LABORATORY OF INFORMATION TECHNOLOGIES

The investigations performed at the Laboratory of Information Technologies during 2015 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 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.

A presentation of the Tier-1 level centre for the CMS experiment at the Large Hadron Collider (LHC) took place at LIT on March 26. This centre is a basic JINR facility, it provides the physicists of the Institute, JINR-participating countries and RDMS-CMS collaboration with the opportunity of a full-scale participation in processing and analysis of data coming from the CMS experiment. When creating the centre, the engineering infrastructure (uninterrupted power supply, climate control, etc.), a high-speed reliable network infrastructure with a dedicated reserved channel to CERN (LHCOPN), a computing system (2400 computing nodes) as well as a storage on the basis of disk arrays (2.4 PB) and tape libraries of big capacity (5 PB) have been developed. These systems provide a 100% reliability and availability of the centre.

The multifunctional centre for storing, processing and analysis of data launched on the base of the JINR Central Information and Computer Complex (CICC) provides a wide spectrum of possibilities for its users on the basis of its components: a grid-infrastructure of levels Tier-1 and Tier-2 to support experiments at the LHC (ATLAS, ALICE, CMS, LHCb), FAIR (CBM, PANDA) and other large-scale experiments (NICA); a general-purpose computing cluster; a cloud computing infrastructure; a computing cluster with heterogeneous architecture HybriLIT; an educational and research infrastructure for distributed and parallel computations.

In 2015, LIT researchers published 155 scientific papers in peer-reviwed journals and presented 30 reports at international and Russian conferences.

INFORMATION AND COMPUTING INFRASTRUCTURE OF JINR

During 2015, work related to the reliable operation and development of the JINR networking and information 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 that on the basis of cloud, grid and hybrid technologies, integrating information resources of the Institute into a unified environment accessible to all users.

JINR Telecommunication Data Links. In 2015, the reliable operation of the high-speed computer communication channel Dubna–Moscow was ensured. The connection with scientific networks and Internet was provided using the following telecommunication links: LHCOPN/CERN (10 Gbps), RBnet (10 Gbps), E-arena (10 Gbps) and Russian scientific networks (10 Gbps), RUNNet and international scientific networks (10 Gbps). The throughput of the reserve data link was increased up to 10 Gbps and was improved at the expense of the additional router Cisco7606-S. The opportunity of modernization of the external data link up to 100 Gbps has been studied. Table 1 shows the distribution of the incoming (more than 3 TB) and outgoing traffics in 2015 over JINR subdivisions.

Table 1

Subdivision	Incoming, TB	Outgoing, TB
DLNP	107.45	48.49
VBLHEP	74.46	66.31
General access servers	60.29	11.11
LIT	52.08	27.19
FLNP	42.98	57.24
JINR Hotel & Restaurant Complex	25.47	4.4
FLNR	23.61	4.12
BLTP	23.22	16.35
JINR Management	20.92	61.44
Node of remote access	19.65	5.09
University “Dubna”	12.12	8.38
VG Computers	11.9	1.64
Joint Stock Company “Dedal”	10.98	4.46
Medical-Sanitary Unit 9	9.84	1.02
LRB	7.01	2.86
Joint-Stock Company “Atom”	3.76	0.33

In 2015, the overall incoming JINR traffic, including the general access servers, Tier-1, Tier-2 and CICC, amounted to 4.3 PB (3.3 PB in 2014). 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). The LHCOPN throughput between Tier-0 and Tier-1 and between Tier-1 and Tier-1 is 10 Gbps.

JINR Local Area Network. In 2015, 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 continued. The work on introduction of the 10 GB network has covered approximately 80% of the networking equipment of the Laboratories.

In the framework of the user’s computer environment support, the scheduled work has been done on enhancement of the mail, webmail, proxy, e-lib and authorization services. Work has been started 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. New rules of work in the network have been prepared and approved for the JINR users. At present, preparation is in progress on transition of the JINR network to a new standard of network addressing 1Pv6.

In 2015, the JINR LAN included 7806 network elements and 12555 IP addresses; 4129 users were registered within the network. There were more than 1500 users of mail.jinr.ru service as well as 1480 users of digital libraries and 641 remote VPN users.

Multifunctional Centre for Data Storage, Processing and Analysis. In 2015, work was progressing on launching a multifunctional information-computer complex at JINR. Its main task is to expand the set of computing services provided for the user. It involves the following elements:

- automated data processing system for the CMS experiment at the LHC of the Tier-1 level;
- grid infrastructure of the Tier-2 level to support LHC experiments (ATLAS, ALICE, CMS, LHCb), FAIR (CBM, PANDA) and other large-scale experiments and projects within the global grid infrastructure;

Table 2

Scientific and educational networks, %	File exchange (p2p), %	Web-resources, %	Social networks, %	Software, %	Multimedia, %
91.33	4.86	2.77	0.67	0.36	0.01

• high-performance computing system (including the parallel ones) outside the limits of heterogeneous and grid systems;
• heterogeneous computer complex;
• cloud environment.

JINR Grid Environment. In 2015, a Tier-1 centre for the CMS experiment at the LHC was launched [1]. It is one of the eight such centres worldwide. It provides the physicists of the Institute, its participating countries, RDMS-CMS collaboration, and the whole CMS collaboration with the opportunity of a full-scale participation in the processing and analysis of data coming from the CMS experiment. The experience gained in LIT at the creation of the Tier-1 centre will be used in the development and introduction of the information environment of storage and data processing of the NICA megaproject and other large-scale projects of the JINR Member States. During 2015, this centre performed 1 362 474 tasks, using a normalized CPU time of 141 753 061 h in HEPSpec06 units. Figure 1 gives the contribution of the Tier-1 global centres to the CMS experimental data processing for the last months of 2015. The JINR Site takes one of the leading ranks in the world as to its productivity.

