LABORATORY OF INFORMATION TECHNOLOGIES

The investigations performed at the Laboratory of Information Technologies in 2017 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 26 themes of the JINR Topical Plan for JINR research and international cooperation. The LIT activity is aimed 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 basis of advanced information and computer technologies.

The implementation of the project on the development of the Multifunctional Information and Computing Complex (MICC) of JINR has been started. It currently comprises the following basic components:

• Central Information and Computing Complex (CICC) of JINR with home built up computing elements (CE) and mass storage elements (SE),

• grid site of Tier-2 level for experiments at the Large Hadron Collider (LHC) and other large-scale experiments and projects within the grid environment,

• grid site of Tier-1 level for CMS experiment,

• heterogeneous cluster HibryLIT for parallel computing,

• cloud infrastructure.

The JINR MICC provides resources needed for different tasks, implied by many projects the JINR researchers take part in, namely: MPD, BM@N, CMS, ALICE, ATLAS, NOνA, BESIII, OPERA, PANDA, STAR, COMPASS, etc. The JINR grid sites of Tier-1 and Tier-2 levels are elements of the Russian Grid Segment of the global Grid infrastructure used within the WLCG project for data processing of ALICE, ATLAS, LHCb and CMS on LHC and other grid applications.

In 2017, construction of a specialized engineering infrastructure for high-performance computing (HPC) was started. It is based on the technology of contact liquid cooling and intended for the development of the heterogeneous cluster HibryLIT with the aim of multiple increase in the computing power needed for a drastic speed-up of complex theoretical research underway at JINR.

In 2017, 213 scientific papers were published by LIT researchers in referred journals, and 61 reports were presented at international and Russian conferences.

INFORMATION AND COMPUTING INFRASTRUCTURE OF JINR

During 2017, the 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, JINR local area network (LAN), Multifunctional Information and Computer Complex as well as the primary software, including 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 2017, the reliable work of the high-speed computer communication channel Dubna–Moscow was secured. The external JINR computer channel is based on the DWDM technology (Dense Wave Division Multiplexing means spectral multiplexing on the wavelength) and uses one lambda of 100 Gbps and two lambdas (two frequencies) of 10 Gbps each. The external distributed network of JINR includes external overlay network LHCOPN (JINR–CERN) passing through MGTS-9 in Moscow, Budapest and Amsterdam to link the centres of Tier-0 (CERN) and Tier-1 (JINR) and external overlay network LHCONE of the same route which is intended for Tier-2 centre at JINR; direct communication links based on EN-VRF technology with the collaboration of research centres RUHEP (Gatchina, NRC "Kurchatov Institute", Protvino and with networks Runnet, RASnet). IPv6 routing for Tier-1 and Tier-2 sites was realized. The throughput of the backup communication channel is 20 Gbps.

Table 1 shows the distribution of the incoming (more than 4 TB) and outgoing traffics in 2017 over JINR subdivisions.

Table 1

Subdivision	Incoming, TB	Outgoing, TB
DLNP	158.23	82.88
VBLHEP	115.36	89.71
LIT	58.15	18.89
FLNP	54.38	37.56
FLNR	41.18	21.1
JINR Management	39.65	74.95
Remote access node	35.96	4.95
JINR's Hotel & Restaurant Complex	30.54	4.05
BLTP	22.75	8.68
Resort Hotel "Ratmino"	15.46	2.41
LRB	7.73	4.39
Procurement and Logistics Service	7.18	2.05
Chief Power Engineer's Department	5.02	0.48
Social Infrastructure Management Office	4.79	0.58
Technical Communication Service	4.12	1.04

In 2017 the overall incoming JINR traffic, including the general access servers, Tier-1, Tier-2, and the computer complex, amounted to 23.5 PB (14.2 PB in 2016). 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, %
97.54	1.34	0.9	0.17	0.05

JINR Local Area Network. In 2017, 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 JINR local area network (LAN) has been transferred to DHCP (Dynamic Host Configuration Protocol). A project was developed of a new link using 4×100 Gbps between the territories of DLNP and VBLHEP with a double redundancy to improve the reliability of the optical transport highway.

