LABORATORY OF INFORMATION TECHNOLOGIES

The investigations performed at the Laboratory of Information Technologies (LIT) during 2014 in the framework of the JINR research field "Networks, Computing, and Computational Physics" were focused on two first-priority themes, namely, "Information and Computing Infrastructure of JINR" and "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data". The cooperation with other JINR Laboratories involved the participation of the LIT staff in research work within 25 themes of the JINR Topical Plan for JINR research and international cooperation. The objective of LIT activity is to provide a further development of the JINR network and information infrastructure asked by the research and production activity of JINR and its Member States using the most advanced information technologies. The existing Central Information and Computing Complex of JINR (CICC JINR) is evolving into the Multifunctional Centre for Storing, Processing and Analysis of Data aimed at providing to its users a wide range of possibilities through its main components: a grid infrastructure at Tier-1 and Tier-2 levels devoted to the support of the LHC experiments (ATLAS, ALICE, CMS, LHCb), FAIR (CBM, PANDA), and other large-scale experiments; a general-purpose computing cluster; a cloud computing infrastructure; a heterogeneous computing cluster HybriLIT; an education and research infrastructure for distributed and parallel computating. Each of the mentioned components can possess its own dedicated equipment and shares equipment with other components using modern virtualization tools.

In 2014, 182 scientific papers were published by LIT staff in refereed journals and 36 invited reports were presented at international and Russian conferences.

INFORMATION AND COMPUTING INFRASTRUCTURE OF JINR

During 2014, an important work, directed to the reliable operation and development of the JINR networking and informational infrastructure, was in progress. The key components of this infrastructure are the telecommunication data links, the JINR local area network, the computing complex and the primary software, also on the basis of cloud and grid technologies, integrating the information resources of the Institute into a unified environment available to all users.

JINR Telecommunication Data Links. In 2014, the reliable work of the high-speed computer communication channel Dubna–Moscow was secured. The connection with scientific networks and Internet used the following telecommunication links: LHCOPN/CERN (10 Gbps), RBnet (10 Gbps), E-arena and Russian scientific networks (10 Gbps), RUNet and international scientific networks (10 Gbps). The throughput of the reserve data link was increased up to 10 Gbps and its reliability was improved at the expense of the addition

Table 1

Subdivision	Incoming, TB	Outgoing, TB
VBLHEP	72.71	36.58
DLNP	61.8	56.81
FLNP	50.27	56.84
LIT	46.28	24.01
General Access Servers	42.49	8.91
LRB	25.22	1.25
BLTP	24.61	9.98
JINR Management	19.17	45.58
FLNR	18.07	4.12
Remote Access Node	15.87	4.5
JINR's Hotel & Restaurant Complex	13.56	2.64
Joint-Stock Company "Dedal"	8.19	1.66
Medical-Sanitary Unit-9	5.56	1.11
University "Dubna"	4.85	5.74
Recreation Centre "Ratmino"	4.2	1.29

Table 2

Scientific and educational networks	File exchange (p2p)	Web resources	Social networks	Software	Multimedia
93.04%	4.18%	1.5%	0.65%	0.63%	0.01%

of a supplementary router Cisco7606-S. The possibility of the gradual modernization of the external data link up to 100 Gbps has been studied. Table 1 shows the distribution of the incoming and outgoing traffics (more than 3 TB incoming traffic) in 2014 over the JINR subdivisions.

In 2014, the overall incoming JINR traffic, including the general access servers, Tier-1, Tier-2, and the general-purpose computing cluster, amounted to 3.3 PB (2.6 PB in 2013). The weights of the various incoming traffic categories are shown in Table 2.

The creation of the Tier-1 centre at JINR required a high-speed reliable network infrastructure with a dedicated reserved channel to CERN (LHCOPN). In 2014, the JINR Tier-1 was included in the LHCOPN subsystem. The LHCOPN throughput between Tier-0–Tier-1 and Tier-1–Tier-1 was 10 Gbps.

JINR Local Area Network (LAN). The construction of the 10 GB network inside the laboratories by upgrading the network equipment in the buildings housing the JINR subdivisions to 10 GB optic interfaces was in progress. In frames of the user support, the scheduled work on the enhancement of the mail, proxy and authorization services was done. Work was carried out on the implementation of a unique authorization for the JINR Web services using the protocol OAuth 2.0. In 2014, the number of the connected objects found outside the Institute area was increased. The unique system of the international academic computer network with a transparent roaming of eduroam (education roaming) has been connected. That allowed the JINR users to connect to the network with the password provided by the JINR network service.

In 2014, the JINR LAN included 7802 network elements and 12292 IP addresses, 4057 users were registered within the network; there were more than 1500 users of mail.jinr.ru service, 1416 users of digital libraries and 861 remote VPN users.

Multifunctional Centre for Data Storing, Processing and Analysis. The centre is currently under development as an extension of the CICC and aiming at the expansion of the set of computational services for users.

For the time being, the basic computing cluster comprises 2560 64-bit central processors and a data storage system of the total capacity of 1800 TB. The central router of the cluster network is connected to the main router of the JINR LAN at a rate of 10 GB Ethernet.

A new version of the monitoring of the computing cluster was implemented. In accordance with the proposed objectives and tasks, a new monitoring system allows a real-time follow-up of the computer resources and their proper provision by the system management team.

