# LABORATORY OF INFORMATION TECHNOLOGIES

The investigations performed at the Laboratory of Information Technologies in 2011 in frames of the JINR field of research «Networks, Computing, and Computational Physics» were focused on two first priority themes, namely, «Information, Computer and Network Support of the JINR's Activity» and «Mathematical Support of Experimental and Theoretical Studies Conducted by JINR». The cooperation with other JINR laboratories involved the participation of the LIT staff in research work within 24 themes of the Topical Plan for JINR research and international cooperation.

At the end of 2011, the computing power of the JINR Central Information Computer Centre (CICC) was doubled in respect to 2010, reaching 5000 kSI2K, the capacity of the data-storage system added 500 TB, reaching 1500 TB at present. The very high value of the productivity vs. resources ratio secured to the CICC JINR grid-site an overall yearly CPU time throughput which places it in the first ten among the more than 160 Tier2 existing sites of the WLCG (Worldwide LHC Computing Grid) infrastructure. The CICC JINR share within the Russian Data Intensive Grid (RDIG) consortium comprising besides JINR other 16 resource centres in institutes from Russia and JINR Member States is lasting $\sim 40\%$. More than 5.3 million jobs were solved at CICC JINR during the whole year 2011.

## NETWORKING, COMPUTING, INFORMATION SUPPORT OF JINR ACTIVITY

During 2011, an important work, directed to the reliable operation and development of the JINR networking and informational infrastructure, was done. The key components of this infrastructure are the telecommunication data links, the JINR local area network, the CICC and the primary software joining information resources of the Institute in a unified environment accessible to all users, the grid-technology environment included.

**JINR Telecommunication Data Links.** In 2011, the reliable work of the high-speed computer communication channel Dubna–Moscow was secured. The connection with scientific networks and Internet used the following telecommunion links: with CERN — 10 Gbps, RBnet — 10 Gbps, GEANT — $2 \cdot 10$ Gbps, Moscow scientific networks — 10 Gbps, RASnet — 10 Gbps, RadioMSU — 10 Gbps, GLORIAD — 1 Gbps, E-arena — 10 Gbps.

Table 1 provides the throughputs of the incoming and outgoing traffic of the most resources consuming (more than 1TB incoming traffic) JINR subdivisions. In 2011 the overall incoming JINR traffic, including the general access servers and CICC, amounted 1525.35 TB (1339.02 TB in 2010). The weights of the various incoming traffic categories are shown in Table 2.

**Table 1**

| Subdivision | Incoming, TB | Outgoing, TB |
|---|---|---|
| LIT | 63.07 | 55.66 |
| DLNP | 51.7 | 76.42 |
| VBLHEP | 48.8 | 89.35 |
| FLNP | 29.91 | 89.12 |
| VPN | 18.51 | 5.95 |
| BLTP | 16.73 | 12.07 |
| Adm | 10.82 | 13.57 |
| FLNR | 7.13 | 1.25 |
| LRB | 5.85 | 1.5 |
| SCAR | 4.43 | 1.27 |
| GRK | 3.6 | 0.6 |
| Uni-Dubna | 3.47 | 5.19 |
| Educational Grid network | 2.47 | 6.62 |

**JINR Local Area Network.** A systematic activity was carried out in LIT with the aim to achieve steady improvement and fault-tolerant operation of the core of the telecommunication structure of the JINR Local Area Network (LAN) as well as substantial increase of the information flows and of the security level. In 2011, the work on the switch off of the JINR Backbone to a 10 Gbps data transfer rate was brought to an end. Figure 1 gives a schematic view of connecting the Institute Laboratories to the JINR Backbone.

**Table 2**

| Scientific & educational networks | File exchange (torrent, ftp) | Web-resources | Social net | Software | Multimedia | Dubna net |
|---|---|---|---|---|---|---|
| 89.46% | 8.07% | 1.66% | 0.5% | 0.11% | 0.17% | 0.04% |