Currently, the main optical highway of the JINR local area network operates at a speed of 10 Gbps. Its transition to 100 Gbps is planned in 2018.

There is a system of network services: DNS, DHCP, SMTP, SNMP, user registration, authorization devices, user authentication, switching, routing, security, videoconferencing communications, VoIP, IPDB (Internet Protocol Data Base), WebMail, etc.

The JINR LAN currently comprises 8008 network elements and 14 129 IP addresses, 4559 users registered at present within the network, 2584 users of mail.jinr.ru service as well as 1597 users of digital libraries and 396 remote VPN users.

JINR Grid Environment. The JINR grid infrastructure is presented by a Tier-1 centre for CMS experiment at LHC and a Tier-2 centre which supports a large number of virtual organizations (VOs) such as ALICE, ATLAS, BES, BIOMED, COMPASS, CMS, LHCB, MPD, NOνA, STAR, etc. The Tier-1 CMS centre at JINR comprises the following basic elements:

1. The data processing system supports 248 64-bit 12- and 20-core worker nodes (WNs) which in total give 4160 cores. Tasks are serviced in a batch mode. To support the batching system, there is a special server with a system for resource distribution of cluster's resources and a scheduler. Software Torque/Maui is used as a resource manager of the task scheduler.

2. The mass storage system is served by dCache and Enstore software as a buffer for work with the tape robot. One of the installations of dCache works only with storage servers and is used for online data storage with fast access to them. The second installation serves special dCache disk servers and tape robot. The disk servers are a buffer zone for the exchange with tapes, while the tape robot is designed for a long, practically eternal storage of CMS data. Totally, two installations have now 6.4 PB of effective disk space, and the tape robot IBM TS3500 has 9 PB of data storage capacity. To support the storage and access to data, 8 physical and 14 virtual machines have been installed.

3. The system for service support ensures the operation of the computing service, storage service, grid service, service of data transmission (File Transfer System (FTS)), distributed computing management system (Portable Batch System (PBS)), information service (monitoring of services, storage servers, data transfer, information sites). Grid-VOBOX service is designed for transferring data between CMS grid sites by means of FTS; the proxy server SQUID is also configured and used, which is necessary when working with specialized CMS databases (conditions DB). The FTS service is used to reliably transfer files between large data stores, primarily between the centres of Tier-0 and Tier-1 levels. Additionally, the services FTS provides control and monitoring of transmission, distribution of site resources between different organizations, and managing user requests. For

calculation a default software stack of the WLCG project is used: $2 \times$ 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 a full-operation mode [1]. During 2017, this centre performed 6 778 864 tasks, using a normalized CPU time of 227 802 717 h in HEPSpec06 units. Figure 1 gives the contribution of the Tier-1 global centres to the CMS experimental data processing (in MEvents) in 2017. The JINR site takes a second place in the world as to its productivity.

Figure 2 shows the number of events processed at the JINR CMS Tier-1 in 2017 for 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 the tape robot during 2017.

Figure 4 illustrates a data transfer rate and amount of data transferred for recording and processing (Fig. 4, a, b) from the Tier-1 and Tier-2 centres to JINR

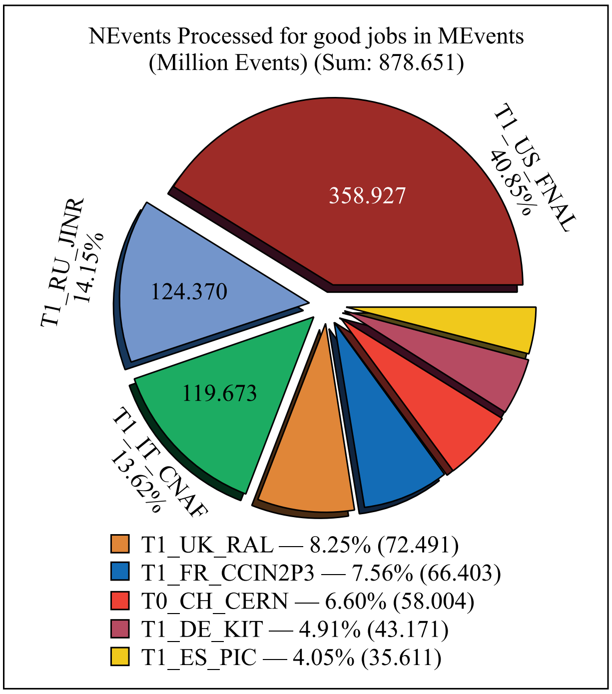

Fig. 1. Number of events processed for all CMS Tier-1 in Million Events in 2017 (Sum: 878.651)

