LABORATORY OF INFORMATION TECHNOLOGIES

The investigations performed at the Laboratory of Information Technologies during 2016 in the scope 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 30 themes of the JINR Topical Plan for JINR research and international cooperation. The LIT activity is intended to provide a further development of the JINR network and information infrastructure, mathematical and software provision for research and production activity under way at JINR and its Member States on the base of advanced information and computer technologies.

For more than a decade, the development of the information and computing infrastructure of JINR created at LIT was done within the Central Information and Computing Complex (CICC) of JINR. In the last few years, in connection with work on the organization of the computing project for NICA, the commissioning of the grid center Tier-1 for the CMS experiment, the implementation of a cloud computing structure and a cluster for hybrid computing, the information-computing environment of JINR evolved in a set of stand-alone structures that have a common engineering infrastructure. Thus, it is possible to identify this structure as a Multifunctional Information and Computing Complex (MICC) of JINR, which currently has the following basic components:

- the Central Information and Computing Complex (CICC) of JINR with home built up compute elements (CE) and mass storage elements (SE);
- the grid center Tier-1 for CMS experiment;
- the grid center Tier-2 site for experiments at the Large Hadron Collider (LHC) and other virtual organizations (VOs) in the grid environment;
- the heterogeneous cluster "HybriLIT" for parallel computing;
- the cloud-based grid infrastructure;
- the training and research grid-cloud infrastructure.

The JINR MICC provides resources needed for different tasks, implied by many projects the JINR researchers take part in, namely: COMPASS, BES-III, DIRAC, HARP, CMS, ALICE, ATLAS, H1, NEMO, OPERA, PANDA, NOνA, STAR, LHCb, etc. The JINR Tier-1 and Tier-2 are elements of the Russian Grid Segment used for LHC computing and other applications. The grid infrastructure at JINR is represented by CMS Tier-1 center and Tier-2 center for ALICE, ATLAS, LHCb, and CMS.

In 2016, 193 scientific papers were published by LIT researchers in referred journals, and 47 reports were presented at international and Russian conferences.

INFORMATION AND COMPUTING INFRASTRUCTURE OF JINR

During 2016, the work related to the reliable operation and development of the JINR networking, informational and computing infrastructure was in progress. The key components of this infrastructure are telecommunication data links, the JINR local area network (LAN), the CICC and the primary software, including the one on the basis of cloud, grid, and hybrid technologies. They integrate information resources of the Institute into a unified environment accessible to all users.

JINR Telecommunication Data Links. In 2016, 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), RUNNet and international scientific networks (10 Gbps).

The throughput of the reserve data link was raised up to 10 Gbps and its reliability was improved at the expense of the addition of a supplementary router Cisco7606-S. The possibility of the gradual modernization of the external data link up to 100 Gbps has been studied and this work was finished at the end of 2016. The new Transmode equipment for this modernization was purchased and put into operation.

Table 1 shows the distribution of the incoming (more than 3 TB) and outgoing traffics over JINR subdivisions in 2016.

Table 1

Subdivision	Incoming, TB	Outgoing, TB
DLNP	125.98	154.99
VBLHEP	102.43	90.68
General access servers	90.99	17.72
LIT	62.13	34.79
FLNP	49.2	63.15
University “Dubna”	48.98	38.43
FLNR	37.6	18.18
JINR Management	26.82	58.2
JINR Hotel & Restaurant Complex	25.47	4.4
Remote access node	24.05	5.74
BLTP	19.71	16.73
Joint-Stock Company “Dedal”	10.78	5.97
Medical-Sanitary Unit 9	10.65	0.82
LRB	8.76	5.26
Resort Hotel “Ratmino”	7.77	2.08
Joint-Stock Company “Atom”	5.13	0.65
Procurement and Logistics Service	4.23	3.07
Chief Engineer’s Department	3.83	0.68

In 2016, the overall incoming JINR traffic, including the general access servers, Tier-1, Tier-2, and CICC, amounted to 14.2 PB (4.26 PB in 2015). The weights of the various incoming traffic categories are shown in Table 2.

Table 2

Scientific and educational networks, %	File exchange (p2p), %	Web resources, %	Social networks, %	Software, %
96.75	2.32	0.53	0.11	0.29

JINR Local Area Network. In 2016, work was in progress on the further development and improvement of the JINR network IT elements intended to increase the working efficiency of the JINR staff. The construction of the 10 GB network inside the laboratories was finished.

In the framework of the user’s computer environment support, the scheduled work has been done on enhancement of the IPDB, mail, webmail, proxy, e-lib, and authorization services. For instance, work is carried out on the transition of the JINR subdivisions to the unified JINR mail service user@jinr.ru. An authorized WiFi has begun its operation on the JINR territory as well as services eduroam and VPN for remote work outside the JINR limits.

The JINR LAN includes 8222 network elements and 13364 IP addresses; 4301 users are registered at present within the network. There are 2341 users of mail.jinr.ru service as well as 1500 users of digital libraries and 371 remote VPN users.

JINR Grid Environment. The Tier-1 center for CMS at JINR was put into a full-operation mode in March 2015. By the end of 2016, the JINR Tier-1 resources comprise: computing power of 55.16 kHS06, 3600 cores/slots (11 Supermicro Twin Blades), disk capacity of 4037 TB (30 Disk servers with hardware RAID6) and 521.88 TB used as a buffer for tape storage (8 Disk servers with hardware RAID6), tape space of 5478.32 TB (IBM TS3500 tape library with $8 \times$ FC8 links to 8 Disk servers). The network is configured as two redundant triangles shared with the NRC “Kurchatov Institute” with 10 Gbit/s LHCOPN connection.

The mass storage systems are built on dCache and Enstore as a tape backend for dCache. Totally, two installations have now 4 PB of effective disk space, and the tape robot has a 5.4 PB of data storage capacity. To support the storage and access to data, 8 physical and 14 virtual machines have been installed.