The management of the computing resources and of the data storage system by means of a new basic software enables sharing and optimization of the resource allocation both for solving international projects involving distributed computing (WLCG, FUSION, BIOMED, HONE, PANDA, CBM, BES, NICA/MPD, etc.) and for sharing tasks of local JINR

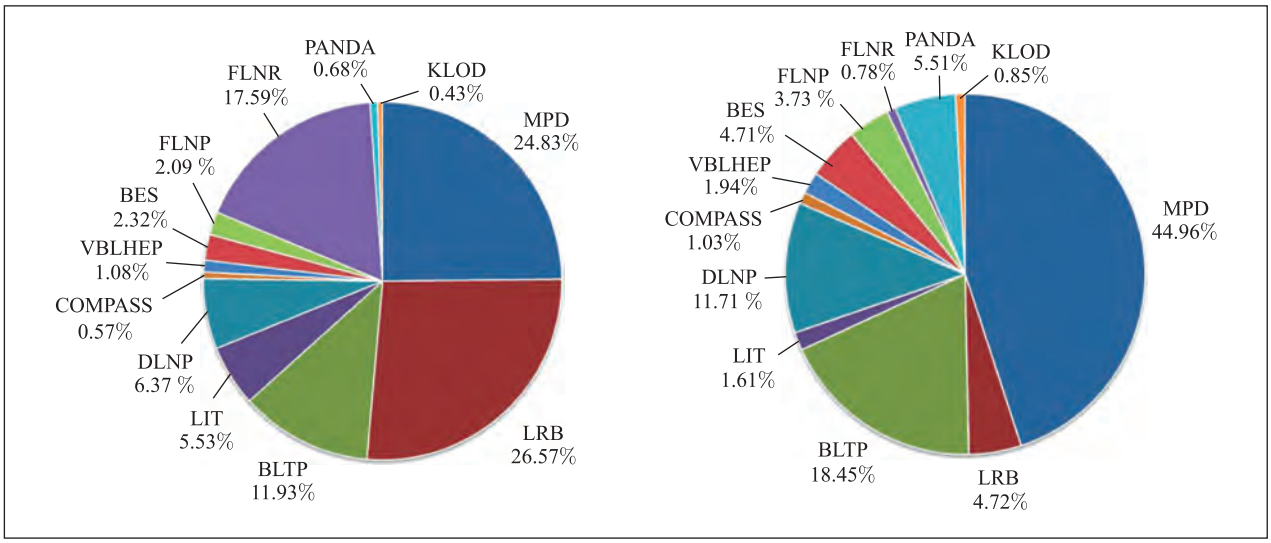

Fig. 1. Sharing of the resources of the computing cluster according to the processing time (left) and to the astronomical time (right) among the divisions of the Institute and user groups

users. To this aim, both the JINR users and the grid users have equal access to all the computer facilities via a unified batch processing system.

The systems of data storage and access dCache and XROOTD ensure data handling both by the local JINR users and by the outer remote users. Two dCache implementations are maintained: dCache-1 for the CMS and ATLAS experiments; dCache-2 for the local users, the user groups and the international projects NICA/MPD, HONE, FUSION, BIOMED, COMPASS. Two implementations of the XROOTD data access system maintain work with data of three international collaborations: ALICE, PANDA, and CBM. All the storage systems are implemented under the hardware data protection mechanism RAID6. Figure 1 shows the distribution of the resources of the computing cluster.

Table 3 provides the 2014 statistics on the CICC use by the JINR subdivisions and user groups, except for the tasks within the grid projects.

Table 3

Laboratory/ group	CPU time, kSi2K · h	Astronomical time, kSi2K · h	Number of jobs
LRB	893701.32	89251.84	1158
MPD	835048.52	850393.16	64120
FLNR	591555.74	14687.34	362
BLTP	401326.39	348956.78	9319
DLNP	214328.90	221485.29	8310
LIT	185922.76	30508.33	468
BES	78183.51	89081.31	32511
FLNP	70211.33	70570.20	392
VBLHEP	36165.57	36715.10	1233
PANDA	22936.75	104304.17	360753
COMPASS	19167.64	19403.42	2582
KLOD	14601.20	16101.93	4368

JINR Grid Environment. In 2014, active work was in progress within the global large-scale grid projects "Worldwide LHC Computing Grid" (WLCG, 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/). The JINR computing cluster supports, under the grid-site name JINR-LCG2 of the global grid infrastructure, computations of 8 virtual organizations (alice, atlas, biomed, cms, dteam, fusion, hone, lhcb) enabling as well possibilities for using grid resources for the experiments BES and PANDA. The main users of the JINR grid resources are the virtual organizations of all the four large LHC experiments.

The servers of the control system of the cluster operation are used for the task distribution (both for local users and WLCG) at various sites of the WLCG project. The service X509 PX (ProXy) stores and updates the user certificates enabling the protection of resources and tasks of users within grid systems. This is the chief method of access control of the registered users within the WLCG project. The CERN distributed file system CVMFS (CernVM File System) is maintained on the cluster to provide and control the access to the software within the ALICE, ATLAS, CMS, LHCb and BES collaborations. Two VOboxes (Virtual Organization box) are used by the ALICE and CMS collaborations to perform their work at the WLCG sites.

The work of the grid site at JINR is maintained by 22 servers under the EMI2/EMI3 system (WLCG middleware). In addition to the support of the operation of the site JINR-LCG2 itself, a part of the servers provide important services and functions for the support of the Russian segment of the WLCG project. Table 4 and Fig. 2 (left) summarize the VO usage of the JINR grid infrastructure within RDIG/WLCG/EGI in 2014. During 2014, Tier-2 has run almost 5 million jobs, with an overall CPU time exceeding 160 million h (in HEPspec06 units). The JINR grid site is one of the most effective Tier-2 level sites within the WLCG infrastructure.

