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LABORATORY OF INFORMATION TECHNOLOGIES

REPORT ON RESEARCH ACTIVITIES IN 2008

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The main directions of the activity of the Laboratory of Information Technologies (LIT) are aimed at the provision of the experimental and theoretical studies conducted at JINR with modern telecommunication, network, information support and new mathematical and computing methods.

The LIT activity is focused on two directions, namely "Information, Computer, and Network Support of the JINR's Activity" (topic 05-6-1048-2003/2010, headed by V.V. Ivanov, V.V. Korenkov, and P.V. Zrelov) and "Mathematical Support of Experimental and Theoretical Studies Conducted by JINR" (topic 05-6-1060-2005/2010, headed by V.V. Ivanov, Gh. Adam, and P.V. Zrelov). These directions are developed in frames of the general JINR topic "Networks, Computing, and Computational Physics". The Laboratory staff involves high-skilled scientists and engineering personnel, including 25 doctors of science and 63 candidates of science. The Laboratory staff participated in research work done within 20 topics of the Topical plan for JINR research and international cooperation.

Following the decision of the JINR Committee of the Plenipotentiary Representatives, on March 14-15 2008, concerning the radical improvement of the computer telecommunication links with major partner laboratories 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.

LIT received a BMBF grant for "Development of the Grid-infrastructure and tools to provide joint investigations performed with participation of JINR and German research centers", CERN-JINR Cooperation Agreement on several topics: PC-based distributed computing NICE, development of LabVIEW applications, and participation of JINR in the LCG. 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 also was progressing 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. Seven grants were afforded by the Russian Foundation for Basic Research and two 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 continued. The promotion of this direction is part of joint propositions of the National Academy of Science of Belarus and Federal Agency of Science and Innovations of the Russian Federation "The development and use of hard- and software in grid-technologies and advanced supercomputer systems SKIF in 2007-2010 (SKIF-GRID)".

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.

The work within the project on the Grid infrastructure development for WLCG financed by the Federal Agency of Science and Innovations of the Russian Federation was in progress, too.

NETWORKING, COMPUTING, INFORMATION SUPPORT

In 2008, the Laboratory provided the reliable operation and development of the JINR networking and informational infrastructure. The key components of this infrastructure comprise JINR telecommunication data links, LAN, JINR Central Information Computing Complex and base software responsible 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.

In 2008, an agreement was concluded between JINR and RSCC on the rent of optical fiber cable for the provision of optical communication links between Moscow and Dubna. The project is realized in cooperation by JINR, RSCC, NORTEL, JET Infosystems, RosNIIROS, the Computer Networks Interaction Center "MCK-IX". A high throughput channel Dubna-Moscow is under construction in frames of this project on the basis of state-of-the-art technologies DWDM and 10Gb Ethernet. The channel is planned to be launched in 2009 with a capacity of 20 Gbps. The mentioned technologies allow one to create up to 72 channels of 10 Gbps each, and to raise the total throughput up to 720 Gbps. To this aim, laying a new single mode optical cable is planned to be done from LIT to "Dubna" Satellite Communications Center.

The Russian national scientific network is designed as an integrated information environment. Its connecting basis is the RBNet network. 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 a substantial increase of the throughput of the channels (from 10 Gbps up to several hundreds Gbps) and to reach a new level of the service.

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 GEANT network. The JINR-participating countries develop regional and national research and educational networks, many of which are being connected to the European network GEANT. 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 GEANT. This is the overall adopted approach to the integration of the regional networks for science and education in Europe.

In 2008, a module was added to the system of the external traffic monitoring that allows one to divide the traffic into categories, for example, a traffic with scientific networks, a traffic with Dubna networks, a multimedia translation traffic, etc. The viewing interface is connected to the JINR users register. The traffic division is performed with the help of the database SQL that contains more than 400 various attributes.

Fig. 1 shows the distribution of the incoming and outgoing JINR traffic from 2003. The sharp growth of the traffic for the last few years is explained by the activity of LHC experiments during the preparation of all computer centers for the moment of LHC startup.

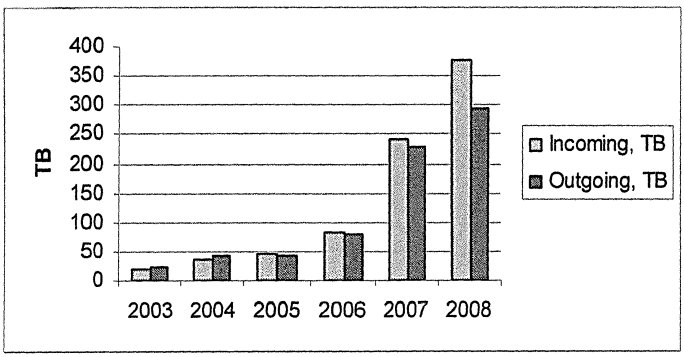


Fig.1.

Table below gives data on the 10 most popular networks, the interaction with which forms the main JINR traffic.

N	Scientific network	Incoming (IN) Tb	Outgoing (OUT) Tb	% IN	% OUT
1	European Organization for Nuclear Research (CH)	73.88	73.0	33.64	72.22
2	Deutsches Elektronen-Synchrotron (DE)	69.3	9.11	31.56	9.01
3	Nationaal Instituut voor Subatomaire Fysica (NL)	16.11	1.17	7.34	1.16
4	Institut National de Physique Nucleaire (FR)	15.27	0.797	6.95	0.77
5	Science Park Watergraaf-smeer Amsterdam (NL)	8.81	5.73	4.01	5.67
6	Joint SuperComputing Centre (RU)	4.82	0.317	2.19	0.31
7	California Institute of Technology (US)	3.45	0.184	1.57	0.18
8	Oxford University (GB)	3.25	0.078	1.48	0.08
9	Gesellschaft fuer Schweri-onenforschung mbH (DE)	2.51	0.181	1.15	0.18
10	SINP MSU (RU)	2.22	0.284	1.01	0.27

Fig. 2 shows the distribution of the incoming traffic over JINR subdivisions. The servers and CICC traffic include the common Grid-traffic of JINR.

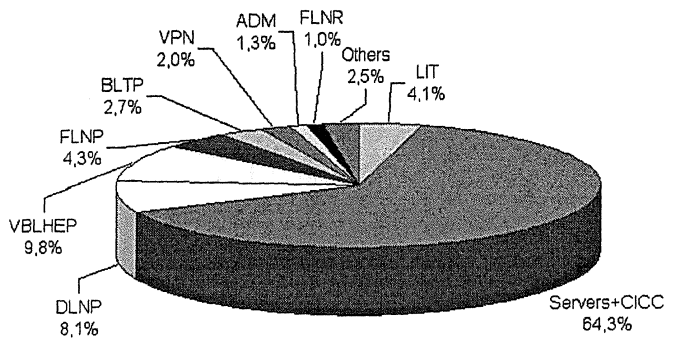


Fig. 2.

JINR LAN

The provision of the fail-safe work of the JINR local area computer network (LAN) is the primary goal of the network service at LIT. At present the JINR LAN includes 6370 computers and nodes (5880 in 2007). In 2008, the JINR LAN included 3562 users, more than 1500 users of mail.jinr.ru service and 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 has allowed us to fix about one million spam – messages a day for central mail-servers.

In 2008, the registration mechanism of access to external libraries was integrated into the JINR user register - the IPDB base. In total, during October 2008, more than 800 users of external electronic libraries were registered. On the average, 20 new users are registered per month.

Central Information and Computer Complex

During the last two years, the development of the computing power of the Central Information and Computer Complex (CICC) in LIT-JINR was done by the acquisitions of multicore processor modules from leading computer providers. Three rackmount modules (two from T-Platforms and one from Hewlett-Packard) each consisting of 40 dual-core 2.66 GHz Intel Xeon 5150 processors, were acquired in 2007. During 2008, an additional amount of four blades was acquired from SuperMicro: three blades involve 20 quad-core 2.66 GHz Intel Xeon E5430 processors each, while the fourth one involves 20 quad-core 3.0 GHz Intel Xeon X5450 processors. Inside each module, the RAM is 2 Gb/core. The information transfer is secured by one Gigabit Ethernet (GbE) in each machine, while every module is connected to the main Backbone Ethernet switch via a four-port GbE trunk, so the aggregated in-between modules rate was upgraded up to 4 Gbps. The fourth blade can work as a dedicated parallel cluster under InfiniBand inter-connect as well.

Thus, the present day CICC JINR cluster is a heterogeneous 560 core structure. Performance assessment using High Performance LINPACK benchmark points to an overall 2.982 TFlops, while the sum of its three homogeneous parts yields 3.3374 TFlops under Gigabit Ethernet interconnect. For the 80-core superblade module having InfiniBand inter-processor connection as well, the performance was 757.5 GFlops. *[Gh.Adam, S.Adam, A.Ayriyan, V.V. Korenkov, V.V. Mitsyn. Performance assessment of the 2008 configuration of the CICC JINR cluster. Proceedings of International Conference "Distributed computing and Grid technologies in science and education, GRID-2008", ISBN 5-9530-0183-5, 2008, pp.283-286].*

The CICC resources are used by participants of the experiments E391a, KLOD, COMPASS, CDF, D0, DIRAC, CMS, ALICE, ATLAS, H1, OPERA,

HERMES, CBM, PANDA, etc. for simulation of physical processes and experimental data analysis.

In the summer of 2008, the CICC conventional performance was equal to 1400 kSI2K (kSI2K units are usually used for computing performance evaluation in accordance with the Spec Integer 2000 special test and the computing power of one core of Intel Xeon 2.8 GHz processor approximately corresponds to 2.5 kSI2K) and the disk storage capacity – 100 TB (82 TB – for user catalogs, software and large data volumes storage). The new equipment was purchased at the end of 2008 under the FASI Contract "Working out the computing system for development of the Grid-complex RuTier2/RDIG for carrying out by the Russian institutes the distributed data analysis for the LHC experiments as a part of global Grid-system WLCG/EGEE" and significant increase of the CICC performance up to 2000 SI2K and the mass storage capacity up to 400 TB will be expected after the equipment installation. Fig.3 shows a new structure of the CICC.