Torque/Maui is used as a scheduler. The standard WLCG software stack was used for computing: $2 \times$ CREAM, $4 \times$ ARGUS, BDII top, BDII site, APEL parsers, APEL publisher, EMI-UI, $220 \times$ EMI-WN + gLExec-wn, $4 \times$ FTS3, LFC, WMS, L&B, glite-proxyrenewal.

The JINR CMS Tier-1 has shown its stable state for the whole period after putting it into the full-operation mode [1]. During 2016, this center performed 8 257 163 tasks, using a normalized CPU time of 237 346 520 h in HEPSpec06 units. Figure 1 gives the contribution of the Tier-1 global centers to the CMS experimental data processing (in MEvents) for the year of 2016. The JINR Site takes one of the leading ranks in the world as to its productivity.

Figure 2 shows the number of events processed at the JINR CMS Tier-1 in June 2016 by the CMS activities (production, reprocessing, analysis, etc.).

One of the main functions of the Tier-1 centres is the archival storage of raw experimental and simulated data. Figure 3 shows the load of our tape robot during 2016. Figure 4 illustrates the requests from the Tier-1 and Tier-2 centres worldwide to the JINR CMS Tier-1 for data in June 2016. The average rate for RAW data transfers to the JINR CMS Tier-1 site is 250–300 MB/s, more than 1 TB/h was transferred.

The JINR Tier-2 center supports a number of virtual organizations (VOs), in particular, ALICE, ATLAS, BES, BIOMED, CMS, HONE, FUSION, LHCb, MPD, NOνA, STAR. The JINR Tier-2 computing resources comprise 2470 cores/slots, 46.72 kHS06; disk capacity:

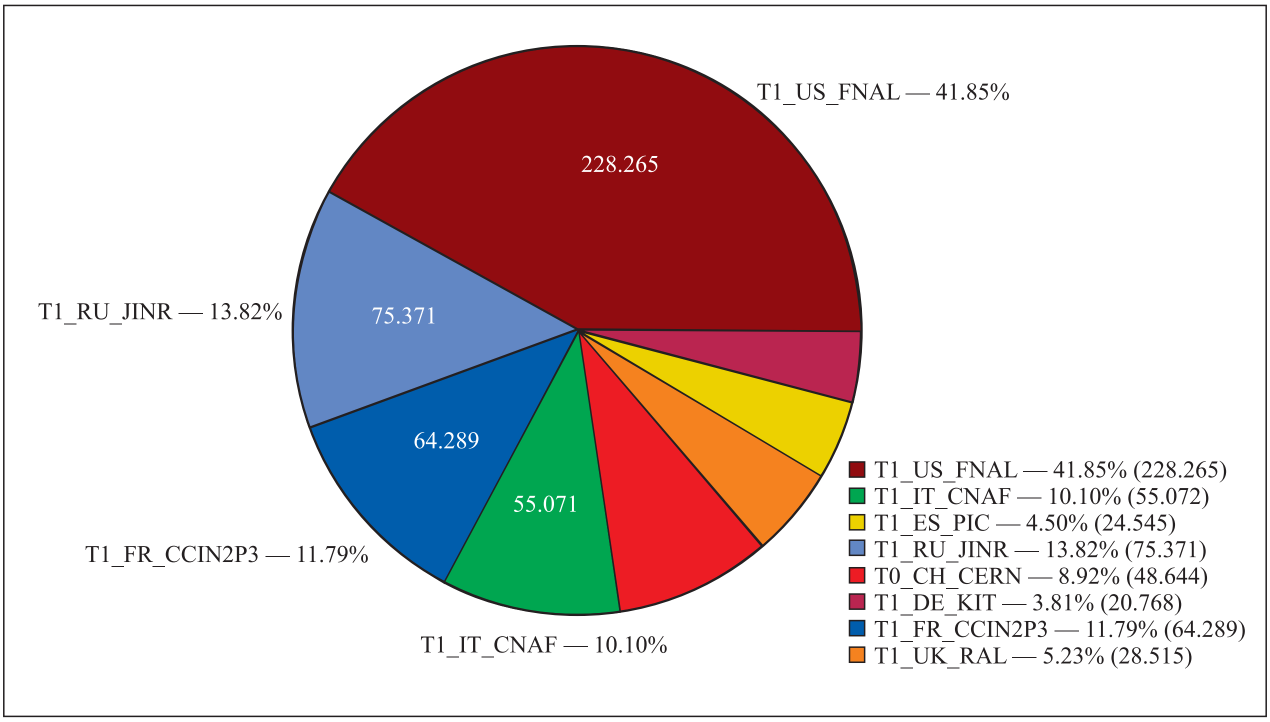

Fig. 1. Number of events processed for all CMS Tier-1 in MEvents in 2016 (sum: 545.470)

