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**REPORT ON RESEARCH ACTIVITIES
IN 2007**

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

The LIT activity is focused on two directions, namely "Information, Computer, and Network Support of the JINR's Activity" (topic 05-6-1048-2003/2007, headed by V.V. Ivanov, V.V. Korenkov, and P.V. Zrelov) and "Mathematical Support of Experimental and Theoretical Studies Conducted by JINR" (topic 05-6-1060-2005/2007, 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 13 topics at the project level and within 23 topics at the cooperation level of the Topical plan for JINR research and international cooperation.

The degree of interest in the LIT activities in the JINR Member States is high. We have a number of collaborators from the JINR Member States: protocols of cooperation with INRNE (Bulgaria), ArmeSFo (Armenia), FZK Karlsruhe GmbH (Germany), IHEPI TSU (Georgia), NC PHEP BSU (Belarus), KFTI NASU (Ukraine), IMIT UAZ (Uzbekistan), WUT (Wroclaw, Poland), etc. LIT have BMBF grant "Development of the Grid-infrastructure and tools to provide joint investigations performed with participation of JINR and German research centers", 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 "Dubna-Grid" started in 2004 on the base of the Agreement between Administration of Dubna, Joint Institute for Nuclear Research and University "Dubna" for creation of a city-wide multi-purpose new generation informational infrastructure based on the Grid technologies. The project "Development of Grid segment for the LHC experiments" was supported in frames of the JINR-South Africa cooperation agreement in 2006-2007.

Some work also was performed in frames of 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 (EGEE) project co-funded by the European Commission (under contract number INFSo-RI-031688) through the Sixth Framework Programme. Six grants were afforded by the Russian Foundation for Basic Research.

Since the year 2007 LIT team participates in SKIF-GRID project - a programme of the Belarusian-Russian Union State. The promotion of this direction is part of joint propositions of NASB 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)”.

During the year 2007, LIT was the main organizer of some workshops and conferences.

A traditional two-day Workshop on Computer Algebra was held in Dubna on May 24-25, 2007. It was the eleventh of the joint seminars on Computer Algebra conducted by the JINR, the Faculty of Computing Mathematics and Cybernetics and SRINP of Moscow State University. The purpose of the workshops was to present topics of current interest and provide a stimulating environment for scientific discussion on new developments in computer algebra. 50 participants from Germany, Finland, Romania, France, Russia (Moscow, St.Petersburg, Pereslavl-Zaleski, Perm, Saratov, Tambov and Dubna) delivered 28 reports. The workshop attendees discussed algebraic methods for nonlinear polynomial and differential equations, symbolic-numeric methods, computer algebra algorithms and software packages; application to theoretical and mathematical physics.

On 10-17 September, Varna, Bulgaria, hosted the 21st International Symposium on Nuclear Electronics and Computing (NEC'2007). For the fourth time JINR organizes this forum in cooperation with the Institute of Nuclear Research and Nuclear Energy of the Bulgarian Academy of Sciences (INRNE BAS) and CERN. Attending were more than 100 participants from 12 countries - Russia, Bulgaria, Switzerland, Great Britain, USA, Germany, Poland, Czech Republic, Romania, Vietnam, Ukraine and Georgia. 57 oral reports and 37 posters, among them 22 oral reports and 25 posters from JINR were submitted. The symposium program comprised the following sections: detector & nuclear electronics, trigger systems and data acquisition systems, automated management systems for experiments and accelerators, information & computing systems, application of network technologies for physical experiments, Grid and LHC computing as well as computer applications and new methods in scientific research. The high level of the Symposium is confirmed by the fact that the status report on the leading global Grid-project EGEE (Enabling Grid for E-science) was submitted by the Project Director Dr. Robert Jones. His personal participation in NEC'2007 testifies the recognition of the success JINR and Russia have achieved in introduction and use of Grid technologies for scientific applications. It should be noted that 20% symposium attendees were young people of 35 years old and younger, and they have made an important contribution to the symposium scientific programme with 13 oral reports and 4 poster presentations. A detailed programme and presentations of the Symposium can be found at the NEC'2007 website <http://nec2007.jinr.ru/programme.asp>

On 15-19 October, LIT was the host of the fourth international workshop “Quantum Physics and Communication”. The purpose of the Workshop was to provide a compact and comprehensive overview of recent advances in quantum information theory and quantum computing, to discuss new experimental and theoretical results, to focus on mathematical and computing aspects of

aspects of quantum information processing as well as to make perspective contacts for the future cooperation. The recent advances in the realization of qubits and elementary quantum logic gates with use of ion traps, QED resonators, nuclear magnetic resonance (NMR) technologies, quantum optical systems, superconducting devices and nanostructures open new horizons in the field of quantum information processing. For example, the report delivered by academician of the Vietnamese Academy of Sciences and Technologies Nguyen Van Hieu, "Quantum information transmission between two qubits through an intermediary photon gas" discussed a theory of quantum information transfer between two semi-conductor two-level quantum points as two qubits through intermediate photons. 31 reports were submitted for the Workshop. The presentations of the reports delivered by the workshop attendees are available on the workshop website at <http://lit.jinr.ru/QPC2007/>. The Workshop was attended by specialists working in different areas of quantum physics and information technologies from Armenia, Belarus, Brazil, Vietnam, Lithuania, Romania, Russian research centres and state universities of Moscow, Novosibirsk, Saint Petersburg, Chernogolovka. Attending were also JINR specialists from LIT, BLTP and FLNP.

NETWORKING, COMPUTING, INFORMATION SUPPORT

JINR telecommunication data links

The 2007 results of the networking activities in JINR provided and coordinated by the LIT specialists include:

- Modernization of JINR Local Area Network (LAN) central telecommunication node was finally accomplished.
- Creation of a direct point-to-point data channel between CERN and JINR Central Information and Computing Center in LIT.
- Working-out the issues of deploying 10 Gbps data link as the external JINR-Moscow data communication channel (fig.1).

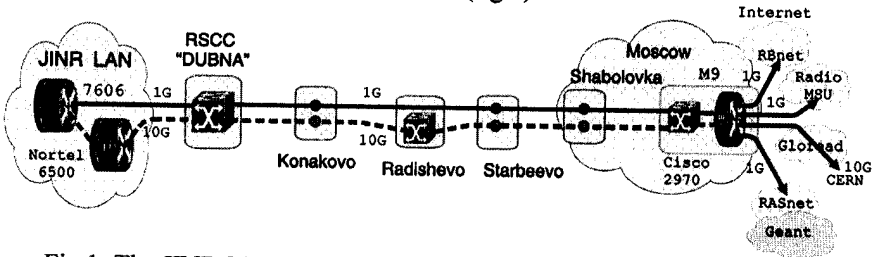


Fig.1: The JINR-Moscow telecommunication channels: solid – current 1Gbps link, dashed – planned 10 Gbps data link

A point of the local network traffic exchange was organized for JINR and Dubna Internet service providers (ISP) on the base of the JINR network facility. The local traffic of Dubna ISPs goes through this point of traffic exchange

without necessity to go through Moscow ISPs. The participants are JINR, LAN-polis, Contact, Telecom-MPK.

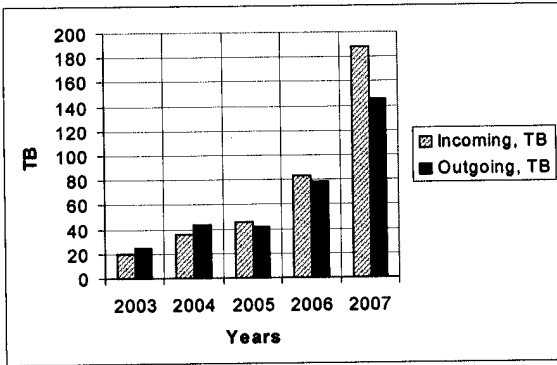


Fig.2: Incoming and outgoing JINR traffic starting from the year 2003

At present, JINR leases 1 Gbps channel to Moscow from RSCC 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). Figure 2 shows increasing of incoming and outgoing JINR traffic starting from the year 2003.

Expected perspectives

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;
- JINR's in the work on realization participation of an international segment creation within project GEANT2; increasing the throughput of the channels up to 10 Gbps in 2008, 40 Gbps in 2010, and 100 Gbps in 2015;
- broadening the Dubna – Moscow channel up to 10 Gbps in 2008, 40 Gbps in 2010, and 100 Gbps in 2015; much preliminary studies to upgrade the JINR external optical communication data link up to 10 Gbps was done. It is expected to have a 10 Gbps data link operational during a first half of 2008;
- integration with the municipal educational network and its development following its transition to advanced technologies (10 Gb Ethernet).