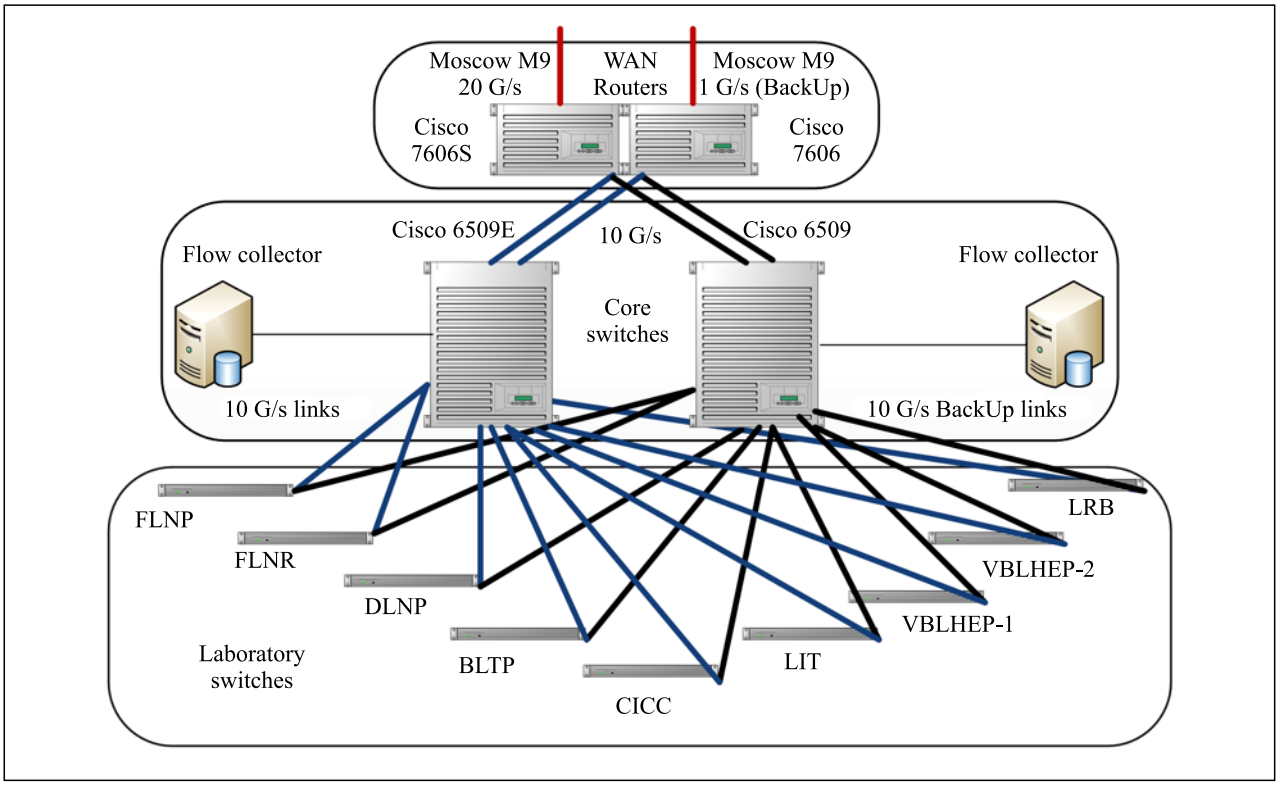


Fig. 1. Scheme of connecting the JINR subdivisions to the backbone

The JINR LAN includes 7119 network elements and 8611 IP-addresses. In 2011, 3563 users were registered within the network, more than 1500 users of the mail.jinr.ru service, 995 users of electronic libraries, and about 1300 remote VPN users.

The LIT specialists continued the modernization and development of the systems for monitoring the JINR LAN infrastructure and authorization, as principal means for provision of reliable and secure functioning of the whole JINR informational–computational environment. The results of the monitoring are displayed on the web-interface NMIS (Network Management Information System), which was adapted for use in the JINR networking environment. By means of NMIS there are realized the permanent monitoring of the state of the JINR network environment, influences of the state of the basic elements of the network (routers and switches), the status and the use of the critical elements of the network. The authorization system is an important component of the safety system. The authorization and the account are organized at JINR on the basis of the IPDB database of the JINR network nodes which is used for unfolding a complex local area network through a web-interface. This system is used for the registration and the authorization of the network elements and users, the visualization of statistics of the network traffic flow, as well as for the support of the remote user database, the electronic library user database, etc.

**JINR Central Information and Computing Complex.** The CICC is organized as a unified informational–computational resource, grounded on the distributed model of data storage and processing and intended for servicing all the spectrum of the JINR activity. In 2011, the growth of the performance and data storage of the CICC significantly advanced. At present, the CICC computing farm comprises 2064 64-bit central processors and a data storage system with the total capacity of 1500 TB. The central router of the CICC network is connected to the main interface router of the JINR network at a rate of 10 Gb Ethernet. In order to ensure a high transfer rate inside the local CICC network and minimal access time to the files and the data, the aggregation of several 1 Gb Ethernet connections into a single virtual channel (trunk) was performed, increasing in this way the transfer rate to a level staying in-bet-

ween 4 and 8 Gb Ethernet. A new CICC climate control system was put into operation to provide the uninterrupted functioning of the hardware components of the complex.

The computing units and the data storage systems are managed by the primary software services that enable the use of the CICC resources both by international projects for distributed computations (WLCG, FUSION, BIOMED, HONE, PANDA, CBM, etc.) and by local JINR users.

The OS Linux (Scientific Linux release — SL5 with x86_64 architecture) is the main CICC operating system. This OS is the basic one in the projects WLCG and EMI (European Middleware Initiative).

The following compilers have been installed at CICC: g77/gcc/g++ — GNU Fortran 77, C and C++ compilers version 3.4.6; gfortran/gcc4/g++4 — GNU Fortran 95, C and C++ compilers version 4.1.2; ifort/icc/icpc — Intel Fortran, C, C++ compilers version 11.1; GCC (GNU Compiler Collection) — a set of freely distributed compilers for various programming languages (C/C++/Fortran, etc.). The Intel compilers were supplied with effective tools for the development of a parallel code supporting the OpenMP standard. To design computer programs with the use of the MPI (Message Passing Interface) package, the MPI libraries have been installed for the programming languages C, C++ and Fortran.

Figure 2 gives the general scheme of the principal CICC elements and their interaction for organizing the work of both the local users and the international collaborations; there are shown the services providing access to the CICC resources from the global network in frames of the international projects. Five machines (Int/UI) provide the interactive access of the JINR users directly to the CICC computing resources and disk storages. From these machines access is possible to all the distributed resources of the WLCG project with the help of the installed user interface of the Grid middleware gLite. The batch server and the WN (Work Node) machines provide the batch processing of numerical jobs: 1) from machines Int/UI lunched by local users, 2) received from the global WLCG system through machines [CREAM] CE (Computing Element). The WMS (Workload Management System) and LB (Logging&Bookkeeping) machines are utilized to assign the jobs (of the local users and WLCG) to various sites of the WLCG project. The WMS machines get the jobs directly from the users submitted from various UIs. The service X509 PX (ProXy) stores and updates the users' certificates (X509 format) for the resource and user task protection in the grid-systems. This is the