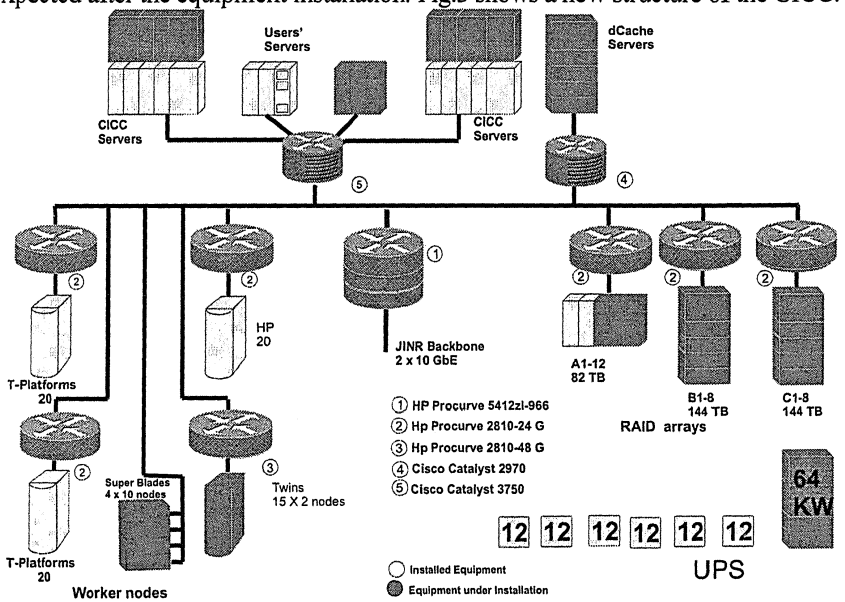


Fig. 3.

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.

The table below shows a batch jobs distribution over JINR Groups excluding WLCG groups in 2008:

Groupname	Jobs number	CPU time (kSi2K*hours)	Wallclock (kSi2K*hours)
DLNP	32435	476237.34	485187.28
VBLHE	13925	35091.82	54066.10
panda	12913	6111.96	84740.23
LIT	3554	66598796.97	202087.02
FLNR	1865	13814.67	3722.98
BLTP	1275	2867175.64	236725.66
FLNP	774	1064906.68	136367.94
foton2	161	9755.24	9996.54
na48	55	20.50	21.61
cbm	1	0.46	0.46
TOTAL	**66958**	**71071911.27**	**1212915.83**

The distribution of Grid Virtual organizations jobs at JINR CICC in 2008 is tabulated as follows:

Grid VO	Jobs number	CPU time (kSi2K*hours)
atlas	342159	1151011.95
cms	327330	1246383.51
alice	161437	1400131.11
biomed	48372	799909.49
lhcb	36433	547456.01
ops	28952	1463.98
hone	23747	447567.90
fusion	10525	376339.26
dteam	7893	23.48
lrgst	200	0.95
rgstest	18	0.01
Total	**987 066 (in 2007 - 220 793)**	**5 970 287.64 (in 2007 - 1 834 466.49)**

Grid-technologies and WLCG project

During the last five years the JINR takes an active part in two large-scale worldwide grid projects: Worldwide LHC Computing Grid (WLCG) project *(http://lcg.web.cern.ch/LCG/)* and Enabling Grids for E-sciencE (EGEE) project *(http://www.eu-egee.org/)*.

The WLCG project has been organized to build and maintain data storage and analysis infrastructure for the high energy physics community that will use the LHC. The modern grid technologies are the basis of the infrastructure building. The JINR staff members participate in three LHC experiments (ALICE, ATLAS and CMS) and it is strongly important to provide the proper conditions for the JINR physicists for their full-scale participation in the experiments at the LHC running phase. The JINR participates in the LCG project in accordance with the Protocol between CERN, Russia and JINR signed and adopted in 2003.

The EGEE project was conceived to create a global infrastructure for a scientific sphere and was supported by the European Community. The aim of the EGEE project is to gather all current national, regional and application grid developments into a common grid-infrastructure for the scientific research. The EGEE project infrastructure provides a 24-hour access to the most high-performance computing resources independently of their geographical location. The worldwide distributed scientific communities can use this infrastructure in accordance with the common access rules. Nowadays the EGEE brings together scientists and engineers from more than 140 institutions in 50 countries world-wide and the EGEE Grid consists of 80,000 CPU at 300 grid sites and currently processes up to 300, 000 jobs per day. 10,000 users are registered and can work in this powerful grid infrastructure. As the EGEE project started in fact at the LCG global infrastructure, the EGEE and LCG projects infrastructures are considered as a common LCG/EGEE infrastructure.

The JINR participation in the LHC experiments and in other large-scale projects asked for a substantial increase of its networking and information resources as well as the deployment of a large volume of work toward the development of the JINR Grid-segment and its integration in the Russian Grid-infrastructure RDIG. For the time being, the RDIG integrates information resources from 15 Russian scientific centers and it is part of the European and global Grid-infrastructures.

To follow the requirements of the global grid projects, a necessary level of all the elements of the JINR telecommunication, network and information infrastructure should be provided including high-throughput telecommunication data links, the JINR local area network (LAN) backbone, central computer complex and grid segment, software support for the physical experiments using grid (at JINR they are ALICE, ATLAS, CMS, PANDA, CBM and H1).

Participation in WLCG includes: WLCG-infrastructure support and development at JINR in accordance with the requirements of the experiments for the LHC running phase; participation in WLCG middleware testing/evaluation; grid monitoring tools development; JINR WLCG portal support and development, MCDB development; user training and induction to grid; support of JINR member states in the WLCG activities.

In 2008, the CICC was switched over from the LCG middleware environment to the gLite new generation middleware (the current version is gLite 3_1_0) and the Scientific Linux 3 operational system has been updated to Scientific Linux 4. Users can access the LCG/EGEE resources via User Interface (UI) service installed at the interactive computers of the JINR CICC. Also the following basic and special grid services are provided at the JINR: Storage Element (SE) service (82 TB dCache disk storage); Computing Element (CE) service as grid batch queue enabling access for 10 Virtual Organizations (VO) including ALICE, ATLAS, CMS, LHCb, HONE (H1 experiment at DESY); Information Service (BDII- Berkley DB Information Index); Proxy service; the advanced service for access to the LCG/EGEE resources (MyProxy); Workload Management System + Logging&Bookkeeping Service (WMS+LB); RGMA-based monitoring system collector service (MON-box); LCG File Catalog (LFC) service and VOboxes special services for ALICE, CMS and PANDA. It should be mentioned here that we have the batch queue enabled for PANDA. Also there are two NFS-servers dedicated to VOs. The software required for Virtual Organizations is currently installing at the JINR LCG/EGEE site including dCache xrootd door, AliROOT, ROOT, GEANT packages for ALICE; ATLAS packages; CMSSW packages for CMS, DaVinchi and Gauss packages for LHCb.

In 2008 for the user support to stimulate their active usage of WLCG resources the special courses, lectures, and trainings (*http://www.egee-rdig.ru/rdig/user.php*) were organized:

- ATLAS data analysis using GANGA (21.01.2008);
- Tutorial on distributed analysis of ATLAS data (17.04.2008);
- User Training (lectures) during GRID'2008 conference (02.07.2008);
- Training courses for users: gLite_3_1_0 (07.07.2008 - 08.07.2008);
- gLite Introduction (in English) for users (09.07.2008-10.07.2008);
- Practical Courses for LCG/EGEE Administrators gLite Installation and Configuration (09 - 19.09.2008);
- Distributed Analysis of Atlas Data (14.10.2008).

In 2008, the Laboratory staff continued

- participation in Service, Data, Software and Analysis Challenges and MC Production for ALICE, CMS and ATLAS in coordination with LHC experiments and Tier1 centers at Karlsruhe (FZK), CERN (CERNPROD) and Amsterdam (SARA);

- participation in CMS Phedex test data transfers; Phedex server for JINR and Russian institutes was supported at the CMS VObox at JINR;
- regular update and testing of ALICE software (AliEn) required for ALICE production Data and Service Challenges and distributed analysis not only at the JINR-WLCG site but also at 12 ALICE sites in Russia;
- support at the JINR-WLCG site of a dedicated Computing Element (lgdce01.jinr.ru) which enables a special short queue (CPU time per job less than 1.5 hour) for any ATLAS VO (Virtual Organization) user;
- the dCache system usage/development/testing (dCacheTestSuit package);
- WLCG middleware testing/evaluation: testing of the gLite Data Management system included testing of LFC (LCG File Catalogue). Firstly, the existing developer's tests were integrated into SAM and then the new tests (35 programs) have been developed for LFC by using CLI commands;
- support and development of monitoring and accounting system (*http://rocmon.jinr.ru:8080*) for the WLCG-infrastructure at JINR and other sites of the Russian Tier2 cluster;
- development of the WLCG MCDB system (WLCG LCG Monte-Carlo physical events Data Base): creation of a set of basic modules, web-interface development, access to MCDB from CMSSW package (*http://mcdb.cern.ch*);
- FTS monitoring and testing (*https://twiki.cern.ch/twiki/bin/view /LCG/TransferOperations*): by now FTS monitoring provides detection of issues affecting the transfers between Tier0/Tier1 WLCG centers, an initial analysis, reports on existing problems to the relevant Regional Operations Centers (generally via service tickets) and solutions recommended; new web-interface to the monitoring system has been developed and implemented in the LHC Dashboard; new version of the FTS monitoring system is under development *[V.Korenkov, A.Uzhinskiy. File Transfer Service Architecture in Grid. Open Systems, 2008, 2, pp.52-56, http://www.osp.ru/os/2008/02 4926522/; A.Uzhinskiy, V.Korenkov. JINR Communication, P11-2008-80, A.Uzhinskiy, V.Korenkov. JINR Communication, P11-2008-82];*
- participation in ARDA activities: CMS Dashboard development, including monitoring of the CMS Monte-Carlo production system and Condor-G job monitoring; the interface to the CMS Dashboard database for GridMap monitoring tool (*http://gridmap.cern.ch/gm)* has been implemented;
- full reconstruction of the GridLab at LIT JINR (in frames of the "Dubna-Grid" project): replacement of the equipment (with the increased number of nodes); creation of fully functional educational lecture-room;
- the analysis and selection of the middleware for the internal information bus of the remote real-time monitoring system (RRTMS) was done. The remote real-time monitoring system conception was implemented. It defines the ar-

chitecture and modules which are essential for the realization of the remote access system to the data tacking and processing systems and it allows remote monitoring system integration with operational monitoring in the Grid- infrastructures. A functional real-time remote monitoring system prototype was implemented. It uses mirror of the online published data from Point1 in the CERN public network. Remote monitoring of this data was implemented *[A.V.Yakovlev. Realization of the services for real-time remote monitoring and data access system in the ATLAS experiment infrastructure. ATLAS Workshop, Dubna, 2008 http://webadm.jinr.ru/cdsagenda//fullAgenda.php?ida=a0825]*. The development and support of ATLAS TDAQ components: Event Dump, Resource Manager, WMI was continued;

- support of the JINR Member States in WLCG activities: work in a close cooperation and provide support to our partners in Ukraine, Belarus, Azerbaijan, Czech, Romania, Poland, Germany, South Africa, and Bulgaria. In particular, technical support is provided for system administrator of NC PHEP BSU (National Scientific and Educational Centre of Particle and High Energy Physics of the Belarusian State University) in their activities on construction, configuration and putting into operation a local grid site at the NC PHEP BSU for its further integration into a world-wide grid infrastructure.