In 2015, 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 computer cluster, as a grid site JINR-LCG2 of the global grid infrastructure, supports computations of eight virtual organizations (alice, atlas, biomed, cms, dteam, fusion, hone, and lhcb) and provides possibilities for using grid resources for the experiments BES and PANDA as well. At the moment, the cluster comprises 2560 64-bit processors and 1800 TB disk data storage. The central CICC network router is connected to the main border router of the JINR network at the Ethernet rate of 10 GB. The main users of the JINR grid resources are virtual organizations of all LHC experiments. In 2015 this site executed 4 666 405 tasks, CPU time being 171 418 826 h in HEPSpec06 units. Figure 2 summarizes data on using the grid site JINR-LCG2 by the virtual organizations within the RDIG/WLCG/EGI in 2015.

During 2015, the data storage systems of the JINR grid centre comprising two grid sites (JINR-LCG2 and JINR-T1 in terms of the WLCG project) of the global WLCG infrastructure performed in the following way: data volume transferred from the JINR to all world grid sites (USA, France, Switzerland, Canada, etc.) is 3215 TB for the CMS experiment and 308 TB for the ATLAS experiment, while the data volume received by the JINR is 3052 TB for the CMS experiment and 351 TB for the ATLAS experiment.

Throughout 2015, JINR grid centre data storage systems were in active use by the users from JINR member and associated states in the framework of their participation in the ALICE, ATLAS and CMS projects. For CMS, 815 TB of data were transferred from the JINR and 654 TB were transferred to the JINR, including Italy — 330 and 348 TB, respectively, Germany — 408 and 286 TB, Russian Federation — 37 and 5 TB, Ukraine — 23 and 3 TB, Hungary — 14 and 9 TB. For ATLAS, 72.5 TB of data were trans-

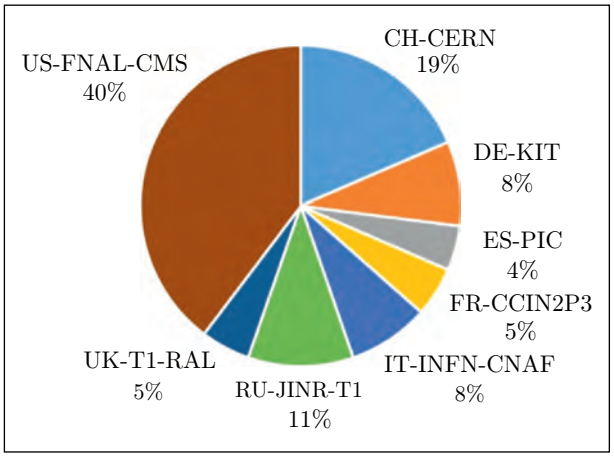

Fig. 1. Usage of the Tier-1 centres by the CMS experiment

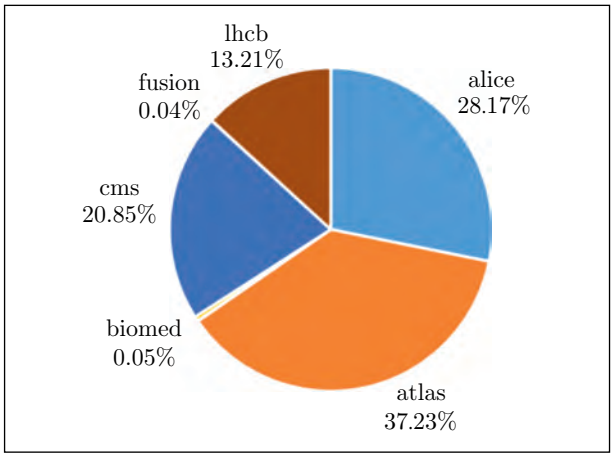

Fig. 2. Using the JINR-LCG2 grid site by virtual organizations within RDIG/WLCG/EGI

ferred from the JINR and 66 TB were transferred to the JINR, including Germany — 24 and 28 TB, respectively, Russia — 32 and 20 TB, Italy — 13 and 14 TB, Czechia — 0.5 and 2 TB, Romania — 1 and 1 TB, Slovakia — 1.5 and about 0.5 TB; also there was data exchange with grid sites from Armenia and South Africa. Data of the ALICE experiment (more than 300 TB) were transferred from the JINR and 2 TB were transferred to the JINR, including Russia — about 300 and 2 TB, respectively; 2 TB were transferred to Italy and 2 TB to Romania, also there was data exchange with grid-sites from Czechia, Germany, South Africa, Slovakia, and the Ukraine.

A new monitoring system of the JINR computer complex has been put into operation, and a centre of control and management over its operation has been launched. For the reliable functioning of the whole computer complex, it is necessary to trace in real time the status of all its units, stating with the power supply and ending the robotized tape library. At present, 690 elements of the computer complex are monitored and 3497 checks are performed in real time. The monitoring allows exhaustive control over the functioning of the system, visualization of the state of the computer complex and sends notifications about failures in the form of e-mail message, SMS, etc. [2]. Figure 3 represents one of the screens of monitoring which shows the functioning of the elements of the computing cluster.

Work on the support and development of services of the PanDA platform includes investigations on using network metrics for decision making (the dynamic clouds mechanism) due to services responsible for the network metrics delivery. The update of services which deliver those metrics to PanDA's information system was performed. The transfer of COMPASS' workflow to PanDA was in progress. In collaboration with Nizhny Novgorod University, works were undertaken on the PanDA server installation at JINR and on running a PanDA queue for job submission to the cluster of this university [3].