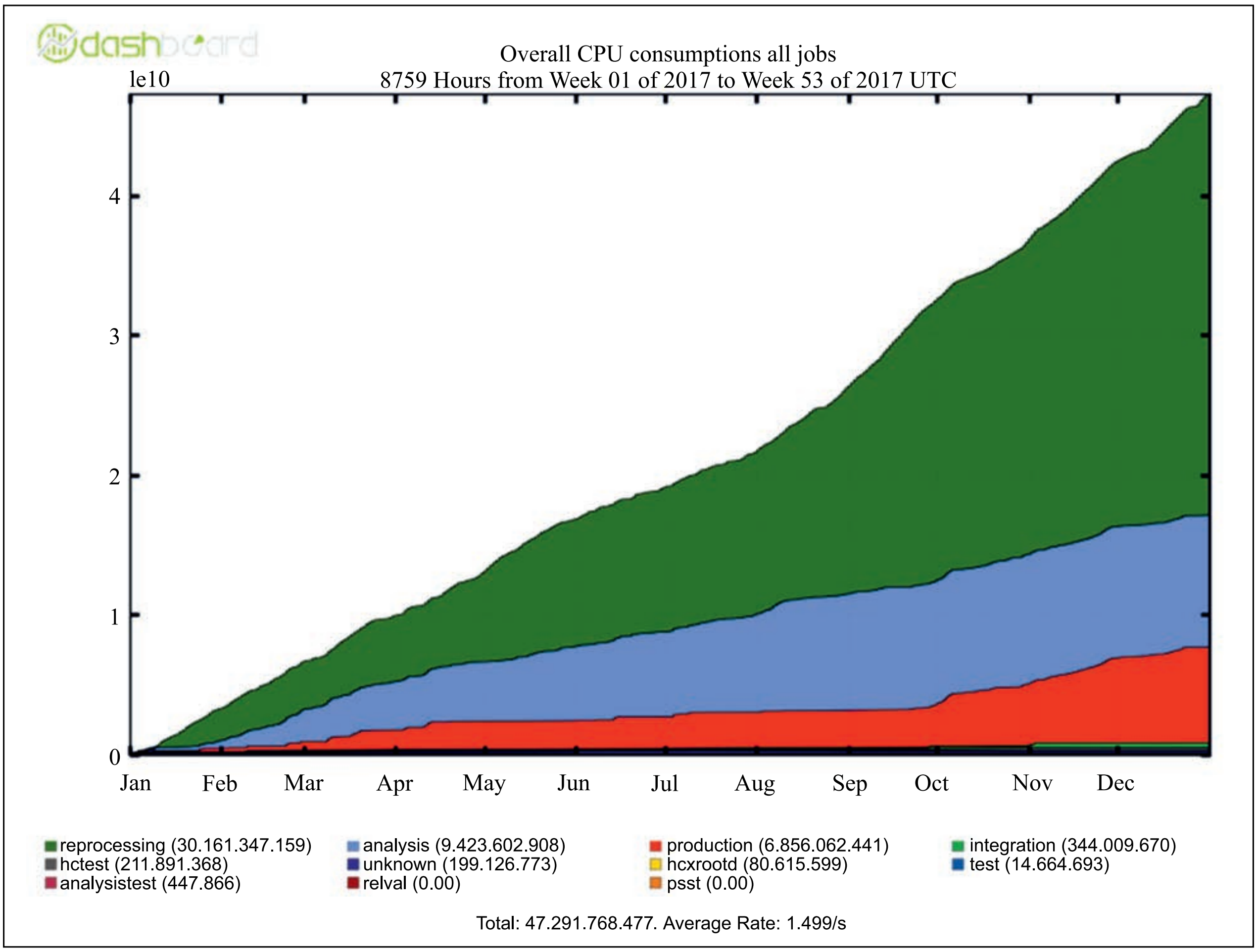

Fig. 2. Number of events processed at the JINR CMS Tier-1 in 2017 for CMS activities (reconstruction, simulation, reprocessing, analysis, etc.)