In frames of participation in Grid activities in cooperation with German centres in 2008 the following work was done:

- FTS test file transfers between FZK and JINR to certificate the link between T1-FZK and T2-JINR. In accordance to the CMS computing requirements, the network links between CMS Tier1 and Tier2 centers should be tested and then be certified at the CMS collaboration if during fixed time intervals transfer rates are not less then 20 MBs. In October 2008 the link between T1-FZK and T2-JINR was successfully tested in frames of CMS Phedex data transfer system (which provides FTS transfers between CMS sites) and certified in CMS. The maximal transfer rates were more than 37 MBs;
- H1 MC production grid monitoring: the common activities with DESY (Hamburg) were started in 2007 year and continued in the 2008 year. The main goal of the work is to provide a reliable way to track down job states in cooperation with the DESY H1 Monte Carlo production group. The statistical monitoring component has been introduced for H1 Monte Carlo production group as an extension to the current job processing framework. It is made as an extension to the current job batch system and can be stopped or removed completely without interrupting job batch system process;

- HONE VO queue configured and enabled at JINR WLCG-site in the 2007 year is in an active use for H1 Monte-Carlo production. From December 2007 to November 2008 more than 23 000 HONE VO jobs have been completed at the JINR WLCG site (it is 4% of a total number of HONE VO jobs during this period) and CPU time usage for their execution forms 7.5 % of the total amount of HONE VO jobs CPU time (normalized to a reference value of 1000 SpecInt2000).

Results of our activities in WLCG/EGEE computing are summarized in the table below, where data on top EGEE/LCG sites for LHC VOs (ALICE, ATLAS, CMS and LHCb) by normalised CPU time obtained from the EGEE accounting portal http://www3.egee.cesga.es/gridsite/accounting/CESGA/egee_view.html for period June-December 2008 (after JINR CICC modernization in June 2008) are presented.

1. FZK-LCG2	7356145
2. GRIF	5866168
3. N2P3-CC-T2	5410861
4. IN2P3-CC	5033304
5. NIKHEF-ELPROD	4985490
6. TRIUMF-LCG2	4491970
7. NDGF-T1	3763150
8. RWTH-Aachen	3634905
9. RAL-LCG2	3436688
10. JINR-LCG2	3340491

The activities on the LHC computing support will become especially important before the LHC start, which is expected in the year 2009. The Russian distributed grid computing infrastructure adopted for the LHC experiments has been successfully built as the RuTier2 (Russian Tier2) distributed cluster. In accordance with the RDIG computing model for the LHC, a distributed RuTier2 cluster operates with the resources located at different institutes and share them between all the LHC experiments. The JINR CICC is an segment of the RDIG infrastructure used for the LHC computing and for different grid Virtual Organizations (VO) for simulation of physical processes and experimental data analysis. These resources have been reliably and successfully used during 2007-2008 years, and their contribution in RDIG was about 44% (see Figs. 4 and 5).

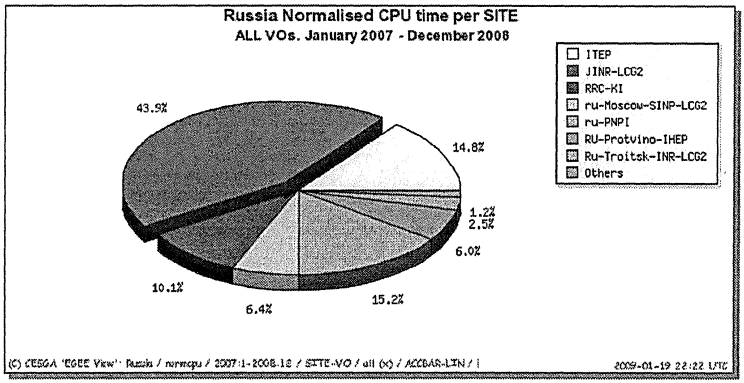


Fig. 4. Distribution of normalised CPU time per RDIG sites (from http://www3.egee.cesga.es/gridsite/accounting/CESGA/tier2_view.html)

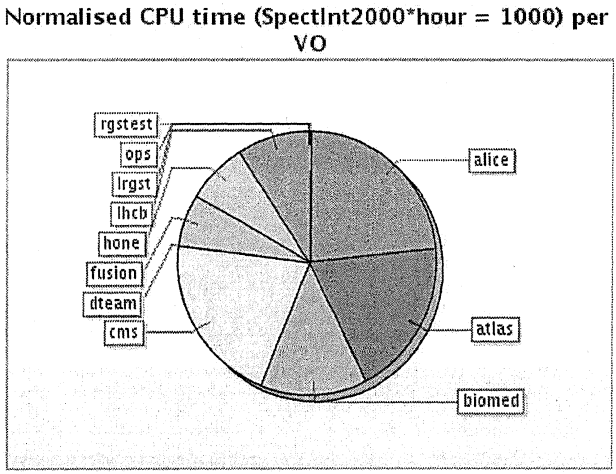


Fig. 5. Distribution of normalised CPU time per VO at JINR site (January - December 2008)

Information and software support

A necessary condition towards the creation of a unified information environment of JINR and its Member States is the provision of information and primary software support of the research-and-production activity of the Institute.

The consecutive development of JINRLIB, a program library for solving a wide range of physical and mathematical problems originated in JINR researcher's scientific activity, is in progress. JINRLIB program packages created

by JINR specialists and corresponding to a wide range of scientific tasks in JINR are renewed and replenished with new programs regularly. There are about 40 such kind of programs subdivided into following classes: high energy theoretical physics, low energy theoretical physics, heavy ion physics, automation of data processing, computational mathematics and technique. The mathematical packages of classic subjects and specific applied problem-oriented packages, each of which has its own range of users are most popular at present.

A part of JINRLIB proposing as object libraries of mathematical programs is developed and supported too. As the JINR Central Information and Computer Complex is continuously renovated and its software is permanently modernized, a complete recollection of this part is often necessary. Object libraries of mathematical programs are prepared in OS Scientific Linux 4 with x86_64 CPU architecture for GNU Fortran 77 compiler, GNU Fortran 95 compiler and Intel Fortran compiler. The maintenance and supplement of the previous object libraries for OS Scientific Linux 3 and Windows 9X/NT/2000/XP also continues.

The maintenance of the program libraries developed by other research centers and organizations (CPCLIB, CERNLIB) as well as the provision of the information and technical help to users continues. The full information on the JINR program libraries is available at the specialized WWW-site http://www.jinr.ru/programs/ and in LIT News Bulletins.

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. In 2008, work was in progress on the regular actualization of the program environment and contents of the central information sites of LIT and JINR (http://wwwinfo.jinr.ru, http://lit.jinr.ru, ftp://faxe.jinr.ru, http://faxe.jinr.ru), on creation and support of databases required for functioning these sites. In cooperation with JINR STD ASM, LIT provided support and modernization of administrative databases, updating and support of software for the central accounting department, translation of programs into version 8.0 1C.

In a hosting mode work was progressing on the development, creation and support of information websites of various conferences, workshops, symposia organized by JINR laboratories (RCDL'2008 – "Electronic libraries: perspective methods and technologies, electronic collections"; 12th CBM Collaboration Meeting "Physics of Compressed Baryonic Matter" (http://cbm2008-oct.jinr.ru/), EXON'2009 (http://exon2009.jinr.ru/); Readings after V.I.Korogodin and V.A.Shevchenko (http://lrb.jinr.ru/Timofeeff/KorShev/Menu/Menu Set_r_09.htm). Work on the information system developed in LIT JINR for the internal paperless document circulation (http://lit.jinr.ru/DoctorDoc/) has been in progress.

The LIT Information Bulletin was prepared and published (http://lit.jinr.ru/Inf_Bul_4/bullet.pdf).

Of paramount importance for the nearest future and of constant concern in a long-term prospect is the development of a clear, well-defined policy on using licensed software products. In particular, it is necessary to work out a special list of maximally needed software products for office computers which are to be secured by centralized support within the Institute, together with the development of rules and means of control over the observance of the licensing policy within the Institute. It is also necessary to develop a version of a program of the alternative development based on the use of freely distributed software products for the OS Linux for office purposes.

MATHEMATICAL SUPPORT OF EXPERIMENTAL AND THEORETICAL STUDIES

The main part of this activity is related to the development of the mathematical description and algorithmic reformulation of the physical models such as to receive significant numerical solutions; development of methods and algorithms able to extract physically insightful information from experimental data; simulation of physical processes within experimental installations; algorithm implementations into effective and reliable hardware adapted program environment.

This subject area covers a wide spectrum of studies in the high energy physics, nuclear physics, solids physics and condensed matter physics, biophysics, information technologies, conducted in close cooperation with all JINR Laboratories.

More than 150 scientific publications and conference proceedings were published in 2008. More than 90 reports were presented at international conferences.

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.

The essential improvements have been done in Fritiof (FTF) model and it was implemented in Geant4 release 9.2beta. New Physics lists which utilize the model (FTFP and FTF_BIC) were proposed for Geant4. The UrQMD model for pion-nucleus interactions was tested. The AMPT model installed at HEPWEB server has been tested for RHIC energies.