High-Performance Computer System. The Multipurpose Information Complex at LIT provides carrying out computations, including the parallel ones, outside the grid environment. These are asked both by the experiments NOVA, PANDA, BES, NICA/MPD, etc. and the local users of the JINR Laboratories. The JINR users and the grid users have access to all the computer facilities via a unified batch processing

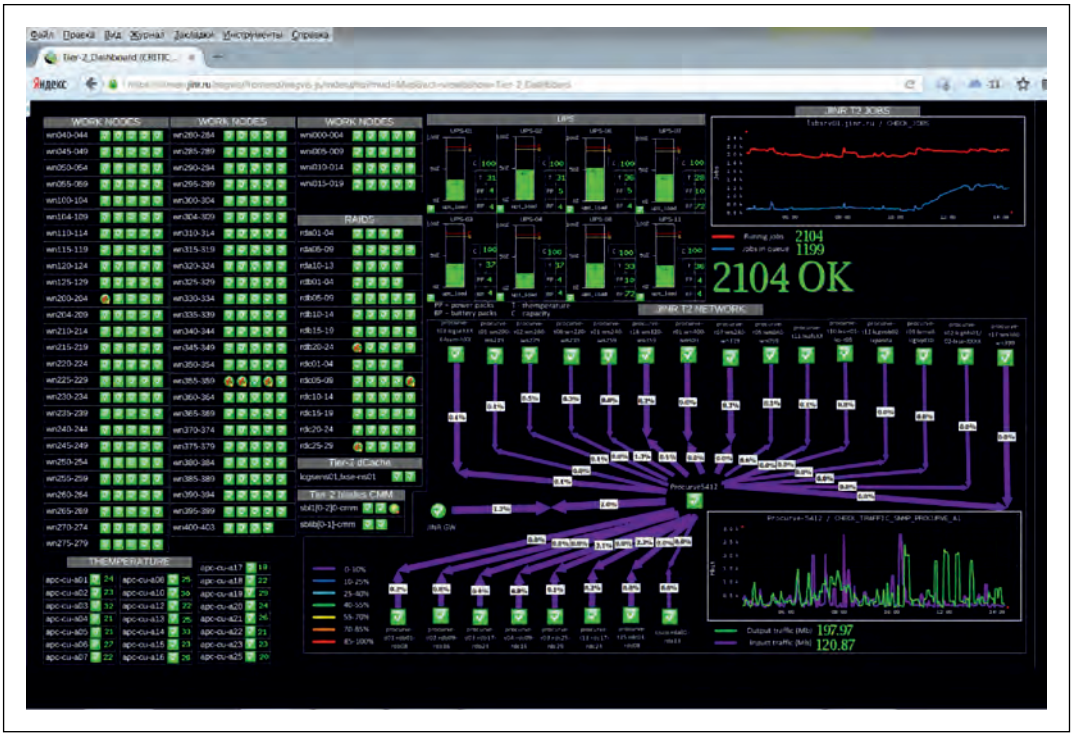

Fig. 3. The cluster component monitoring screen that shows in real time the current state and provides check-up of the computing servers (WN), disc arrays (RD), cooling panels (APC) switches and routers as well as the load of the network of the computing complex and the load of the uninterrupted power supply (UPS), a number of tasks executed by the complex (2104) and a job queue (1199)

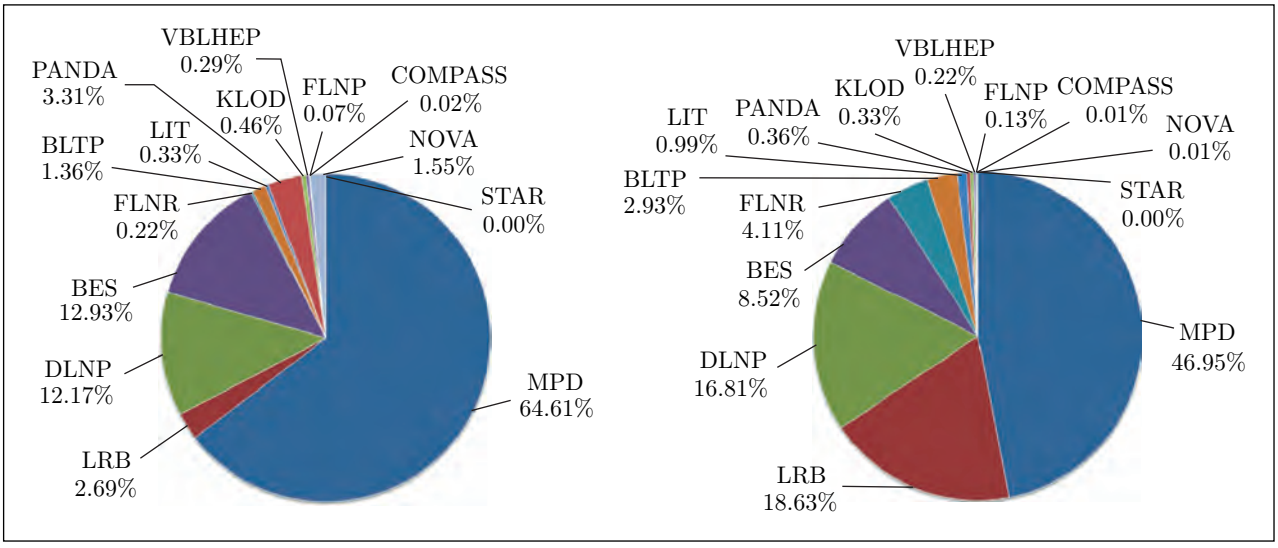

Fig. 4. Statistics of using astronomic (left) and processor time (right) of the computing cluster by the subdivisions and experiments of JINR without grid users

system — batch. In 2015, 903 staff members were registered as users of the computing cluster (apart from the grid users). Figure 4 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 (64.6% of astronomic time and 46.9% 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 the experiments CMS and ATLAS; dCache-2 for local users, groups of users and the international projects NICA/MPD, HONE, FUSION, BIOMED, COMPASS. Two installations of the XROOTD data access arrangement maintain work with data of three international collaborations: ALICE, PANDA and CBM. All the storage systems are constructed under the hardware data protection mechanism RAID6.