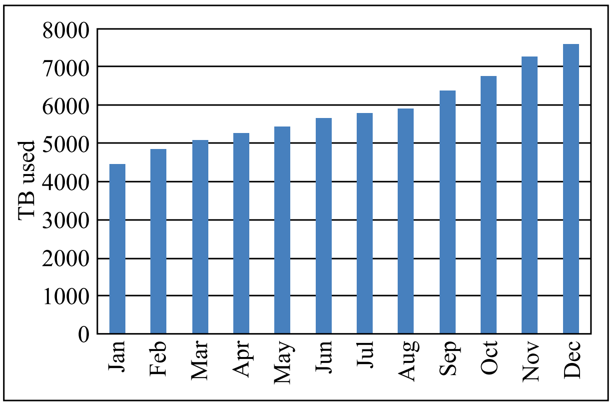

Fig. 3. JINR CMS Tier-1 tape robot load in 2017

CMS Tier-1 as well as a data transfer rate and amount of data transferred from JINR CMS Tier-1 for recording and processing to centres Tier-1 and Tier-2 (Fig. 4, c, d) during 2017. The average speed of raw data transfer to JINR CMS Tier-1 is 280–380 Mbps.

The Tier2 level centre at JINR [1] allows the data processing for all the four LHC experiments (ALICE, ATLAS, CMS, and LHCb) and, in addition, supports a number of VOs that are not included in the LHC (BES, BIOMED, COMPASS, FUSION, MPD, NOνA, STAR, etc.). The computational resources of the Tier-2 centre consist of 3640 cores. The data storage system is installed in two versions of software: two dCache installations and two XROOTD installations. One of the dCache installations is used by CMS and ATLAS. The other dCache is used by the JINR users and user groups as well as for the NICA experiment (MPD). Besides, this installation is used to store data of several third-party experiments (BIOMED, BES, FUSION). One XROOTD installation is used by ALICE, and the other within the FAIR project of the PANDA collaboration. The size of the storage system is 1909.8 TB. The storage systems support 19 servers that organize data distribution, authorization of access to data and protocols to work with the data.

For VO to work, special servers have been installed that support the WLCG grid environment. Part of the WLCG services was installed on physical machines, some of them on virtual ones. The WLCG services use software UMD for compatibility with the grid software environment in WLCG. Currently, 23 WLCG services are installed. These services provide the entire infrastructure for remote work with grid: user and VO authorization, job run from remote VO services, WLCG information system, and various algorithms for remote testing and checking the service environment on the local resources. There are five settings of user interface (UI) for job run into a distributed grid environment.