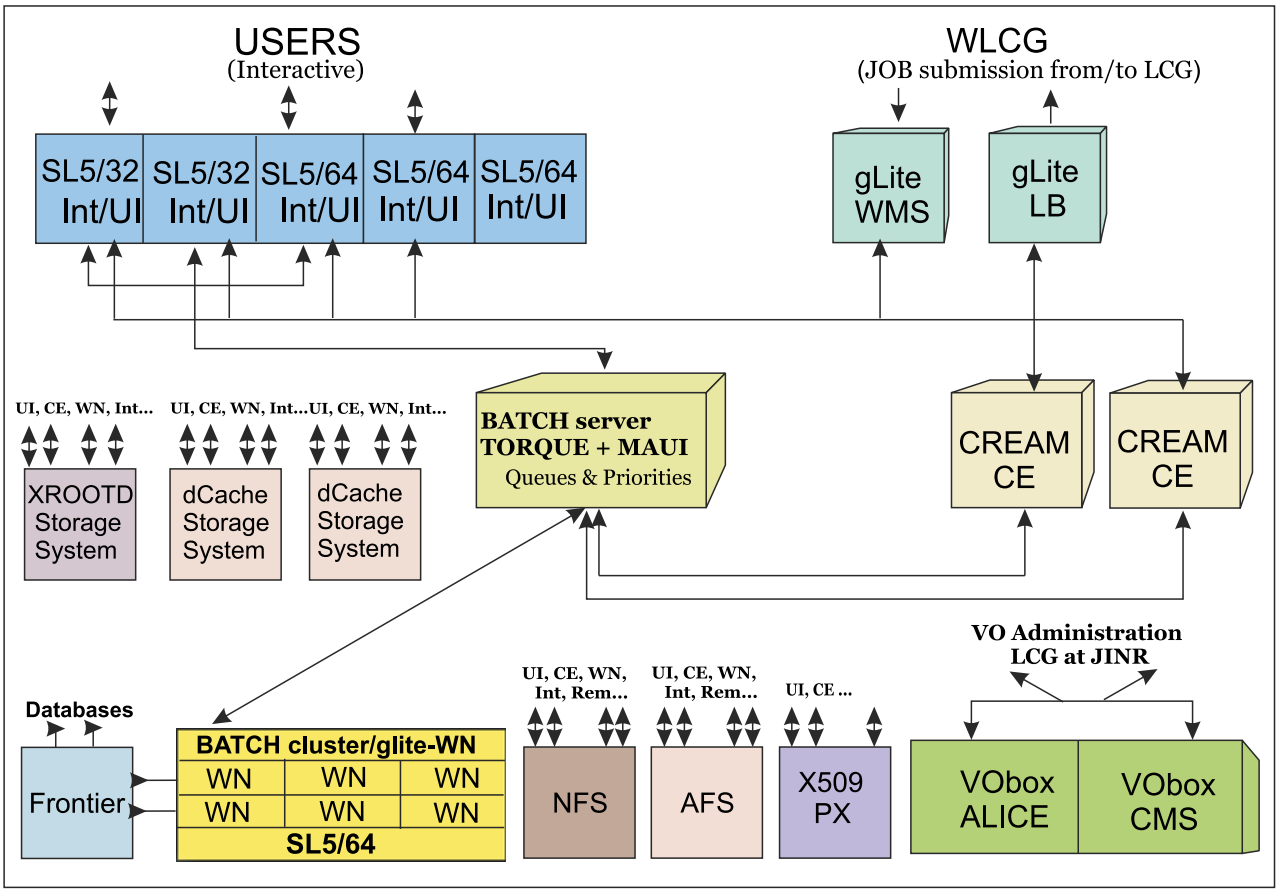


Fig. 2. A general scheme of the JINR CICC main components and their interoperation

main method of monitoring the registered users within the WLCG project. The Frontier machine provides the cache access service to remote data from WN. In particular, it maintains the distributed file system CVMFS (CernVM File System) which provides the access (under the https protocol) to the software of the collaborations ATLAS, LHCb, and BES which is installed and stored on servers at CERN. Two VOboxes (Virtual Organization box) are used by the collaborations ALICE and CMS to perform their work on the WLCG site. The storage and access systems dCache and XROOTD secure the work with data both for the local JINR users and for the users and the collaborations (virtual organizations) within WLCG.

Several servers support the work of the users and services of JINR: batch, WWW, DB MySQL and Oracle, e-mail, DNS, Nagios monitoring, etc. The mentioned servers mainly operate on 64-bit hardware platforms Xeon and Opteron.

The hard- and software complex dCache manages the storage and manipulation of large volumes of data in CICC. Two dCache installations are maintained: dCache-1 — for the CMS and ATLAS experiments, and dCache-2 — for local users, groups of users and the international projects NICA/MPD, HONE, FUSION, BIOMED, and COMPASS. These dCache installations manage 9 servers of the main interfaces of the dCache system and 40 data storage systems (Pool). Several CICC user groups make use of the system XROOTD of remote access to information. All the storage systems are built up with the help of a RAID6 hardware mechanism.

The CICC comprises several special-purpose machines for the support of local users and international collaborations — the projects NICA/MPD, PANDA-GRID, and CBM. These machines are set for the dedicated software of the mentioned collaborations and for running jobs through batch processing. These machines also support the NFS-service for the dedicated software for WN.

**Table 3**

| Laboratory/ Group | Number of jobs | CPU time, kSi2K · h | Astronomical time kSi2K · h |
|---|---|---|---|
| MPD | 44345 | 102850.88 | 108541.71 |
| PANDA | 19662 | 57679.36 | 74545.53 |
| VBLHEP | 12615 | 19982.22 | 26392.33 |
| DLNP | 9126 | 308877.99 | 141539.47 |
| COMPASS | 6957 | 29034.42 | 30310.09 |
| LIT | 1712 | 1383856.71 | 99700.55 |
| BLTP | 1041 | 196524.91 | 197218.56 |
| FLNP | 800 | 118544.73 | 105121.83 |
| LRB | 53 | 16696.36 | 4190.24 |

Table 3 shows the distribution of the batch tasks in 2011 (more than 50) over the Institute subdivisions and user groups, except for the tasks within the grid-projects. The total number of jobs increased more than five times as compared to the 2010 year.

**JINR Grid-Environment.** JINR actively participates in the large-scale global grid-projects: «Worldwide LHC Computing Grid» (WLCG project, http://lcg.web.cern.ch/LCG/) and «European Grid-infrastructure» (EGI-InSPIRE — Integrated Sustainable Pan-European Infrastructure for Researchers in Europe, http://www.egi.eu/projects/egi-inspire/).

In order to maintain the WLCG site in JINR (the JINR-LCG2 site) and other international collaborations, 22 servers under the gLite system (WLCG middleware) have been installed. Besides supporting the operation of the site JINR-LCG2 itself, part of the servers provide important services and functions for the support of the Russian segment of the WLCG project. At present, the share of the CICC computing resources with respect to the whole Russian WLCG community is in the range of 40–50% and a little bit less as concerns the data storage tools. In view of its reliability and availability, the JINR site is one of the most effective Tier2 sites in the world. The participation in these projects includes the support and development of the JINR grid-infrastructure in accordance with the requirements of the LHC experiments, the participation in WLCG middleware testing and evaluation, the development of grid-monitoring tools, the development of a database of the simulated physical events, the user training, the support of the JINR Member States in their WLCG activity, etc. The LIT specialists continue participating in the check-up and estimation of the middleware of the WLCG project (gLite MPI, gLite 3.2, EMI, UMD, etc.).

**Table 4**

| VO | CPU time, (kSi2K · h) | Jobs |
|---|---|---|
| ATLAS | 9.713.186 | 3.025.294 |
| ALICE | 5.804.598 | 943.830 |
| CMS | 5.389.518 | 1.059.918 |
| LHCb | 2.993.831 | 156.445 |
| Fusion | 53.443 | 11.858 |
| BioMed | 61.189 | 17.504 |
| HONE | 105.897 | 22.614 |
| ops | 398 | 50.709 |
| dteam | 0 | 399 |
| bes | 0 | 68 |
| rgstest | 0 | 68 |
| Total | **24.122.060** | **5.288.707** |

In 2011, a large amount of work was done on data receipt and processing for the experiments ALICE, ATLAS, and CMS at JINR. Table 4 presents the results of using the JINR CICC grid-infrastructure by the virtual organizations (VO) within RDIG/WLCG/EGI in 2011.