JINR Local Area Network

Systematic work on the JINR LAN management was performed by the Network Operation Centre (<http://noc.jinr.ru/>). At present the JINR LAN comprises 5880 computers and nodes (5681 in year 2006). There are 3322 network users, 689 modem pool users, and 500 JINR staff members use VPN connection. About 1500 JINR staff members use @jinr.ru for e-mailing.

In 2007 the following work was performed:

- configured was a specialized server flow.jinr.ru to have a system to collect/account/analyze of the overall JINR network traffic;

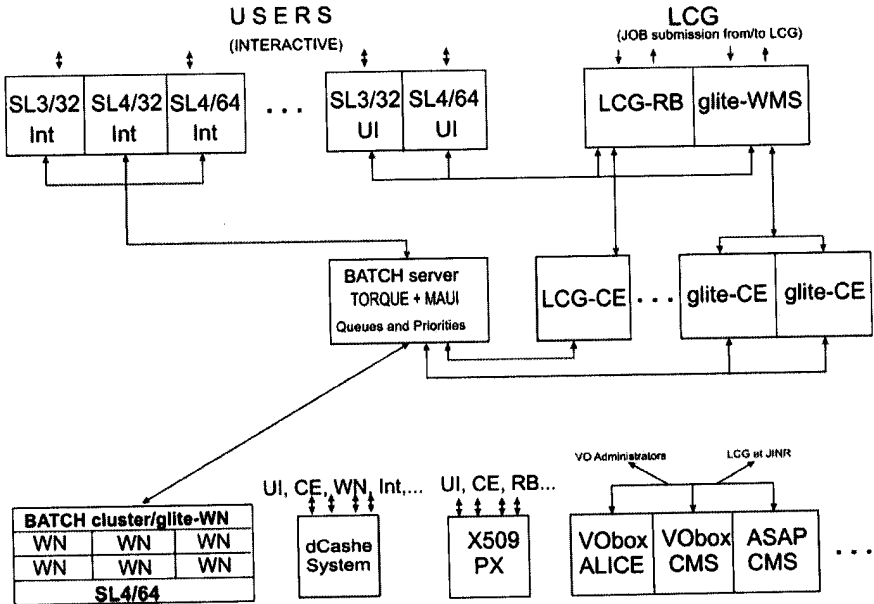


Fig.4: CICC computing resources, access and maintenance scheme:

SL3/32 Int/UI – Interactive nodes/User Interface at 32-bit architecture with Scientific Linux 3 (SL3), SL4/32 Int/UI - Interactive nodes/User Interface at 32-bit architecture with Scientific Linux 4 (SL4), SL4/64 Int/UI - Interactive nodes/User Interface at 64-bit architecture with SL4, LCG-RB - LCG Resource Broker, LCG-CE - LCG Computing Elements, WN - Worker Nodes, X509 PX - Proxy, VObox - special node where experiments (ALICE, CMS, etc.) or Virtual organizations (VO) can run specific agents and services to provide a reliable mechanism to accomplish various tasks specific for VO, AFS - AFS servers, dCache - dCache servers

The former CICC structure represented a number of special-purpose clusters allowing two ways of each cluster resources usage: either local or global. Since June 2007, the CICC resources and services have been integrated into a unified information and computing structure (Fig.4). The CICC logical and software structure was substantially restructured. The main changes concerned the security and the batch systems. All the CICC computing and data storage resources can now be used both locally and globally (for distributed computations in the LCG/EGEE grid infrastructure) 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. Access to the general-purpose software and user home catalogs is pro-

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

A new configuration of the CICC computing resources has been entered too. Instead of the resource separation into a farm for WLCG and a farm for local use, all computing resources became general. This has demanded significant changes in the LCG standard software - gLite, because gLite standard foresees allocation of resources only under LCG/EGEE needs.

Currently, there are the following computing nodes at the CICC:

- 53 special-purpose servers (29 for main the CCIC and JINR information infrastructure support and 24 for the JINR-LCG2 site support in RDIG, WLCG and EGEE);
- 4 interactive nodes;
- 60 computers of 64-bit architecture (2 Xeon 5150 dual-core processors, 8 GB RAM, 160 GB disk, 1 Gb Ethernet);
- 5 computers of 32-bit architecture (2 Athlon 2400+ processors, 2 GB RAM, 40 GB disk, 1Gb Ethernet, Myrinet network adapter).

The internal CICC network for the most part makes use Gigabit Ethernet. All the basic computing and data storage resources are connected to internal network routers at the rate of 1 Gbps. The internal CICC network is also connected to the JINR backbone network and the border router at the rate of 1 Gbps.

The special-purpose servers are used to support the work of users and JINR services: batch, WWW, MySQL and Oracle DBs, e-mail, DNS and some others.

The AFS distributed file system with a highly secure data access is used at JINR for user home catalogs and general-purpose software. The total AFS space is about 1.45 TB (1.40 TB – at CICC servers). There are 8 AFS servers installed and supported at the CICC.

Information stored at the CICC disk servers can be subdivided into 2 categories: user home catalogs and software products in different forms; “physical” information, i.e. data obtained at physical experiments and simulated data samples stored in the dCache system.

The dCache system has finally replaced the Castor system. We have chosen the dCache system instead the Castor, because dCache responds the best to the requirements which are demanded by the JINR as part of distributed Ru-Tier2 center in the WLCG hierarchy. dCache hardware and software complex serves to store large data volumes. It includes a server for hardware control, 5 front-end servers for system monitoring and work with data, and 14 data storage systems (back-end or pool). All storage systems are constructed with the usage of RAID5 hardware. Internal sub-connections are implemented at the 1Gb Ethernet technology. All the front-end systems are also connected to the 1 Gb Ethernet. Now the volume of dCache data storage pools is about 82 TB.

The table below shows a batch jobs distribution over JINR divisions on June-December 2007:

Division	Jobs number	CPU time (kSi2k*hours)
LIT	284	51421.30
FLNR	1062	11823.26
LPP	3667	10606.44
VBLHE	363	9762.61
Foton2	195	6992.83
DLNP	735	5206.62
BLTP	26	315.36
TOTAL	6332	96128.42

The distribution of Grid Virtual organizations jobs at JINR CICC in June-December 2007 is tabulated as follows:

Grid VO	Jobs number	CPU time (kSi2k*hours)
ALICE	90 441	1 370 820.40
ATLAS	15 643	48 980.43
CMS	52 249	51 883.18
LHCb	10 484	6 604.50
BIOMED	25 103	164 102.07
FUSION	9 208	145 053.80
Others	17 665	47 022.10
TOTAL	220 793	1 834 466.49

To increase the performance of the JINR CICC in December 2007 a Contract was prepared for two SuperBlade systems (40 CPU Xenon 5430 2.66 GHz Quad Core ~ 400 kSi2K). Thus, total expected performance in the year 2008 will consist ~ 1070 kSi2K.

In frames of Hulubei-Meshcheryakov programme, common investigation of the present status of the SIMFAP parallel computing cluster at IFIN-HH Bucharest was performed. The peak performance assessment and outputs of parallel computing case studies were done. They point to an effective and reliable operation of the open MPI version for high performance parallel computing implemented on the cluster within the present collaboration, in the frame of Hulubei-Meshcheryakov programme. Comparison with the High-Performance Linpack benchmark outputs obtained on the new supercomputing system installed at LIT-JINR sheds light on the effective use of parallel computing resources. [Gh. Adam, S. Adam, A. Ayriyan, E. Dushanov, E. Hayryan, V. Korenkov, A. Lutsenko, V. Mitsyn, T. Sapozhnikova, A. Sapozhnikov, O. Streltsova,

F. Buzatu, M. Dulea, I. Vasile, A. Sima, C. Visan, J. Busa, I. Pokorny: Performance assessment of the SIMFAP parallel cluster at IFIN-HH Bucharest. Submitted to Romanian Journal of Physics, December 2007.]

Expected perspectives

The future development of the JINR CICC is summarized in the following programme:

- Development of JINR CICC and Grid segment in accordance with experiments requirements:

	2007	2008	2009	2010
CPU (kSI2K)	Plan – 1000; Real – 670; Contract – 400	1250	1750	2500
Disk (TB)	Plan - 150-200; Real – 100	400	800	1200
Tapes (TB)	-	-	100	200

- raising computing cluster performance;
- raising disk storage system;
- creation data storage system of Active tape type;
- Transfer of the CICC local network to 10 Gbps;
- Development of the servers maintaining the JINR Grid segment and computing cluster;
- Development and modernization of servers of the JINR information structure and the general storage system (dCache, WEB, database servers).

