus-nucleus collisions in terms of the amplitudes of lepton-nuclear scattering is obtained. From it the approximate compact expression for this amplitude valid with accuracy up to terms of order $(Z\alpha)^5$ is derived. 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 ampli-

tude valid up to terms of ninth order in finite structure constant is obtained. A new approach for calculation of form factors of relativistic elementary atoms is proposed. Explicit expressions for form factors of transitions from bound nS-states to continuum are derived. It is shown that these form factors can be represented in terms of the classical polynomials and may be evaluated numerically with arbitrary degree of accuracy. A general formula for bound-continuous transition form factors of dimesoatoms is derived. It is shown that these form factors can be represented in the form of a finite sum of terms with a simple analytical structure and may be calculated numerically with arbitrary degree of accuracy. *[O. Voskresenskaya and S. Bakmaev. arXiv: nucl-th/06100010. О.О.Воскресенская, А.Н.Сисакян, А.В.Тарасов, Г.Т.Торосян. Ватсоновское представление для амплитуды образования лептонных пар в ядро-ядерных соударениях. Письма в ЭЧАЯ, 2006, Т.3, №4(133) cc.43-47. O. Voskresenskaya and S. Bakmaev. Analytic form factors of hydrogenlike atoms for diskrete-continuum transitions. Particles and Nuclei, Letters, 2006, V. 3, No. 6(135) pp. 33-37. O.O. Voskresenskaya, A.N. Sissakian, A.V. Tarasov and H.T. Torosyan. A Structure for the Amplitude of $Z_1Z_2 \rightarrow l^+ l^- Z_1Z_2$ Reaction Beyond the Born Approximation. Particles and Nuclei, Letters, 2007, V. 4. No. 1(137), pp. 36-41 (in press)].*

A system of minimally coupled nonlinear spinor and scalar fields within the scope of a Bianchi type-I (BI) cosmological model in presence of a perfect fluid and a cosmological constant (Λ term) is studied and solutions to the corresponding field equations are obtained. The problem of initial singularity and the asymptotical isotropization process of the Universe are thoroughly studied. The role of Λ term on the character of evolution is analyzed. It is shown that some special choice of spinor field nonlinearity generates regular solution, but the absence of singularity results in violating dominant energy condition in Hawking-Penrose theorem. It is also shown that a positive Λ, which denotes an additional gravitational force in our case, gives rise to an oscillatory or a non-periodic mode of expansion of the Universe depending on the choice of some problem parameter. The regular oscillatory mode of expansion violets the dominant energy condition, if the spinor field nonlinearity occurs as a result of self-action, whereas, in case of a linear spinor field or nonlinear one that occurs due to interaction with a scalar field the dominant condition remains unbroken. A system with time varying gravitational (G) and cosmological (Λ) constants is also studied to some extent. The introduction of magneto-fluid in the system generates nonhomogeneity in the energy-momentum tensor and can be exactly solved only under some additional condition. Though in this case one indeed deals with all four known fields, i.e., spinor, scalar, electromagnetic and gravitational, the over-all picture of evolution remains unchanged. *[Saha, Bijan: Spinor fields in Bianchi type-I Universe. Physics of Elementary Particles and Atomic Nuclei. 37 Suppl. 1, S13-S44, (2006)].*

Within the framework of Bianchi type-I space-time, the Bel-Robinson tensor and its impact on the evolution of the Universe have been studied. Different definitions of the Bel-Robinson tensor existing in the literature were used and the results were compared. Finally the so called "dominant super-energy property" for the Bel-Robinson tensor as a generalization of the usual dominant energy condition for energy momentum tensors was investigated. *[Saha, Bijan, V. Rikhvitsky, M. Visinescu: Bel-Robinson tensor and Dominant Property in the Bianchi type I universe. Modern Physics Letters A 21(11) 847-861, (2006)].*

A self-consistent system of interacting nonlinear spinor and scalar fields within the scope of a Bianchi type-I cosmological model filled with perfect fluid is considered. The role of spinor field in the evolution of the Universe is studied. It is shown that for some special choice of nonlinearity the spinor field can explain the late time accelerated mode of expansion of the Universe. *[Saha, Bijan: Spinor field and accelerated regimes in cosmology. Gravitation & Cosmology. 12. N. 2-3 (46-47), 215-218 (2006)].*