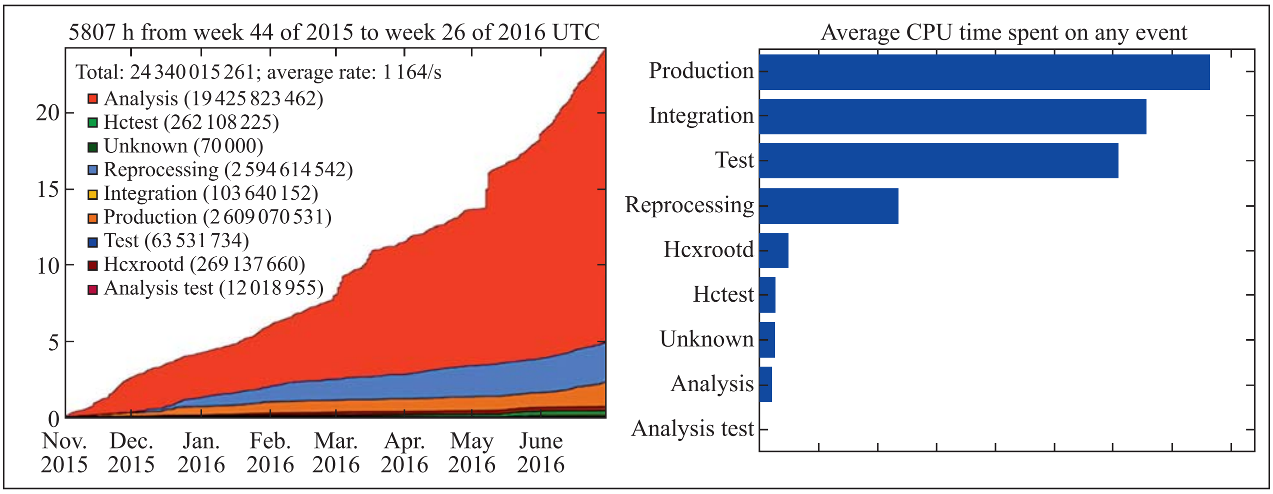

Fig. 2. Number of events processed at the JINR CMS Tier-1 in June 2016 by the CMS activities (production, integration, reprocessing, analysis, etc.)

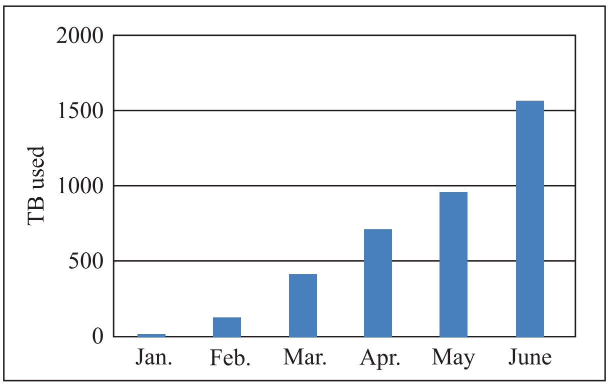

Fig. 3. JINR Tier-1 CMS tape robot load

587.46 TB for ALICE, 641.87 TB for ATLAS, 659.31 TB for CMS.

We are working on integration of OSG type Computing Element — HT-CONDOR in our WLCG Tier-2 infrastructure. At the moment, it is for STAR VO mainly but can be extended for supporting other VOs in the future.

The main users of the JINR grid resources are virtual organizations of all LHC experiments [2]. In 2016, this site executed 4 185 956 tasks (3 912 779 for LHC), CPU time being 186 711 011 h in HEPSpec06 units. Figure 5 summarizes data on using the grid site JINR-LCG2 by the virtual organizations within the RDIG/WLCG/EGI community in 2016.

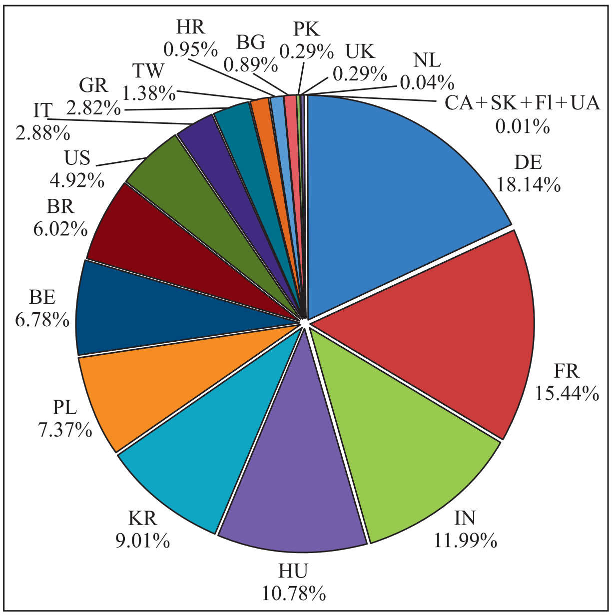

Fig. 4. The requests from the Tier-1 and Tier-2 centres to the JINR CMS Tier-1 for data in June 2016

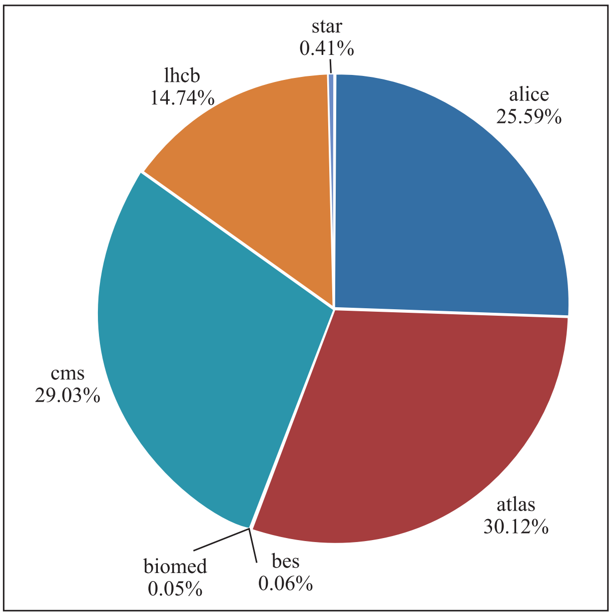

Fig. 5. Using the JINR-LCG2 grid site by virtual organizations within RDIG/WLCG/EGI

PanDA, production and distributed analysis system, manages tasks for ATLAS since 2005. Since that time the system has grown, and in 2013 the BigPanDA project started, aiming to prepare packets of PanDA which can be used outside the LHC. One of the experiments to which production management PanDA is being applied is COMPASS at CERN. The workflow of the experiment has to be changed to enable grid for production and user jobs. This year JINR as a computing site for COMPASS was connected through PanDA, i.e., the task was to allocate the space and define PanDA queue at JINR's computing infrastructure; define PanDA queues in other institutes participating in COMPASS and make their data analysis distributed [3].