Grid-technologies and WLCG project

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

In 2006 the LCG project entered a new phase, i.e. the construction of a global infrastructure of the regional centers intended for processing, storage and analysis of data for a moment of the accelerator start-up. The project is referred to as WLCG (Worldwide LHC Computing Grid), document WLCG TDR has been developed and approved. In cooperation with the managing body of the WLCG project, a three-power agreement MoU has been prepared between CERN, Russia and JINR on participation in this project and obligations on its

financing by Russia and JINR. In September 2007 the document was signed from the Russia side by the Head of the Federal Agency on Science and Innovations S.N. Mazurenko and by JINR Director A.N. Sissakian. The signing of this document provides a legal and financial basis for the development of the WLCG infrastructure in Russia and JINR required for the full-value participation of Russian physicists in processing and analysis of experimental data on LHC. The created global infrastructure can also be used for solving other large-scale problems.

The CICC provides the following services in the WLCG environment:

- Basic services: top level BDII for Russian WLCG community; site BDII; Computing Element (CE); Proxy Server (PX); Resource Broker (RB); Workload Management System + Logging & Bookkeeping Service (WMS+LB); RGMA-based monitoring system collector server (MON-box); LCG File Catalog (LFC); Storage Element (SE), 42TB dCache.
- Special Services: VO boxes for ALICE and for CMS; ROCMON.
- PS and testing infrastructure: Pre-production gLite version; xrootd door in dCache for ALICE.
- Software for VOs: dCache xrootd door, AliROOT, ROOT, GEANT packages for ALICE; ATLAS packages; CMSSW packages for CMS; DaVinci and Gauss packages for LHCb.
- Several versions of ALICE, ATLAS and CMS software are installed at the CICC locally at the AFS system.

In 2007 the following work was performed:

- participation in Service, Data, Software and Analysis Challenges 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 installed and supported at the CMS VObox at JINR;
- CMS DBs activities: further improvement and development of CMS offline DBs;
- regular update and testing of ALICE software (AliEn) required for ALICE production Data and Service Challenges and distributed analysis not only at the JINR-LCG2 site but also at 12 ALICE sites in Russia;
- a dedicated Computing Element (CE) was installed at the JINR-LCG2 site (lgdce01.jinr.ru) enabling a special short queue (CPU time per job less than 1.5 hour) for any ATLAS VO (Virtual Organization) user;
- the local CICC computing infrastructure was made ready for a full-scale simulation of Higgs boson decay carried out by the JINR ATLAS team;
- the Data Quality Monitoring framework (online and offline) was installed on the farm and tested with real data from ATLAS Point1;
- LCG middleware testing/evaluation: testbed infrastructure for testing in the gLite3.X environment was installed at JINR local nodes; development of

- certification tests for VOMS: 60 program tests were developed and integrated into the automated system SAM (Service Ability Monitor) and are in regular use;
- monitoring and accounting system (<http://rocmon.jinr.ru:8080>) was modernized and developed for the LCG-infrastructure at JINR and other sites of the Russian Tier2 cluster; in particular, a special web-page on RDMS CMS PhEDEx transfer statistics has been developed (<http://rocmon.jinr.ru/scripts/phedex>), it provides access to the information on data transfer rates and amount of data transferred during different time periods (hours and days);
 - evaluation of new Grid technologies in context of their usage in LCG (Globus Toolkit 4 testing&evaluation);
 - MCDB development (<http://mcdb.cern.ch>): creation of a set of basic modules; web-interface development; integration of MCDB data and information access facilities to CMSSW package [S. Belov et al.: *LCG MCDB - Knowledge Base of Monte Carlo Simulated Events, Proceedings of ACAT07 conference, Amsterdam, The Netherlands, Proceedings of Science, PoS(ACAT)(2007)030*];
 - FTS monitoring and testing (<https://twiki.cern.ch/twiki/bin/view/LCG/TransferOperations>) providing Daily logs with tracking of current problems and open issues; Daily logs are kept in the Daily log archive representing a history of situation on channels;
 - the Multi-Phase Transport Model (AMPT) adapted for the LHC energies has been installed at the HEPWEB server (<http://hepweb.jinr.ru>);
 - participation in ARDA project activities: CMS Dashboard development, including monitoring of the CMS Monte-Carlo production system and Condor-G job monitoring [J. Andreeva, S. Belov, ... , I. Sidorova, ... , E. Tikhonenko et al.: *Dashboard for the LHC Experiments, to be published in Journal of Physics: Conference Series - CHEP'2007 Proceedings*];
 - participation in the EGEE project: modernization and steady renewal of WEB-portals for EGEE (<http://www.egee-rdig.ru>); participation in the SA1 (organization and support of grid-services) and NA2 (dissemination of information) activities and testing/evaluation of new middleware;
 - the fully operable gLite site has been created on the basis of the GridLab of LIT JINR in frames of the "Dubna-Grid" project. The Worker Nodes of the site operate on virtual machines (VMWare Player), while the Computing Element and the Storage Element are represented by ordinary PCs. The site will be used for educational purposes as well as for testing of various configurations;
 - support of the JINR Member States in LCG activities: close cooperation with partners in Ukraine, Belarus, Czech Republic, Poland, Romania, South Africa and Bulgaria, in particular, consultations and support in LCG software, workshop and grid tutorials for Romanian system administrators for

ATLAS and ALICE at JINR, a special agreement in grid activities between JINR and Wrocław University is in preparation;

- user's support to stimulate their active usage of LCG resources (courses, lectures, trainings, publication of user guides in Russian): Courses "CMS user analysis using EGEE/LCG infrastructure" - January 19, 2007; Tutorial on distributed analysis of ATLAS data - April 19, 2007; Translation of "LCG2-Manual-Install" guide into Russian (http://lcg.jinr.ru/section.asp?sd_id=76).

The results of the work were presented at ACAT'2007 conference in Amsterdam, NEC'2007 symposium in Varna and the conference "Physics at the Future Colliders" in Tbilisi.

In frames of participation in Grid activities in cooperation with German Centres in 2007 the following work was done:

- HONE VO (Virtual Organization for H1 experiment at DESY) queue was configured and enabled at JINR LCG-2-site and is in an active use. As the result, from July 2007, the JINR LCG farm has been in active use for H1 MC production and by the November, 2007 more than 7 millions simulated events produced at JINR (for comparison: during this period at the DESY LCG site there were produced about 56 millions simulated events);
- In July-August of 2007, ALICE group and JINR system administrators made tests to estimate the parameters of the data communication link between FZK and JINR to check-up functionality, reliability and possible bottlenecks of all the services involved in such communications as well as transfer rate.

The activities on the LHC computing support will become especially important before the LHC start, which is expected in the year 2008. A distributed grid computing infrastructure adopted for the LHC experiments has been successfully built as the RuTier2 (Russian Tier2) distributed cluster. This has undergone a long time testing at JINR and Russian institutes – members of Russian Data Intensive Grid (RDIG) consortium. In accordance with RDIG computing model for the LHC, a distributed RuTier2 cluster operates with resources located at different institutes between all the LHC experiments. The JINR CICC is element of the RDIG infrastructure used for LHC computing and for other applications.

The distribution of Normalized CPU time per RDIG sites (June 2007 - December 2007) is shown at fig.5.

Expected perspectives

Establishment and development of JINR's Grid infrastructure as a segment of the Russian and worldwide system of distributed computations:

Normalised CPU time (SpectInt2000 = 1000) per Site

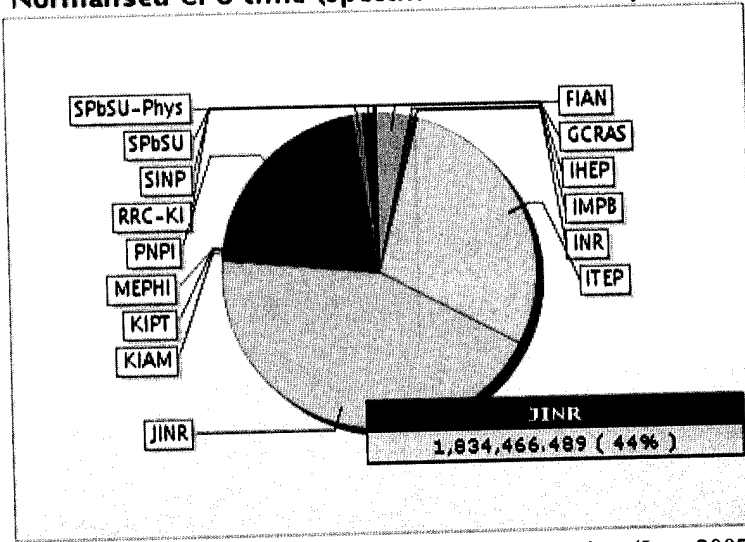


Fig.5: Distribution of normalised CPU time per RDIG sites (June 2007 - December 2007)

- development of JINR's Grid segment with a fully functional set of services;
- participation in international, national, and regional projects of developing Grid technologies (WLCG, EGEE, OSG, NorduGrid, DubnaGrid, etc.);
- participation in developing the technologies of application "gridification" that will allow applied software packages to be adapted to the Grid environment.