A self-consistent system of Bianchi type-I (BI) gravitational field and a binary mixture of perfect fluid and dark energy has been considered. The perfect fluid is taken to be the one obeying the usual equation of state, i.e., $p = \zeta\epsilon$, with $\zeta \in [0; 1]$ whereas, the dark energy is considered to be obeying a quintessence-like equation of state. The modification of the ordinary quintessence lies in the fact that its pressure becomes positive if the (dark) energy density exceeds some critical value. Exact solutions to the corresponding Einstein equations are obtained. The model under consideration gives rise to a Universe which is spatially finite. Depending on the choice of problem parameters the Universe is either close with a space-time singularity, or an open one which is oscillatory, regular and infinite in time. Role of the Λ term in the evolution of the BI Universe has been studied. *[Saha, Bijan: Anisotropic cosmological models with perfect fluid and dark energy reexamined. International Journal of Theoretical Physics.*

45(5) 983-995, (2006); Saha, Bijan: Anisotropic cosmological models with a perfect fluid and a Λ term. Astrophysics and space science 302, 83-91, (2006)].

The nature of cosmological solutions for a homogeneous, anisotropic Universe given by a Bianchi type-I (BI) model in the presence of a Cosmological constant Λ is investigated by taking into account dissipative process due to viscosity. The system in question is thoroughly studied both analytically and numerically. It is shown that the viscosity, as well as the Λ term exhibit essential influence on the nature of the solutions. In particular a positive Λ gives rise to an ever-expanding Universe, whereas, a suitable choice of initial conditions plus a negative Λ can result in a singularity free oscillatory mode of expansion. For some special cases it is possible to obtain oscillations in the exponential mode of expansion of the BI model even with a positive Λ, where oscillations arise by virtue of viscosity. [Saha, Bijan and V. Rikhvitsky: Bianchi type I universe with viscous fluid and a Λ term: A qualitative analysis. Physica D 219, 168-176, (2006)].

Condensed matter physics

At present the thermal spike description of heavy ion track formation in high-T superconductors is confronted with serious difficulties caused by a high sensitivity of theoretical track radii to a small change of the electron diffusivity value. This sensitivity is caused by a bifurcation point found numerically in the model and resembles the impossibility of the classical gas description in the mechanics framework due to a dramatic dependence of particle trajectories on small variations of the initial conditions. For solution of the problem, we suggested a thermal explosion model which takes into account such a non-equilibrium process as superheating known from laser-induced phase transformations in solids. This allows us to stabilize essentially the theory. For the first time we give a quantitative description of tracks in $YBa_2Cu_3O_{7-x}$ with both elliptical and circular cross sections. [B.F.Kostenko, J.Pribis, I.N.Goncharov. Thermal Spike Model of Track Formation in $YBa_2Cu_3O_7$. PEPAN Letters, v.3, 2006, pp. 31-44].

A nonlinear system of equations for electron gas and lattice around and along the trajectory of a 700MeV uranium heavy ion in nickel at the constants of heat capacity and heat conductivity taken at room temperature, is solved numerically in the cylindric axial-symmetric coordinate system. Based on the temperature dependence upon radius and depth around the ion trajectory, one can conclude that the ionizing energy loss is enough for the melting and evaporation processes in the target. The maximal sizes of radius and depth in target where the melting and evaporation processes can take place, have been estimated. [И.В.Амирханов, А.Ю.Дидык, Е.В.Земляная, И.В.Пузынин, Т.П.Пузынина, Н.Р.Саркар, И.Сархадов, В.К.Семина, З.А.Шарипов, А.Хофман. Численное исследование температурных эффектов в материалах при облучении их тяжелыми ионами высоких энергий в рамках уравнений теплопроводности для электронов и решетки. Письма в ЭЧАЯ, 1[130], 2006, сс.63-75. I.V.Amirkhanov, A.Yu.Didyk, D.Z.Muzafarov, I.V.Puzynin, T.P.Puzynina, N.R.Sarkar, I.Sarhadov, Z.A.Sharipov. Investigation of thermal processes in one- and two-layer materials under irradiation with high-energy heavy ions within the thermal peak model. Crystallography reports, 2006, Vol.51 Suppl. 1, pp.S32-S43].