Presently, the JINR grid site is the best among the RDIG sites. Our 2011 contribution to the job processing for RDIG and for the experiments ALICE, ATLAS, and CMS is presented on the diagrams of Fig. 3.

The activity started in 2010 in cooperation with CERN was continued on the design of one of the central services the ATLAS (DQ2) — the Deletion experiment

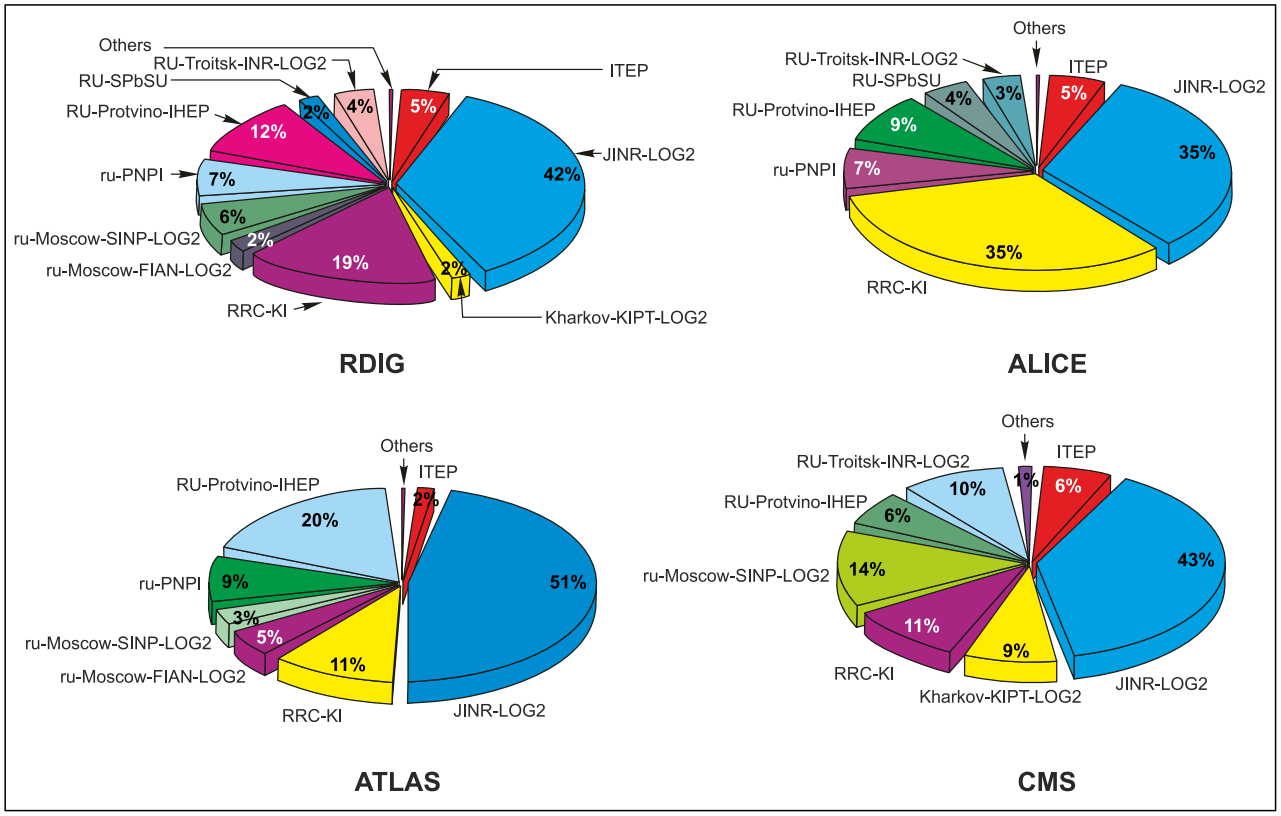


Fig. 3. Contribution of the JINR CICC Grid site (JINR-LCG2) to the job processing of RDIG and of experiments ALICE, ATLAS, and CMS in 2011

Service, of the data management system for which is intended for centralized deletion of data of the ATLAS experiment on the Tier0, Tier1, and Tier2 sites. The design and maintenance of this service, which is responsible for the replication, access and accounting of the data of the experiment in more than 100 distributed Grid-sites, have become one of the important contributions of the LIT team to the ATLAS experiment.

There is ongoing work on the design and implementation of a monitoring system of the Tier3 sites of the ATLAS experiment, which have already been established or are in train of being planned in several institutes and organizations within the ATLAS Collaboration. These sites consist of various resources, are intended for the data analysis by local scientific groups, and are not always supplied with a grid middleware. The LIT participates in the T3mon project directed at the design and implementation of a software suit for monitoring the Tier3 sites both from the point of view of the local site administrator and from the point of view of the administrator of the whole ATLAS VO, thus providing a global scrutiny of the contribution of the Tier3 sites to the computing process. For this purpose, a virtual test infrastructure has been designed and implemented at JINR which allows the simulation of various Tier3 clusters and solutions for data storage. These issues were of particular interest at the official ATLAS Computing Technical Interchange Meeting that was held in Dubna in May, 2011.

An important component of the participation in the processing and analysis of the data obtained from the LHC experiments is the creation at JINR of a real time remote access system (SRART) and its integration into the global service-oriented grid architecture of data acquisition and processing within the LHC experiments. The design and start-up of the system of the real time remote access to monitoring the data gathering and processing in the ATLAS Control Room is a result of the long-term JINR–CERN cooperation under the TDAQ ATLAS project. The service-oriented architecture of the composite service integrates the main services of the SRART infrastructure (online-services TDAQ Software and Grid-services) thus providing the remote user with an effective tool for further processing and analysis of the quality of the data received within the ATLAS experiment.

JINR participates, in cooperation with nine resource centres in different regions of Russia, in the project GridNNN (Grid National Nanotechnological Network) which is carried out within the federal target programme «Development of a Nanoindustry Infrastructure in the Russian Federation». In frames of this project the JINR specialists have solved tasks concerning the monitoring and accounting, support of the registration system of grid-services and sites, support of the virtual organizations. Significant efforts were also undertaken for the design of web-interfaces and the adaptation of the applied problem-oriented packages to facilitate their

use in the grid-environment. A JINR team has developed problem-oriented interfaces for three applications: DL_POLY (a parallel version of the multipurpose software package for computations in the field of molecular dynamics), Elmer (a fully functional mathematical package for the mathematical simulation of physical processes and structure calculation by the finite element method), and GEANT4-DNA (extension of the GEANT4 package to the simulation of the biological damages induced by the ionizing radiation at the cellular and subcellular scale).