An updated versions of Fitter - a C++ program aimed to fit a chosen theoretical multi-parameter function through a set of data points was installed. The Fitter is designed to be used for SANS data processing first of all. Thus,

SANS theoretical models are implemented in it. Moreover, some standard mathematical models and minimization module are added for wider applicability. It provides a safe call of MINUIT procedures in the current version. The important feature of Fitter's design is its expandability: both new models and new minimizing algorithms can easily be added to the existing ones. A long write-up description of the new version of Fitter was published *[A.G. Soloviev, A.V. Stadnik, A.H. Islamov, A.I. Kuklin Communication of JINR E10-2008-2, Dubna, 2008, http://wwwinfo.jinr.ru/programs/jinrlib/fitter/indexe.html].*

A new version of the SAS package for small-angle neutron scattering data treatment was added to the JINR Program Library too. Data visualization is provided by the Gluplot package.

Also, a new version of the Gluplot - the data plotting package, was included in JINR Program Library. It was originally intended both as graphical library and as standalone program which would allow scientists and students to visualize data. (The "GLU" in gluplot means that it is OpenGL/GLU/glut based.) The Gluplot handles both curves (2D) and surfaces (3D). For 2D plots, there are many plot styles, including lines, points, lines with points, error bars and impulses. Surfaces are plotted as a color map on the x-y plane. The Gluplot supplies both linear and logarithmic axes. Moreover, any other axis distortion is available using a Gluplot library. The axis scale and also many other settings are changeable by Gluplot command-line options or by menu items and hot-keys after it runs. After all, Gluplot supports high quality plot output to PostScript, Encapsulated PostScript and Portable Document Format files. Figures 6 and 7 give some Gluplot usage examples. *[A.G. Soloviev: http://www.jinr.ru/programs/jinrlib/gluplot/indexe.html]*

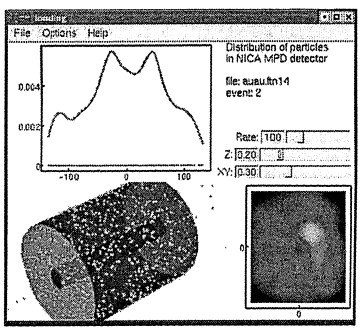


Fig. 6. Example visualization of particles distribution in NICA/MPD detector

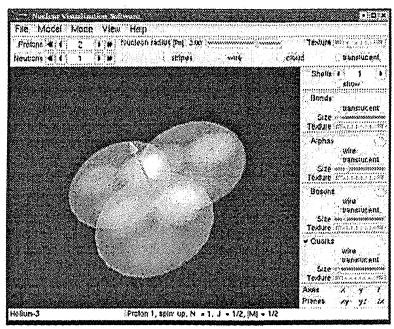


Fig. 7. Visualization of some nuclear model

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

In frames of the work performed at LIT on mathematical support of the CBM experiment (GSI) the track-finding routines were developed for the Transition Radiation Detector (TRD). The track-finding algorithm is based on the 3D track-following method with the Kalman Filter use. Two different algorithms have been developed: a standalone TRD track-finder (using only TRD information) and algorithm based on the information from tracks found in the STS detectors. A detector layout study has been performed, in order to optimize the detector setup while keeping high reconstruction efficiency. All developed algorithms were tested on large statistics of simulated events and were included into the CBM ROOT framework for common use *[A.A. Lebedev, G.A. Ososkov. JINR Preprint E10-2008-3, Dubna, 2008].*

Algorithms for charged particles track reconstruction and their identification by the Transition Radiation Detector (TRD) have been developed at LIT for CBM experiment. The algorithm for track reconstruction is based on a track-following method with the Kalman filter application. An artificial neural network, that uses as input samples the particles energy losses in the TRD layers, is applied for electron/pion identification. First results on the optimization of the TRD geometry taking into account the efficiencies of track reconstruction, electron identification and pion suppression, are presented *[V.V. Ivanov et al. JINR Communication P10-2008-152, Dubna, 2008].*

The work performed by researchers of LIT and GSI, Darmstadt, Germany, describes a 3D finite elements mesh generator based on the "Mapping" approach. In order to improve the quality of the mesh generation, a special standard subdividing elements library is used for mesh refinement. A user-friendly interface for defining the input geometry has been developed. A set of tools to describe the curvature of standard and non-standard current windings curvature with various cross-sections is designed. This also covers the currently requested coil windings made for coaxial cables. At all stages of the mesh generation process a visual control of the quality is available including a final refinement stage. The proposed generator can be used as a preprocessor for solving a wide range of problems based on the finite elements method *[P.G. Akishin et al. JINR Communication P11-2008-149, Dubna, 2008].*

Calculation of the 3D Field of SIS 100 Main Magnets was performed in collaboration with GSI. Checking the obtained results with the elliptic multipoles revealed that the increased number of elements produced artifacts. Increasing the number of nodes allowed obtaining a field quality with a deviation to the interpolation of less than 100 ppm. The elliptic multipoles and comparing the calculation to the data of the interpolation proved as a very sensitive tool to show the physical validity of the obtained results *[P. Schnizer, B. Schnizer, P. Akishin, E. Fischer, "Field Representation for Elliptic Apertures", Technical Report, GSI, January 2008; P.*

Schnizer, B. Schnizer, P. Akishin, E. Fischer. Theoretical field analysis for superferric accelerator magnets using plane elliptic or toroidal multipoles and its advantages. Proc. of EPAC08, P. 1773-1775; A. Mierau, P. Akishin, E. Ficher, P. Schnizer. Impact of mechanical imperfections on the field quality. study for SIS 100 single layer dipole. Technical report, Gesellschaft fur Schwerionenforschung mbH, October 2008].

Particle physics

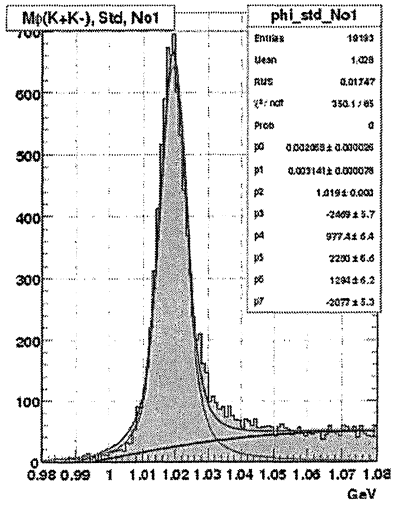


Fig. 8. Elastic phi-meson photoproduction in H1 experiment (DESY) on 2005-2007 data

The work within the activities on phi-meson cross-section and F_2^D proton structure function calculations on H1 experimental data with FPS (Forward Proton Spectrometer) are in progress. The results have been reported to the H1 meetings at DESY (Hamburg). Elastic phi-meson photo-production obtained on 2005-2007 experimental data is presented in Fig. 8 *[M. Kapishin, D. Nikitin, V. Palichik, V. Spaskov. FPS F2D3 Analysis. Diffractive Working Group Meeting, 01/07/2008 https://www-h1.desy.de/icgi-h1wiki/ moin.cgi/ DiffractiveWorking Group / DiffractiveMeeting2008-07-01; M. Kapishin, D. Nikitin, V. Palichik, V. Spaskov. FPS F2D3 Analysis and t-slopes. Diffractive Working Group Meeting, 15/07/2008 https://www-h1.desy.de/icgi-h1wiki/moin.cgi/ DiffractiveWorking Group /DiffractiveMeeting2008-07-15].*

An excellent Dubna Cathode Strip Chamber spatial resolution (46 microns) has been obtained from CMS muon cosmic data with 3.8 T magnetic field in the actual version of CMSSW (several improvements with additional cross-talk corrections) (Fig.9) *[V. Palichik. ME1/1 spatial resolution from CRAFT data MU Endcap CSC/ME1/1 Meeting, CMS Week, 08/12/2008 http://indico.cern.ch/contributionDisplay.py?contribId = 10& confide = 46650].*

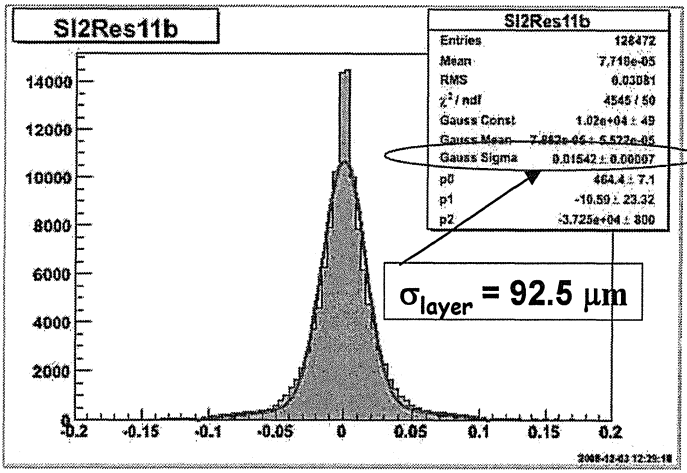


Fig. 9. Dubna Cathode Strip Chamber (CSC) Single Layer Spatial Resolution from Muon Cosmic Data (CMS, LHC). CMS Technical Proposal requirement for Dubna CSC spatial resolution: σ(CSC) = 75 μm, obtained σ(CSC) = σ_{layer}/(number of Degrees of Freedom) = 46 μm

A hybrid method of pion energy reconstruction in ATLAS calorimeter was developed and investigated. The method uses the modified Local Hadronic Calibration scheme (developed in DLNP) and the Artificial Neural Net procedure (developed in LIT) for reconstruction of energy losses in the "dead" material of the ATLAS calorimeter. The method was tested on the combined test beam 2004 data (CTB04) in the range of 10 – 350 GeV, $\eta = 0.25$. The test results show that the new method has a high energy resolution (about 1.5 times better than in the Hadronic Calibration method used by the Oxford-Stockholm group and slightly better than the H1 method results for CTB04 obtained by the Pisa group). The obtained characteristics of the new method reach the requirements of the ATLAS project for energy resolution for hadrons *[Y.Kulchitsky, V.Shigaev, P.Tereshko, V.Vinogradov. "Update of CTB04 Pion Energy Reconstruction by the Local Hadronic Calibration Method", Int. Atlas Conf., CERN February 12 2008, http://indico.cern.ch/conferenceDisplay.py? confId=27301; Yu.A. Budagov, J.I. Khubua, Yu.A. Kulchitskii, N.A. Rusakovitch, V.N. Shigaev, P.V. Tsiareshka, Artificial Neural Networks for reconstruction of energy losses in dead materials between barrel LAr and Tile calorimeters: exploration and results, CERN, ATL-COM-TILECAL-2008-002, 1-24, 02.2008]*