The results of sputtering coefficient measurements for pure metals, alloys, amorphous alloys, semiconductors, and highly oriented pyrolytic graphite under irradiation by high energy ions are considered. The possible mechanisms of strong sputtering of materials with high defect concentrations are discussed. The threedimensional thermal spike model ("hot ion track") with the temperature dependence of thermodynamic parameters (specific heat thermal conductivity) is formulated for single-layer mono- and polycrystals and multilayer systems (materials). The results of a numerical solution to the introduced system of partial differential equations are considered for the lattice and electronic subsystem temperatures around and along the fast heavy ion trajectory as a function of the time t, as well as radial r and longitudinal z coordinates, taking into account possible phase transitions such as melting and evaporation. [I.V. Amirkhanov, Yu. N. Cheblukov, A. Yu. Didyk, A. Hofman, I.V. Puzynin, V. K. Semina, and Z. A. Sharipov Sputtering of Solids by Heavy Ions and Temperature Effects in Electronic and Lattice Subsystems. Physics of Particles and Nuclei, 2006, Vol. 37, No. 6, pp. 837–866].

Small angle neutron scattering (SANS) on the unilamellar vesicle (ULV) populations (diameter 500Å and 1000Å) in D_2O was used to characterize lipid vesicles from dimyristoylphosphatidylcholine (DMPC) at three phases: gel $L_{\beta'}$, ripple $P_{\beta'}$, and liquid L_α. Parameters of vesicle populations and internal structure of the DMPC bilayer were characterized on the basis of the Separated Form Factor (SFF) model (see Fig.9) For vesicles prepared via extrusion through pores with the diameter 500Å, it is shown that the vesicle shape changes from nearly spherical in the L_α

phase to elliptical in the $P_{\beta'}$ and $L_{\beta'}$ phases. Parameters of the internal bilayer structure (thickness of the membrane and the hydrophobic core, hydration, and surface area of lipid molecule) were determined. DMPC membrane thickness in the L_α phase ($T = 30°C$) demonstrates a dependence on the membrane curvature for extruded vesicles. The dependence of the DMPC membrane thickness on temperature was restored from the SANS experiment *[M.A.Kiselev, E.V.Zemlyanaya, V.K.Aswal, R.H.H.Neubert. What can we learn about the lipid vesicle structure from the small-angle neutron scattering experiment? Investigation DMPC vesicle structure by small angle neutron scattering. European Biophysics Journal, Vol. 35, No 6, 2006, pp. 477 - 493].*
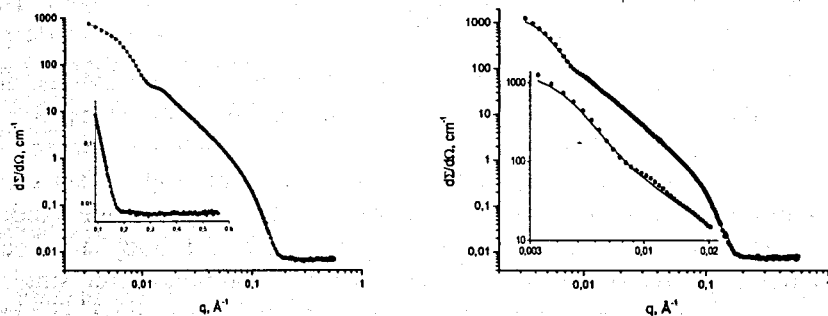

Fig.9. Experimental cross-sections of the ULVs population at $T = 30°C$ (dots) for vesicles extruded through pores of 500Å (left panel) and 1000Å (right panel) diameter and the fitting curves (solid line). The inset on the left panel shows the magnified curve for large q. The right panel inset shows the magnified curve for small q

Partial critical dependences of the form current–magnetic field in a two-layered symmetric Josephson junction are modeled. A numerical experiment shows that, for the zero interaction coefficient between the layers of the junction, jumps of the critical currents corresponding to different distributions of the magnetic fluxes in the layers may appear on the critical curves. This fact allows a mathematical interpretation of the results of some recent experimental results for two-layered junctions as a consequence of discontinuities of partial critical curves. *[P.Kh.Atanasova, T.L.Bojadjiev and S.N.Dimova. Numerical Simulation of Critical Dependences for Symmetric Two-Layered Josephson Junctions. ЖВМиМФ, Т46, №4, 666-679].*