Computing Cluster with a Heterogeneous Architecture HybriLIT. In 2015, the heterogeneous structure of the computer complex was actively developed. Its computing capacity was increased to enable parallel applications for solving a wide range of mathematical resource-intensive tasks with the use of all possibilities of multicore components and computation accelerators. For instance, in 2015 the performance of the cluster increased 1.5 times at the expense of including two computing nodes with graphic accelerators of the last generation NVIDIA K80. Figure 5 shows the current configuration of the cluster which consists of two computing nodes with two graphic processors NVIDIA Tesla K80, four units with three GPU NVIDIA Tesla K40 (Atlas) in each, a unit with two co-processors Intel Xeon Phi 7120P as well as a unit containing NVIDIA Tesla K20x and a co-processor Intel Xeon Phi 5110P. Each computing node contains two 12-core processors Intel Xeon E5-2695v2. In total the

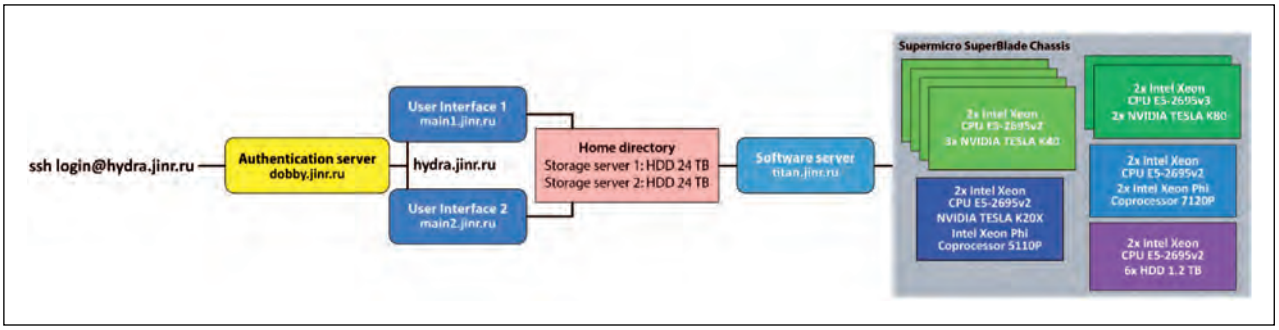

Fig. 5. The structure of the HybriLIT heterogeneous computing cluster

cluster contains 216 CPU cores, 57 216 GPU cores, 182 PHI cores; 896 GB RAM; 57.6 TB HDD. The cluster's full productivity is 111 TFLOPS for single-precision computation and 240 TFLOPS for double-precision computation. During 2015, the number of users doubled to reach 120 researchers from JINR and its Member States as well as from Russian universities. The HybriLIT cluster was intensively used for computations using computational accelerators for dedicated software development as well as for performing resource-demanding computations with the use of the packages of applied software and mathematical libraries already adapted to hybrid architectures.

Now HybriLIT is used not only for parallel calculations but also as a polygon for training students, postgraduate students and young scientists in the field of parallel programming technologies. During 2015, on the basis of the cluster, training courses were carried out in the framework of conferences and schools held by LIT (MMCP'2015, NEC'2015, AIS GRID'2015) within programs on international cooperation at Sofia University and the Mongolian State University. On its basis, regular training courses and tutorials for the JINR employees are held. As part of the regular training courses on parallel computing technologies organized at LIT for the JINR employees, students and postgraduates of the University "Dubna", the heterogeneous computations team HybriLIT held tutorials on C/C++ program languages, ROOT/PROOF program packages parallel programming technologies CUDA, OpenMP, OpenCL, MPI as well as on the user-friendly GitLab web-interface for mutual parallel development of applications.

Cloud Environment. In 2015 the modernization and upgrade of the JINR cloud infrastructure was continued (http://cloud.jinr.ru). The LIT JINR cloud infrastructure is based on OpenNebula software. In order to minimize the service downtime by increasing its reliability and availability, the JINR cloud was built in a highly available (HA) configuration (Fig. 6).

Currently the JINR cloud has 40 servers running 200 cores, 400 GB RAM and 16 TB disk space. The JINR cloud usage [4] is developed in three main areas:

- for testing, educational and research tasks as part of participation in various projects;
- systems and services deployment with high reliability and availability requirements; and
- extension of computing capacities of the grid infrastructures.

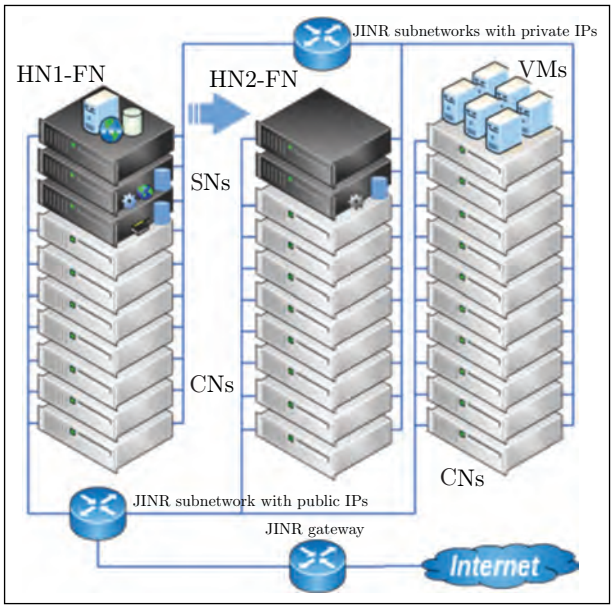

Fig. 6. The scheme of the JINR cloud in configuration of high reliability and availability: HN1-FN, HN2-FN — physical servers with components of the cloud front-end machine (FN), CNs are cloud working nodes on which the virtual machines (VMs) are placed; SNs — datastore units