A new scheme for the introduction of formfactors for the SU(4) chiral meson Lagrangian approach to the J/psi breakup cross sections by pion and rho meson impact was suggested. This mesonic formfactor scheme respects the fact

that on the quark level of description the contact and the meson exchange diagrams are constructed by so-called box and triangle diagrams which contain a different number of vertex functions for the quark-meson coupling. The model calculation for Gaussian vertex functions within the meson formfactor scheme was performed and compared with those of the usual global formfactor model. The new meson formfactor model was calibrated with results for the pion impact processes from a relativistic quark model and present predictions for the rho-meson induced processes. A fit formula for the resulting energy-dependent cross sections has been provided for practical use in future model calculations *[D.B. Blaschke, H. Grigorian, Yu.L. Kalinovsky. Meson formfactor scheme for J/psi breakup cross sections in the Chiral Lagrangian approach. arXiv:0808.1705, 2008, subm. Phys.Rev.C].*

Two photon decays of scalar mesons $f_0(980)$, $a_0(980)$, $\sigma(600)$ in the quark Nambu - Jona - Lasinio (NJL) model are calculated. The contributions of the meson loops are taken into account along with the quark loops (Hartree - Fock approximation). This corresponds to the next order of the $1/N_c$ expansion, where $N_c=3$ is the number of quark colors. It is shown that the meson and quark loops give comparable contributions to the amplitude. Moreover, in the process $f_0(980) \to \gamma\gamma$ the kaon loop plays the dominant role. A similar situation takes place in the decay $\phi \to f_0(980)\gamma$. The results are in satisfactory agreement with the recent experimental data *[Yu.L. Kalinovsky, M.K. Volkov. Two photon decays of scalar mesons in the quark NJL model. arXiv:0809.1795, 2008].*

A software complex KANTBP 2.0 has been designed for computing the wave functions of a discrete and continuous spectrum of multi-dimensional quantum systems by Kantorovich method (KM). Kantorovich method is applied to calculate the wave functions of a discrete and continuous spectrum of a hydrogen atom in a magnetic field and the cross-sections of photoionization of the linearly polarized light along the axis *z* from an initial state of the discrete spectrum into a final state of the continuous spectrum. A method of effective computation of potential curves and matrix elements for coupled radial equations describing the behaviour of a hydrogen-like atom in a homogeneous magnetic field has been developed and realized in the Fortran 77 programming language. The efficiency of the method is essentially based on the developed and realized in the MAPLE system algorithms of computation in an analytical form of asymptotics of basic functions, matrix elements and radial solutions. A numerical research on the photoionization model and speeds laser-induced recombination of a hydrogen atom in a homogeneous magnetic field of a suitable magnetic optical trap has been conducted. The effects of resonant passage and full reflection of the unlike charged particles in the homogeneous magnetic field have been predicted for the first time *[O. Chuluunbaatar, A. Gusev, S.I. Vinitsky, A.G. Abrashkevich. KANTBP2.0: New version of a program for computing energy levels, reaction*

matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach. Comput. Phys. Commun., 179, pp.685–693(2008); O. Chuluunbaatar. Variation-iteration algorithms of a numeric solving of bound state problems and a scattering problem for systems of coupled radial equations. Vestnik RUPF: Series Mathematics. Informatics. Physics. 2, pp.40–56 (2008); O. Chuluunbaatar, V.P. Gerdt, A.A. Gusev, S.I. Vinitsky, A.G. Abrashkevich, M.S. Kaschiev, V.V. Serov. POTHMF: A program for computing potential curves and matrix elements of the coupled adiabatic radial equations for a Hydrogen-like atom in a homogeneous magnetic field. Computer Physics Communications, 178, 301-330, 2008; O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky, V.L. Derbov, L.A. Melnikov, V.V. Serov. Photoionization and recombination of a hydrogen atom in a magnetic field. Phys.Rev. A77, pp.034702-1-4(2008); O. Chuluunbaatar, A.A. Gusev, V.L. Derbov, M.S. Kaschiev, L.G. Mardoyan, V.V. Serov, T.V. Tupikova, S.I. Vinitsky. Adiabatic representation for a hydrogen atom photoionization in a uniform magnetic field. Physics of Atomic Nuclei 71, pp.844–852 (2008); Nuclear Physics 71, pp.871–878 (2008)].

An anisotropic Bianchi type-I string cosmological model in the presence of a magnetic field is investigated. Some exact solutions are produced using a few tractable assumptions usually accepted in the literature. The analytical solutions are supplemented with a numerical and qualitative analysis. In frames of the present model the evolution of the Universe and other physical aspects are discussed. Figs. 10 and 11 illustrate the potential and evolution of the Universe in presence of a cosmic string and magnetic fluid *[B. Saha, M. Visinescu. String cosmological model in the presence of a magnetic flux. Astrophysics and Space Science 315, 99-104 (2008)].*

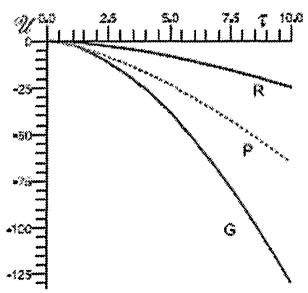


Fig. 10. Evolution of the Universe for different equations of state in presence of a magnetic field

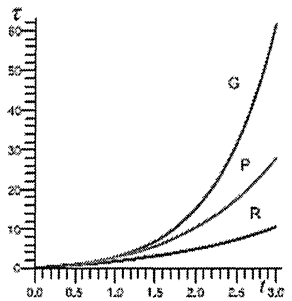


Fig. 11. Potential corresponding to the different equations of state in presence of a magnetic field

A self-consistent system of interacting spinor and scalar fields within the scope of a Bianchi type I gravitational field in presence of a viscous fluid and L term was studied. A corresponding system of equation has been derived

and thoroughly studied qualitatively. A complete qualitative classification of the mode of evolution of the universe given by the corresponding dynamic system has been illustrated. In doing so all possible values of the problem parameters are considered independent to their physical validity. The system is studied from the view point of blow up. It has been shown that in absence of viscosity the blow up does not occur. It should be emphasized that the phenomena similar to that in question can be observed in other discipline of physics and present enormous interest from the view point of catastrophe, demography etc *[B. Saha, V. Rikhvitsky. Anisotropic cosmological models with spinor and scalar fields and viscous fluid in presence of a L term: qualitative solutions. Journal of Mathematical Physics 49, 112502(2008)].*

Nuclear physics

Interactions of relativistic heavy ions with total energy above 30 Gev have been studied in thick Cu and Pb targets (>2cm) based on computer simulation using the Dubna Cascade Model (DCM) (and other available computer codes – MCNPX) (Fig. 12).

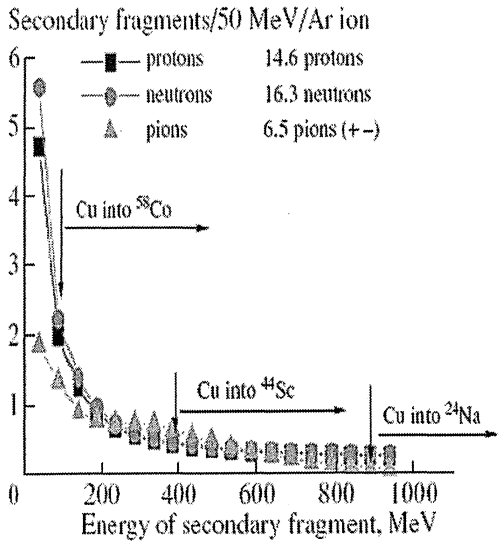


Fig. 12. Calculated energy spectra for secondary protons, neutrons and pions produced by 72 GeV ^{40}Ar in thin Cu target using the Dubna DCM code

A comprehensive review of the experiments on irradiation of extended heavy targets with relativistic ion beans carried out in the last decades is given. Calculated data are compared to the available experimental data acquired at JINR, LBL, Sacley etc. Open unresolved problems are pointed out, e.g. neutron production by 44 GeV ^{12}C ions with thick Cu and Pb targets *[R. Brandt, V.A. Ditlov, K.K. Dwivedi, H.A. Khan, W. Ensinger, E. Ganssauge, Guo Shi-Lun, M.I. Krivopustov, ..., A.N. Sosnin et al,. Interactions of relativistic heavy ions in thick heavy element targets and some unresolved problems. Physics of Particles and Nuclei, 2008, v.39, N 2, 259-285; R. Brandt, V.A. Ditlov,*

K.K. Dwivedi, W. Ensinger, E. Ganssauge, Guo Shi-Lun, M. Haiduc, S.R. Hashemi-Nezhad, H.A. Khan, M.I. Krivopustov, R. Odoj, E.A. Pozharova, V.A. Smirnitsky, A.N. Sosnin, W. Westmeier, M. Zamani-Valasiadou. Studies with SSNTD and nuclear chemistry on nuclear reactoions induced by relativistic heavy ions in thick targets: a Review. Radiation measurements 43 (2008), 132-138].