Based on the method of molecular field dominated by magnetic component, it is shown that a homogeneous magnetically aligned nematic liquid crystal can respond to a circularly polarized optical field by transverse nemato-magnetic wave in which velocity of incompressible flow and director undergo coupled oscillations slowly traveling along the axis of magneto-optical anisotropy. The effect may be of practical interest for the magnetically controlled information processing and storage. *[S. Bastrukov, Pik-Yin Lai, D. Podgainy, I. Molodtsova. Optical response of magnetically aligned nematic soft matter by transverse nemato-magnetic waves. Journal of Magnetism and Magnetic Materials, V 304, September 2006, Pages e353-e355].*

It is argued that in the long wavelength limit of electromagnetic, far infrared, field optical response of an ultrafine metal particle threaded by uniform magnetic field can be properly modeled by equations of semiclassical electron theory in terms of the surface inertial-wave-like oscillations of free electrons driven by Lorentz restoring force. The detailed calculation of the frequency of size-independent gyromagnetic plasmon resonances computed as a function of multipole degree of electron cyclotron oscillations is presented. This spectrum is derived in juxtaposition with the canonical Mie's spectral formula for the surface plasmon resonances caused by the Coulomb-force-driven plasma oscillations of conduction electrons. *[Bastrukov S.; Lai Pik-Yin. On the Surface Gyromagnetic Plasmons in a Metal Sphere. Surface Review and Letters, V 13, Issue 01, pp. 81-86 (2006)].*

Quantum systems and computational physics

Two variational wave functions of helium have been developed. They give accurate energy values and satisfy Kato's cusp conditions adapted to the variational procedure. These wave functions are utilized in calculations for reproducing the electron-helium double-ionization experimental data involving both the small and large momentum transfer. A comparison of the present numerical results for the differential cross sections with experiment indicates a minor role of the cusp conditions. *[O.Chuluunbaatar, I.V.Puzynin, P.S.Vinitsky, Yu.V.Popov, K.A.Kouzakov and C.Dal Cappello. Role of the cusp conditions in electron--atom double ionization. Phys. Rev. A 74, pp. 014703(1-4) (2006)].*

A Kantorovich approach is used to solve for the eigenvalue and the scat-

tering properties associated with a multi-dimensional Schroedinger equation. It is developed within the framework of a conventional finite element representation of solutions over a hyper-spherical coordinate space. Convergence and efficiency of the proposed schemes are demonstrated in the case of an exactly solvable 'benchmark' model of three identical particles on a line, with zero-range attractive pair potentials and below the three-body threshold. In this model all the 'effective' potentials, and 'coupling matrix elements', of the set of resulting close-coupling radial equations, are calculated using analytical formulae. Variational formulations are developed for both the bound-state energy and the elastic scattering problem. The corresponding numerical schemes are devised using a finite element method of high order accuracy. *[O.Chuluunbaatar, A.A.Gusev, M.S.Kaschiev, V.A.Kaschieva, A.Amaya-Tapia, S.Y.Larsen and S.I.Vinitsky. Benchmark Kantorovich calculations for three particles on a line. J. Phys. B 39, pp. 243—269, 2006].*

A new effective method of calculating the wave functions of discrete and continuous spectra of a hydrogen atom in a strong magnetic field is developed based on the Kantorovich approach to the parametric eigenvalue problems in spherical coordinates. The two-dimensional spectral problem for the Schroedinger equation with fixed magnetic quantum number and parity is reduced to a spectral parametric problem for a one-dimensional equation for the angular variable and a finite set of ordinary second-order differential equations for the radial variable. A canonical transformation is applied to approximate the finite set of radial equations by means of a new radial equation describing an open channel. The rate of convergence is examined numerically and illustrated with a set of typical examples. The results are in good agreement with calculations by other authors. *[O.Chuluunbaatar, A.A.Gusev, V.L.Derbov, M.S.Kaschiev, V.V.Serov, T.V.Tupikova and S.I.Vinitsky. On an effective approximation of the Kantorovich method for calculations of a hydrogen atom in a strong magnetic field. Proceedings of SPIE 6165, pp. 66-82 (2006)].*