Of great importance for the development of both the JINR informational–computational infrastructure as a whole and its grid-segment is the collaboration with the NRC «Kurchatov Institute» on the design, in 2011–2013, of an automated system for the LHC data processing at the Tier1 level and provision of the grid-services for distributed data analysis. The work is carried out within the federal programme «Research and Development on the Priority Directions of the Scientific–Technological Complex Development in Russia for 2007–2013».

In 2011, LIT started (in collaboration with VBLHEP) the design of a model of grid computing for the NICA project. Together with other Russian organizations, LIT participates in the development of the Russian national grid-network.

**Information and Software Support.** The information, software and algorithmic support of the research-and-production activity of JINR is a traditional direction of research performed at LIT. In particular, it includes the development and support of the informational WWW/FTP/DBMS servers of JINR and LIT, the creation and storage of electronic documents related to the scientific and administrative activities of the Institute. The administrative databases are maintained and upgraded on a regular basis in cooperation with STD AMS of JINR.

In 2011, work was conducted on the design and support of various information sites, such as sites of conferences, workshops, symposia organized by JINR Laboratories (upon request). For instance, web-portals were created for the FLNP International Seminar on Interaction of Neutrons with Nuclei (ISINN) http://isinn.jinr.ru and the FLNP International Meeting «Stress and Texture Investigation by Means of Neutron Diffraction» http://sti2011.jinr.ru/, the FLNR 4th International Conference on Physics and Chemistry of the Transactinide Elements (TAN'2011) http://tan11.jinr.ru/, the FLNR 6th International Symposium on Exotic Nuclei (EXON-2012) http://exon2012.jinr.ru/, etc. The modernization and upgrade of the websites of the weekly newspaper «Dubna: Science, Community, Progress» and of the JINR Museum of the history of science and technology were performed on a new technological ground. The information system of electronic document circulation DoctorDoc, developed at LIT for the internal paperless document circulation, has been upgraded and its opportunities have been expanded (http://lit.jinr.ru/DD/) [1].

The open access JINR Document Server (JDS) (http://jds.jinr.ru/) electronic archive-repository has been developed at JINR in frames of the international programme Open Access Initiative (OAI). One of the purposes of the repository is to put together on a single site all the publications of the JINR staff [2].

Another traditional direction of LIT activity is the development and the support of the program library JINRLIB as well as support of program libraries (CERNLIB, CPC Program Library) developed by other research centres and organizations. New additions to the JINRLIB in 2011 are the new versions of the software programs SAS, FITTER, RC, Gluplot, together with new computer programs: Clebsch2 — parallelization of the calculation of the simplest form Clebsch–Gordan coefficients; GridCom — Grid Commander: a graphic interface for work with tasks and data in the grid-environment; TPIKL — a program for the numerical solution of a linear system of equations of the thermal spike model by the method of alternating directions; BIBasis – a package for computing Boolean involutive and Grцbner bases within the REDUCE and Macaulay2 computer algebra systems; ASYMPT — a program for calculating asymptotics of hyperspherical potential curves and adiabatic potentials; LINA01 and GITA — REDUCE programms for the normalization of polynomial Hamiltonians; KANTBP — a package for the solution of two-dimensional discrete and continuum spectra boundary-value problems within the Kantorovich (adiabatic) approach.

In 2011, work was underway on the adaptation of the EVM system (Earned Value Management) designed at CERN with the purpose of evaluating the expenses and monitoring the activities on the implementation of the JINR projects.

## MATHEMATICAL SUPPORT OF EXPERIMENTAL AND THEORETICAL STUDIES

The main objective of this research field at LIT is to provide the mathematical, algorithmic and software support of the experimental and theoretical research underway at JINR. In 2011 the obtained results were reported in more than 250 papers, 135 works being published in referred journals. Two monographs were published.

More than 70 reports were presented at international conferences. Below there is a brief report about a few of the obtained results.

The development of fast algorithms for event reconstruction is of special importance for the CBM (Compressed Baryonic Matter) experiment (GSI, Darmstadt). In cooperation with colleagues from GSI, parallel algorithms of particle identification with the help of Cherenkov detector (RICH), transition radiation detector (TRD), and muon system (MUCH) have been developed. The realized software using opportunities of the modern processors as vector data processing (SIMD) and multithreading allows one to increase considerably the recognition rate [3].

An important work has been done by researchers in LIT and VBLHEP on the analysis of elastic and inelastic scattering of antiprotons by protons and nuclei. In particular, an exhaustive analysis of the existing experimental data on the absorption cross sections of the antiproton by nuclei was performed. It is shown [4] that they are well reproduced within the Glauber approximation. A software package for the calculation of the cross sections and the simulation of the elastic scattering of the antiprotons and antinuclei scattering on protons and nuclei has been developed and was subsequently included in the Geant4 simulation toolkit. The differential cross sections of the elastic antiproton–nucleus and antinucleus–nucleus scattered are well described by a strong absorption model. It is shown that the model is also applicable to antiproton-proton scattering data [5] as well as to proton–proton data. Moreover, it resulted in an excellent description of the Totem Collaboration data (Fig. 4) recently obtained at the Large Hadron Collider (CERN, Geneva) [6].