Table 4

VO	CPU time, HEPspec06 · h	Number of jobs
atlas	41 876 104	2 677 075
cms	46 230 972	1 003 803
alice	45 093 312	786 849
lhcb	21 135 604	141 346
biomed	1 650 056	237 252
bes	300 552	40 456
hone	266 944	20 016
fusion	46 348	16 624
ops	572	80 438
Total	156 600 464	5 003 859

A Tier-1 site for the experiment CMS was created in LIT. At the moment, Tier-1 comprises 1200 64-bit processors, a 660 TB storage system and a 72 TB tape storage. During 2014, almost 1 million tasks were run at the JINR Tier-1 site, with an overall processor time of 65 million h (HEPspec06 units). Figure 2 (right) summarizes data on the usage of the Tier-1 centres of the CMS experiment. The contribution of the JINR's Tier-1 prototype was 4.82%.

By the state of the LHC run, the build-up of the first-level configuration of the fully functional Tier-1 center in JINR should be brought to an end. To this purpose, a 5 PB tape robot (IBM) was already installed, while the works on commissioning the uninterrupted power supply source and the installation of inter-row air-conditioning for new Tier-1 modules have reached the final stage.

In 2014, work continued on building up the parameters of the network connections between the sites of the ATLAS collaboration infrastructure to the targets established within the PanDA (Production and Distributed Analysis System) task processing system. In particular, a service has been created that transfers only necessary data from ATLAS SSB (Site Status Board), which

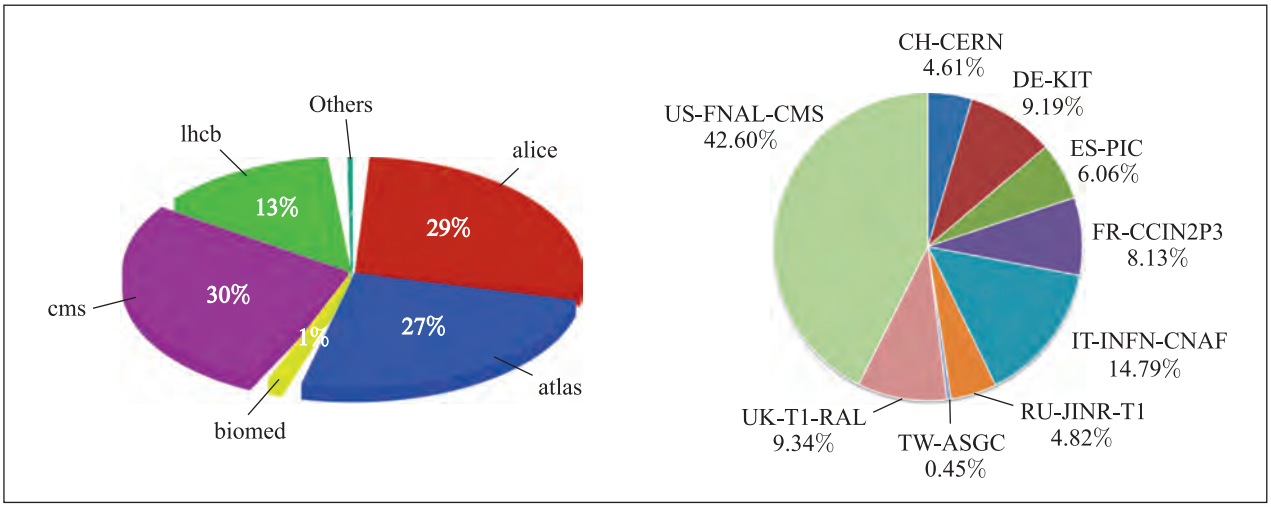

Fig. 2. Summary of the use of the JINR Tier-2 grid infrastructure by virtual organizations that are a part of RDIG/WLCG/EGI (left). Usage of the Tier-1 centers by CMS experiment (right)

stores both the current information and historical data, into AGIS (ATLAS Grid Information System), the unified information system for all systems of the ATLAS collaboration. Also, the service SchedConfig was developed in 2014 to carry out network metrics as well as additional information to the internal information system PanDA. SchedConfig is a database containing configuration parameters required for PanDA operation; partial duplication is made such that to keep the PanDA to serviceability under unviability of inaccessibility of the AGIS information system [1].

Heterogeneous Computing Cluster HybriLIT. In 2014, the computing cluster HybriLIT (http://hybrilit.jinr.ru) was put into operation. It comprises four computing nodes: two nodes containing three graphical accelerators NVIDIA Tesla K40 (Atlas) each, a node containing two co-processors Intel Xeon Phi 7120P, as well as a node containing NVIDIA Tesla K20x and a co-processor Intel Xeon Phi 5110P. Moreover, each computing node includes two processors Intel Xeon E5-2695v2. The HybriLIT cluster also includes a control unit and a data storage unit. Figure 3 shows the structure and the main characteristics. Inclusion of the HybriLIT cluster in the computer infrastructure of the Multipurpose Center of Data Storage, Processing and Analysis provides the specialists from JINR and the JINR Member States with the possibility to create their own software asked by research that needs resource-intensive computations, to use software packages already adapted for hybrid architectures, as well as mathematical libraries. In 2014, on the base of