(e,2e) and (e,3-1e) experiments on the double processes of He, i.e. single ionization with simultaneous excitation and double-ionization, were analyzed. The symmetric noncoplanar geometry combined with high incident electron energies has made it possible to study at large momentum transfers. The results are compared with plane wave impulse approximation (PWIA) calculations using He wavefunctions of various levels of sophistication. It is shown that shapes of the momentum dependent (e,2e) and

(e,3-1e) cross sections are well reproduced by the PWIA calculations when highly correlated wave functions are employed, but noticeable discrepancies between experiment and theory remain in magnitude. The discrepancies are, however, reduced with increasing impact energies, suggesting higher excitation energies may be required to analyze these double processes in terms of the PWIA. *[N.Watanabe, Y.Khajuria, M.Takahashi, Y.Udagawa, P.S.Vinitsky, Yu.V.Popov, O.Chuluunbaatar and K.A.Kouzakov. (e,2e) and (e,3-1e) studies on double processes of He near the Bethe ridge. AIP Conference Proceedings 811, pp. 96-101 (2006)].*

The boundary-value problem in spherical coordinates for the Shroedinger equation describing a hydrogen-like atom in a strong magnetic field was
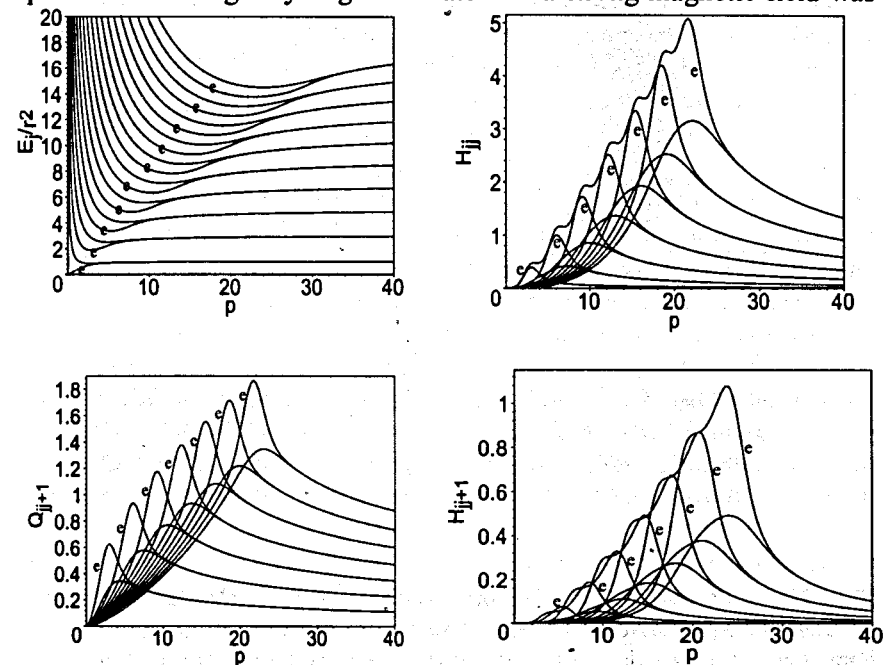

Fig. 10. Some effective potentials $H_{ij}(r)$, $Q_{ij}(r)$ and potential curves $E_j(r)/r^2$ versus the parameter $p=\gamma r^2/2$ for even (marked by symbol 'e') and odd parity states at $|m|=0$ and $\gamma=1$

reduced to the problem for a set of radial equations in the framework of the Kantorovich method. The effective potentials of these equations are given by integrals over the angular variable between the oblate angular spheroidal functions depending on the radial variable as a parameter and