Calculations of microscopic optical potentials (OP's) (their real and imaginary parts) are performed to analyze the ^{6}He+p elastic scattering data at a few tens of MeV/nucleon. The OP's and the cross sections are calculated using three model densities of ^{6}He. Effects of the dependence of the NN-forces on nuclear density are investigated (Fig. 13). The role of the spin-orbital terms and the non-linearity of the OP's and also the role of its renormalization are studied. The sensitivity of the cross sections to these effects is tested *[K.V. Lukyanov, E.V. Zemlyanaya, V.K. Lukyanov, A.N. Antonov, M.K. Gaidarov. Calculations of the ^{6}He+p elastic scattering cross sections within the folding approach and the high-energy approximation for the optical potential. Bulletin of the Russian Academy of sciences: physics, 2008, Vo.72, pp.854-858. ISSN 1062-8738 Allerton Press Inc.].*

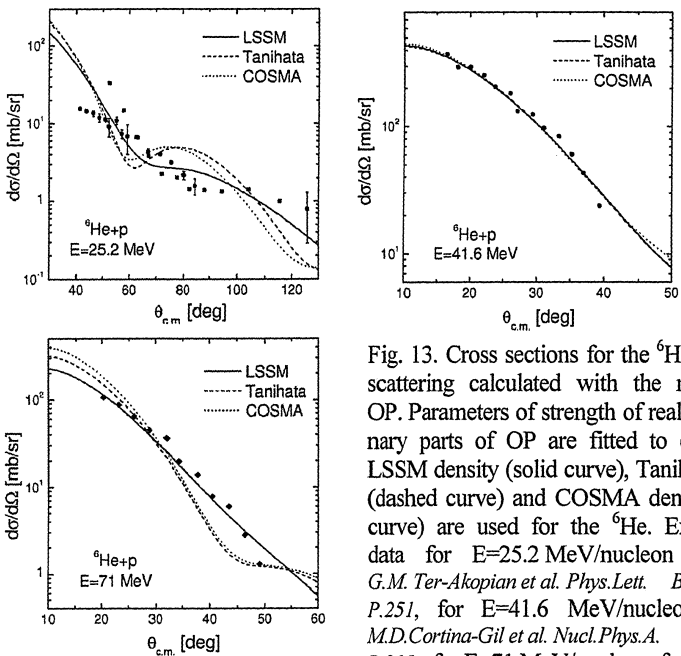


Fig. 13. Cross sections for the ^{6}He+p elastic scattering calculated with the microscopic OP. Parameters of strength of real and imaginary parts of OP are fitted to experiment. LSSM density (solid curve), Tanihata density (dashed curve) and COSMA density (dotted curve) are used for the ^{6}He. Experimental data for E=25.2 MeV/nucleon are from *G.M. Ter-Akopian et al. Phys.Lett. B.1999,V.426. P.251*, for E=41.6 MeV/nucleon – from *M.D.Cortina-Gil et al. Nucl.Phys.A. 1997.V.616. P.215c*, for E=71 MeV/nucleon–from *A.Kor--sheninnikov et al. Nucl.Phys. A.1997.V 616, 189c.*

It is shown that the neutron production of 44 GeV ^{12}C within thick Cu and Pb targets is beyond the estimated extrapolated yield determined in experiments with 12 GeV ^{12}C which is promising when applied to enhanced transmutation capacity of subcritical assemblies.

Fluxes of secondary particles were further studied in the Gamma-2 spallation source where neutron and proton distributions were determined using natCd activation detectors. It is shown that calculated relative neutron and proton production is in good agreement with the acquired experimental data *[M. Manolopoulou, S. Stoulos, M. Fragopoloulou, R. Brandt, W. Westmeier, M.I. Krivopustov, A.N. Sosnin, S.R. Hashemi-Nezhad, M. Zamani-Valasiadou. Proton and neutron production from GAMMA-2 spallation source irradiated with relativistic proton beams. Nuclear Instruments and Methods in Physics Research A, 586 (2008), 239-245].*

MCNPX 2.6C code was used to study yields of natU(p,f), natU(pi,f) and natU(gamma,f) reactions, which are possibly imposing the decisive impact on the neutron yield and in particular the neutron spectrum in the "Energy+Transmutation" assembly. Possible sources of errors both in experiments and calculations are shown *[S.R. Hashemi-Nezhad, I. Zhuk, M. Kievets M.I. Krivopustov, A.N. Sosnin, M.W. Westmeier, R. Brandt. Nuclear Instruments and Methods in Physics Research A, 591 (2008), 517-529].*

Condensed matter physics

On the basis of the solution of a nonlinear diffusion equation with initial and boundary conditions, a transport coefficient of moisture in a sample of a porous material is found by minimization of a functional, which expresses diversion of the computed profile of moisture concentration in well defined time moments from their experimental values for the defined moisture transport coefficient by the Newton method. In this case the transport coefficient as opposed to the previous works is found as a sum of the degree and exponential functions of the moisture concentration. The exponent of the power function depends on time. Thus, a more accurate coincidence of the computed profiles of the moisture concentration to their experimental profiles is gained in comparison to previous works performed by other authors. The exponential term provides a good coincidence of the mentioned profiles for big times nearby the boundary of the sample, where evaporation of the moisture to the atmosphere takes place *[I.V. Amirkhanov, E. Pavlušová, M. Pavluš, T.P. Puzynina, I.V. Puzynin, I. Sarhadov. Numerical method for determination of moisture transfer coefficient according to the diffusion moisture profiles, PEPAN Letters, 2008. V.5, №3(145). P.479-484; I.V. Amirkhanov E. Pavlušová, M. Pavluš, T.P. Puzynina, I.V. Puzynin, I. Sarhadov. Numerical solution of an inverse diffusion problem for the moisture transfer coefficient in a porous material. Materials and Structures (2008) 41:335-344].*

The research related to producing nanostuctures in materials exposed to high-energy heavy ions was performed in collaboration with FLNR. The numerical results obtained in frames of a thermal spike model for an anisotropic material on an example of highly-oriented pyrolytic graphite are represented. The experimental data are compared to the calculated ones, new experiments and theoretical approaches are suggested *[I.V. Amirkhanov et al. "Research in radiation processes resulting in formation of nanosize objects in materials" in Book "Nuclear Physics and nanotechnologies: nuclear physics aspects of formation, study and application of nanostructures", P18-2008-33, JINR, Dubna, 2008, pp. 339-349].*

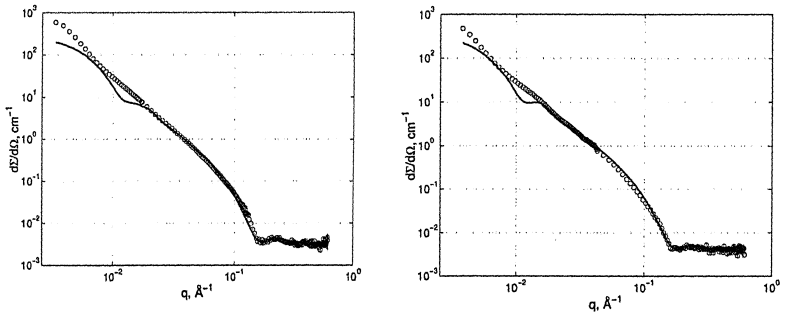


Fig. 14. Results obtained by the fitting of the measured small-angle neutron scattering spectra of the polydispersed population of the ceramide 6 / cholesterol / palmitic acid /cholesterol sulfate unilamellar vesicles at a temperature 32°C (left panel) and 60°C (right panel) in the framework of the separate-form-factor method within the hydrophobic-hydrophilic approximation. The fitting was performed in the range of scattering vectors $q \geq 0.02$ Å^{-1}

In collaboration with FLNP and co-authors from the Martin Luther University (Halle, Germany) and PSI (Villigen, Switzerland), a numerical analysis of the small angle neutron scattering data has been performed 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 in frames of the separated form factors model show 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 (Fig.14) 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, R. Neubert, J. Kohlbrecher, V.L. Aksenov. Investigation of structure and properties of the stratum corneum model membranes by the small angle neutron scattering. Journal of Surface Investigation.*

X-ray, Synchrotron and Neutron Techniques. 2008, Vol.2, No. 6, pp.884-889. ISSN 1027-4510 Pleiades Publishing Ltd.].

A method of entanglement production is suggested, based on the resonant generation of topological modes in systems with Bose-Einstein condensates trapped in optical or magnetic lattices. The method allows one to regulate the strength of entanglement production as well as to govern its time variation. This method can serve as a practical tool for quantum information processing and quantum computing *[V.I. Yukalov and E.P. Yukalova. Entanglement production with Bose atoms in optical lattices. J. Phys. Conf. Ser. 104, 012003-11 (2008); V.I. Yukalov and E.P. Yukalova. Nonlinear dynamics of ultracold gases in double-well lattices. Laser Phys. Lett., DOI: 10.1002/lapl.200810111].*

The peculiarities of coherent spin radiation by magnetic nanomolecules is investigated by means of numerical simulation. The consideration is based on a microscopic Hamiltonian taking into account realistic dipole interactions. Superradiance can be realized only when the molecular sample is coupled to a resonant electric circuit. The influence on the level of radiation, caused by sample shape and orientation, is analysed. The most powerful coherent radiation is found to occur for an elongated sample directed along the resonator magnetic field *[V.I. Yukalov, V.K. Henner, P.V. Kharebov, and E.P. Yukalova. Coherent spin radiation by magnetic nanomolecules and nanoclusters. Laser Phys. Lett. 5, 887-893 (2008); V.K. Henner, V.I. Yukalov, P.V. Kharebov, E.P. Yukalova. Collective spin dynamics in magnetic nanomaterials. J. Phys. Conf. Ser. 129, 012015-5 (2008)].*

A numerical simulation of a non-isothermal glass fiber drawing process has been conducted at LIT in cooperation with the Institute of Mechanics of BAS, Bulgaria, and the Polytechnic Institute in Marseille, France. A mathematical model of the process is a boundary-value problem for a system of differential equation including a one-dimensional version of the equations of motion coupled by the heat transfer equation. The effects of the temperature-dependent viscosity, gravity, surface tension and air-drag, as well as that of axial heat conduction, heat convection and radiative heat transfer are taken into account. The numerical algorithm is based on the Continuous analog of Newton's method together with a spline-collocation scheme of a higher-order of accuracy for the solving of linearized problems on each iteration. Numerical results for the fiber radius, axial velocity and temperature are shown, illustrating the cooling effects of Stanton and radiation numbers *[S.P. Radev, T.L. Boyadjiev, F. Onofri. Preprint JINR, E11-2008-161; "All-Russian seminar on aerohydro-dynamics", Saint-Petersburg, Febr. 5-7, 2008, pp. 14-18].*

New methods of mathematical simulation of Josephson structures have been suggested at LIT in collaboration with the universities of Sofia and Plovdiv, Bulgaria. A new effective numerical algorithm for solving a nonlinear

system of ODE's describing the static distributions of the magnetic flux in N–stacked Josephson junctions (JJ). The algorithm is based on the continuous analog of the Newton's method. The linear boundary-value problems arising at each iteration are solved numerically with a finite element method. A corresponding matrix Sturm-Liouville problem for studying their global stability is proposed. To solve the problem, a sub-space iteration method is used. As an example, the existence, stability, lack of stability and some physical characteristics of two kinds of magnetic flux distributions in 3-layered JJs are analyzed *[I. Hristov, S. Dimova, T. Boyadjiev. Preprint JINR E11-2008-160; Subm. in Lect. Notes in Comp. Sci.].*