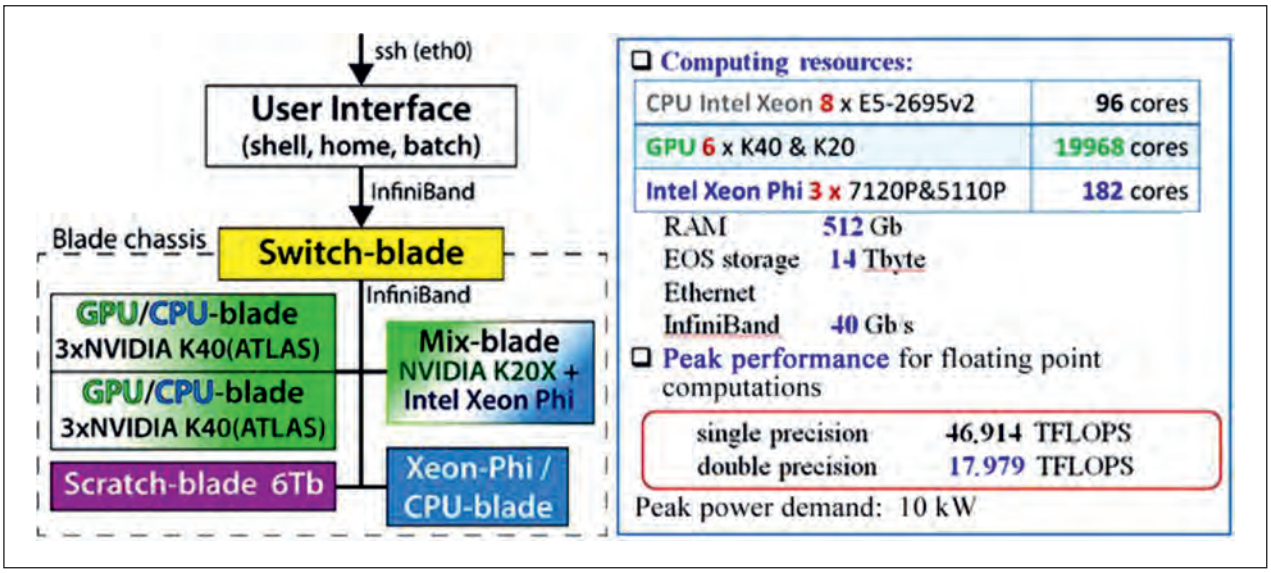

Fig. 3. The structure of the heterogeneous computing cluster HybriLIT (left). The main parameters of the computational elements of the cluster and its efficiency (right)

the HybriLIT cluster, training courses were held on the parallel programming technologies in the framework of the GRID'2014 conference, the International youth conference MPAMCS'2014, as well as within the Helmholtz International Summer School "Lattice QCD, Hadron Structure and Hadronic Matter". The overall number of participants in the training courses exceeded more than 60 people from Germany, Mongolia, Russia, Romania, etc.

For the efficient use of the heterogeneous cluster HybriLIT, an information-software environment that includes services for applications development, debugging and profiling is being developed and implemented by LIT staff together with colleagues from the Institute of Experimental Physics and the Technical University in Košice (Slovakia).

Cloud Environment. During the first half of 2014, a cloud infrastructure was brought into service (http://cloud.jinr.ru). Presently, the cloud resources include 138 cores, 260 GB RAM and 10 TB disk space. At the moment, 67 accounts are registered in the cloud.

The cloud service resources are utilized by users for various activities within the themes of the JINR Topical Plan for JINR research and international cooperation as well as for the fulfillment of LIT and JINR obligations under various projects:

- two test beds for the PanDA Application Software (AS): the first is for development, the second is to estimate its suitability for construction of the computing infrastructure of the NICA project;
- test bed based on the DIRAC AS for experiment BES-III and computing resources for it;
- test beds for the project management (JPMS) services and the document server (JDS).

Figure 4 shows the distribution of the cloud resources over JINR Laboratories and groups in 2014.

Migration of services of education for the research and test grid infrastructure on virtual machines to the JINR cloud service was performed.

A virtual organization NICA has been created on the VOMS-server to perform corresponding investigations under the project with the same name.

Information and Software Support. A new grid- and cloud-service simulation system for the future NICA accelerator complex data storage and processing setup was developed in 2014. Within the new system, the assessment of the quality of the already developed grid- and cloud-service simulation is done together with the design of the further development by combining the simulation code with the monitoring of grid-cloud service through a dedicated database [2].

A comparative analysis of these packages for modeling cloud infrastructures — CloudSim, iCanCloud, and CReST, has been done. These program packages allow the development of models of cloud systems with definite functionality and configuration. The output of the simulation done via the final model consists of statistical information on the most important features of the cloud infrastructures: execution time, virtual machine lifecycle, the use of resources. From the analysis of this information, the developer can reveal bottlenecks in the model and foresee their solution, the validity of the implementation of which being checked at the next iteration of the simulation [3].

Approaches have been developed for ensuring the content integration and interoperability of the information systems assisting the research activities at JINR, namely, the JINR Document Server (JDS), the information-analytical system "Personal Information about JINR employees" (PIN) and the scientific activities management Indico [4].

During 2014, work was in progress on the transition to the unified information platform 1C 8.2 UPP: the 1C 8.2 UPP and ADB2 components regarding operational performance of the JINR budget; a specialized constructor of multiline documents was developed; the module "Budgeting", including the "Application Mechanism", was brought into service. During 2014, courses for users were also organized; for instance, training on the new functional "Mutual Settlement of Accounts with Self-Supporting Divisions". Weekly meetings with users from the Accounting Department were held regularly for revealing and solving urgent tasks and problems arising during the 1C software usage.