The JINR MICC monitoring system provides real-time information about: work nodes, disk servers, network equipment, uninterruptable power supply elements, and cooling system. It can also be used for creating network maps and network equipment load maps, for drawing state tables and different plots. Special Control Room was equipped for operators of the MICC (see Fig. 6).

HappyFace monitoring system was installed and configured for the purposes of JINR Tier-1. It is a product developed in KIT for monitoring grid sites of CMS and ATLAS experiments. Currently, it is one of the key elements of JINR Tier-1 services monitoring (http://happyface.jinr.ru).

Development of the new service monitoring system for CMS Tier-1 at JINR was initiated. The system has a modular structure. The following modules were developed: Job Status — to determine the number of executed and aborted jobs; SSB Status — to collect monitoring results performed by WLCG Dash-

Fig. 6. Video Wall with HappyFace monitoring system at Control Room

board; PhedexQuality — to determine transfers quality from other grid sites and T1_RU_JINR; PhedexErrors — to determine Phedex errors connected to T1_RU_JINR. The test version of the service monitoring system was launched at lcgsens01o.jinr.ru. Now it aggregates and displays on the web page the data related to Phedex, dCache, and WLCG monitoring [4]. The system is developing as a general-purpose tool which can be adapted for other Tier-1 centers and experiments.

High-Performance Computer System. The multipurpose information complex at LIT provides carrying out computations, including the parallel ones, outside the grid environment. They are asked both by the experiments NOνA, PANDA, BES, NICA/MPD, etc., and the local users of the JINR laboratories. The JINR users and the grid users have an access to all the computer facilities via a unified batch processing system. Figure 7 gives the time distribution of the tasks executed on the computing cluster by the JINR subdivisions and the user groups. The main user of these resources is NICA/MPD (61.07% of astronomic time and 55.53% of processor time).

Systems of storage and access to data dCache and XROOTD ensure work with the data both for local JINR users and for the WLCG users and collaborations. Two dCache installations are supported: dCache-1 for experiments CMS and ATLAS; dCache-2 for local users, groups of users and international projects NICA/MPD, HONE, FUSION, BIOMED, COMPASS. Two installations of the XROOTD data access arrangement maintain work with the data of three international collaborations: ALICE, PANDA, and CBM. All the storage systems are constructed under the hardware data protection mechanism RAID6.

A system for grid and cloud services simulation of contemporary HENP experiments of the Big Data scale was developed. This simulation system is focused on improving the efficiency of the grid/cloud structures development by using the work quality indicators of some real system to design and predict its evolution. For these purposes the simulation program is combined with a real monitoring system of the grid-cloud service through a special database (DB). The DB accomplishes acquisition and analysis of monitoring data to carry out dynamical corrections of the simulation. Such an approach allows us to construct a general model pattern which should not depend on a specific simulated object, while the parameters describing this object can be used as input to run the pattern. The development of such kind software is very important for making a new grid/cloud infrastructure for such big scientific experiments as the NICA/MPD/SPD Tier-0/Tier-1 distributed computing [5, 6]. The NICA includes the BM@N experiment the first run of which is planned to be performed in 2017. Therefore, it is necessary to develop a computing system for distributed data storing and processing for the experiment. The simulation program SyMSim is used to choose a proper architecture of the BM@N computing system infrastructure. SyMSim facilitates making a decision regarding a required equipment [7].

Heterogeneous Computing Cluster HybriLIT. During 2016, the total performance of the HybriLIT cluster increased 1.8 times. At the moment, the computing component of the cluster contains four nodes with NVIDIA Tesla K80 graphical processors and four nodes with NVIDIA Tesla K40 accelerators, a node with Intel Xeon Phi 7120P co-processors, and a node with two

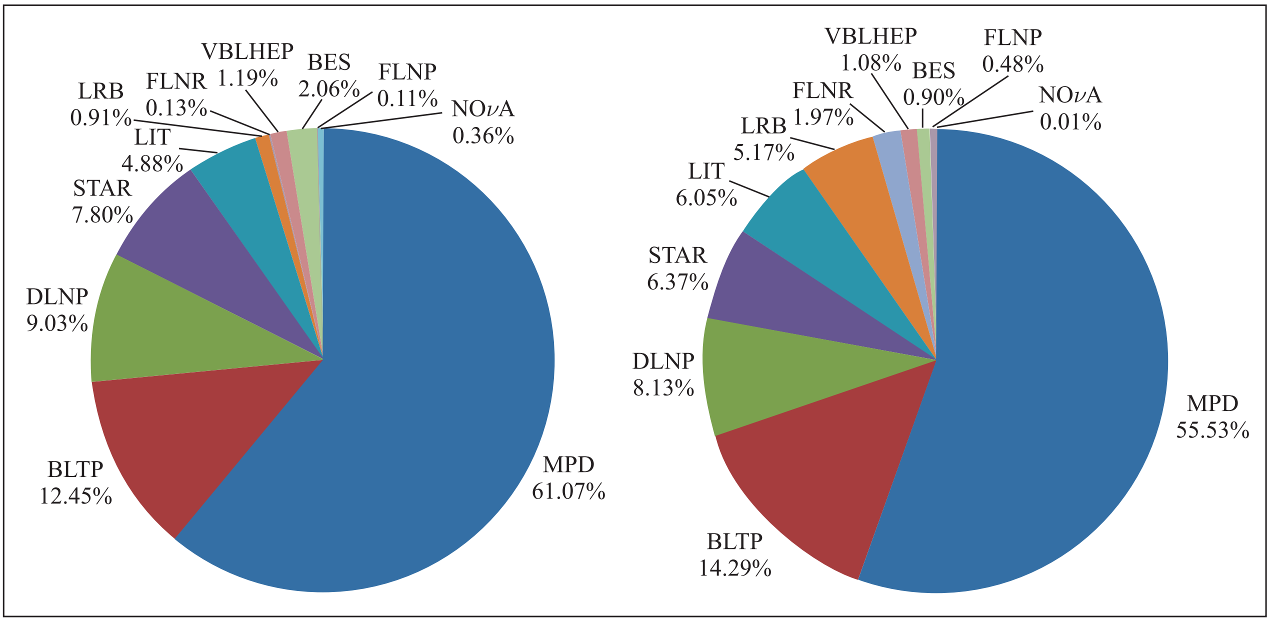

Fig. 7. Statistics of using astronomic (left) and processor time (right) of the computing cluster by the subdivisions and experiments of JINR without grid users