their derivatives with respect to the parameter (Fig. 10.). A symbolic-numerical algorithm for evaluating the oblate spheroidal functions and corresponding eigenvalues which depend on the parameter, their derivatives with respect to the parameter and matrix elements is presented. The efficiency and accuracy of the algorithm and of the numerical scheme derived are confirmed by computations of eigenenergies and eigenfunctions for the low-excited states of a hydrogen atom in the uniform magnetic field (Fig. 11). ionization rate of the left-hand side state and the right-hand side state will occur by the linear and circular polarized light,
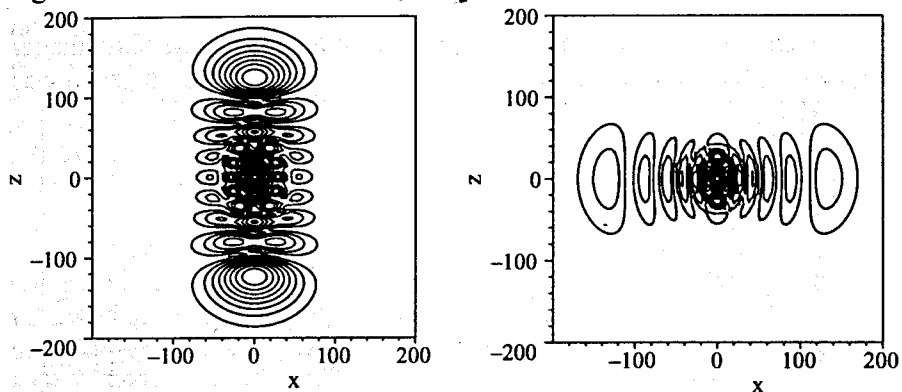
j_{max}	E	j_{max}	E
2	-0.00781242971347	2	-0.00499982705326
4	-0.00617279526323	4	-0.00499993540325
6	-0.00617279808777	6	-0.00617243586258
8	-0.00617279808777	8	-0.00617243586258

Fig. 11. The probability density isolines of the Zeeman wave states $|N=9,N_r=0,m=0>$ (lhs) and $|N=9,N_r=8,m=0>$ (rhs) with even parity $\sigma=+1$ in a homogeneous magnetic field. In down panel is shown convergence of the method for these states versus number j_{max} of basis functions in the Kantorovich method at $\gamma=1.472\cdot10^{-5}$

respectively. From the picture (Fig. 11) one can see that the maximal ionization rate of the left-hand side state and the right-hand side state will occur by the linear and circular polarized light, respectively. The developed approach yields a good tool for calculation of threshold phenomena

in formation and ionization of (anti)hydrogen like atoms and ions in magnetic traps. One can calculate the dynamics of the Zeeman states in time-dependent external electric fields with help of the algorithm for unitary decomposition of the time evolution operator. The latter has a certain perspective for computer simulation of the ion motion in the trapped models of quantum computers. *[V.Gerdt, A.Gusev, M.Kaschiev, V.Rostovtsev, V.Samoylov, T.Tupikova, S.Vinitsky. LNCS 4194, Springer-Verlag, Berlin, 2006, pp. 205-218].*

Theoretical calculations for the evolution of Zeeman states have been performed in a train of short electric half-cycle pulses (kicks). For the numerical solution of the corresponding time-dependent Schroedinger equation (TDSE) the high accuracy splitting scheme based on the unitary approximations of the evolution operator is developed. The finite element method is used for determining the spatial form of the solution. The efficiency and stability of the developed computational method is shown for 1D models in the cases of second-, forth-, and sixth-order accuracy with respect to the time step. Numerical calculations for the kicked hydrogen atom in the presence of magnetic field are performed using the scheme of the sixth-order accuracy with respect to a time step and both Galerkin and Kantorovich reductions of the problem with respect to the angular variables. For a particular choice of the electric- and magnetic-field parameters and the initial Zeeman state the corresponding results exhibit a two-state resonance picture. *[O.Chuluunbaatar, A.A.Gusev, V.L.Derbov, M.S.Kaschiev, K.A.Kouzakov, V.V.Serov, V.N.Samoylov, T.V.Tupikova and S.I.Vinitsky. On the Kantorovich approach for calculations of the hydrogen atom states in laser pulses. Proceedings of SPIE 6165, pp. 83-98 (2006)].*