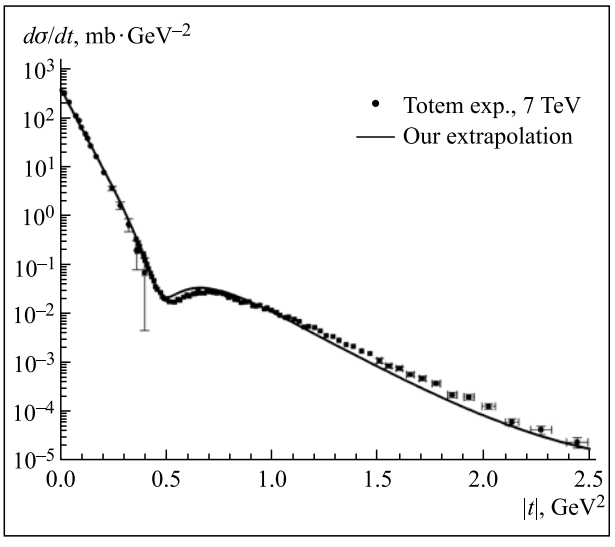


Fig. 4. Differential cross section of $pp$ elastic scattering (points) obtained by Totem experiment at 7 TeV, and computations (line) presented in [6]

Further implementations were performed on the system HepWeb (http://hepweb.jinr.ru) which allows a user to perform the most popular calculations in high energy physics: the calculations of hadron–hadron, hadron–nucleus and nucleus–nucleus interaction cross sections as well as calculations of the secondary particle characteristics in the above-mentioned interactions by use of Monte Carlo event generators. The List of the generators includes the Dubna version of the intranuclear cascade model CASCADE, the FRITIOF model, the ultrarelativistic quantum molecular dynamic model UrQMD, the HIJING model, and the AMPT model. The inputs to colliding particle properties (the collision energy, the mass numbers and charges of the nuclei, the impact parameters of the interactions, and the number of generated events) are introduced via a WEB interface. A query is processed by a server, and results are presented to the user as a WEB-page [7].

The Hamiltonian reduction of the Yang–Mills theory with the structure group $SU(2)$ to a nonlocal model of self-interacting $3\times3$ positive semidefinite matrix field is presented. Analysis of the field transformation properties under the Poincare group action is given. It is shown that in the limit of a strong coupling the classical dynamics of the reduced system can be described within the local theory of interacting nonrelativistic spin-0 and spin-2 fields. A perturbation theory in powers of the inverse coupling constant $g^{-2/3}$, which allows one to calculate corrections to the leading long-wave approximation, is suggested [8].

New types of equations for Feynman integrals are found. It is shown that Feynman integrals satisfy functional equations connecting integrals with different kinematics. A regular method is proposed for obtaining such equations. The derivation of functional equations for one-loop two-, three- and four-point functions with arbitrary masses and external momenta is given. It is shown that the functional equations can be used for the analytic continuation of Feynman integrals to different kinematic domains [9].

The $^6\mathrm{He} + {}^{12}\mathrm{C}$ elastic scattering data at three beam energies $E = 3$, 38.3, and 41.6 MeV/nucleon are analyzed using a microscopic optical potential (OP) model. In this approach two or three parameters are fitted, renormalizing the depth of the real, imaginary and surface parts of the computed OP. In this case there is still an ambiguity in the obtained set of fitting parameters which, however, can be narrowed by introducing an additional selection criterion — the dependence of the OP volume integrals upon energy. The structure of the obtained OP, the role of the nuclear matter in the formation of the OP imaginary part as well as a relationship of the surface potential and the breakdown channels $^6$He are discussed [10].

A computational program for the quantum-chemical cluster calculations of the local electronic structure of systems with strong electron correlations was developed and applied to several 3D-metal oxides. The computational strategy employed relies upon the cluster-in-solid embedding technique with the use of the quantum-

chemical MOLPRO package together with the CRYSTAL program combined into a unique code with the CRYSTAL-MOLPRO interface developed by authors at the first stage of the project. The calculated electronic structure has been directly compared with experimental data obtained by resonant inelastic X-ray scattering (RIXS) measurements. The computational scheme and the presented results point to a promising route to the modeling and reliable interpretation of the RIXS spectra as well as to a quantitative description for the intrinsic electronic properties of strongly correlated 3D-metal oxides [11].

The LAP LAMBERT Publishing House released a book «Spinor Field in the Evolution of the Universe. Spinor Field as a Source of Isotropization and Accelerated Expansion of the Universe» [12] which contains a theoretical study of the evolution of the Universe at different stages within the scope of an integrated approach based on anisotropic cosmological model, defined by different sources of gravitation fields. Nonlinear spinor fields, viscous fluid, Van der Waals gas, and dark energy as a source of the gravitational field have been considered. In this study for the first time the characteristics of matter, influencing the evolution of the Universe, are modeled by means of nonlinear spinor fields.

The progress obtained within the Bayesian approach to the computation of Riemann integrals by automatic adaptive quadrature was reviewed in [13]. The construction of both the binary tree and the priority queue controlling its advancement has been shown to be dramatically changed by the conditioning diagnostics derived inside close proximity neighbourhoods of the tentative discretization abscissas of the integration domain into subranges.

To study discrete dynamical systems of different types — deterministic, statistical, and quantum — various approaches were developed. The concept of a system of discrete relations on an abstract simplicial complex was formulated, and algorithms were developed for the analysis of the compatibility and the construction of canonical decompositions of such systems. The developed algorithms and programs exploiting discrete symmetries were used to study microcanonical ensembles and to search for phase transitions in mesoscopic lattice models. An approach was proposed to the quantization of the discrete systems based on the introduction of gauge connectivity with values in unitary representations of some finite groups — the elements of the connectivity are interpreted as amplitudes of quantum transitions. Tools of the computer algebra and computational group theory methods were used to perform this study [14].

In order to provide the theoretical description of the double ionization of two simple diatomic molecules, $H_2$ and $N_2$, for which experiments are currently performed, it has been defined the correlation wave function of the continuous spectrum of the two ejected electrons from the diatomic molecule. It was shown that the taking into account of the correlation significantly changes the final output and results in good agreement with the experimental cross sections (Fig. 5). New computational approaches have been proposed with the aim to decrease the computing time and to improve the precision of the computations [15].

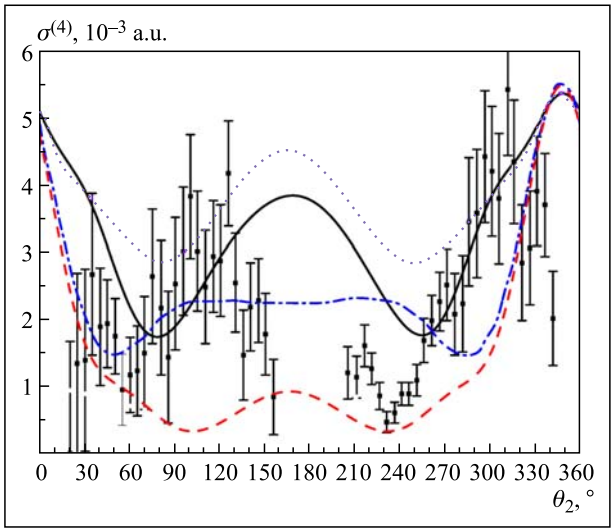


Fig. 5. Quadruple differential cross section of ionization $H_2$ as a function of corner $\theta_2$ of emitted electron. Solid line is the given work. Experimental results are scaled in the field of a maximum of binary peak (about 300°). Dotted line is the result without taking into account electronic correlations; dashed line is the result with using extended spheroidal coordinates and complex scaling; dash-dotted line is the result with using the first Born approximation and a 3C model (are normalized to a solid line in 345°)

The solution of the undamped nonlinear Schrödinger equation driven by a periodic external force was investigated. A diagram of stability and bifurcations of the moving solitons on the plane of parameters of the rate and damping power has been built (Fig. 6). It is shown that at definite rates the moving waves can produce stable two-soliton structures [16].