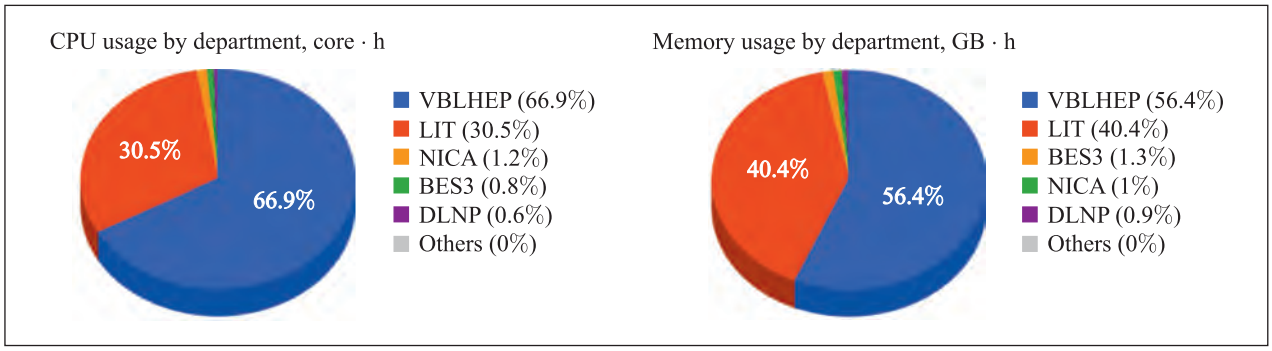

Fig. 4. Distribution of cloud resources among the Laboratories and JINR groups in 2014

In 2014, the system of electronic document circulation (EDC) "1C:DocumentCirculation" EDC was debugged; the document "Turnkey contract" (Contractor's agreement) with corresponding procedures of electronic confirmation was put into commercial operation. Relevant instructions for users were prepared as well, and the users were trained on the creation and confirmation of documents "Turnkey contract" in EDC "1C:DocumentCirculation".

In 2014, work was done on updating the project plans in the information control system of the NICA project (ADB2-EVM), a separate version of the CERN module APT-EVM was prepared, the integration of the APT-EVM functional with the information system (IS) of the NICA project management (ADB2-EVM) was done, APT-EVM was installed on the JINR area, and the functional of integration with the information system of the NICA project management was tested. In the framework of the development of the IS for the NICA project management, the following modules have been elaborated: on the work with baselines; on the input of the parameters of the budgeted cost of the performed work (EV); the notification system; account forms with the ADB2-EVM were tested; the directories of the work breakdown structure (WBS) between IS of the NICA project management (ADB2-EVM) and 1C were synchronized. Further, in 2014, the modernization and development of the module on the verification of actual data on payment of accounts/orders within 1C and ADB2 were carried out together with organization of sessions of leaders of 1-2 WBS ranks for the work with the ADB2-EVM system.

During 2014, work was in progress on the update of the software environment and databases of the LIT/JINR websites http://lit.jinr.ru, http://www.jinr.ru, http://wwwinfo.jinr.ru. Also, an active work was conducted on the creation and storage of electronic documents related to scientific and administrative activity of LIT and the Institute as a whole at the request of the JINR Scientific Organizational Department (information on the operation of the JINR basic facilities, the sessions of the JINR Scientific Council, etc.), and the internet access was ensured to the relevant information concerning the JINR Prizes — a retrieval system (data since 1960) http://wwwinfo.jinr.ru/search_award_dbs.htm; information on conferences and the JINR workshops http://wwwinfo.jinr.ru/confer-e.htm; information on the JINR dissertation councils (http://wwwinfo.jinr.ru/dissertation/JINR_DCs.htm), as well as announcements on defending PhD theses and Doctor's theses at JINR on proposals of the scientific secretaries of the councils. Maintenance and modernization of the web-portal of the journals "Physics of Elementary Particles and Atomic Nuclei" (PEPAN) and "Particles and Nuclei, Letters" (http://pepan.jinr.ru/) were done. Traditional regular work was conducted on the design and support of various information websites, sites of conferences, workshops, symposia organized by JINR Laboratories, as well as organization of a website hosting (upon request). Instances: FLNP (CMR@IBR-2), DLNP (RCRC-2014), FLNP (EXON-2014), LRB (MPGRRE-2015), LIT (RCDL-2014), etc.

METHODS, ALGORITHMS AND SOFTWARE FOR MODELING PHYSICAL SYSTEMS, MATHEMATICAL PROCESSING AND ANALYSIS OF EXPERIMENTAL DATA

One of the main directions of the research activity at LIT is to provide a mathematical, algorithmic and software support of the experimental and theoretical research underway at JINR. Below there is a brief report on some results.

A new algorithm for constructing the segments in endcap cameras of the CMS setup on the LHC has been developed. By means of specially developed programs for finding the parameters of simulated MC objects, there has been carried out the analysis of the results obtained with the use of various algorithms, and the efficiency of the new algorithm over the standard one for particles obtained as a result of collisions and for cosmic rays has been proved.

Within the works on the modeling and optimization of the setup of Baryonic Matter at Nuclotron (BM@N) project, a number of problems have been carried out; in particular, the analysis of the data obtained from the GEM-detector prototype, in the course of which the efficiency and a number of other parameters in the work of the detector have been estimated. The results of the analysis were provided to the specialists for further improvement of the geometry of the prototype. The code for information readout obtained from the GEM-detector has been developed and provided for the implementation into the basic software package of the experiment. The efficiency of the DC-detector at low values of the electric potential has been estimated; and a software for dealing with data obtained from the 8 planes of the detector has been developed.

An algorithm for the real-time charged particles trajectory reconstruction of the CBM experiment (GSI, Darmstadt, Germany) has been developed on the basis of the Kalman filter. The problems related to the reconstruction of charged particle trajectories require high-performance computing resources, so a software implementation of the suggested algorithm was carried out on the basis of various technologies of parallel pro-

gramming adapted to hybrid computing architectures. To solve the considered problem numerically, the hybrid server of LIT JINR with two central processors Intel Xeon X5660 and graphic card NVIDIA GTX 480 was used [5].