The services and testbeds currently deployed in the JINR cloud are the following: EMI-based testbed (it is used for trainings, testing, development and research tasks related to grid technologies as well as for fulfilling the JINR obligations in local, national and international grid projects such as, e.g., WLCG); PanDA testbed which is used for PanDA software validation and extensions, developments for the ATLAS and COMPASS experiments; DIRAC-based testbed (it is used for monitoring tools development for BESIII experiment distributed computing infrastructure and also as its computing facility); a set of VMs of NOvA experiment users for analysis and software development; NICA testbed for grid middleware evaluation for the 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; HybriLIT services (Indico — a service for event organization, archival and collaboration; FreeIPA — an integrated identity and authentication service used for user accounts management in HybriLIT; Git — local Git repository (well-known distributed revision control system) for HybriLIT team); Helpdesk (a web application for the day to day operations of an

IT environment including user technical support of JINR IT services); DesktopGrid testbed based on BOINC software (to estimate the volunteers' computing technology for possible use in solving JINR users' tasks); web-service HepWep (provides opportunities to use different tools for Monte-Carlo simulation in high-energy physics); test instances of the JINR document server (JDS) and JINR Project Management Service (JPMS); CT for web-sites development including new JINR web-portal; JINR GitLab — local GitLab installation for all JINR users; Hadoop testbed; a set of users' VMs and CTs which are used for their own needs; a set of CTs for evaluation of various monitoring software to be used for the JINR Tier-1 grid site monitoring system development.

In order to join resources in the framework of cooperation on joint projects, integration of the JINR cloud with the cloud of the Plekhanov Russian University of Economics, the Institute of Physics of Azerbaijan National Academy of Sciences (Baku) and the Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine (Kiev) has been done, and the work is in progress with the European cloud infrastructure EGI Federated Cloud.

Information and Software Support. Within the NICA project the information control system of the NICA project, (ADB2-EVM) is actively developed at LIT. A flexible instrument was created for expansion of the existing system ADB2-EVM for the NICA project, it was elaborated during the work on the APT EVM system. In the framework of the development of an IS of the NICA project management, functional opportunities have been implemented: control over a hierarchical structure of the project (WBS), planning and re-planning activities on the project; work with baselines; tracing the process of the project realization on indices of actual costs (AC), on input of parameters of the budgeted cost of work performed (EV — the earned value or the volume of the work fulfilled); regular notification of users by e-mail (for timely reporting the progress of the work); account forms (graphics) according to ADB2-EVM (earned value management) procedure; financial statements on the project due to the "annual window" as a basic structure of the JINR budget and schedules of payments on the project activities, a hierarchical structure of users access rights, Web-interface. Also, in 2015 work was in progress on the expansion of the functional opportunities of the scheduling unit by way of integrating the ADB2 and MS Project Prof. The possibility of selecting alternative variants of profiles of the work schedule has been added.

Another direction of the project NICA support at LIT is related to the dynamic simulations of all the processes included in the store, transfer and analysis of data for the computer infrastructure of this project. The SyMSim (Synthesis of Monitoring and SIMulation) program has been designed for modeling a grid-cloud environment. The originality of this approach consists in integration of the process of modeling the information computing environment with real data monitoring of grid-cloud environments (example — the Tier-1 centre at JINR) in the framework of one program. The results of modeling the computer system for NICA experiments consisting of Teir-0 and Tier-1 centres allow one to draw conclusions about the optimal relationship between the number of processors and the storage systems for data processing. Solutions are aimed at modeling problems and subsequent development of data storages [5]. Within the project, a new system of modeling grid and cloud services has been created which integrates monitoring, analysis of its results and simulation itself. The objects of the simulations are the computing facilities intended for processing information of tens of petabytes per year [6].

The main work within the development of the unified information platform 1C 8.3 UPP was directed toward the inclusion into the system of the self-supporting subdivisions of JINR. In 2015 the following subdivisions were added to 1C 8.3 UPP: Department of Chief Power Engineer (DCPE), Motor Transport Service (MTS), Repair-Building Management (RBM), Social Infrastructure Management, Hotel-Restaurant Complex Management (HRCM), and the boarding house "Dubna". The primary book-keeping, time-keeping and human resources records management have been started simultaneously. Automatic calculation of the cost price of release in RBM, MTS and DCPE was adjusted. During 2015 the calculation of the wages was centralized which in turn allowed one to increase the rate of preparing the reporting in various funds (Pension Fund of Russia, Social Insurance Fund). In the HRCM a module of accounting the available housing facilities of the Institute was started. The human resources management was provided with a module on accounting cards of special estimation of working condition (SEWC); a unified electronic database of cards was generated. There were modernized all personnel documents and documents of the

Department of Labor Protection and Wages for accounting the results of SEWC cards.

In 2015, a subsystem of the electronic coordination of orders on the basic activity was developed and put into operation as part of the system "Base of JINR Documents". Besides, in 2015, a first run of the high-grade system of electronic document circulation (EDC) "Dubna" was developed and put in trial operation. In the development of the EDC "Dubna" applied were technologies and tools earlier developed in cooperation with CERN and successfully used for the creation of the systems of automating administrative activity in CERN and JINR. These tools allow one to create, in a short period of time, complex and flexible web-applications with friendly user interfaces. A document "Application for purchase of production" has been started in the system.

The support and development of the software for the automation of information and JINR library activities was continued in 2015. This includes filling and support of digital collections of JINR STL newsletters, support of digital catalogs, support of the on-line service "Electronic Mailing STL Weekly Newsletters". In 2015 the support of Open Access repository JINR Document Server was in progress: filling and verification of collections, output format settings, Authority Records module setting and testing.