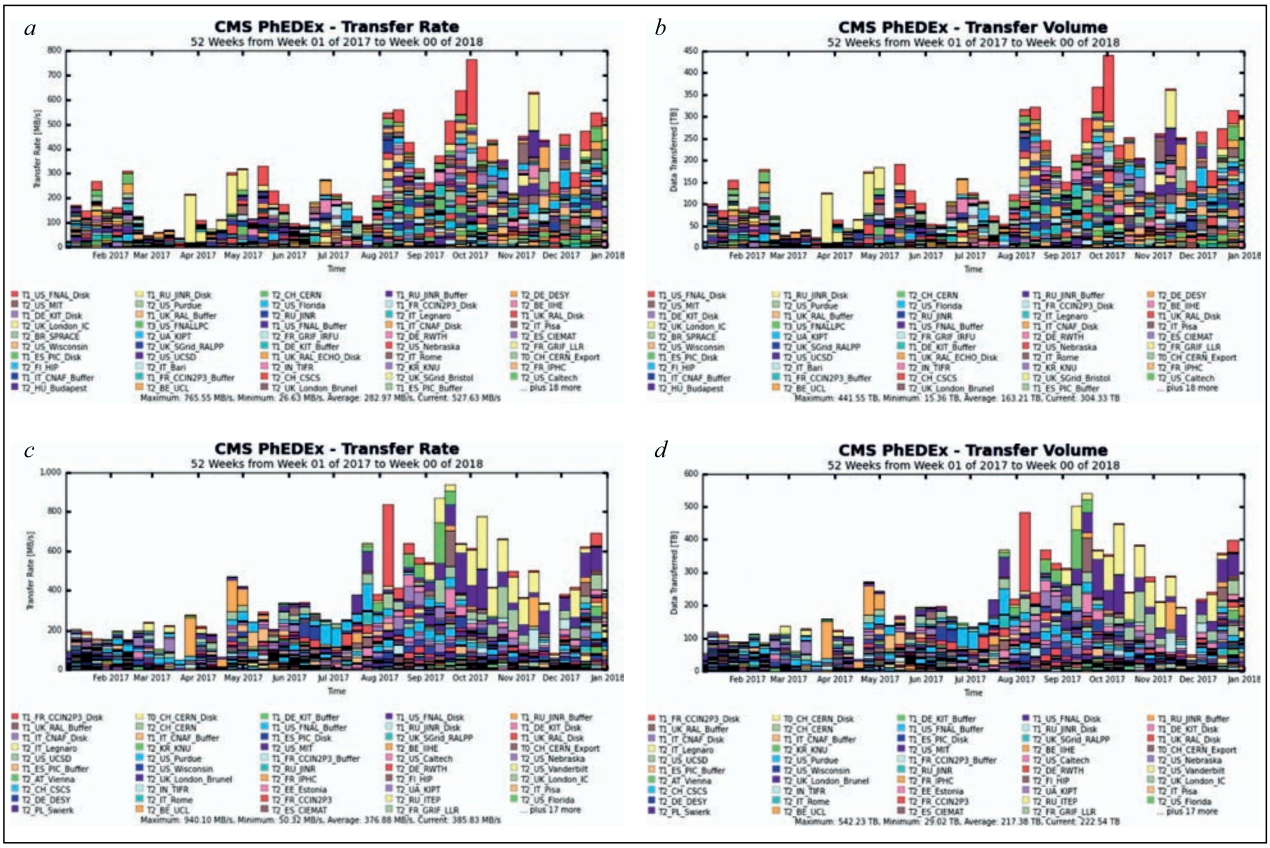

Fig. 4. The data transfer rate and amount of data transferred for recording and processing (a, b) from Tier-1 and Tier-2 centres to CMS Tier-1 at JINR and the transfer rate and amount of data transferred from JINR CMS Tier-1 for recording and processing to centres Tier-1 and Tier-2 (c, d) in 2017

The computing element OSG HT-CONDOR has been integrated in the Tier-2 centre infrastructure. This provides a way for VO STAR to process data using JINR Tier-2.

The main users of the JINR grid resources are virtual organizations of all LHC experiments. During 2017, the Tier-2 site performed 6 682 112 tasks, CPU time was 236 405 186 h in HEPSpec06 units. Figure 5 gives data on using the Tier-2 site (JINR-LCG2) at JINR by the virtual organizations within projects RDIG/WLCG/EGI in 2017.

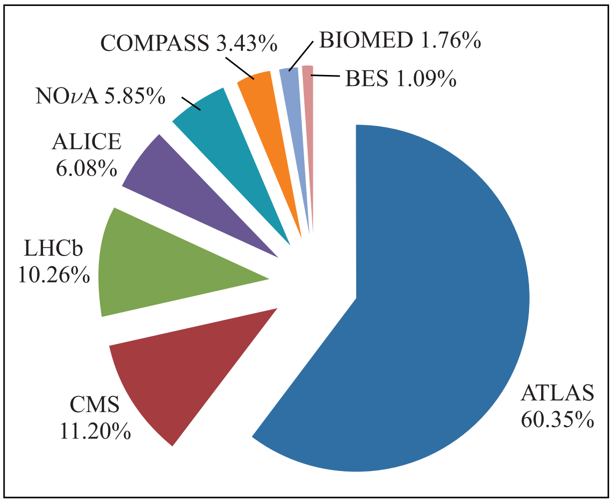

Fig. 5. The use of the JINR-LCG2 grid site by virtual organizations within RDIG/WLCG/EGI