Information and software support

The modernization of CICC software and its installation in a 64-bit variant required a full recompilation of programs from JINRLIB library. The object libraries of mathematical general-purpose programs have been 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 old object libraries for OS Scientific Linux 3 and Windows 9X/NT/2000/XP are also maintained and filled.

JINRLIB program packages created by JINR specialists are renewed regularly. These programs serve a wide range of scientific tasks under way at JINR – from experimental data processing automation to low energy theoretical physics. A specialized WWW site provides an electronic access to the descriptions of the programs, compiled libraries and source texts.

The program libraries developed in other research centres (CPCLIB, CERNLIB) are also maintained. The full information on the JINR program libraries is available at the specialized WWW-server <http://www.jinr.ru/programs/> and in LIT Information Bulletins.

Work is in progress on the re-engineering technology for distributed computing in a local area network. [A.P. Sapozhnikov, A.A. Sapozhnikov, T.F. Sapozhnikova: *Re-engineering Technology and Software Tools for Distributed Computations with Using Local Area Network. Proceedings of the 6th International Conference "Large-Scale Scientific Computing"* (Sozopol, Bulgaria, June 5-9, 2007). Springer, LNCS, Volume 4818, pp..700-707.]

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 2007 work was in progress on the regular actualization of the program environment and contents of the central information sites of LIT and JINR (<http://www.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 provided was support and modernization of administrative databases, updating and support of software for the central accounting department, accounting departments of the Experimental Workshop, and the power engineering head division; 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 (QPC2007 - the 4-th International workshop "Quantum physics and communications"; RCDL'2008 – "Electronic libraries: perspective methods and technologies, electronic collections"; <http://www.jinr.ru/esna2007>; <http://www.jinr.ru/sarantsev07>; <http://www.jinr.ru/pontecorvo07>). A prototype of the information system developed in LIT JINR for the internal paperless document circulation (<http://lit.jinr.ru/DoctorDoc/>) has been created.

The portal technology is a key performance technology for all modern investigation projects due to the large-scale and world-wide nature of the most scientific and especially experimental collaborations in nuclear and particle physics. Special software for design, development and support of special and general-purpose web-servers based on modern portal service-oriented technologies has been worked out. Using this software does not require special Internet technology knowledge or skills. This software includes a specific database and a set of adjustable web-interfaces (online participant registration, initial abstract submission and upload of presentation files of various formats, web-site structure dynamic creation its files management, keeping news, forming mailing lists and setting up e-mail distribution service, extracting and sorting information on participants and their papers, providing access of different level for work with database). In 2007, the following web sites were developed using this software: <http://newuc.jinr.ru/> - site of the JINR University Centre; <http://nec2007.jinr.ru/>

- site of the XXI International Symposium on Nuclear Electronics and Computing (NEC'2007).

MATHEMATICAL SUPPORT OF EXPERIMENTAL AND THEORETICAL STUDIES

Performance of top research in computational mathematics and computational physics, aimed at solving specific problems arising in experimental and theoretical research carried out with the direct participation of JINR is the main scientific activity of LIT. The basic part of this activity covers: the mathematical description and algorithmic reformulation of the physical models such as to meet the requirement of computing solution in polynomial time; development of methods and algorithms, capable to extract physically insightful information from experimental data; simulation of physical processes within experimental installations; algorithm implementation into efficient and reliable hardware adapted programs.

More than 130 scientific publications and proceedings of conferences were published in 2007. More than 70 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. In addition, this includes creation of specially designed computer complexes, for example, computer clusters and farms.

The creation in LIT of the specialized physical server HEPWEB can serve as an example (<http://hepweb.jinr.ru>). The aim of the project is to provide physicists with informational and mathematical support of their investigations with use of WEB access to LIT computing resources for Monte Carlo simulations. Additional aim is to test Monte Carlo generators of physical processes for the LHC Computing Grid project. The web-page allows one to estimate the main properties of hadron-nucleus and nucleus-nucleus interactions (includes FRITIOF model, HIJING model, and tools for Glauber and Reggeon theories calculation). A WEB-page containing materials of comparing experimental data and Quantum Molecular Dynamics model (UrQMD) model calculations has been designed. The page can be useful for new experimental data analysis, or new experimental research planning.

A new version of Fitter - a C++ program aimed to fit a chosen theoretical multi-parameter function through a set of data points was installed. The method of fitting is chi-square minimization. Moreover, the robust fitting method can be applied in Fitter. It was designed to be used for a small-angle neutron

scattering data analysis. Respective theoretical models are implemented in it. Some commonly used models (Gaussian and polynomials) are also implemented for wider applicability. [A.G. Soloviev, A.V. Stadnik, A.H. Islamov, A.I. Kuklin: <http://www.jinr.ru/programs/jinrlib/fitter/index.html>]

Also, a new version of Gluplot - data plotting package was included in JINR Program Library. It was originally intended both as a graphical library and as a standalone program, which would allow scientists and students to visualize data. Gluplot handles both curves (2D) and surfaces (3D) (fig.6). [A.G. Soloviev: <http://www.jinr.ru/programs/jinrlib/gluplot/indexe.html>]

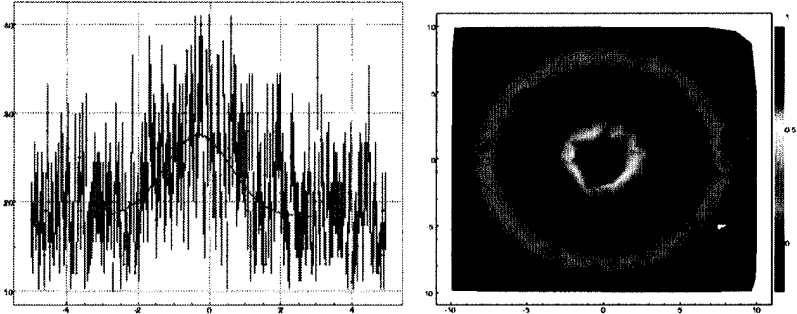


Fig 6: Examples of Gluplot 2D and 3D

In order to increase the efficiency of a local smoothing of surfaces, a bicubic model has been suggested where a biquadratic component is fixed by coordinates of reference points of the surface, a bicubic one remains free, and basic functions depend on parameters. Such an approach has allowed one to reduce more than twice the dimension of the matrix of normal equations, to increase essentially the speed and stability of computations. The algorithms constructed on the basis of the suggested model, are focused both on practical applications and on the development of more efficient global methods of approximation and smoothing of surfaces. [N. Dikoussar, Cs. Török: "Kybernetika", V. 43, No. 4, pp. 533 - 546, 2007.]

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

The problem of electron/pion identification in the CBM experiment based on the measurements of energy losses and transition radiation in the TRD detector was studied. A possibility to solve such a problem by applying an artificial neural network (ANN) was considered. As input information for the network, both the samples of energy losses of pions or electrons in the TRD absorbers and the "clever" variable obtained on the basis of the original data were used. It is shown that usage of this new variable permits one to reach a reliable level of particle recognition no longer than after 10-20 training epochs, there are practi-

cally no fluctuations against the trend, and the needed level of pions suppression is obtained under the condition of a minimal loss of electrons. [E.P. Akishina, T.P. Akishina, V.V. Ivanov, A.I. Maevskaya, O.Yu. Afanas'ev: *Electron/pion identification in the CBM TRD applying a multilayer perceptron, JINR Communication, E10-2007-17, JINR, Dubna, 2007.*]

The opportunity of solving the specified problem of electron/pion identification in the CBM experiment with the help of nonparametric goodness-of-fit criterion ω_n^k is investigated and compared with the method on the basis of an artificial neural network (ANN). It is shown that both approaches provide a comparable level of pion suppression and electron identification; moreover, the criterion ω_n^k is simple in use, while the ANN provides a required level of pion suppression only if using "clever" variables. It is shown that application of the ω_n^k criterion to the J/ψ reconstruction procedure provides a high-level suppression of a pion background and essentially improves a signal/background ratio. [E.P. Akishina, T.P. Akishina, V.V. Ivanov, A.I. Maevskaya, O.Yu. Denisova: *PEPAN Letters, Volume 5, No. 2(144), 2008, pp. 202-218.*]