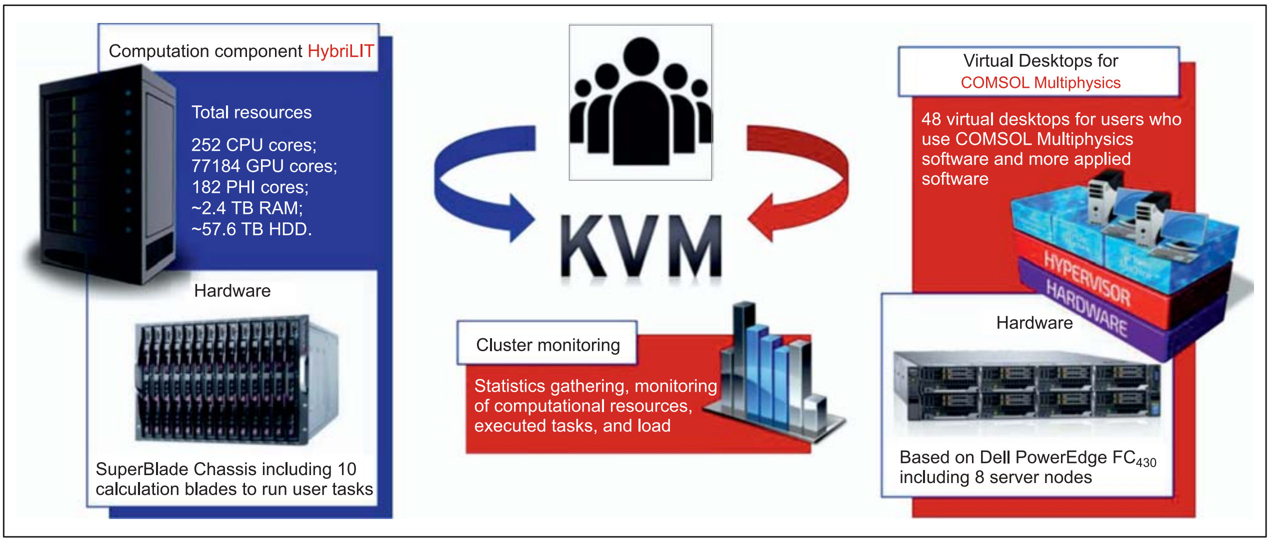

Fig. 8. The new component of the cluster to work with applied packages

types of computing accelerators NVIDIA Tesla K20x and Intel Xeon Phi 5110P. All the nodes have two multicore processors Intel Xeon. Overall, the cluster contains 252 CPU cores, 77184 GPU cores, 182 PHI cores; it has 2.4 TB RAM and 57.6 TB HDD, and its total capacity is 142 TFLOPS for operations with single precision and 50 TFLOPS for double precision.

In 2016, a new component was included in the cluster structure — a virtual desktop system to support users work with applied packages. Deployed was a polygon of eight servers where on the basis of KVM (Kernel-based Virtual Machine) virtual desktops with remote access to the package COMSOL Multiphysics for user groups have been designed. The developed new cluster's component allows the users to effectively utilize the cluster's resources conducting intensive calculations from the applied software packages on the computing nodes of the cluster (Fig. 8).

In 2016, the software and information environment of the cluster was actively maintained and developed allowing its users to develop software applications, to perform calculations with the help of the latest computational architectures. The total number of its users is 450 people from the JINR laboratories and the JINR Member States. In particular, the cluster resources are used for calculations in the field of quantum chromodynamics, quantum mechanics, and molecular dynamics. In addition, software PandaRoot, MpdRoot installed on the cluster allows one to perform calculations in high energy physics.

The heterogeneous cluster HybriLIT is used both to perform massively parallel computations and to learn how to use applied software packages and parallel programming technologies. During 2016, over 20 training courses were held, which were attended by over 200 specialists from various departments of the Institute, young scientists from the JINR Member States and Russian universities. The tutorials were dedicated to using applied packages MCTDHB-Lab, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), VMD (Visual Molecular Dynamics), and parallel programming technologies CUDA, OpenMP, OpenCL, and MPI. Tutorials and master classes were held during the 7th International Conference “Distributed Computing and Grid Technologies in Science and Education” (GRID'2016) and the JINR–CERN School “Grid and Advanced Information Systems”.

Cloud Environment. In 2016, the JINR cloud infrastructure [8] has been developing in the following directions: increasing the number of resources its users have access to; increasing the number of tasks it is used for; reimplementing an aggregation and visualization statistics on the cloud resources utilization using InfluxDB and Grafana software. The amount of the resources available for the JINR cloud users has been increased due to 1) maintaining additional servers as cloud nodes and 2) integration of part of computing resources of partner organizations clouds.