The scientists of LIT and VBLHEP involved in the Geant4 Collaboration have performed a research work entitled "The Effect of uu Diquark Suppression in Proton Splitting in Monte-Carlo Event Generators". Most of the Monte-Carlo event generators of multiparticle production assume that nucleons split into diquarks and quarks in strong interactions. In particular, protons split into (ud) diquarks and u quarks with a probability of $2/3$ and into (uu) diquarks and d quarks with a probability of $1/3$. It was demonstrated that using a value of $1/6$ for the last probability allows one to describe at a semi-quantitative level the NA49 Collaboration data for $p + p \to p + X$ reactions at 158 GeV/c. A suppressed weight of (uu) diquarks in protons is expected in the instanton model of the QCD vacuum. According to that model, quark–quark interactions are flavor-dependent. For example, they are nonzero only if quarks are of different flavors. Thus, (uu) diquarks must be suppressed in protons. The Fritiof (FTF) model of Geant4 was used to simulate the $p + p \to p + X$ reactions. Good results were obtained. The suppression of diquarks is included in the last release of Geant4 [6].

The FORTRAN 77 program POTHEA is presented for calculating with a predetermined accuracy of eigenvalues, surface eigenfunctions and their first derivatives with respect to a parameter of the parametric self-adjoined 2D elliptic partial differential equation with the Dirichlet- and/or Neumann-type boundary conditions in a finite two-dimensional region. The program also calculates potential matrix elements that are integrals of the products of the surface eigenfunctions and/or the first derivatives of the surface eigenfunctions with respect to a parameter. Eigenvalues and matrix elements computed by the POTHEA program can be used for solving the bound state and multichannel scattering problems for a system of the coupled second-order ordinary differential equations with the help of the KANTBP program [7].

The analysis of cross sections of inelastic scattering of π mesons by nuclei Si, Ni, Pb at the energy of 291 MeV has been performed on the basis of a microscopic optical potential (OP). These OPs were determined on the basis of a pion–nucleon amplitude and a nucleus density distribution. In doing so, used were parameters of the πN amplitude in nuclear matter obtained earlier from the analysis of data on elastic scattering on the same nuclei. Calculation of cross sections was conducted on the basis of the relativistic wave equation. Parameters of the nuclei deformation were received from a comparison with experiment of cross sections of inelastic scattering [8].

A method and a software complex have been elaborated for numerical simulation of the process of formation of polaron states in condensed matter. Numerical study of this process was carried out for aqueous medium exposed to laser irradiation in a ultraviolet range. It was shown that within the suggested approach one can numerically reproduce the experimental data on formation of hydrated electrons. A scheme was presented of a numerical solution to the system of nonlinear differential equations in partial derivatives describing a dynamic polaron model. Software realization was executed with the use of parallel programming technology MPI [9].

Direct proof of the role of the CuO_2 planes in the occurrence of the high-temperature superconductivity in cuprates was got experimentally from the investigation of the behaviour of the critical temperature T_c under gradual substitution of the in-plane Cu^{2+} ions by divalent metal ions M^{2+}. Functional dependencies $T_c = T_c(y)$ on the y content of M ion are inferred from the existing experimental evidence on $La_{1.85}Sr_{0.15}Cu_{1-y}M_yO_4$ (LSCO) for M^{2+} denoting either Zn^{2+} or Ni^{2+}. Data processing and analysis point, in both cases, to a sharp linear decrease of T_c under the increase of y, with an M ion-dependent slope. The result substantiates the basic hypothesis of the effective two-dimensional two-band Hubbard model (*Plakida N. M. et al.* // Phys. Rev. B. 1995. V. 51. P. 16599; JETP. 2003. V. 97. P. 331; Eur. Phys. J. B. 2013. V. 86. P. 115; *Plakida N. M.* High-Temperature Cuprate Superconductors. Experiment, Theory, and Applications, 2nd Ed. Berlin, Heidelberg: Springer, 2010) of searching the origins of the high-T_c superconductivity in cuprates inside individual CuO_2 planes [10].

For the first time formulas for the polynomial coefficients represented as basic elements (MBE) that depend on the parameters of a three-point grid have been obtained. The use of MBE polynomials of high degrees for piecewise-polynomial approximation (PPA) and smoothing improves the quality of approximation and increases the efficiency of the data processing algorithms [11].

The methods of computation invariant theory together with those of computer algebra have been used to describe the space of separable and entangled states for composite quantum systems. In particular, such quantum systems as a pair of qubits and a three-level quantum system (qudit) have been considered. It has been shown that their state space is uniquely determined by a semi-algebraic set (e.g., set of equations and inequalities) in terms of polynomial invariants of the global unitary group, $SU(4)$ for 2-qubit systems and $SU(3)$ for qutrits [12].

Finite-element-method (FEM) simulations have been performed to determine the current and field distributions and to calculate the AC losses in cables made of MgB_2 superconductors. For current capacities of 2–5 kA (peak), the power cables are assembled from a relatively small number of MgB_2 strands. The performance of such cables strongly depends on the cur-

rent and field distributions, which are, in turn, influenced by the number and the arrangement of the superconducting components and also by the magnetic properties of supporting materials. Numerical simulations can help to test different cable configurations and provide important insights for optimizing the cable's design. The numerical model includes the field dependence of the superconductor's critical current density and the nonlinear properties of magnetic materials [13].

The ground state of a homogeneous Bose gas of hard spheres has been treated in self-consistent mean-field theory. It has been shown that this approach provides an accurate description of the ground state of the Bose–Einstein condensed gas for arbitrarily strong interactions. The results are in good agreement with Monte-Carlo numerical calculations. Since all other mean-field approximations are valid only for very small gas parameters, the present self-consistent theory is a unique mean-field approach allowing for an accurate description of Bose systems at arbitrary values of the gas parameter [14]. It has also been shown that, contrary to all other variants of mean-field theory, which incorrectly describe the condensation phase transition exhibiting instead of the necessary second-order transition a first-order transition, the self-consistent mean-field approach is the sole mean-field theory that provides the correct second-order condensation transition for Bose systems with atomic interactions of arbitrary strength, whether weak or strong [15].