A comparative study of two methods for a circle fitting over measured points was performed. A method, optimal from the accuracy viewpoint for estimating circle parameters, has been chosen. On the basis of the selected method a robust algorithm has been developed. The program implementing this algorithms is used to estimate the parameters of the Cherenkov radiation rings obtained in the RICH (Ring Imaging Cherenkov) detector of the CBM experiment, and it is included in the CBM software framework. [A. Airiyan, S. Baginyan, G. Ososkov, C. Hoehne: *Fast algorithms for parameter estimating of Cherenkov radiation ring in RICH detectors, Tver Univ.Herald, N 17(45), 2007, pp 15-26.*]

Two algorithms of ring recognition, a standalone ring finder (using only RICH information) and an algorithm based on the information from vertex tracks are worked out. The fake ring problem and its solution using a set of 2 dimensional cuts or an artificial neural network was studied. A comparative study of two algorithms was performed. All developed algorithms were tested on large statistics of simulated events and were then included into the CBM framework for common use. [S. Lebedev, G. Ososkov, C. Hoehne: *Ring Recognition in the CBM RICH detector. JINR Commun. E10-2007-88.*]

In 2007, in course of computational experiments with Monte Carlo events for CTB04 setup, a new class of procedures based on Artificial Neural Networks (ANN) technique was developed for reconstruction of energy losses (EDM) in the LAr/Tile dead materials of the ATLAS calorimeter. The developed ANN procedures exploit as their input vectors the information content of different sets of variables (parameters) which describe particular features of the hadronic shower of a particular event in the ATLAS calorimeter. It has been shown that application of ANN procedures allows one to reach 40% reduction of the

EDM reconstruction error compared to the conventional procedure ($EDM = C \sqrt{E_{LAr3} E_{HC1}}$) used in the ATLAS collaboration. Impact of various features of a shower on the precision of EDM reconstruction was investigated in detail. It was found that the use of information on the longitudinal shower profile of an event brings a greater improvement in EDM reconstruction accuracy than the use of cell energies information in the central samplings LAr3 and Tile1. [Y. Kulchitsky, P. Tsiareshka, V. Shigaev: "Artificial Neural Networks for reconstruction of energy losses in Lar/Tile dead material: exploration and results" JINR/ATLAS Data Preparation Workshop, December 28 2007, <http://indico.cern.ch/conferenceDisplay.py?confId=27029>; Y. Kulchitsky, P. Tsiareshka, V. Shigaev: "Application of artificial neural networks to reconstruction of the energy lost in Lar/Tile dead material (first steps)" Int. Atlas Conference, section: Hadronic Calibration of ATLAS calorimeters. CERN October 10 2007, <http://indico.cern.ch/conferenceDisplay.py?confId=22213>]

The Neural Networks scheme of DM energy loss evaluation was incorporated into a pion energy reconstruction procedure at 250 and 350 GeV. As a result, precision of the pion energy reconstruction has substantially increased for both MC-events and real events of CTB04 experiment. The attained precision fulfills requirements of the ATLAS technical project. [Y. Kulchitsky, P. Tsiareshka, V. Shigaev: "Incorporation of Neural Networks scheme of DM energy loss evaluation into pion energy reconstruction procedure". JINR/ATLAS Data Preparation Workshop, December 28 2007, <http://indico.cern.ch/conferenceDisplay.py?confId=27029>]

Particle physics

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

A resummation of the perturbative series for the amplitude of lepton pair production in the nucleus-nucleus collisions is performed on the basis of the Watson theorem and hypothesis of the infrared stability. An explicit expression for this amplitude valid up to terms of ninth order in finite structure constant is obtained. [O.O. Voskresenskaya, A.N. Sissakian, A.V. Tarasov, H.T. Torosyan: *A Structure for the Amplitude of $Z_1 Z_2 \rightarrow l^+ l^- Z_1 Z_2$ Reaction Beyond the Born Approximation. Physics of Elementary Particles and Atomic Nuclei, Letters, 2007,*

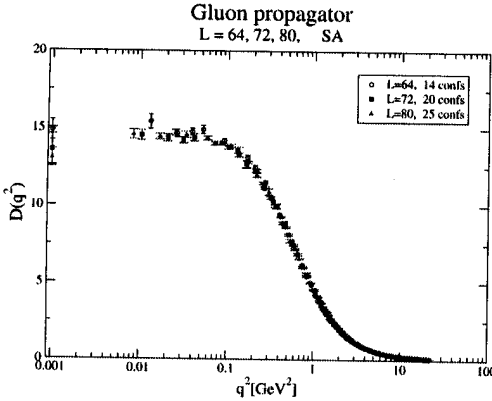


Fig.7: The gluon propagator from different lattices sizes for $\beta = 5.7$. The data points drawn at $q^2=0.001$ represent the zero-momentum gluon propagator $D(0)$

relaxation was employed. It was found, that the gluon propagator for the largest volumes and at $q^2 \sim 0.01 \text{ GeV}^2$ becomes flat (fig.7). Although not excluded by obtained data, there is still no clear indication of a gluon propagator tending towards zero in the zero-momentum limit. New data for the ghost propagator are reported, too. [I. L. Bogolubsky, E.-M. Ilgenfritz, M. Müller-Preussker, A. Sternbeck: *The Landau gauge gluon and ghost propagators in 4D SU(3) gluodynamics in large lattice volumes. PoS(LATTICE-2007)290. e-Print: arXiv:0710.1968.*]

The recent results of the Landau gauge gluon and ghost propagators in $SU(3)$ pure gauge theory at Wilson $\beta = 5.7$ for lattice sizes up to 80^4 corresponding to physical volumes up to $(13.2 \text{ fm})^4$ were presented. In particular, the focus on finite-volume and Gribov copy effects was investigated. A gauge - fixing method, that combines a simulated annealing algorithm with finalizing over

A software complex has been designed for computing the wave functions of a discrete and continuous spectrum of quantum systems by Kantorovich method. The eigenvalue problems obtained with the help of this method for the systems of ordinary differential second-order equations with variable coefficients are solved by a finite element method. The efficiency and stability of the algorithm has been demonstrated with 2-dimensional exactly solvable quantum models. The software complex has been applied to computation of the wave functions of the discrete and continuous spectrum of a hydrogen atom in a magnetic field which are required for computing a photo-ionization cross-section and the rate of a forced recombination under the influence of laser pulses and ultimately for determining the conditions when the yield of the recombining atoms will be the highest. [S.I. Vinitzky, V.P. Gerdt, A.A. Gusev, M.S. Kaschiev, V.A. Rostovtsev, V.N. Samoilov, T.V. Tupikova, O. Chuluunbaatar: *Programming and Computer Software* 33, pp. 105-116 (2007); O. Chuluunbaatar,

A.A. Gusev, V.P. Gerdt, V.A. Rostovtsev, S.I. Vinitsky, A.G. Abrashkevich, M.S. Kaschiev, V.V. Serov: *accepted in Comput. Phys. Commun.* doi:10.1016/j.cpc.2007.09.005 (2007); O. Chuluunbaatar, A.A. Gusev, V.L. Derbov, M.S. Kaschiev, V.V. Serov, T.V. Tupikova, S.I. Vinitsky: *Proceedings of SPIE 6537*, pp. 653706-1-18 (2007).]

A FORTRAN 77 program is presented which calculates energy values, reaction matrix and corresponding radial wave functions in a coupled channel approximation of the hyperspherical adiabatic approach. In this approach, a multi-dimensional Schroedinger equation is reduced to a system of the coupled second-order ordinary differential equations on the finite interval with homogeneous boundary conditions of the third type. The resulting system of radial equations which contains the potential matrix elements and first-derivative coupling terms is solved using high-order accuracy approximations of the finite-element method. As a test desk, the program is applied to the calculation of the energy values and reaction matrix for an exactly solvable 2D-model of three identical particles on a line with pair zero-range potentials. [O. Chuluunbaatar, A.A. Gusev, A.G. Abrashkevich, A. Amaya-Tapia, M.S. Kaschiev, S.Y. Larsen, S.I. Vinitsky: *KANTBP: A program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach*, *Comput. Phys. Commun. Vol. 177*, pp. 649-675 (2007)].

A new efficient method for calculating the photoionization of a hydrogen atom in a strong magnetic field is developed based on the Kantorovich approach to the parametric boundary problems in spherical coordinates using the orthogonal basis set of angular oblate spheroidal functions. The progress consists of the development of the Kantorovich method for calculating the wavefunctions of a continuous spectrum, including the quasi-stationary states imbedded in the continuum. Resonance transmission and total reflection effects for scattering processes of electrons on protons in a homogenous magnetic field are manifested. The photoionization cross sections found for the ground and excited states are in good agreement with the calculations by other authors and demonstrate correct threshold behavior. The estimates using the calculated photoionization cross section show that due to the quasi-stationary states the laser-stimulated recombination may be enhanced by choosing the optimal laser frequency. [O. Chuluunbaatar, A.A. Gusev, V.L. Derbov, M.S. Kaschiev, V.V. Serov, L.A. Melnikov, S.I. Vinitsky: *Calculation of a hydrogen atom photoionization in a strong magnetic field by using the angular oblate spheroidal functions*, *J. Phys. A, Vol.40*, pp. 11485-11524 (2007).]