A new method for numerical solution of non-linear boundary value problems for systems of ODE's given on the embedded intervals has been proposed. The algorithm is based on the continuous analog of Newton method. A numerical solution to corresponding linear boundary-value problems at each iteration is performed with a spline-collocation scheme. As a particular example, a problem is considered about possible distributions of the magnetic flux in a system of two magnetically coupled long Josephson junctions with different layers lengths. The influence of the length's ratio on the main physical properties of basic bound states is studied numerically. The existence of bifurcations by changing the lengths of the layers for some class of solutions is proved *[H. Melemov, T. Boyadjiev, Preprint JINR, E11-2008-143; Subm. in Lect. Notes in Comp. Sci.].*

The problem of optimal biosensor development was analized. The electrostatic properties of a number of enzymes and nucleic acids have been calculated. The results obtained reveal a number of patterns in interaction of enzymes with charged nanostructures, which can be directly utilized in biosensor development, provided that new software aimed at systematization and generalization of data on immobilized proteins should be developed, such as an appropriate database and an expert system. Such software will be able to become a first step towards implementation of computational nanotechnology, aimed at the development of biosensors with predetermined properties *[V.V. Ivanov et al. "About computing biosensor technology, electrostatic properties of enzymes and polyelectrolytes" in Book "Nuclear Physics and nanotechnologies: nuclear physics aspects of formation, study and application of nanostructures", P18-2008-33, JINR, Dubna, 2008, pp. 293-311].*

The modern development of microelectronics allows one to make nanodevices with almost nuclear accuracy. One of the important tasks of quantum engineering is the designing of various quantum structures possessing desirable spectral properties. This problem arises at the creation of various heterogeneous structures, lattices, quantum computers, etc. Basic elements of the modern micro- and nano-electronics are structures of low dimension which are generated

from quantum wells, dots, wires. From a theoretical viewpoint, the problem of determining the potentials of quantum wells which would support the desirable spectrum, arises. A positive solution to this problem would make the quantum engineering more effective and flexible, thus providing conditions for the development of new quantum objects. The generalized Schroedinger equation with effective mass dependent on a spatial variable has been widely used lately to simulate the electronic properties of nano-objects *[A.A. Suzko, A. Schulze-Halberg, "Intertwining operator method and supersymmetry for effective mass Schrodinger equation", Phys. Lett. A (2008), V.372, pp 5865-5871; A. Suzko, I. Tralle, "Reconstruction of quantum well potentials via the intertwining operator technique", Acta Physica Polonica, B (2008), V.39, No.3, pp 545—567].*

The macroscopic solid-mechanical continuum model of electric pygmy dipole resonance (PDR) is proposed, in which its origin is attributed to perturbation-induced effective decomposition of nucleus into two spherical domains - undisturbed inner region treated as a static core and dynamical layer undergoing elastic shear vibrations. The obtained analytic equations for the energy of E1 vibrational soft mode and its excitation strength lead to the following estimates for the PDR energy centroid $E_{PDR}(E1)=[31\pm1]A^{-1/3}$ MeV and the total excitation strength $B_{PDR}(E1)=[1.85\pm0.05]10^{-3}\ Z^2\ A^{-2/3}e^2$ fm^2 throughout the nuclear chart exhibiting fundamental character of this soft dipole mode of nuclear resonant response (Fig.15) *[S.I. Bastrukov, I.V. Molodtsova, S. Misicu, H-K. Chang, D.V. Podgainy. Elasticity of nuclear continuum as a principal macrodynamical promoter of electric dipole pygmy resonance. Phys.Lett.B 664 (2008), p.258].*

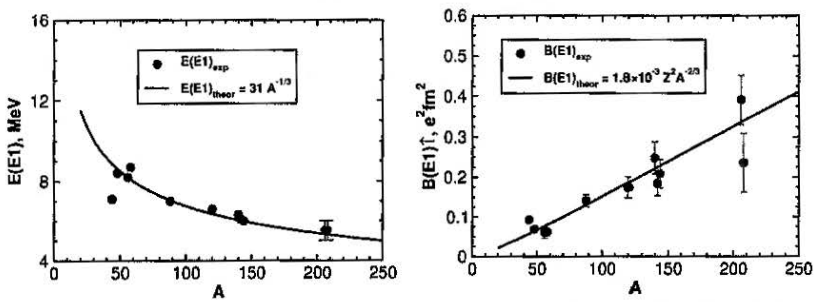


Fig. 15. Computed energy E(E1) and excitation strength B(E1) of low-energy dipole electromagnetic nuclear resonant response (lines) in juxtaposition with experimental data on energy centroid and E1 excitation strength of the dipole electric soft mode (symbols)

The scrutiny of the complete mean field Green function solution of the effective two-dimensional two-band Hubbard model of the high-Tc superconductivity in cuprates unveils three important features of this model. (i) While the conjecture of the spin-charge separation in cuprates, repeatedly stressed by

P.W. Anderson, is at variance with the existence of the Fermi surface in these compounds, the main findings of the present investigation point towards its actual occurrence and to an alternative explanation. (ii) The two-band Hubbard model recovers the superconducting state as a result of the minimization of the kinetic energy of the system, in agreement with ARPES data. (iii) The anomalous pairing correlations may be consistently reformulated in terms of localized Cooper pairs both for the hole-doped and the electron-doped cuprates *[Gh. Adam, S. Adam. Separation of the spin-charge correlations in the two-band Hubbard model of high-Tc superconductivity. Journal of Optoelectronics and Advanced Materials, Vol. 10, No. 7, July 2008, pp. 1666-1670].*

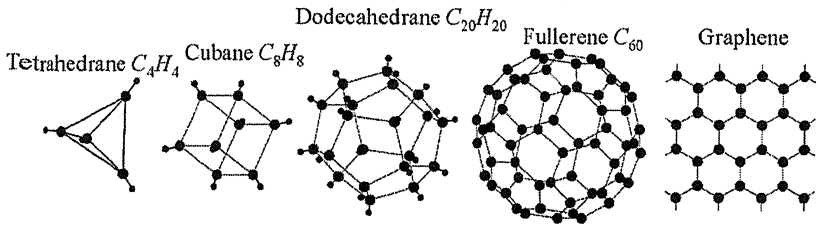
Computer algebra and applications

An algorithm was developed for decomposition of multivariate algebraic polynomial equations into triangular subsystems with disjoint solution space. The algorithm is a part of the general algorithmic approach to completion of nonlinear partial differential systems to involution *[V.P. Gerdt. On decomposition of algebraic PDE systems into simple subsystems. Acta Appl. Math. 101, 2008, 39-51].*

The Gröbner bases technique was applied to reduction of multiloop Feynman integrals and to automatic generation of finite difference schemes for linear partial differential equations *[V.P.Gerdt. Gröbner bases applied to systems of linear difference equations. Physics of Particles and Nuclei, Letters Vol.5, No.3, 2008, 425-436. arXiv:cs.SC/0611041].*

The SU(n) Yang-Mills light-cone mechanic studied in detail *[V.P. Gerdt, A.M. Khvedelidze, Yu.G .Palii. Light-cone Yang-Mills mechanics: SU(2) vs. SU(3). Theoretical and Mathematical Physics, 155(1), 2008, 557-566; Yu.G. Palii, A.M. Khvedelidze. On the homogeneous Gröbner basis for tensors. Programming and Computer Software, Vol. 34, No. 2, 2008, 101-106].* In the framework of the Dirac constraint formalism for degenerate Hamiltonian the complete set of constraints was computed and classified for the cases of SU(2) and SU(3) symmetry groups. All underlying computations were done by means of the Gröbner bases technique in the polynomial ideals theory.

Discrete dynamical systems and mesoscopic lattice models are studied in *[V.V. Kornyak. Discrete dynamical systems with symmetries: Computer analysis. Programming and Computer Software, Vol.34, No. 2, 2008, 84-94]* from the standpoint of their symmetry groups. Universal specific features of the dynamical system behavior associated with nontrivial symmetries of these systems are specified. A program in C for the group analysis of such systems was also developed. In particular, the program constructs and investigates phase portraits of discrete dynamical systems modulo symmetry group and seeks dynamical systems possessing special features, such as, for example, reversibility. Typical examples of discrete systems with high symmetry are (hydro)carbon nanostructures:



Nontrivial connections between symmetries and dynamics of discrete systems have been revealed. In particular, it is shown that formation of moving soliton-like structures is typical for discrete dynamical systems with nontrivial symmetry group. These structures are analogs of "spaceships" in cellular automata and "generalized coherent states" in quantum physics.

The highly efficient specialized computer algebra system GINV was described *[V.P. Gerdt, Yu.A. Blinkov. Specialized computer algebra system GINV. Programming and Computer Software, Vol. 34, No. 2, 2008, 112-123].* The system is oriented to investigation and solving multivariate systems of equations by their completion to involution.

Based on the general involutive approach to systems of polynomial equations, specialized algorithms for computing Gröbner bases in Boolean rings were designed and implemented in C++ *[V.P. Gerdt, M.V. Zinin. Involutive method for computing Gröbner bases over F_2. Programming and Computer Software, Vol.34, No. 4, 2008, 191-203; V.P. Gerdt, M.V .Zinin. A Pommaret division algorithm for computing Gröbner bases in Boolean rings. Proceedings of ISSAC 2008, ACM Press, pp.95-102].* The designed algorithms and their implementation are applicable, in particular, to simulation of quantum computation and to the logical analysis of technical systems.

On the basis of the involutive approach the C program was developed *[D.A. Yanovich. Efficiency estimate for distributed computation of Gröbner bases and involutive bases. Programming and Computer Software, Vol.34, No. 4, 2008, 210-215]* for distributed computation of involutive and Gröbner bases that in a network consisting of heterogeneous machines. The effectiveness of such an approach estimated and verified by means of computer experiments.

A method to describe dynamics of a composite system interacting with a strong laser field is suggested *[P. Jameson, A. Khvedelidze. Classical dynamics of a charged particle in a laser field beyond the dipole approximation. Phys. Rev. A 77, 053403, 2008].* The suggested method takes into account the relativistic and quantum effects caused by a high intensity of the laser field. Based on this method, a new quasi-classical approach was developed in *[V.P. Gerdt, M.V. Zinin. On role of involutive criteria in computing Boolean Gröbner bases. Programming and Computer Software, Vol.35, 2009]* which allows one to describe the dynamics of the composite systems in strong laser

fields. As quite a promising application of the developed approach, one can consider control over the spin entanglement for particles by variation of the laser radiation.