INTERNATIONAL COLLABORATION

In 2014, in cooperation with the Chinese colleagues, a system of distributed computations was designed for experiment BES-III (Beijing Spectrometer III) on the electron–positron collider in Beijing. For the BES-III distributed computations system, the DIRAC infrastructure (Distributed Infrastructure with Remote Agent Control) has been chosen that allows realization of required functionalities. The LIT specialists actively participated in all tasks of the development of grid systems for the BES-III experiment, especially in engineering data and grid-monitoring management systems. Considerable progress was made towards the creation of a data storage infrastructure; also, the first version of the BES-III monitoring system was developed and put into operation.

In collaboration with the University of Plovdiv (Bulgaria) and the University of Cape Town (South Africa), a numerical investigation of complexes of localized states has been performed in two dynamical systems: a directly driven nonlinear Schrödinger equation (NLS) and a double sine-Gordon equation (2SG). Both systems have a wide range of physical applications. In both cases, the numerical approach is based on a numerical continuation with respect to the control parameters of the quiescent (stationary) solutions and stability and bifurcation analysis of the linearized eigenvalue problem. Multisoliton complexes of the NLS equation are studied in the undamped and weak damping regimes. It has been shown that in the weak damping case, the directly driven NLS equation holds stable and unstable

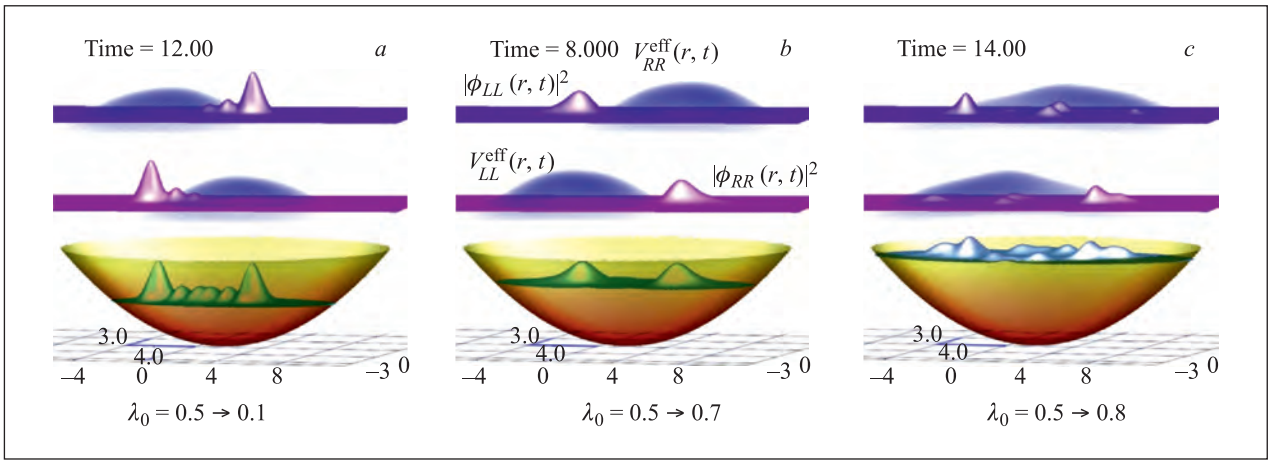

Fig. 5. Visualization of the concept of interaction-induced time-dependent barriers to interpret the two generic dynamical regimes of strongly-interacting trapped bosons; 2D case. Evolutions of a two-fold fragmented initial state induced by a sudden displacement of the harmonic trap $V(x,y) \to V(x-1.5,\, y-0.5)$ with the simultaneous quench of the interparticle repulsion: (*a*) strong decrease $\lambda_0 = 0.5 \to 0.1$, snapshot at $t = 12$; (*b*) moderate increase $\lambda_0 = 0.5 \to 0.7$, snapshot at $t = 8$; (*c*) strong increase $\lambda_0 = 0.5 \to 0.8$, snapshot at $t = 14$

multisoliton complexes. The obtained numerical results have been confirmed by means of direct numerical simulations of the time-dependent NLS equation. The properties of the multifluxon solutions of 2SG equation have been studied depending on the parameter of the second harmonic. It has been shown that the second harmonic changes properties and increases the complexity of coexisting static fluxons of 2SG equation. The results have been discussed in the framework of the long Josephson junction model [16].

In cooperation with the Slovak colleagues, an algorithm of modeling a process of heat conductivity has been developed at the design and optimization of a cryogenic cell, pulse feeding working gases (in a msec range) into an electron-string source of high-charge ions. To speed up the calculations, a parallel algorithm realized in the OpenCL language has been developed. Results of the calculations have shown that the selected characteristics and the configuration of the device meet necessary requirements to the mode of its work [17].

In the framework of ongoing collaboration between Many-Body Theory of Bosons group at the Center for Quantum Dynamics, Heidelberg University (Germany) and the Laboratory of Information Technologies, JINR (Russia), theoretical investigations of the highly-nonequilibrium quantum dynamics realized in trapped systems of ultracold atoms and molecules were in progress. In particular, the development and optimization of the Multiconfigurational Time-Dependent Hartree for Bosons (MCTDHB) package designed to solve the many-body Schrödinger equation for bosons was continued. The program modules designed for the MCTDHB package are intended to perform 1D, 2D and 3D computations on hybrid computing systems including multicore CPU and graphical accelerators. Parallel modules have been realized on the basis of the present-day parallel programming technologies MPI + CUDA (MPI + PGI CUDA). The modules developed will be included into a new version of the package. Examples of the results of the MCTDHB package calculations are shown in Fig. 5. The development, implementation and preliminary computations were performed on the heterogeneous computing cluster HybriLIT (LIT JINR) and on the hybrid K100 cluster (Keldysh Institute of Applied Mathematics) [18].