Based on the developed adaptive algorithms, investigated was a supercritical system of nonlinear evolutionary equations, namely, a coupled system of interaction Yang-Mills and dilaton fields. Decay of regular static spherically symmetric solutions in the $SU(2)$ Yang-Mills-dilaton (YMd) system of equations under independent excitation of their unstable eigenmodes has been studied self-consistently in a nonlinear regime. The considered regular YMd solutions form a

discrete family and can be parametrised by the number $N=1,2,3,4\dots$ of their unstable eigenmodes in linear approximation. The strong numerical evidences have been obtained in favour of the following statements: all static YMd solutions are distinct local threshold configurations, separating blowup and scattering solutions; the main unstable eigenmodes are only those responsible for the blowup/scattering alternative; excitation of higher unstable eigenmodes always leads to finite-time blowup; the decay of the lowest $N=1$ static YMd solution via excitation of its unique unstable mode is an exceptional case because the resulting waves propagate as a whole without energy dispersion revealing features peculiar to solitons. [E.E. Donets, E.A. Hayryan, O.I. Streltsova: *Blowup/scattering alternative for a discrete family of static critical solutions with various number of unstable eigenmodes*. ArXiv: 0711.3994v1 [gr-qc]. *Submit. to Phys.Rev. D.*]

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. Exact self-consistent solutions to the corresponding field equations are obtained. The role of spinor field in the evolution of the Universe is studied. It is shown that the spinor field gives rise to an accelerated mode of expansion of the Universe. At the early stage of evolution the spinor field nonlinearity generates the acceleration while at the later stage it is done by the nonzero spinor mass. [Bijan Saha: *Nonlinear spinor field in Bianchi type-I cosmology: accelerated regimes*. *Romanian Reports in Physics*, Vol. 59, No. 2, P. 655–666, 2007.]

The study of a self-consistent system of nonlinear spinor and Bianchi type I gravitational fields in presence of a viscous fluid and Λ term with the spinor field nonlinearity being some arbitrary functions of the invariants I and J constructed from bilinear spinor forms S and P , generates a multi-parametric system of ordinary differential equations. A qualitative analysis of the system in question has been carried out. A complete qualitative classification (fig.8) of the mode of evolution of the universe given by the corresponding dynamic system has been done. [B. Saha, V. Rikhvitsky: *Anisotropic cosmological models with spinor field and viscous fluid in presence of a Λ term: qualitative solutions*. *J.Phys. A: Math.Theor.* v.40, 14011-14027 (2007), arXiv: 0705.3128v1[gr-qc].]

A time-dependent periodic Hamiltonian admitting exact solutions are applied to construct a universal set of gates for quantum computation. The approach is based on transformation of soluble time-independent equations into time-dependent ones by employing a set of special time-dependent transformation operators. A class of periodic time-dependent Hamiltonians with cyclic solutions is constructed in a closed analytic form and the non-adiabatic geometric phase and evolution matrices are determined in terms of the obtained solutions. [A.A. Suzko, G. Giorgadze: *Quantum Computing in Exactly Solvable models and Geometric Phases*. *Contemporary Mathematic and its Applications*, Vol.44, 2007, pp.141-151.]

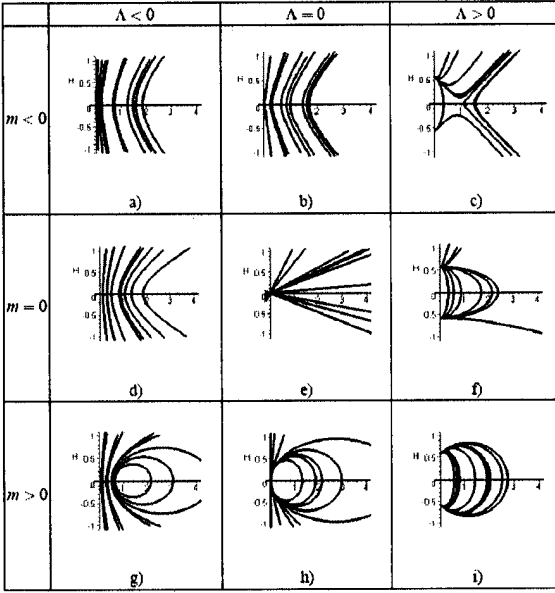


Fig.8: Classification of qualitatively different types of evolution (phase portrait) on $\epsilon=0$ plane for $n=2$

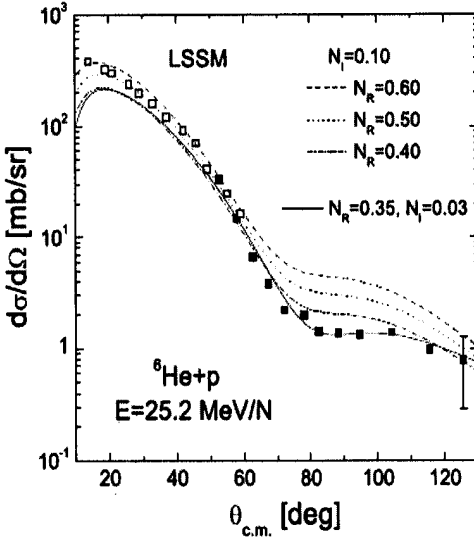


Fig. 9: Elastic ${}^6\text{He}+p$ scattering cross sections for $E = 25.2 \text{ MeV/N}$ calculated by using the large-scale shell-model (LSSM) density for ${}^6\text{He}$. The curves exhibit results for $U_{\text{opt}} = N_R V^F + i N_I W^H$ with different values of N_R and fixed value of $N_I=0.1$. The solid curve is for $N_R=0.35$ and $N_I=0.03$. The experimental data were obtained in FLNR JINR (G.M. Ter-Akopian et al., Phys. Lett. B426, 251 (1999); R. Wolski et al., Phys. Lett. B467, 8 (1999); S. Stepanyov et al., Phys. Lett. B 542, 35 (2002))

Nuclear physics

Calculations of microscopic optical potentials (OP's) (their real and imaginary parts) are performed to analyze the ${}^6\text{He}+p$ elastic scattering data at a few tens of MeV/nucleon (MeV/N). The OP's and the cross sections are calculated using three model densities of ${}^6\text{He}$. Effects of the regularization of the NN forces and their dependence on nuclear density are investigated. Also, the role of the spin-orbital terms and of the non-linearity in the calculations of the OP's, as well as effects of their renormalization are studied. The sensitivity of the cross sections to the nuclear densities was tested and one of them that gives a better agreement with the data was chosen (fig.9). [K.V. Lukyanov, V.K. Lukyanov, E.V. Zemlyanaya, A.N. Antonov, M.K. Gaidarov: *Calculations of ${}^6\text{He}+p$ elastic scattering cross sections using folding approach and high-energy approximation for the optical potential. Arxiv: 0708.3586[nucl-th]. European Physical Journal A, vol. 33, 389-400, 2007.*]

Excitations of low-lying collective states of nuclei in the heavy-ion scattering are studied at energies about tens MeV/nucleon. The interaction potential, responsible for excitations, is taken as a derivative of the microscopic (or semi-microscopic) double-folding nucleus-nucleus optical potential. The cross sections of elastic and inelastic scattering are calculated in the framework of the high-energy approach, and the amplitude of inelastic scattering is obtained in the first order in the deformation parameter. Comparisons are made with the experimental data on scattering of the ${}^{17}\text{O}$ projectiles on different nuclei with excitations of 2^+ rotational state. [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. Bul. Rus. Acad. Sci. Phys., Vol. 72, No. 3, 2008, pp.386-390, 2008 (in print).*]

The existing experimental data on the total cross sections of the ${}^6\text{He}$, ${}^6,7\text{Li} + {}^{28}\text{Si}$ reactions at energies $E=5-50$ A MeV are analyzed in the framework of a microscopic optical potential with real and imaginary parts obtained with the help of the double-folding procedure and by using the current models of densities of the projectile nuclei. Comparisons are made of cross sections calculated within the microscopic double-folding Coulomb potential and with when one applies the traditional Coulomb potential of the uniform charge distribution. The semi-microscopic potentials are constructed from the renormalized microscopic potentials and with addition of their derivatives to take into account collective motion effects and to improve an agreement with experimental data. [K.V. Lukyanov, I.N. Kukhtina, V.K. Lukyanov, Yu.E. Penionzhkevich, Yu.G. Sobolev, E.V. Zemlyanaya: *Microscopic model analysis of the ${}^6\text{He}$, ${}^6\text{Li} + {}^{28}\text{Si}$ total reaction cross sections at the energy range 5-50 A MeV. Bul. Rus. Acad. Sci. Phys., Vol. 72, No. 3, pp. 381-385, 2008 (in print).*]