During 2015, work was in progress to update the software environment, databases and contents of the LIT and JINR information sites http://lit.jinr.ru, http://www.jinr.ru, http:/wwwinfo.jinr.ru, faxe.jinr.ru, ptp.jinr.ru, and pkp.jinr.ru. In cooperation with JINR STD AMS, work continued on modernization of software related to scientific and administrative activity. Also, within theme 05-8-1037-2001/2019 work was in progress to update the 2015 database for "The System of the Interactive Formation of a Topical Plan for Research in Scientific Organizations" (with reference to JINR): the site ptp.jinr.ru. Maintenance and modernization of the web-portal of journals "Physics of Elementary Particles and Atomic Nuclei" and "Particles and Nuclei, Letters" continued in 2015 (http://pepan.jinr.ru/). Regular work was traditionally conducted on the design and support of various information websites, sites of conferences, workshops, and symposia organized by JINR Laboratories as well as organization of a website hosting (upon request). Among them are web-portals for FLNP (ISINN), FLNR (EXON-2016), LRB (MPGRRE-2015), etc.

Since May 2015, works have been underway (in cooperation with the JINR International Department) on launching a specialized information system User Office that provides online support of the process of receiving visitors to 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 program code widely applied at RHIC and LHC for calculations of geometrical properties of nucleus–nucleus interactions has been adapted for the experiments NICA/MPD and CBM. A parameterization of *pp* elastic scattering amplitude proposed earlier is used for setting the nucleon–nucleon collision profile. An approach well known in physics of low and intermediate energies is used for determination of nuclear parameters. The code is enlarged by a possibility to account for Gribov inelastic screening [7].

A new algorithm of the track-segment reconstruction in the cathode-strip chambers of the CMS experiment has been developed and tested. As seen from Fig. 7, on the Monte Carlo data with TeV muons the efficiency of the track-segment reconstruction of the suggested algorithm is 4–7% higher. It practically does not decrease with the growth of the pseudorapidity in contrast to the standard algorithm [8].

Estimations of the spatial resolution in the CMS cathode-strip chambers have been obtained using the LHC experimental data of 2015, in agreement with the results obtained in 2012. The resolution (from 64 down to 50 μм) in the bottom part of the chamber ME1/1 after separating the coupled signals from the strips has been significantly improved. The computations performed based on Monte Carlo data for the future collider HL-LHC have shown that the trigger loadings in ME1/1 chambers due to hadron penetrating radiation will increase 30 times as compared to the experimental data of 2012. This will demand additional technical

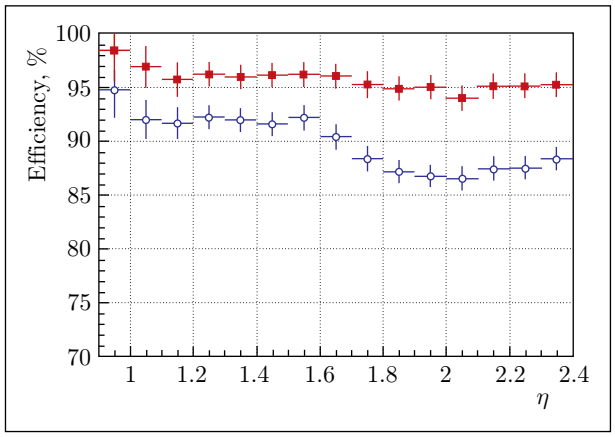

Fig. 7. Efficiency of the track-segment reconstruction in cathode-strip chambers depending on the pseudorapidity for simulated TeV muons: the results of reconstruction with a standard algorithm (blue), with a new algorithm (red)

solutions, for instance, increase in the thickness of the calorimeter absorber [8].

An algorithm of the particle trajectories reconstruction in drift chambers has been developed and implemented for the BM@N experiment so the "noisy" channels were eliminated. Besides, the geometrical alignment of the chambers was achieved (at the software level). Estimations of the spatial resolution and efficiency of the drift chambers, as well as of the Nuclotron beam pulse, were given.

An algorithm of the charged particle track reconstruction based on Kalman filter has been proposed. This algorithm is used for solving one of the key tasks of the CBM (Condensed Baryon Matter) experiment, i.e., recognition of the charged particle trajectories and their parameters. Since within the CBM experiment the full reconstruction of signal events in real-time experiments is planned, the developed algorithms should be fast and they have to maximize the capabilities of present-day multi-core processors and GPU architectures. Computations were performed with a high-performance server with two processors Intel Xeon X5660 and a graphic card Nvidia GTX 480 [9].

A model of microscopic optical potential (OP) has been applied to construct the pion-nucleus differential cross sections of elastic and inelastic scattering on the nuclei ^{28}Si, ^{58}Ni, ^{208}Pb at $T_{\rm lab} = 291$ MeV. The density distributions of ^{10}Be and ^{11}Be nuclei obtained within the quantum Monte Carlo model and the generator coordinate method are used to calculate the microscopic optical potentials (OPs) and cross sections of elastic scattering of these nuclei on protons and ^{12}C. To analyze the inelastic scattering cross sections, the parameters of the πN amplitude in a nuclear medium obtained earlier from the analysis of data of elastic scattering on the same nuclei have been used. The well-known energy dependence of the volume integrals is used as a physical constraint to resolve the ambiguities of the parameter values. The potentials can be used in further calculations of cross section of the reactions with these participating nuclei [10].