The development of a new service monitoring system for CMS Tier-1 at JINR was begun. The system has a modular structure. The following modules have been developed: Job Status — number of completed and emergency-ended jobs; SSB Status — results of the monitoring performed by Dashboard; Phedex-Quality — quality of transfers between other sites and T1_RU_JINR; PhedexErrors — errors associated with T1_RU_JINR. The test version of the service monitoring system was lunched at lcgsens01o.jinr.ru. Now it aggregates and displays on the web page the data related to Phedex, dCache and WLCG monitoring. The system is developed as a general-purpose tool which could lately be adapted for other Tier-1 centres and experiments.

A new data processing system of the COMPASS experiment in a grid environment (Grid COMPASS Production System) has been developed and commissioned [2]. The management infrastructure is located in the cloud of JINR. Data processing is performed with the help of PanDA, which allows one to send a job to any available computational resource: Condor, LSF, PBS, etc. Most of the processing is executed on the grid resources of CERN and JINR.

High-Performance Computer System. The MICC 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 by 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 system. Figure 6 gives the time distribution of the tasks executed on the computing cluster by the JINR subdivisions and the user groups.

The systems of storage and access to dCache and XROOTD data ensure work with 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 a hardware data protection mechanism RAID6 and a software mechanism

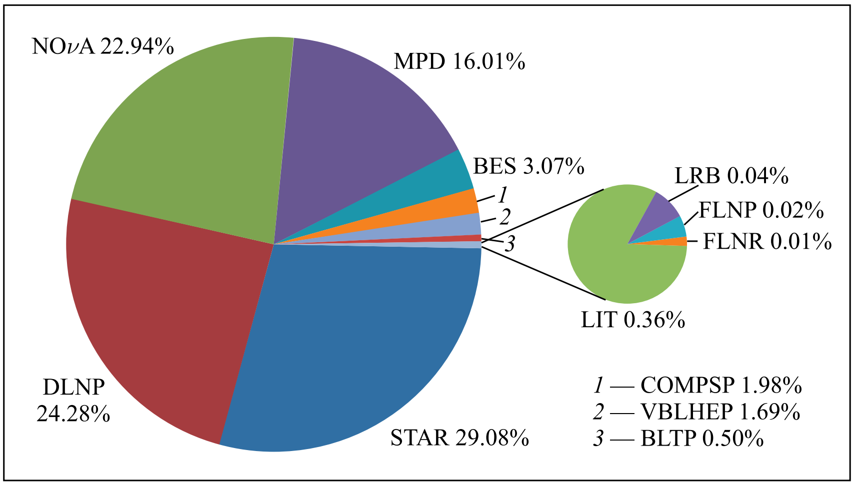

Fig. 6. Statistics of using the computing cluster by the subdivisions and experiments underway at JINR in 2017 without grid users

RAIDZ2, which is not inferior to the reliability of the RAID6 hardware.

Cloud Environment. In 2017, the cloud infrastructure of JINR was equipped with 14 servers Dell PowerEdge R630 with the total number of CPU cores 336 and total RAM size of 1792 GB, 6 servers Dell PowerEdge R730xd with 16 8TB disks in each for a cloud storage based on ceph, 2 Dell PowerEdge R630 servers for head machines of the cloud. In order to support the computing infrastructure of the NOνA experiment, five Dell PowerEdge R430 servers with 120 CPU cores and total RAM size of 640 GB were commissioned as well as one Dell PowerEdge R730xd server with 16 8TB disks to expand the cloud storage for the needs of the NOνA experiment.

In 2017, a new fault-tolerant cloud architecture of JINR was designed on the basis of the Raft-algorithm implemented on a new version of cloud platform OpenNebula. The work was done with a purpose to optimize the architecture of the cloud storage based on ceph [3].