Monte Carlo method is used to estimate production of secondary proton and neutron fluxes in different subcritical assemblies (k_{eff} in the range from 0.15 to 0.98) under irradiation with protons in the energy range from 660 MeV up to 2.0 GeV. Neutron and proton spectra emitted from the surface of these assemblies are calculated using the CASCADE and MCNP-X codes (fig.10). Results of Monte Carlo calculations demonstrate that even after passing the bulk of several dozen centimeters of cased heavy material arranged in a dense grid in the presence of coolants proton fluxes are accounting for up to several percent of the

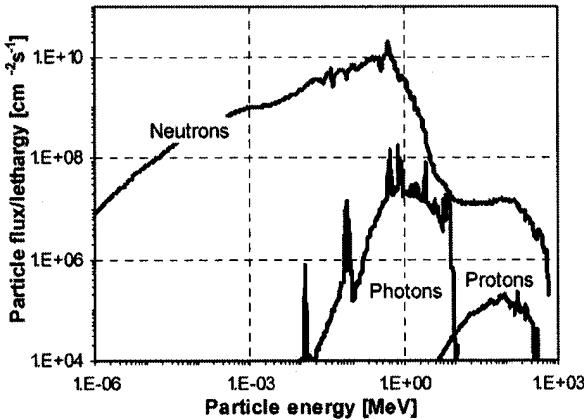


Fig. 10: Neutron, photon and proton fluxes emitted from the assembly under irradiation with 660 MeV protons

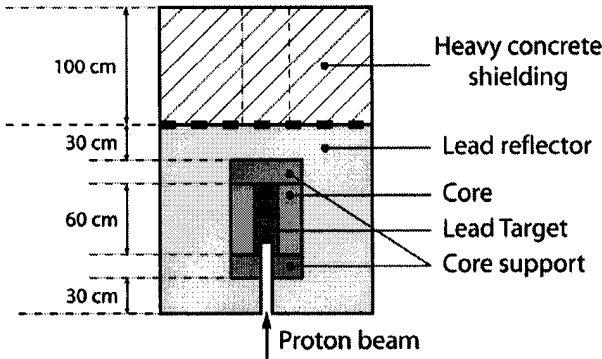


Fig. 11: General scheme of the assembly under investigation

high energy neutron flux which may show some effect on the choice of materials, size of the primary target and construction of the assemblies. The scheme of the assembly under study is shown in fig.11. The assembly under investigation is built from the BN-350 MOX fuel elements, external lead reflector and concrete shield. The assembly is cooled with the flow of air. Estimated multiplication factor of the assembly is $k_{\text{eff}}=0.951-0.974$. Energetic gain (ratio of the energy produced in the assembly to the energy spent on the proton beam) is equal to 30-50 kW correspondingly to the value of the multiplication factor. Beam power is

I kW. [A.A. Polanski, A.N. Sosnin: *The 20-th International Conference on Transport Theory ICTT-20, July 22-28, 2007, Obninsk, Russia, pp. 212-213, subm. to "Transport Theory and Statistical Physics".*]

Condensed matter physics

The neutron scattering length density across the membrane is simulated on the basis of the fluctuated model of a lipid bilayer. The use of a separated form factors method has been applied to the identification of the structural features of the polydispersed unilamellar DMPC vesicle system. The hydration of vesicle is described by a sigmoid distribution function of water molecules. The application of the model to the obtained SANS spectra allows determination of the main parameters of the system, such as a average vesicle radius (and its polydispersity), a membrane thickness, a thickness of the hydrocarbon chain region, a number of water molecules located per lipid molecule, and a phospholipid surface area. Moreover, the approach allows calculation of some relevant parameters connected with the water distribution function across the bilayer system. The main features of the obtained results furnish an explanation of why lipid membrane is easily penetrated by the water molecules of the solution. [M.A. Kiselev, E.V. Zemlyanaya, N.Y. Ryabova, T. Hauss, S. Dante, D. Lombardo: *Water distribution function across the curved lipid bilayer: SANS study. To be published in Chemical Physics, 2008, Online first: DOI 10.1016/j.chemphys.2007.09.051*]

Interactions between the dark solitons of the parametrically driven defocusing nonlinear Schroedinger equation have been studied. This equation is derived in a broad variety of physical situation in the fluid dynamics, nonlinear optics and ferromagnetic theory. The Bloch-Bloch and Neel-Neel interactions of solitons (domain walls) was considered. Two distant Neel walls and two distant Bloch walls are shown to attract, repel, or form a stable bound state in dependence on the parameters of driving and dissipation. Regions of existence and stability of two-wall complexes have been found, numerically and analytically. It is established that in the low driving strength case two well-separated Neel walls can repel or attract in dependence on their initial separation. For intermediate driving strength, two Neel walls can evolve into a stable stationary bound state. The Neel walls with the driving greater than the threshold driving strength attract and annihilate irrespective of their initial separation. The collision of two Bloch walls or two nondissipative Neel walls typically produced a quiescent or moving breather. [I.V. Barashenkov, S.R. Woodford, E.V. Zemlyanaya: *Interactions of Parametrically Driven Dark Solitons. I: Neel-Neel and Bloch-Bloch interactions. Phys. Rev. E, Vol.75, 026603 (2007).*]

The temperature effects have been studied in an anisotropic material of highly-oriented pyrolytic graphite (HOPG) exposed to 253 MeV heavy ions ^{86}Kr and 710 MeV ^{209}Bi ions in frames of a nonlinear (i.e. with the account of temperature-dependent thermo-physical parameters) 3-D model of the thermal peak.

A comparative analysis in a linear model has been made. Research of the temperature effects are conducted in the model, when changing the coefficient of the electron-phonon interaction g . It is shown that in case of irradiation of HOPG by bismuth ions, the temperature on the target surface can exceed the melt temperature at the values of the constant of the electron-phonon interaction $g \geq 440 \times g_k$, where $g_k = 3.12 \times 10^{12} \text{ Wt/cm}^3 \times K$, that is two order greater than in the linear model ($g \approx 1.5 \times g_k$). On the basis of the calculations one can explain qualitatively the experimental data about the presence of crater type structures on the HOPG surface exposed to ^{209}Bi ions or their absence in case of irradiation by ^{86}Kr ions. [I.V. Amirkhanov, A.Yu. Didyk, D.Z. Muzafarov, I.V. Puzynin, T.P. Puzynina, N.R. Sarkar, I. Sarhadov, Z.A. Sharipov: Temperature effect studies in frame of thermal spike model at highly-oriented pyrolytic graphite under irradiation by ^{86}Kr and ^{209}Bi heavy ions with high energy. Preprint JINR, P11-106-2007, subm. to "Surface".]

Within the thermal peak model in a three-dimensional case, calculated were temperatures in two-layer structures representing a massive substrate and quite a thin put layer from another material exposed to fast heavy ions with high ionizing energy losses. The temperature changes on the bounds of separation of such a two-layer structure on an example of Ni-W are investigated in detail depending on the size of the convective heat exchange coefficient Θ , characterizing the changing of a temperature gradient on the bounds of the separation, and consequently, determining also a thermal contact type. Calculations are performed both for a nonlinear case with thermo-physical temperature-dependent constants and for a linear case with temperature-independent thermo-physical constants. It has been found that, if taking into account the dependence of thermo-physical parameters on temperature, the calculated temperatures of electronic gas and crystal lattice are much less than in case of constants of the thermo-physical parameters taken at room temperature. A special feature of the nonlinear model is that the thermal processes in the crystal lattice are much slow than in the linear case. It is shown, that when increasing the coefficient Θ , transition from a case of non-ideal contact to ideal contact takes place. [I.V. Amirkhanov, A.Yu. Didyk, D.Z. Muzafarov, I.V. Puzynin, T.P. Puzynina, N.R. Sarkar, I. Sarhadov, Z.A. Sharipov: The use of nonlinear thermal spike model for calculations of temperature effects at two layer structures under their irradiation by high energy heavy ions. Preprint JINR, P11-105-2007, subm. to "Surface".]