A new Bayesian analysis was suggested using independent mass and radius constraints for extracting probability measures for realistic models of cold dense nuclear matter equations of state. One of the key issues of such an analysis is whether a deconfinement transition in core of compact stars proceeds as a crossover or rather first-order transition. The latter is relevant for the possible existence of a critical endpoint in the QCD phase diagram under scrutiny in present and upcoming heavy-ion collision experiments such as MPD (NICA) and CBM (FAIR). Due to this problem, the question of the existence of mass twins (the third-family stars) — two stars with the same mass but different structures — is getting interesting. Using the constructed hybrid EoS based on APR-type hadronic models (without and with baryonic excluded volume effect) and bag model for the quark phase, a probabilistic estimation has been made on the basis of observational constraints. For the analysis used were the constraints for the mass of configuration taken from observation of one of the massive pulsar PSR J0348+0432 and for radius of PSR J0437-4715. Calculations show that the high-mass twin stars configurations have the highest probability measure [11].

A theoretical approach earlier used to calculate double photoionization of a binuclear nitrogen molecule N_2 was extended to grasp the processes of photoionization of the three-centered molecule CO_2 in which a dissociation dication $CO_{22}+$ is generated. The electron bound states are described in terms of Dyson orbitals, and the emitted electrons are simulated by a parametrized correlated three-center function of continuum. Differential scattering cross sections are studied when detecting emitted electrons on concurrence. Orientation of the internuclear axis of CO_2 molecule is left arbitrary. A comparison of the obtained results with a Gaussian parametrized model demonstrates similarities and distinctions between monoatomic targets and molecule CO_2 [12].

Nonrelativistic quantum mechanics considers the motion of a charged particle with spin

in a weak field of a monochromatic electromagnetic wave in the framework of the dipole approximation and predicts the particle's spin precession. However, with increasing intensity of electromagnetic radiation the relativistic effects come into force and violate the adiabatic spin dynamics. For their quantitative calculation a model of spin-laser interaction beyond the dipole approximation has been formulated. The evolution of state of the spin-1/2 particle was described in a quasi-classical approach based on the Pauli equation and modified by relativistic corrections taking into account the effect of the interaction delay, the influence of the magnetic component of the Lorentz force, and the Thomas precession. When computing transitions in an elliptically polarized laser field, the Pauli equation was reduced to the Riccati equation. Its numerical analysis allowed one to establish the resonant character of the spin-flip probability depending on the intensity, polarization and the gyromagnetic ratio of the charged particle [13].

APPLIED RESEARCH

Algorithms of numerical simulations of the evolution of the heat conductivity processes with a time-periodic source have been developed at LIT in cooperation with VBLHEP (JINR) and realized in the OpenCL language to calculate with the help of graphic processor devices. A model of the multilayered cylindrical device with a nontrivial computational domain and nonlinear thermodynamic properties of materials at cryogenic temperatures is considered. This model describes the so-called cryogenic cell designed for pulsing working gases into the multiply charged ion source chamber. The surface is heated by passing a pulsed electrical current through one of the conductive layers of the cell. The algorithm makes possible the further optimization of the design of the cryogenic cell [14].

Scientists of LIT and FLNP performed investigation on the structure of a polydispersed population of the unilamellar DMPC vesicles in sucrose solutions by methods of small-angle neutron scattering (SANS) and X-ray scattering (SAXS). The calculations based on a unified approach in the framework of the separated form factors model (SFF) show that the structure of the vesicle system essentially depends on the sucrose concentration [15].

Research on the physical processes in porous materials is in progress at LIT. Penetration and moisture transfer leads to chemical and physical damages of materials. A new system of equations has been proposed in which three physical processes are included: transfer of heat, liquid and vapor in porous materials. The proposed equations are solved with a splitting scheme. The results of numerical experiments are in good agreement with observable data [16].

A method of forecasting the passenger traffic in Moscow metro with the help of artificial neural networks has been developed at LIT and FTI "Rostransmodernizatsiya", Moscow. The analysis and the selection of those factors that have a major impact on the passenger traffic in the subway were done. The data corresponding to the daily volumes of the passenger traffic on weekdays demonstrated the fundamental possibility of a short-term forecasting with acceptable accuracy. It is shown that the use of the wavelet filtering for the realized values of daily traffic allows one to improve significantly the prediction accuracy and to expand the time horizon [17].

INTERNATIONAL COOPERATION

The work performed by specialists of LIT and the National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM, Cluj-Napoca, Romania) analyzes an approach to the efficient satellite image processing which involves two steps. The first step assumes the distribution of the steadily increasing volume of satellite collected data through a Grid infrastructure. The second step assumes the acceleration of the solution of the individual tasks related to image processing by implementing execution codes which make heavy use of spatial and temporal parallelism. An instance of such an execution code is the image processing by means of the iterative Perona–Malik filter within FPGA application specific hardware architecture [18].

In the framework of collaboration between a heterogeneous computations HybriLIT cluster team and a group of the theory of multiparticle boson systems of the Centre for Quantum Dynamics of Heidelberg University, work was in progress on the software development for research in the dynamic properties of quantum systems, including those realized on the basis of super-cold atoms and the molecules in external magnetic-optical potentials (traps). In 2015, a software package MCTDHB-Lab (http://qdlab.org) was presented which is based on solving a nonstationary Schrödinger equation by the MCTDHB (MultiConfigurational Time-Dependent Hartree for Bosons) method. This is a cross-platform package (i.e., it works under operating systems Windows, Linux, OS X), a freely distributed and convenient graphic interface (see Fig. 5). On the basis of this package, systematic studies of the dynamic properties of multiparticle quantum systems have been conducted [19].