CONFERENCES AND MEETINGS

On 3–8 February, JINR hosted the 21st International Conference "Mathematics. Computer. Education" (MCE). The Conference was organized by the JINR Laboratory of Information Technologies, "Dubna" University, Lomonosov Moscow State University, Puschino Scientific Center of RAS, Keldysh Institute of Applied Mathematics (Moscow, RAS), MSU Centre of National Intellectual Reserve, Foundation "National Intellectual Development", as well as the Interregional Public Organization "Women in Science and Education". Traditionally for the MCE conferences there were organized presentations and discussions of research projects developed by high-school students within the "FOROS" project, which were held at the International University of Nature, Society and Man "Dubna". The students came from Moscow and Moscow region, the cities of Tver and Izhevsk. For the pupils who were not able to come to Dubna, a television space bridge was organized.

A traditional two-day Workshop on Computer Algebra was held at the Laboratory of Information Technologies on 21–22 May. More than 40 scientists from universities and scientific institutes of Bucharest (Romania), Sofia (Bulgaria), Tbilisi (Georgia), Moscow, St. Petersburg, Ivanovo, Pereslavl-Zalesskiy, Petrozavodsk, Saratov, Tambov, and Dubna took part in this Workshop. Thirty-four reports were presented. This year, a number of new promising results on: analysis and solving of the algebraic, differential and difference equations; increase of computational efficiency of algorithms of computer algebra; study of algebraic properties of the qubits in entangled states in quantum informatics, as well as computer algebra applications to physics and mathematics, were presented.

The 6th International Conference "Distributed Computing and Grid Technologies in Science and Education" was held at the Laboratory of Information Technologies on 30 June – 5 July. This year marked the tenth anniversary of the first conference in 2004. It should be noted that the Conference has become a unique forum for the discussions of a wide range of questions related to the use of distributed and grid technologies in different fields of science, education, industry and business, and of fresh ideas and results. The Conference was attended by more than 200 participants from the following scientific centers: Armenia, Belarus, Bulgaria, Hungary, Mongolia, etc. Russia was presented by participants from more than 30 universities and research centers. Within the Conference, there were organized eight sections, which included discussions on the current and future role of grid technologies, cloud technologies, Big Data in the models of computing for megaprojects such as NICA and FAIR. During the Conference, there was also held a meeting "Computing Models, Software and Data Processing for the Future HENP Experiments". During the work of the Conference, there were made 30 plenary reports, more than 65 sectional reports and 13 poster presentations. Within the Conference, there was held a tutorial on parallel programming technologies. Participants from

Mongolia, Romania and Russia listened to the lectures on the following technologies: MPI, OpenMP, CUDA, and OpenCL. The practical trainings were held on the basis of the heterogeneous computing cluster HybriLIT (http://hybrilit.jinr.ru/).

On 25–29 August, the Joint Institute for Nuclear Research (JINR) under the auspices of the National Committee of the Society for Industrial and Applied Mathematics (SIAM), the International Coordinating Committee for Computational Mathematics of the CIS Academies of Sciences hosted the International conference for young scientists "Modern Problems of Applied Mathematics and Computer Science". The Conference was organized by the KIAM RAS, LIT JINR, INM RAS, and RCC MSU. The Conference was attended by participants from Russia, Belarus, Tajikistan, Armenia, Mongolia, Slovakia, etc. The total number of the Conference participants was 132, 108 persons being students, postgraduates and young scientists under 35 years of age (more 80%). The Conference for young scientists MPAMCS'2014 provided a way for young scientists to get acquainted with the present-day methods and approaches to solving problems of science and technology with the help of high-performance computing systems, with methods of developing large program complexes, modern parallel programming techniques, as well as with the latest achievements in the field of exaflops computations and Big Data. The best reports presented by young scientists will be published in the journal "Mathematical Modeling".

On 13–16 October, the Laboratory of Information Technologies hosted the 16th Conference in a series of annual scientific conferences "Digital Libraries: Advanced Methods and Technologies, Digital Collections" RCDL-2014. Alongside with the Russian employees of scientific research institutes, teachers and postgraduate students, specialists in the field of library affair and industry of information technologies from Moscow, St. Petersburg, Kazan, Yaroslavl, etc., the RCDL-2014 Conference was attended by the representatives of Great Britain, India, Kazakhstan, and France. Fourteen sessions were organized, which, alongside with the invited talks, included 28 reports and 19 communications. By the tradition of the last few years, in the framework of the Conference, a dissertational seminar of young scientists was organized to discuss the directions and results of scientific studies performed by the authors of reports to the seminar.

On 20–24 October, the 5th School on information technologies "Grid and Advanced Information Systems" was held under the auspices of the LIT JINR, CERN and NRNU MEPhI. The 5th School was devoted to the management of scientific complexes and information systems. In total, students from 12 leading universities were invited: Saint-Petersburg State University, MSU, Lobachevsky State University (Nizhni Novgorod), PFUR, Plekhanov Russian University of Economics, Tver State University, NRNU MEPhI, BMSTU, MPEI, and "Dubna" University. Also, students from Slovakia and Georgia took part in work of this School. The participants heard lectures on database, cloud computing, digital library, grid technologies, software development, the NICA accelerator complex, Tier-1 in Dubna, etc. The organizers of the School held a competition among the participants. On the first day of the School the students were given the tasks which they could decide and realize during a week. The best result was shown by Kirill Korepanov from Bauman Moscow State Technical University, the second prize went to a group of students from Tver State University and the third prize went to "Dubna" University. All the winners were presented the prizes.

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