At present, the total number of CPU cores available for users in the JINR cloud is 330 (200 in 2015) and the total RAM is 840 GB (400 GB in 2015). The spectrum of tasks solved with the help of JINR increases. For this purpose, the following components have been installed on this infrastructure:

• PanDA testbed was deployed for PanDA software validation and extensions development for ATLAS and COMPASS experiments;

• DIRAC-based testbed (it is used for monitoring tools development for BES-III experiment distributed computing infrastructure as well as its computing facility);

• a set of VMs of NOνA experiment users for analysis and software development;

• NICA testbed for grid middleware evaluation for NICA computing model development;

• EOS testbed for research on heterogeneous cyber-infrastructures, computing federation prototype creation and development based on high-performance computing, cloud computing and supercomputing for Big Data storage, processing, and analysis;

• a standalone Spark instance for Machine Learning and Big Data analysis.

At present, one of the most important trends in the cloud technologies is the development of method of integrating various cloud infrastructures [9]. In order to join the cloud resources of partner organizations from JINR Member States for solving common tasks as well as to distribute a peak load across them, a cloud bursting driver has been designed by the JINR cloud team. It allows one to integrate the JINR cloud with the partner clouds either OpenNebula-based one (and in this case it is possible to enable real time external cloud resources monitoring) or any other cloud platform which supports Open Cloud Computing Interface (OCCI). The clouds of the following partner organizations from JINR Member States are integrated into the JINR cloud: Institute of Physics of Azerbaijan National Academy of Sciences (Baku, Azerbaijan); Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine (Kiev, Ukraine); Plekhanov Russian University of Economics — PRUE (Moscow, Russia). The geographical location of the partner organizations from JINR Member States whose cloud resources are integrated into the JINR cloud following the so-called "cloud bursting" model are shown in Fig. 9.

Besides, the JINR cloud is integrated into EGI Federated cloud thus enabling a possibility to use part of the JINR computing resources by EGI FedCloud Virtual Organizations.

Currently, one of the most important directions of the JINR cloud development is a reimplementation of an aggregation and visualization statistics on resources utilization. Initially it was done by JINR cloud team as an additional item in a menu of OpenNebula graphical web-interface (which is called "Sunstone"). However, a drawback of the implementation was a necessity to check the compatibility of that aggregation and visualization add-on against each new release of OpenNebula because its web-interface might be changed. It was needed to adopt the code of visualization module for the new Sunstone in case of its incompatibility. So in order to avoid such extra steps before software update on the JINR cloud as well as to store a collecting metrics in a database for further analysis against their changes over time and to obtain the dynamics for the selected period, it was decided to implement aggregation and visualization statistics on JINR cloud resources utilization using such tools as InfluxDB and Grafana software [10].

Information and Software Support. A traditional direction of the LIT activity in 2016 is the development and support of the program library JINRLIB as well as support of the program libraries (CERNLIB, CPC Program Library) developed by other research centres and organizations. The JINRLIB Web-site was renovated. A special section for parallel programs was added together with educational programs on parallel programming (MPI). The H-Utils package that is being developed at LIT for the HybriLIT users was included in the JINRLIB (http://wwwinfo.jinr.ru/programs/jinrlib/h-utils/index.html). This package contains a number of libraries and is aimed at help in solving general difficulties that the developers often face while creating software complexes for solving problems in the field of physics, chemistry, biology, etc. on high-performance computational platforms.

In the scope of the development of the JINR corporate information systems (CIS) [11], a subsystem of electronic coordination of orders on the basic activity has been developed and put into operation in the struc-

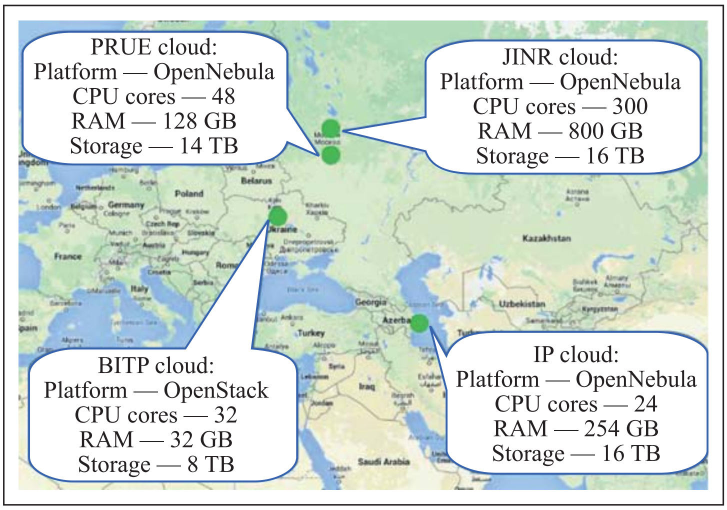

Fig. 9. Geographical locations of the partner cloud infrastructures from JINR Member States which provide part of their computational resources being integrated into the JINR cloud

ture of the system "Base of JINR documents"; a universal gateway for data exchange between different CIS subsystems 1C, EDH "Dubna", ADB2, ISS, PIN was implemented in 2016; work was in progress on enhancing the functionality of the information system of the NICA project management based on ADB system, implementation of functionality on the formation of Cost Book for the NICA project, realization of functionality on the formation of various consolidated reports on the project [12]; the development of the unified system 1C 8.2 UPP was in progress, a regular support of the end-users of the system also continued in 2016.

In 2016, the improvement of the software for the JINR Document Server (JDS) was in progress, namely, tools have been developed to speed up data entry, the quality of the content and efficient data reuse was improved. The work is carried out on the test server jds-test3 (http://jds-test3.jinr.ru), deployed in the cloud infrastructures of LIT JINR.

METHODS, ALGORITHMS AND SOFTWARE SUPPORT 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 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 of searching for tracks — candidates for event reconstruction in the experiment BM@N (Baryonic Matter at Nuclotron) — has been proposed. The event reconstruction is one of the most important tasks for experimental data processing in high energy physics. It consists of the tracks and their parameters evaluation in the tracking detectors of the experiment, which requires a huge number of searches of all the hits (reconstructed responses of the detector) to find those belonging to one track (see Fig. 1). The authors propose a new coordinate transformation that maps experimental data to the normalized coordinate space in which the hits corresponding to one track are grouped into compact horizontal segments. In order to estimate the parameters, the found tracks — the candidates — are approximated by Archimedes spirals. Due to the compactness of data in the space of normalized coordinates, the proposed algorithm can be effectively parallelized on modern computing architectures [13].