The specialists of LIT and the Institute of Cybernetics of Georgia conduct joint research in the field of quantum mechanics and quantum computations.Using a method of transformation of soluble time-independent problems of quantum mechanics into time-dependent ones, periodic potentials with a complex dependence on time and coordinate variables are employed. The problem of evolution of spins of a particle in a heterogeneous T periodic magnetic field, a special case of which is a dynamics of spin states in a homogeneous magnetic field, is under study. The matrices of the evolution received in an explicit form are used to construct a universal set of gates needed for quantum computations. Non-adiabatic geometrical phases are determined in terms of the cyclic solutions obtained. In the suggested approach, the geometrical phase effect at construction of

one-cubit gates is naturally taken into account. A way of obtaining entangling operators is discussed too. *[Suzko A.A., Giorgadze G. - Submitted to "Contemporary Mathematics and its Applications", 2006].*

It is known that the interwining operator technique (Darboux transformations) as well as the method of supersymmetry in quantum mechanics provides a set of exactly soluble stationary models. Each of these models with time-independent Hamiltonian can be generalized to receive a corresponding family of time-dependent exactly soluble Hamiltonians. The method of interwining operators provides a universal approach for obtaining new exactly soluble equations and can be applied to operators of general kind. The interwining operator technique is applied to the generalized Schroedinger equation with an additional functional dependence h (r) in the right-hand side of the equation. The suggested generalized transformations turn into the Darboux transformations both for fixed and variables values of energy and angular momentum. A relation between the Darboux transformation and supersymmetry is considered. *[Suzko A.A., Giorgadze G. - "Atomic Nuclei", Vol. 69, No.10, 2006].*

A system of traps was considered, each containing a large number of Bose-condensed atoms. This ensemble of traps was subject to the action of an external modulating field generating nonequilibrium nonground-state condensates. It was found that when the frequency of the modulating field was in resonance with the transition frequency between two different topological coherent modes, each trap became an analog of a finite-level resonant atom. Then, similarly to the case of atoms in an electromagnetic resonant field, one can create entanglement between atomic traps subject to a common resonant modulating field generating higher coherent modes in each of the traps. A method was suggested for regulating entanglement production in such a system of multitrap and multimode Bose-Einstein condensates coupled through a common resonant modulating field. Several regimes of evolutional entanglement production, regulated by manipulating the external field, were illustrated by numerical calculations. The suggested method can be used for information processing and quantum computing. *[V.I. Yukalov and E.P. Yukalova, Laser Phys. 16, 354-359 (2006). "Entanglement production with multimode Bose-Einstein condensates in optical lattices". V.I. Yukalov and E.P. Yukalova, Phys. Rev. A 73, 022335-10 (2006). "Regulating entanglement production in multitrap Bose-Einstein condensates"].*

Distributions of phosphate backbone-produced electrostatic potentials around several tRNAs were calculated by solving the nonlinear Poisson-Boltzmann equation. The tRNAs were either free or bound to the proteins involved in translation: aminoacyl-tRNA and elongation factor EF-Tu identified several regions of strong negative potential related to typical structural patterns of tRNA and invariant throughout the tRNAs. The patterns are conserved upon binding of tRNAs to the synthetase and the EF-Tu. Variation of tRNA charge in our theoretical calculations of electrostatic potential-mediated pK shifts of pH-dependent labels attached to tRNA, compared to experimentally observed pK shifts for those labels, shows that the total charge of tRNA is large, within the interval from -40 to -70 proton charges. The electrostatic field of tRNA is sufficient to cause ionization of histidine residues of ARSase, causing additional free energy of ARSase-tRNA interaction of at least several kcal/mol. This may discriminate proteins with respect to the particular tRNA at large distances. Two types of tRNA-protein electrostatic recognition mechanisms are discussed. One, more specific, involves charges induced on protein by the large electrostatic potential of tRNA, while the other, less specific, does not involve induced charges. *[R.V.Polozov, M. Montrel, V.V. Ivanov, Yu. Melnikov, V.S. Sivozhelezov: Transfer RNAs: Electrostatic Patterns and an Early Stage of Recognition by Synthetases and Factor EF-Tu, Biochemistry, 45(14), 4481- 4490, 2006].*