The method of self-similar factor approximants is completed by defining the approximants of odd orders, constructed from the power series with the largest term of an odd power. It is shown that the method provides good approximations for transcendental functions. In some cases, just a few terms in a power series make it possible to reconstruct a transcendental function exactly. Numerical convergence of the factor approximants is checked for several exam-

ples. A special attention is paid to the possibility of extrapolating the behavior of functions, with arguments tending to infinity, from the related asymptotic series at small arguments. Applications of the method are thoroughly illustrated by the examples of several functions, nonlinear differential equations, and anharmonic models. [V.I. Yukalov, E.P. Yukalova: *Method of self-similar factor approximations. Phys. Lett. A* 368, 341-347 (2007).]

A system with Bose-Einstein condensate is considered in the frame of the self-consistent mean-field approximation, which is conserving, gapless, and applicable for arbitrary interaction strengths and temperatures. The main attention is paid to the thorough analysis of the condensate and superfluid fractions in a wide region of interaction strengths and for all temperatures between zero and the critical point T_c . The normal and anomalous averages are shown to be of the same order for almost all interactions and temperatures, except the close vicinity of T_c . However, even in the vicinity of the critical temperature, the anomalous average cannot be neglected, since only in the presence of the latter the phase transition at T_c becomes of second order, as it should be. Increasing temperature influences the condensate and superfluid fractions (fig.12) in a similar way, by diminishing them, but their behavior with respect to the interaction strength is very different.

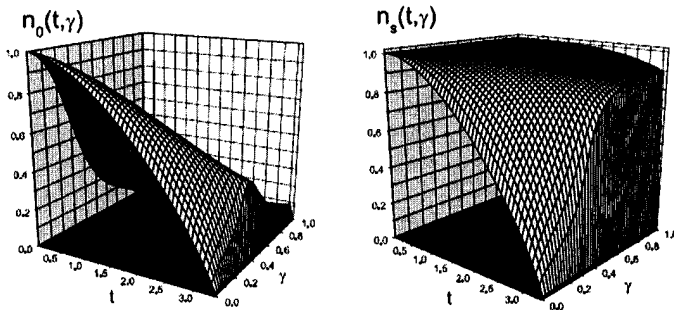


Fig.12: Condensate fraction $n_0=n_0(t,\gamma)$ (left) and superfluid fraction $n_s=n_s(t,\gamma)$ (right) as functions of the variables t and γ

For all temperatures, the superfluid fraction is larger than the condensate fraction. These coincide only at T_c or under zero interactions. For asymptotically strong interactions, the condensate is almost completely depleted, even at low temperatures, while the superfluid fraction can be close to one. [V.I. Yukalov, E.P. Yukalova: *Condensate and superfluid fractions for varying interactions and temperature Phys. Rev. A* 76 (2007) 013602-9.]

Bose-Einstein-condensed gases in external spatially random potentials are considered in the frame of a stochastic self-consistent mean-field approach. This method permits the treatment of the system properties for the whole range of the interaction strength, from zero to infinity, as well as for arbitrarily strong

disorder. Besides a condensate and superfluid density, a glassy number density due to a spatially inhomogeneous component of the condensate occurs. For very weak interactions and sufficiently strong disorder, the superfluid fraction can become smaller than the condensate fraction, while at relatively strong interactions, the superfluid fraction is larger than the condensate fraction for any strength of disorder. The condensate and superfluid fractions, and the glassy fraction always coexist, being together either nonzero or zero. In the presence of disorder, the condensate fraction becomes a nonmonotonic function of the interaction strength, displaying an antidepletion effect caused by the competition between the stabilizing role of the atomic interaction and the destabilizing role of the disorder. With increasing disorder, the condensate and superfluid fractions jump to zero at a critical value of the disorder parameter by a first-order phase transition. [V.I. Yukalov, E.P. Yukalova, K.V. Krutitsky, R. Graham: *Bose-Einstein-condensed gases in arbitrarily strong random potentials. Phys. Rev. A* 76, 053623-11 (2007).]

Computer algebra and applications

The methods on simulation of quantum computation in the framework of circuit model were further developed in the form of a Mathematica package [V.P. Gerdt, V.M. Severyanov: *A C# Package for Assembling Quantum Circuits and Generating Associated Polynomial Sets. Particles and Nuclei, Letters, Vol. 4, No.2, 2007, pp.225-230*; V.P. Gerdt, R. Kragler, A.N. Prokopenya: *On Simulation of Quantum Circuits with Mathematica. In: "Computer Algebra Systems in Teaching and Research / CASTR 2007", University of Podlasie, Scioldce, Poland, 2007, pp.135-144*]. The package has a user-friendly interface to input an arbitrary quantum circuit. It contains the built-in data base of one-, two- and three-qubit quantum gates that are widely used for implementation of quantum algorithms. Besides, the package exploits the linear algebra library of Mathematica to compute the unitary matrix determined by the input circuit. In addition, for a circuit constructed from the Toffoli and Hadamard gates and in accordance to the observation made, for such a circuit its unitary matrix can be computed by counting the number of common solutions of the multivariate polynomial equations associated with the circuit, the package explicitly constructs this polynomial system. After that it is possible to exploit the built-in Groebner basis module of Mathematica to count the number of solutions, and, thus, to find the circuit unitary matrix. [V.P. Gerdt, R. Kragler, A. Prokopenya: *A Mathematica Package for Construction of Circuit Matrices in Quantum Computation. Computer Algebra and Differential Equations, Acta Academiae Aboensis, Ser. B, Vol. 67, no. 2, 2007, pp.28-38*.]

Improvement of methods, algorithms and programs for solving topical problems of physics by using Groebner bases proposed [V.P. Gerdt, Yu.A. Blinkov: *On Selection of Nonmultiplicative Prolongations in Computation of Janet Bases. Programming and Computer Software, 33, № 3, 2007, pp.147-153*.]

New heuristically good selection strategies were discovered for nonmultiplicative prolongations that is important to speed-up computation of Groebner bases by involutive methods, and computational efficiency of the new strategies was investigated. Due to their implementation into the specialized computer algebra system GINV this system became the fastest open source software in the world with respect to speed of computation of Groebner bases. [V.P. Gerdt, Yu.A. Blinkov: *On selection of nonmultiplicative prolongations in computation of Janet bases. Programming and Computer Software*, 33, № 3, 2007, pp.147-15.]

Some important algorithmization issues for the Dirac constraint formalism for degenerate dynamical systems with polynomial Lagrangians were studied. As an important application, the full set of constraints was obtained and their classification in the first and second classes was done for the SU(3) Yang-Mills light-cone mechanics. [V.P. Gerdt, A.M. Khvedelidze, Yu.G. Palii: *Deducing the constraints in the light-cone SU(3) Yang-Mills mechanics via Gröbner bases. "Computer Algebra in Scientific Computing / CASC 2007"*, LNCS 4770, Springer-Verlag, Berlin, 2007, pp. 145-159.]

Discrete dynamical systems and mesoscopic lattice models have been studied from the standpoint of their symmetry groups. Universal specific features of behavior of deterministic dynamic system associated with nontrivial symmetries of these systems were specified. Group nature of soliton-like moving structures analogous to the "spaceships" in cellular automata was revealed. Study of lattice models is also considerably simplified when their symmetry groups are taken into account. A program in C for group analysis of systems of both types has been developed. The program, in particular, constructs and investigates phase portraits of discrete dynamic systems modulo symmetry group and seeks dynamical systems possessing special features, such as, for example, reversibility. For mesoscopic lattice models, the program computes microcanonical distributions and looks for phase transitions. [V.V. Kornyak: *Discrete Symmetries and Dynamics of Cellular Automata. In: "Computer Algebra Systems in Teaching and Research / CASTR 2007"*, University of Podlasie, Scieldce, Poland, 2007, pp.192-201; V.V. Kornyak: *Symmetries and Dynamics of Discrete Systems. "Computer Algebra in Scientific Computing / CASC 2007"*, LNCS 4770, Springer-Verlag, Berlin, 2007, pp. 236—251; V.V. Kornyak: *Symmetric Cellular Automata. Programming and Computer Software*, Vol. 33, No. 2, 2007, pp. 87–93; V.V. Kornyak: *Symmetry Analysis of Discrete Dynamical Systems. Computer Algebra and Differential Equations, Acta Academiae Aboensis, Ser. B, Vol. 67, no. 2, 2007, pp.155-167.]*

An analytical numeric algorithm has been developed for computing coefficients of discrete two-dimensional elliptic equation on the given eigenvalues and some symmetry conditions for basic eigen-functions. [S.I. Serdyukova: *Journal of Computing Mathematics and Mathematical Physics*, No.2 (2007).]

Отпечатано методом прямого репродуцирования
с подготовленного лабораторией оригинала.

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