A computer program of the Glauber calculations for the NICA experiments has been proposed. It should be noted that all contemporary experiments with relativistic nuclear beams (RHIC, LHC, NICA, CBM) use and will use various methods of determining the geometrical properties of interactions, especially collision impact parameter. No impact parameter can be measured directly. That is why the experimental observable quantities are connected, in one or another manner, with the geometrical properties calculated within the Glauber approach. However, the existing methods of the Glauber calculations do not meet modern requirements. The proposed approach allows one to calculate the geometrical properties of interactions of gold nuclei with gold nuclei at RHIC and NICA energies (5–10 GeV in the center of mass of NN collisions) and to improve the result by 5–7% as compared to the currently used software. The changes of the physical characteristics of the NICA collisions can be related to changing the interaction physics [14].

A new segment building algorithm for the cathode-strip chambers has been developed. Results of comparison of the standard and new algorithm for various types of simulated data were obtained. Track segments are reconstructed with higher precision and efficiency using the new algorithm, especially for high luminosity on the LHC and high transverse momentum of particles passing through the muon endcap system. In July 2016, the algorithm was implemented in the official CMS reconstruction software package [15].

Effects of vector interaction in Nambu–Jona-Lasinio model with Polyakov loop have been studied in combination with entanglement interaction between quark and pure gauge sector. The QCD phase diagram was investigated. It has been found that the first-order chiral phase transition at the finite baryon chemical potentials and its critical point disappear at sufficiently large values of the vector interaction constant G_v. The presence of entanglement interaction between the quark and pure gauge sector leads to the increasing of value G_v when the first-order phase transition in the thermodynamic system disappears. The influence of nonzero G_v on the curvature of the crossover boundary in the $T-\mu$ plane nearby $\mu = 0$ is also examined for the cases of additional quark–gluon interaction and without it [16].

The Asynchronous Differential Evolution (ADE) method is applied to research on the drug delivery Phospholipid Transport Nano System (PTNS) in the scope of the Separated Form Factor model. Basic parameters of PTNS unilamellar vesicles are fitted to experimental data of the small-angle synchrotron X-ray scattering. The structure of PTNS nanoparticles has been analyzed depending on the maltose concentration in water. Numerical results confirm the efficiency of parallel MPI-implementation and the preference of the ADE-based global minimization in comparison to other popular optimizing procedures [17].

A new approach to the higher-order polynomial approximation (smoothing) based on the basic elements method (BEM) is proposed. The design of the BEM-polynomial is built on a three-point grid and depends on the control parameters x_0, $\alpha = x_\alpha - x_0$, $\beta = x_\beta - x_0$ related to the independent variable $\tau = x - x_0$ by a cross-ratio rule. The BEM polynomial of degree n is expressed using four basic elements given on the three-point grid: $x_0 + \alpha < x_0 < x_0 + \beta$, $\alpha\beta < 0$. Formulas for calculating the coefficients of the polynomial model of order 12 were obtained, depending on the interval length, the parameters α, β, and the derivatives $f^{(m)}(x_0 + \nu)$, $\nu = \alpha, \beta, 0$, $m = \overline{0, 3}$. Application of the higher-degree BEM polynomials for piecewise polynomial approximation of functions and data smoothing enhances the stability and accuracy of calculations when increasing the grid step and reduces the computing complexity as well [18].

Two conceptual developments in the Bayesian automatic adaptive quadrature approach to the numerical solution of one-dimensional Riemann integrals (*Adam Gh., Adam S. //* Springer LNCS. 2012. V. 7125. P. 1–16) are reported. First, it is shown that the numerical quadrature, which avoids the overcomputing and minimizes the hidden floating point loss of precision, asks for the consideration of three classes of integration domain lengths endowed with specific quadrature sums: microscopic (trapezoidal rule), mesoscopic (Simpson rule), and macroscopic (quadrature sums of high algebraic degrees of precision). Second, sensitive diagnostic tools for the Bayesian inference on macroscopic ranges, coming from the use of Clenshaw–Curtis quadrature, are derived [19].

A research was in progress at LIT on the problem of mathematical description of quantum correlations in composite systems. A problem of classification and correlations in systems being in the so-called X-states was studied within the mathematical framework of the classical theory of invariants by means of advanced methods of computer algebra. Quantum entanglement properties of a mixed two-qubit system in mixed X-states were analyzed in terms of local unitary invariant polynomials in the elements of the density matrix [20]. The structure of the ring of invariant polynomials was studied, and it is shown that for the X-states there is an injective ring homomorphism of the quotient ring of $SU(2) \times SU(2)$-invariant polynomials modulo its syzygy ideal and $SO(2) \times SO(2)$-invariant ring freely generated by five homogeneous polynomials of degrees 1, 1, 1, 2, 2. The separable mixed 2-qubit X-states are classified in accordance with degeneracies in the spectrum of density matrices [21].

APPLIED RESEARCH

LIT researchers, in cooperation with VBLHEP scientists, conduct the investigation on the behavior of the solution to the nonlinear boundary-value magnetostatic problem in the vicinity of the “corner point” (the intersection of two environments — vacuum/iron) of ferromagnet. The upper estimate for the acceptable growth of the magnetic field in the vacuum region near the corner point of the ferromagnet has been obtained. It is shown that under certain conditions imposed on the magnetic permeability the magnetic field within the vacuum region in the vicinity of the corner points is limited. An algorithm of thickening differential grid near the corner point has been developed. It allows one to significantly reduce the computation time and simultaneously increase the accuracy of the solution of the boundary value problem. The results of modeling the magnetic system containing corner points are presented. The problems of creating a homogeneous map of the field of possible solenoid-type magnetic systems of the NICA installation are analyzed. The computations were performed with the help of two software products, i.e., TOSCA and MFC (Magnetic Field Calculation), developed by the authors [22].