The evolution of the polarons in a homogeneous medium was investigated in terms of the parameters of the model and the initial conditions chosen as combinations of stationary polaron states. The computational scheme and the results of the numerical modeling are presented [17].

A software package for the study and visualization of a wide class of protein complexes at various levels (atoms, bases, chains, relief) has been designed at LIT in cooperation with researchers of ITEB RAS, ICB RAS, and IPR RAS (Puschino). For the first time it provides a way to investigate the molecular surfaces of quite a complex shape with utmost precision in frames of a full-functional mapping complex. This package comprises programs with a graphic interface as well as console programs for large scale computation of the maps in a distributed computing environment. The ob-

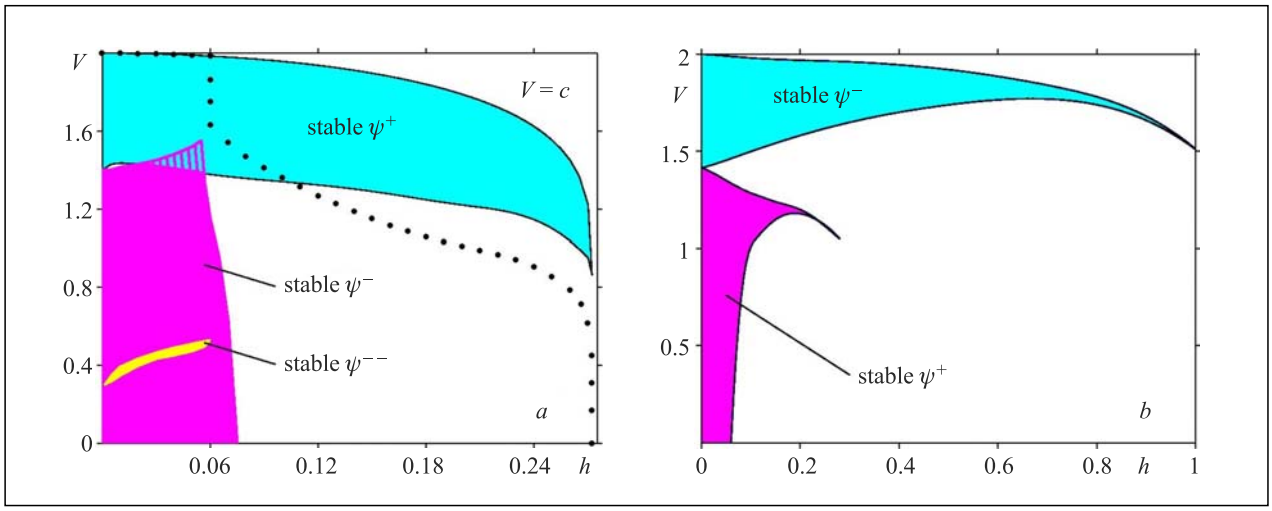


Fig. 6. (*a*) Diagram of existence and stability of travelling solitons in the externally driven, damped nonlinear Schrödinger equation on the plane of parameters of velocity $V$ and pumping $h$. Solid curve $V = c$ and dotted curve correspond to the top border of existing two types of one-soliton solutions: $\psi^-$ and $\psi^+$. The stability regions of these two types of travelling waves are shown by different shades of grey. The two domains overlap over a bistability region (shaded with parallel lines). The light inclusion in the dark grey domain represents the area where both the $\psi^-$ soliton and the $\psi^{(--)}$ bound state are stable. (*b*) The same attractor chart for parametrically driven damped nonlinear Schrödinger equation

tained results, developed algorithms, methods and codes as well as their implementation in the distributed computing environment can be used for designing proteins and peptides, purposefully modifying the expression of damaged genes, as a basis of effective gene therapy [18].

It is shown that the recognition of DNA by the recognizing $\alpha$-helix of protein is governed by two groups of contact. The invariant protein-DNA group of contacts includes six contacts, formed by the atomic groups of the coding and noncoding DNA chains with the groups of amino acids. The recognizing $\alpha$-helix forms contacts with the polar groups of residues Trp2 (NE1), Asn5, and Lys9 with the canonical sequence $T_1A_2A_3T_4$ of the coding DNA chain, and contacts with the residues Lys0, Arg7 and Lys11 with the sequence $A_4X_5X_6X_7$ from the noncoding DNA chain, where X is any nucleotide. A variable protein-DNA group of contacts comprises two groups bound with the sequence $T_3A_4X_5X_6$ of the noncoding DNA-chain. These contacts are mainly formed with the bases and they define the binding pattern of each individual homeodomain. The invariant contact group represents a recognition pattern for transcription factors of the homeodomain family: a few adenine-asparagine contacts and six position-specific phosphate contacts mainly with lysine or arginine. Within this group, three most significant invariant contacts have been found which allow the inference of recognition rules for the homeodomains. These rules are the same within the different taxonomic groups of the homeodomain family and they can distinguish the members of this family from any other family of transcription factors [19].

A new approach to the clustering of large amounts of data was developed in the course of research into clustering geographic and graphical data. The algorithm is based on the so-called neural gas, i.e., such a self-propagating generalization of the artificial neural network which allows one to separate the feature space into polyhedrons, the algorithm speed being independent on the volume of the data. The research provides a brief theoretical description of this clustering algorithm as well as recommendations for choosing suitable neural-net methods. Simulated and air-photography data are used to exemplify the approach to applications [20].

## INTERNATIONAL COOPERATION

The research work at the Laboratory is carried out in close cooperation with scientists and specialists of the JINR Member States as well as a number of research centers of other countries. Some examples of such cooperation should be particularly stressed.