Conferences and Workshops

During the year 2008, LIT was the main organizer of several workshops and conferences.

On January 28 - February 2, 2008 the 15-th interdisciplinary conference "Mathematics. Computer. Education" (MCE) was held. The MCE conferences are organized on a regular basis at the Laboratory of Information Technologies (LIT) during winter student's holidays every two years. The organizers of the Conference are JINR, Moscow State University, Puschino scientific centre of biological studies of RAS, University "Dubna", Interregional Public Organization "Women in Science and Education". The specificity of the conferences is that they have a scientific-educational and interdisciplinary character. They provide a way for professional scientific dialogue at sectional sessions and allow scientific youth to communicate with experienced researchers and lecturers and to discuss their results. At the last conference more time was dedicated to sectional sessions to provide a more detailed professional discussion of issues of mathematical modelling in various fields of knowledge, techniques of teaching various disciplines at school and higher school and to share experience of using information technologies in science and education with colleagues.

Attending were more than 400 participants, young people being a good few of them. The participation of 50 students and post-graduates on a competitive basis was provided in frames of the Presidential Programme by the State Club "Personnel reserve".

A traditional 12-th Workshop on Computer Algebra was held at the Laboratory of Information Technologies (JINR) on May 14-16, 2008. More than 50 scientists from universities of Weingarten (Germany), Turku (Finland), Limoges (France), Bucharest (Romania), Chicago (USA), Brest (Belarus) and Russian scientific centres of Moscow, St. Petersburg, Saratov, Tambov, Tver and Dubna attended the Workshop. 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. A number of new promising results were presented on increase of computing efficiency of algorithms for solving systems of algebraic, differential and difference equations; modelling of quantum computations and research of entanglement of multi-particle quantum systems important for problems of quantum computer science; solution to the boundary-value problems arising in nuclear physics and engineering sciences.

The international conference «Distributed Calculations and Grid Technologies in Science and Education» was held on 30 June – 4 July. The conference is organized every two years by the Laboratory of Information Technologies. This conference is the only event in Russia dedicated to the issues of development and application of Grid technologies and other related aspects of information technologies. Organized by JINR LIT for a third time under the support of the Russian Foundation for Basic Research, the conference year by year attracts more and more specialists. The programme included not only the issues on the establishments and operation of Grid infrastructures, but also theoretical and practical aspects of application of distributed calculation media, distributed data processing, etc. Sponsors of the conference — representatives of the companies T-platform, Niagara, EtegroTech., and IBM — informed the participants about their produce and activities. This year the conference gathered 228 participants from 20 countries: Armenia, Azerbaijan, Belarus, Bulgaria, Czechia, France, Germany, Georgia, Kazakhstan, Moldova, Poland, Romania, Russia, Slovakia, Spain, Sweden, Switzerland, Ukraine, the USA, and Uzbekistan, as well as from CERN and JINR. Russia was represented by participants from 49 universities and research centres. Representatives of the companies T-platform, IBM, Niagara, Etegro, Linux Ink, Nortel, Samsung, Intel, and JetInfosystems took part in the conference. For the period passed since the second conference, considerable success has been achieved in the implementation of regional and local Grid projects. The number of Grid resource centres of the RDIG has been almost doubled. There were the following sections at the conference: «Grid Applications», «WLCG — Worldwide LHC Computing Grid», «Grid Service and Architecture», «Personnel Training in Advanced IT Trends». LIT staff members organized a special lecture session on Grid technologies for beginning users. The traditional plenary reports at the conference dwelt on modern status and prospects of foreign Grid centres development. 38 plenary reports, 65 section reports and 9 poster presentations were delivered to the conference. The participants were unanimous in their opinion that such conferences should be continued. This type of the events is a powerful tool for consolidation, experience sharing and attraction of new participants. Each time, it becomes more and more useful and important for Grid development and its applications both in Russia and in JINR Member States.

On October 7 -10, LIT hosted the All-Russian scientific conference "Digital libraries: perspective methods and technologies, electronic collections" (RCDL'2008) that celebrated its anniversary in a decennial series of annual Russian conferences. The RCDL Conferences have always been open to Russian as well as to foreign leading specialists in the specified area that allowed them to exchange experience, ideas and results for setting up contacts for close cooperation in the future. As a result, for the last ten years a few hundred specialists in

various fields of science, education and application have attended them. The anniversary conference RCDL'2008 was attended by 107 participants from Moscow, Saint Petersburg, Sosnovy Bor, Petrozavodsk, Puschino, Ekaterinburg, Perm, Kazan, Yaroslavl, Murom, Novosibirsk, Tomsk, Omsk, Kaspiysk, Voronezh, Taganrog, Tula, Troitsk, Dubna, Obninsk, Kharkov and Kiev.

The conference programme included full texts of 33 papers, 14 short talks and 6 poster presentations which have been selected from 56 submissions. It summed up the achievements in the mentioned area focusing on the possibility to apply semantic representation of information and knowledge in distributed and hybrid DL and scientific collections, ontological modelling, and integration of heterogeneous resources. Besides, other general issues of creating facilities of forming, analysis and search in the repositories of text and multimedia data of different structure were considered. Traditionally special attention was paid to the work on the electronic collections created within the RFBR projects and other programs on digital libraries. In frames of the RCDL'2008 a specialized Russian seminar on the data retrieval methods estimation ROMIP'2008 was organized where the developers of algorithms and specialists - analysts of the well-known companies Yandex, Mail.ru, Galaxy Soft, KM.RU, HeadHanter, etc. presented their reports.

Expected perspectives

Strategic items of LIT activity within JINR Roadmap:

- A well developed, corresponding to the nowadays requirements, telecommunication, networking, and computing infrastructure.
- The data analysis will require massively distributed CPU power with huge data storage facilities connected together through high bandwidth links, as well as new mathematical methods for extracting insightful information from experimental data.
- The home made implementations of open software, together with their quality assessment through specific validation procedures, are cornerstones of an activity devoted to the minimization of the financial effort. This is particularly important for successful realization of new JINR home projects and participation of JINR in future large scale projects such as FAIR complex, Super-LHC, International Linear Collider (ILC), etc.
- Training of high-skilled IT specialists:
  - user training and support;
  - student specialization, preparation of diploma and master theses at the 2 MIREA chairs and 1 chair of Dubna University working on the LIT basis;
  - preparation of PhD and DSc theses;
  - organization of dedicated periodic Schools, Conferences, Workshops, tutorials.

The formation of a unified Grid-environment of the JINR Member States is a cornerstone of the 7-year plan within the direction "Networks. Computing. Computational Physics".

There can be distinguished three main levels within the JINR Grid-environment: network, resource and applied. **The network level** deals with high-speed backbones and telecommunication links; **the resource level** consists of highly-efficient computing clusters, supercomputers, and data storage systems joined in a unified Grid-environment with the help of basic software and middle-ware. **The applied level** encompasses sets of research topics the solutions of which have been adapted to the Grid-environment in the frame of corresponding virtual organizations. The sound approach to the development of each level is to consider the correlations with the other two.

Network level:

- JINR-Moscow channel - on the basis of state-of-the-art technologies DWDM and 10Gb Ethernet, to create up to 72 channels of 10 Gbps each, and to raise the total throughput up to 720 Gbps;
- development with the RBNet - main JINR service-provider for access to the Internet, 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;
- for the effective participation in the processing and analysis of the data from the LHC experimental facilities, a devoted computer communication link joining the Russian research centers with CERN (of 10 Gbps and above) is needed;
- upgrade of the JINR backbone to a data transfer rate of 10 Gbps; connection to the 10 Gbps backbone of LIT, DLNP and VBLHE, and, as the need arises, of other JINR laboratories.

Resource level

Today the requirements of the LHC experiments stimulate the development of a global Grid-infrastructure, together with the resource centers of all the cooperating organizations. First of all, this is of primary importance for such large research centers as the JINR. To reach effective processing and analysis of the experimental data, further increase in the JINR CICC performance and disk space is needed.

The table below gives estimates of the JINR CICC resources increase based on the rates of their growth in 2007-2008.

	2010-2011	**2012-2013**	**2014-2015**	**2016**
CPU (kSI2K)	3500	5000	8000	12000
Disk systems (TB)	1500	2500	4000	8000
Mass storage (TB)	1000	2000	5000	10000

In order to manage the joint Grid-infrastructure, it is planned to set up a center of primary Grid-services (CPGS) that will provide the coordinated functioning of geographically distributed resource centers.

Applied level

The applied level covers the user applications working in a virtual organization environment which comprises both users and owners of computing resources. In the existing Grid-systems, a VO defines a collaboration of specialists in some area, who combine their efforts to achieve a common aim. The virtual organization is a flexible structure that can be formed dynamically and may have a limited life-time.

Instances of VOs working within the WLCG project are the VOs on the LHC experiments: ATLAS, CMS, Alice, LHCb, the first three being carried out with the noticeable and direct participation of the JINR. Nowadays, as a Grid-segment of the EGEE/RDIG, the JINR CICC supports computations of the virtual organizations registered in RDIG. Alongside with the LHC experiments, the main users of the JINR Grid-segment are currently VOs BioMed, PHOTON, eEarth, Fusion, HONE, Panda.

In the future, as the interest arises at a large-scale level, VOs can be organized at JINR in the fields of nuclear physics and condensed matter physics and, most probably, in the new promising direction related to the research of the nanostructure properties.

The creation of new VOs gets possible and necessary under maturation of the algorithmic approaches to the problem solution, the development of corresponding mathematical methods and tools. This subject area covers a wide spectrum of studies in the high energy physics, nuclear physics, solids physics and condensed matter physics, biophysics, information technologies, conducted in close cooperation with all JINR Laboratories. It includes the following key directions:

- methods and tools for simulation of physical processes and analysis of experimental data software and computer complexes for experimental data processing;
- numerical methods, algorithms and software for modeling complex physical systems;
- methods, algorithms and software of computer algebra;
- new computing paradigms;
- development of specialized software for solving problems within the Grid-environment.

Formation of the Grid environment of the JINR-Member States

This direction covers a wide spectrum of works aimed at the creation of the Grid environment of the JINR-participating countries. It will allow to bring out the research underway at JINR in the field of high energy physics, nuclear physics, solid state physics and condensed matter physics, biophysics, biosensor (nano)technologies, etc., on a qualitatively new level.

Отпечатано методом прямого репродуцирования
с подготовленного лабораторией оригинала.

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