INTERNATIONAL COOPERATION

In cooperation with scientists from South Africa, the inclusive reaction ^{59}Co(p, α) at an incident energy of 100 MeV has been studied. A theoretical analysis based on a statistical multistep mechanism indicates that the terminal step leading to emission of an α particle can be a pickup or knockout process, in which both are very prominent. This is a conclusion which is in agreement with an earlier study of the ^{93}Nb(p, α) reaction. This inspires an investigation of the reason why a mixture of knockout and pickup is present at incident energy of 100 MeV, whereas at both higher and lower incident energies the knockout appears to dominate for the target nucleus ^{93}Nb. It has been found that the different dynamics of the two competing reaction mechanisms provides explanation for the observed phenomenon. It is speculated that for ^{59}Co at both lower and higher incident energies the trend is likely to be similar to that of ^{93}Nb [23].

In collaboration with scientists from research centers of the USA, the development of the workflows management system PanDA (Production and Data Analysis) has been proposed, which allows one to send tasks to HPC platforms. This development was tested on the Titan supercomputer (Oak Ridge Leadership Computing Facility, USA), supercomputer of the National Research Center "Kurchatov Institute", supercomputer IT4 (Ostrava, Czech Republic), and others. The testing has shown the possibility of using the modified PanDA WMS as a portal, independent of a computing infrastructure which can be used not only for solving intensive tasks of high energy physics and nuclear physics but also in other fields such as bioinformatics and astrophysics [24].

In 2016, in collaboration with colleagues from China and France work was in progress on the creation of a distributed computing environment for the experiment BES-III, which currently joins 12 resource centers from China, USA, Italy, JINR, and providing access to more than 3000 CPU cores and 0.5 PB disk space. In the current year, more than half a million tasks were executed in this distributed system. To date, the distributed data processing system of the BES-III experiment is reliable, it is a significant part of the computing power for experimental data processing [25].

CONFERENCES, WORKSHOPS

On 25–30 January, LIT hosted the 23rd International conference "Mathematics. Computer. Education". The conference has been held since 1993 and manifested itself as a productive form of exchanging experience between specialists in various scientific areas including mathematicians, biologists, economists, and teachers. 250 scientists from the JINR Member States and 32 cities of Russia, Ukraine, Belarus, and Kazakhstan attended the conference. A symposium "Biophysics of Complex Systems. Molecular Modeling. System Biology" was organized in the framework of the conference. Some sessions on mathematics, mathematical simulation and computing methods, biology, economy and pedagogy included oral and poster reports. Alongside with the traditional round tables, 11 master classes were organized to acquaint the conference participants with the bases of the modern high-level programming languages and their applications to modeling in solving research problems. The conference was traditionally brought to an end with a discussion of the work of the sections and awarding young participants with certificates for the best reports.

A traditional 19th two-day Workshop on Computer Algebra was held at LIT on 24–25 May. More than 40 scientists from universities and scientific institutes of Bucharest (Romania), St. George (Grenada), Tbilisi (Georgia), Turku (Finland), Moscow, Petrozavodsk, St. Petersburg, Saratov, Tambov, and Dubna took part in this workshop. Twenty-four reports were presented. The main goal of these workshops is to provide a forum for researchers on computer algebra methods, algorithms and software and for those who use this tool in theoretical, mathematical, and experimental physics. A number of new promising results on the development of algorithms for investigating and solving systems of algebraic, differential and difference equations, on symbolic-numeric simulation of quantum-mechanical systems, as well as on computation of multiloop Feynman integrals by computer algebra methods and on various computer algebra applications to physics and mathematics, were presented.

On 4–9 July, LIT hosted the 7th international conference "Distributed Computing and Grid Technologies in Science and Education" (GRID'2016). The conference is held every two years and is traditional for the Laboratory. This year the conference was dedicated to the 60th anniversary of JINR and the 50th anniversary of LCTA/LIT. Note that the GRID'2016 conference is a unique platform for discussing a wide range of issues related to the use and development of distributed grid technology, heterogeneous and cloud computing in various fields of science, education, industry, and business. The conference attracted a large community of Russian and foreign specialists ready to discuss emerging challenges and prospects of the development of advanced information technology. The conference was attended by more than 250 scientists from the research centers of Azerbaijan, Belarus, Bulgaria, Germany, Georgia, China, Moldova, Mongolia, Romania, Slovakia, Czech Republic, Chile, France, Sweden, etc. Russia was represented by participants from more than 30 universities and scientific research centers. The conference was organized in ten sections which discussed the issues related to the development of grid technologies, heterogeneous computing, volunteer computing, cloud computing, big data analytics. Also, during the conference a school for young scientists, postgraduates and students was organized, where tutorials on heterogeneous and cloud computing were conducted. In total, the conference participants heard 35 plenary, more than 120 oral, and 43 poster reports. Forty students and young scientists from Mongolia, Romania, and the Russian universities (MEPhI, St. Petersburg State University, and University "Dubna") attended the school.

On 24–28 October, the 7th school on information technologies "Grid and Advanced Information Systems at CERN" organized by the Joint Institute for Nuclear Research and the European Organization for Nuclear Research (CERN) and supported by the National Research Nuclear University "MEPhI" and the Plekhanov Russian University of Economics was held at LIT. The School was attended by over 90 students as well as masters and post-graduates from Russia and Kazakhstan. The students attended lectures on modern information technologies delivered by the leading specialists of CERN and JINR. On the basis of the materials of the lectures, trainings and competitions were organized, the winners were awarded with prizes.

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