CONFERENCES AND MEETINGS

The workshop "Big Data Processing and Analysis Challenges in Mega-Science Experiments" was held at the NRC "Kurchatov Institute" and LIT on 29–30 February. The main objective of the workshop was to discuss big data challenges in mega-science experiments. The workshop was attended by well-known specialists from Russia, USA, CERN, European centres and Taiwan. Much attention was given to the modeling of cloud infrastructures and the discussion of the further development of modern computer infrastructures for solving tasks on processing data from LHC experiments and other mega-projects as well as problems in the field of biology, chemistry, climate, and social problems. There were also presented reports on the development of Tier-1 centres in Taiwan, Kurchatov Institute and LIT. The workshop was concluded with a discussion on the development of the global computer infrastructure that is used in the current and future mega-projects.

On 26–27 May, LIT hosted the scientific practical forum "Distributed Information and Computing Systems and Data Processing in the 21st Century" (DICS-XXI) which was organized by the JINR Laboratory of Information technologies and the Skobeltsyn Scientific Research Institute of Nuclear Physics of MSU (SRINP MSU). The DICS-XXI forum was dedicated to the present-day tendencies in the field of design, creation and application of modern and promising distributed information and computing systems and the technologies of big data processing on their basis. Reports of leading specialists in the field of distributed computer systems, including supercomputer and grid technologies, were presented to the forum participants. The forum was attended by more than 50 representatives from the following institutions and companies: Joint Institute for Nuclear Research, SRINP MSU, National Research Centre "Kurchatov Institute", state budgetary educational institution of the Moscow Region "International University of Nature, Society and Man 'Dubna'", state educational institution of the higher professional education "St. Petersburg State University of Information Technologies, Mechanics and Optics", joint-stock company "Niagara Computers", Russian agency of corporation "American Power Conversion", and Russian branch of IBM. A round-table session "The Future of Distributed Technologies for Big Data Processing" was held when the forum was over.

A traditional two-day Workshop on Computer Algebra was held at LIT on 26–27 May. More than 30 scientists from universities and scientific institutes of Bucharest (Romania), Minsk (Belarus), Tbilisi (Georgia), Moscow, St. Petersburg, Rostov-on-Don, Saratov, and Dubna took part in this workshop. Twenty-eight reports were presented. A number of new promising results on developments of algorithms for investigating and solving systems of algebraic and differential equations, symbolic-numeric simulation of quantum-mechanical systems, computation of the multiloop Feynman integrals by computer algebra methods and various computer algebra applications to physics and mathematics were presented.

On 13–17 July, the eighth international conference "Mathematical Modeling and Computational Physics" (MMCP'2015) was held in High Tatra Mountains, Stará Lesná, Slovakia. The conference was devoted to the 60th anniversary of the Joint Institute for Nuclear Research. It was organized by LIT, IFIN-HH (Bucharest, Romania), the Institute of Experimental Physics of the Slovak Academy of Sciences (Košice), the Technical University of Košice, the Pavol Jozef Šafárik University (Košice), and the Slovak Physical Society (Košice). The scientific

area of the conference covered a wide spectrum of questions including: mathematical methods and tools for modeling complex physical and technical systems, computational chemistry, biology, and biophysics; methods, software and computer complexes for experimental data processing; computer algebra and quantum computing methods, algorithms and software; distributed scientific computing and big data; parallel and hybrid calculations, extra massive parallelism. Attending were 90 scientists and specialists from Belarus, Bulgaria, Germany, Canada, Russia, Romania, Slovakia, Ukraine, USA, Taiwan, etc. A large number of Russian scientific centres and universities such as NRC "Kurchatov Institute", Institute of Mathematical Problems of Biology of RAS (Pushchino, Russia), Institute of Theoretical and Applied Mechanics of SB RUS, St. Petersburg State University, Novosibirsk State University, PFUR, etc., were presented. In total, there were heard 17 plenary and 62 oral reports. The young conference attendees were especially interested in the training course on parallel programming technologies CUDA and OpenCL, conducted on the basis of the HybriLIT heterogeneous computing cluster.

On 27–30 August, LIT hosted the workshop "Computational Modeling in Complex Systems". Twenty-two scientists from JINR, Russia, Slovakia, China and Taiwan attended the meeting. The participants heard 16 reports on computational methods, algorithms and tools of modeling complex physical phenomena and technical systems. The reports presented the results of investigations obtained with simulations of biophysical and astrophysical systems, processes of stochastic dynamics, optics and accelerator techniques.

On 28 September – 2 October, the XXV International Symposium on Nuclear Electronics and Computing (NEC'2015) was held in Budva, Montenegro. The symposium has been traditionally held by JINR since 1963, and for the eighth time JINR and CERN became its organizers. The scientific programme of the symposium covered a wide spectrum of questions and included the following sections: detector and nuclear electronics, computer applications for physical research, triggering and data acquisition, automation and control in scientific research, big data, grid technologies and cloud computations, computing for experiments on large-scale accelerator installations (LHC, FAIR, NICA, etc.), problems of computations on hybrid platforms as well as such traditional subjects as innovations in training with the use of information technologies. This year the symposium is devoted to the 60th anniversary of JINR. Attending were 120 leading specialists in modern computer and network technologies, distributed computing and nuclear electronics from 15 countries. In the framework of the symposium, a workshop, a round-table session and an international students school on modern information technologies were organized. The school was attended by more than 40 students from leading Russian universities.

On 2–6 November, the sixth school on information technologies "Grid and Advanced Information Systems" was held under the auspices of the Joint Institute for Nuclear Research, the European Organization for Nuclear Research (CERN) and the National Research Nuclear University "MEPhI". It was devoted to the management of scientific complexes and information systems in reference to the technologies developed at JINR and CERN. The school was attended by over 60 students from leading universities of Moscow, Moscow Region, Tver and St. Petersburg (National Research Nuclear University "MEPhI", Lomonosov Moscow State University, Saint Petersburg State University, University "Dubna", the Plekhanov Russian University of Economics, and Tver State University). A tutorial on the parallel programming technologies on hybrid architectures was organized on the basis of the HybriLIT cluster.

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