At present, after 120 years of the theoretical and experimental works, the issue of the genome macroarchitecture as the highest level of interphase chromosome organization in somatic cell nuclei remains still unresolved. The problem of the spatial arrangement of interphase chromosomes in haploid germ cells has never even been studied. A 3D simulation of packaging of the entire second chromosome in Drosophila mature sperms has been performed by using mathematical approaches and visualization methods to present macromolecular structure data. As genetic markers for simulation, frequency and location of the second inversion breakpoints for 72 structural *vg* mutants induced by ionizing radiation were used supposing that both ends of each inversion are topologically brought together forming loop of appropriate size. For the account of a degree of spatial affinity and visualization of chromosomal loops modern 3D-modeling methods with application of splines, libraries OpenGL, language Delphi, program Gmax were used. According to the model proposed, the entire second chromosome within mature sperm nuclei seems to be packaged in the form of a megarosette-loop structure which may be a basic principle

of organization of the genome macro-architecture in animal haploid germ cells. *[I.D. Alexandrov, M.V. Alexandrova, N.S. Zaikin, V.V. Koren'kov, O.V.Pervushova, V.A. Stepanenko. 3D Modeling of Genome Macroorganization on the Basis of Its Structural Changes after Action of Radiation. PEPAN Letters, 2006, v. 3, n. 6(135), pp. 58-73].*

Computer algebra and applications

The investigation "Discrete relations on abstract simplicial complexes" discusses an approach to research of a system of discrete relations based on set-theoretical and topological constructions. On the one hand, a system of discrete relations is a generalization of cellular automaton and, on the other hand, it is a set-theoretical analog of a system of polynomial equations. The proposed approach is implemented as a C program. The results of application of this approach to some binary cellular automata are presented. In the binary case, cellular automata can be represented by systems of polynomial equations, which are normally studied by the Gröbner basis method. The approach is compared with this method on some examples. *[V.V. Kornjak "Programming", 2006, No.2].*

Computational efficiency of applying involutive criteria for avoiding some useless reductions in construction of Groebner bases by the Janet division algorithm was investigated by means of computer experiments. *[V.P.Gerdt, D.A.Yanovich. Effectiveness of Involutive Criteria in Computation of Polynomial Janet Bases. Programming and Computer Software, Vol. 32, No. 3, 2006, 134—138].*

Algorithm was designed and implemented in Maple for automatic generation of finite difference schemes for linear partial differential equations with two independent variables and for uniform and orthogonal grids. The algorithm is based on construction of difference Groebner bases. *[V.P.Gerdt, Yu.A.Blinkov, V.V.Mozzhilkin. Groebner Bases and Generation of Difference Schemes for Partial Differential Equations. Symmetry, Integrability and Geometry: Methods and Applications (SIGMA) 2 (2006) 051, 26 pages. arXiv:math.RA/0605334].*

A new parametrization of the SU(3) group manifold was found which can be considered as a generalization of the classical parametrization of group SU(2) by the Euler angles. The new parametrization can be used, in particular, for Hamiltonian reduction of gauge field theories with SU(3) symmetry and for quantum computation based on the use of qutrits – quantum particles with three classical states. *[V.Gerdt, R.Horan, A.Khvedelidze, M.Lavelle, D.McMullan, Yu.Palii. On the Hamiltonian reduction of geodesic motion on SU(3)to SU(3)/SU(2). Journal of Mathematical Physics, Vol.47, No. 10, 2006, 112902 (27 pages). arXiv:hep-th/0511245].*

A numerical and analytical algorithm for reconstructing the two-dimensional discrete elliptic equation of a part of spectrum and pre-scribed symmetry conditions was developed. The right problem is solved in the rectangle MxN with the zero-boundary conditions. If the given symmetry conditions are satisfied, the eigenfunctions can be prolonged from the rectangle to the whole plain with reserving continuity of the first derivatives. The problem is reduced to reconstruction of a symmetric five-diagonal matrix. It is proved that when the prescribed symmetry conditions are satisfied, the considered block three-diagonal matrix and all its blocks are persymmery. This matrix has L<MN different elements and can be reconstructed of L given eigenvalues. The matrix elements and lacking MN-L eigenvalues are determined by solving a polynomial system constituted of the Vieta relations for 4 multipliers of the characteristic polynomial of the matrix. Numerical experiments were produced. The polynomial systems were derived and solved by using CAS REDUCE. *[S.I.Serdyukova. Inverse Problem for discrete elliptic equation with prescribed symmetry conditions. DAN, Mathematica, v.406, n.2, pp.160-164, 2006].*