In cooperation with SRI NP BSU (Minsk, Belarus), work was in progress on the integration of the cloud infrastructure with the JINR cloud. Similar work [4] is underway with the following organizations:

- Nazarbayev University and the Institute of Nuclear Physics (Astana, Kazakhstan);
- Georgian Technical University (Tbilisi, Georgia);
- Yerevan Physics Institute (Yerevan, Armenia);
- Institute for Nuclear Research and Nuclear Energy and Sofia University (Sofia, Bulgaria);
- University “St. Kliment Ohridski” in Bitola (Bitola, Macedonia).

The geography of organizations of the JINR Member States which provide part of their resources to integrate with the JINR Cloud is presented in Fig. 7.

In 2017, work was complete on refactoring the driver of JINR LIT Cloud on the platform OpenNebula to deploy an OpenVZ container. For the task to be solved, a test polygon has been deployed and configured which consists of two virtual machines, one of which is equipped with a host system OpenNebula, and the other has its work node. For a correct operation of the test polygon, synchronization is required for the driver data between the host system and its work node. During the execution of the work, a unified class OneDriver was created which includes all the container management methods required for the correct operation of the driver as well as some auxiliary methods and functions that are involved in the work of the container. In OpenNebula, the rules for third-party driver developers provide calls of the container management functions from the same-name scripts. For example, the command to create and deploy the container “deploy” needs to be called from the same-name file. So, all necessary scripts were set up to create an object of class OneDriver and then to call a container management method. The driver is based on the Ruby programming language.

In 2017, a smart scheduler for the cloud was developed that proposes using an overcommitment mechanism (assigning more virtual resources than physically available) with the automated virtual machine migration to de-allocated resources. A necessary part of this project is to collect current and historical information on the load distribution in the cloud. The default monitor-