For the purpose of training users and system administrators for work in the grid-environment, the educational infrastructure at LIT (http://gridedu.jinr.ru) is vigorously developed. In 2011, a new grid-site of the Euroasian National University (Astana, Republic of Kazakhstan) was included in this distributed infrastructure, and at present this system comprises 7 grid-sites in the JINR-participating countries and three sites located at JINR. The cooperation on the grid-infrastructure de-

velopment in the JINR Member States is progressing. In 2011, the first successful steps in this direction were taken at the Institute of Informatics of the Mongolian Academy of Sciences: with the active assistance of LIT an educational grid-site was launched which will become part of the education&research grid-infrastructure of the JINR-Member States. In frames of training users and system administrators for the JINR Member States, tutorials were organized in 2011 for the employees of the Institute of Theoretical Physics (ITP, Kiev, Ukraine) and the National Technical University of the Ukraine «Kiev Polytechnic Institute» (KPI, Kiev, Ukraine) as well as for the system administrators from Azerbaijan, Kazakhstan, and Mongolia.

Research on the statistical properties of classical spin-glasses and simulations of «spin-glass» systems are performed at LIT in collaboration with Armenian scientists (IIAP NAS and IM NAS of Armenia). The statistical properties of the classic 3D spin-glass layer of a certain width and of infinite length have been studied. The 3D spin glass is represented as an ensemble of disordered 1D spatial spin chains (SSC) where the spin chains randomly interact among themselves (nonideal ensemble of 1D SSCs). It has been proved that the 3D spin glasses can be generated by the Hamiltonian of a disordered 1D SSC with random environment at the limit of Birkhoff ergodic hypothesis performance. The disordered 1D SSC is defined on a regular lattice. Recurrent transcendental equations are obtained on the nodes of the lattice. On the basis of these equations, a high-performance parallel algorithm was developed for 3D spin glasses simulations [21].

In frames of the RSA-JINR collaboration, a numerical analysis has been performed on stability and bifurcation of temporally periodic particle-like excitations described by the damped-driven nonlinear Schrödinger equation. New solutions to this equation have been obtained which represent temporally periodic two-soliton complexes coexisting with temporally periodic one-soliton structures, with stationary one- and two-soliton solutions as well as with quasi-periodic solitons. A finite-dimensional approximation of the solutions to the equation under study is proposed which allows one to qualitatively reproduce a diagram of bifurcation of oscillating solitons [22].

A model for the description of the heat and moisture transfer in a porous material is proposed by LIT researchers and Slovak colleagues. The density of saturated vapor and transfer coefficients depend on the temperature. At the same time the conductivity coefficient of the porous material depends on the moisture. On the basis of the proposed model, a numerical simulation of heat and moisture transfer for three different initial and boundary conditions was performed [23].

Fundamental and applied aspects of the quantum computing were analyzed in cooperation with our Belarus colleagues. Attention was focused on the simulator of quantum computations QuantumCircuit implemented in the language Mathematica as well as on a whole set of its applications for modelling quantum computations [24].

A numerical simulation of the magnetic nanoparticle motion in a blood vessel exposed to the magnetic field produced by a focused magnet, has been performed in collaboration with Slovak researchers. In order to get the particle motion trajectories, distributed computations on the JINR grid-cluster were used. The developed programs allow one to determine the parameters of the magnetic nanoparticles for their capture and confinement in a predefined area. This allows the derivation of a solution to the task of medications delivery over the blood system in a desired area [25].

## CONFERENCES, MEETINGS

A traditional two-day Workshop on Computer Algebra was held at the Laboratory of Information Technologies (JINR) on June 2–3, 2011. More than 30 scientists from the universities of Weingarten (Germany) and Western Ontario (London, Canada), IMI BAS (Sofia, Bulgaria) and Russian scientific centres of Ivanovo, Moscow, St. Petersburg, Petrozavodsk, Saratov, and Dubna took part in this Workshop. 33 reports were presented. This Workshop was the 14th in a series of workshops which was jointly started in 1997 by the Joint Institute of Nuclear Research, the Computer Science Department and the Skobeltsyn Institute of Nuclear Physics of Moscow State University.

The international conference «Mathematical Modeling and Computational Physics» (MMCP'2011) devoted to the 55th anniversary of the Joint Institute for Nuclear Research was held in High Tatras Mountains, Stará Lesná, Slovakia, on July 4–8, 2011. The Organizers of the Conference were the JINR Laboratory of Information Technologies, the Institute of Experimental Physics of the Slovak Academy of Sciences, University of Pavol Šafárik and the Technical University (TU), Košice, and the Union of Slovak Mathematicians and Physicists. The Conference was the sixth one organized by LIT under this name.

The coverage of MMCP'2011 included: mathematical methods and tools for modeling complex physical and technical systems; methods, software, and computer complexes for experimental data processing; methods, algorithms, and software of computer algebra; computational chemistry, biology, and biophysics; distributed scientific computing; computing tools of a new generation. Twelve plenary lectures and nearly fifty contributed talks covered a broad range of topics, the com-

mon feature of which was the mathematical modeling of various topics within attempts to secure both rigorous and efficient algorithms within the hardware and software environments at hand. A number of 72 participants from 13 countries (Algeria, Belarus, Bulgaria, Finland, Germany, Netherlands, Poland, Romania, Russia, Slovakia, Taiwan, Turkey, USA) attended the conference. A number of 42 papers have been published in Lecture Notes in Computer Sciences (LNCS) series of Springer-Verlag, Berlin, after passing the refereeing process.

On September 12–19, Varna, Bulgaria, hosted the 23rd traditional international symposium on nuclear electronics and computing (NEC'2011) organized jointly by JINR, CERN and the Institute of Nuclear Research and Nuclear Energy of the Bulgarian Academy of Sciences (INRNE, BAS, Sofia). Almost 100 scientists from 15 countries attended the event: Azerbaijan, Belarus, Bulgaria, Germany, Georgia, Italy, Kazakhstan, Poland, Russia, Romania, USA, Ukraine, France, Czech Republic and Switzerland, more than 30 participants being 36 years old or younger (from Azerbaijan, Belarus, Bulgaria, Georgia, Poland, Russia, Romania, Ukraine and Czech Republic). The Symposium programme covered the following topics: detector&nuclear electronics, accelerator and experiment automation control systems, trigger systems and data acquisition systems, computer applications for measurement and control in scientific research, methods of experimental data analysis, data and storage management, information and database systems, Grid computing, cloud computing, LHC computing, computer networks for scientific research; innovative IT education: experience and trends. 61 oral report and 28 poster presentations, among them 25 oral reports and 13 posters made by JINR participants, were delivered.

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