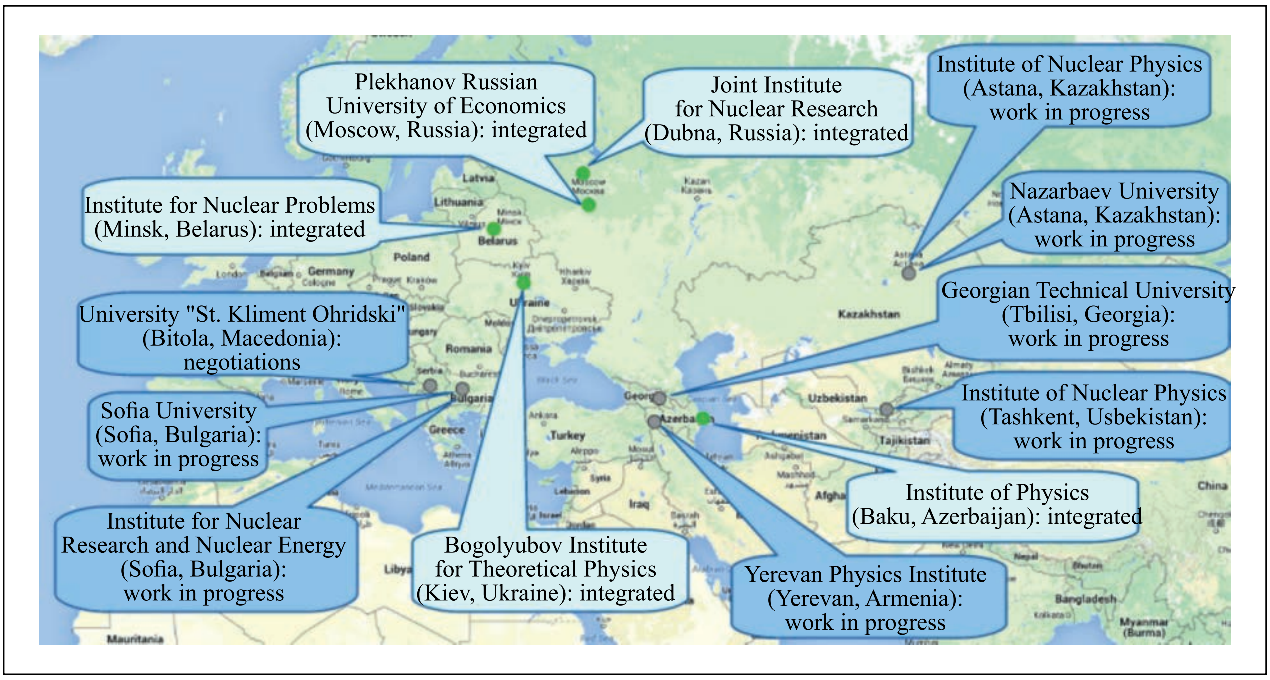

Fig. 7. Geographical location of cloud infrastructures of the JINR-participating organizations which provide part of their resources for integration with JINR Cloud

ing system embedded into the OpenNebula cloud platform possesses limited possibilities as to data collection and data processing options. Therefore, the problem of choosing the most suitable external monitoring system gets urgent. Another important aspect to be considered is its performance and scalability as in large clouds it can be a critical limiting factor for the scheduler. Based on the test results and the experience gained with the systems Ganglia, Icinga2, NetXMS, NMIS and Zabbix, Icinga2 has been chosen as a load information collection system for the smart cloud scheduler project [5].

Heterogeneous Computation Cluster HibryLIT. The development of the information and software environment of the heterogeneous computing cluster HibryLIT [1] that is a component of MICC of LIT [2] was in progress in 2017. The cluster is intended for carrying out massive parallel computations using modern computing architectures such as GPUs (Nvidia Tesla K40, K80) and Intel Xeon Phi coprocessors/processors. At the moment, the computing component of the cluster contains 10 nodes with NVIDIA Tesla K80 graphical processors, NVIDIA Tesla K40 accelerators, Intel Xeon Phi7120P coprocessors and two types of computing accelerators NVIDIA Tesla K20x and Intel Xeon Phi 5110P. All the nodes have two multi-core processors Intel Xeon. Overall, the cluster contains 252 CPU cores, 77 184 GPU cores, 182 PHI-cores; it has 2.5 TB RAM and 57.6 TB HDD, and its total capacity is 140 Tflops for operations with single precision and 50 TFlops for double precision. HibryLIT infrastructure allows developing modern software along with providing JINR Member States with possibilities for carrying out resource-demanding computations. SLURM is being used in the structure of the cluster as a workload manager. SLURM settings allow distributing computation nodes by partitions formed according to computation architectures used in the process of carrying out computations. In order to get information about available resources in different SLURM partitions, characteristics of the nodes and a status of running tasks — in other words, information for more efficient organization of computing on the cluster, a MobiLIT mobile application has been developed. It provides the following possibilities:

- user's jobs monitoring;
- quick view of user's files (*.out, *.dat, *.in or *.sh);
- possibility to kill jobs directly via the app;
- monitoring of the expected computation time;
- monitoring of available resources on different nodes and partitions of the cluster which are meant for using different computing architectures;
- full information on jobs launched on the cluster, the resources they require, etc.

The MobiLIT application is developed using NativeScript framework. It is available in Google Play Store [5] for users of smartphones and tablets under Android; for iOS users the application is available in App Store in test mode. To sign in, users need authorization data for the HibryLIT cluster. The developed mobile application MobiLIT for users of HibryLIT enriches its information-software environment with a convenient and modern IT service, which makes it simpler to carry out parallel computations and provides additional optimization while using computation resources of the cluster.

A new service HLIT-VDI has been developed for shared use of applied software packages on the HibryLIT cluster using GUI (graphical user interface). By means of this service, it is now possible to work with applied software packages such as Wolfram Mathematica, Maple, Matlab, COMSOL, GEANT4, etc., via remote access to the virtual machines (VMs) in the framework of the HibryLIT cluster. The developed service allows carrying out computations in frames of VMs and massive computations using the resources of the cluster (Fig. 8).

The cluster's resources are widely used not only for massive-parallel computations to solve the problems underway at JINR, but also to train how to work with high-performance computing systems (HPC). On the basis of the cluster HibryLIT that is a dynamic,

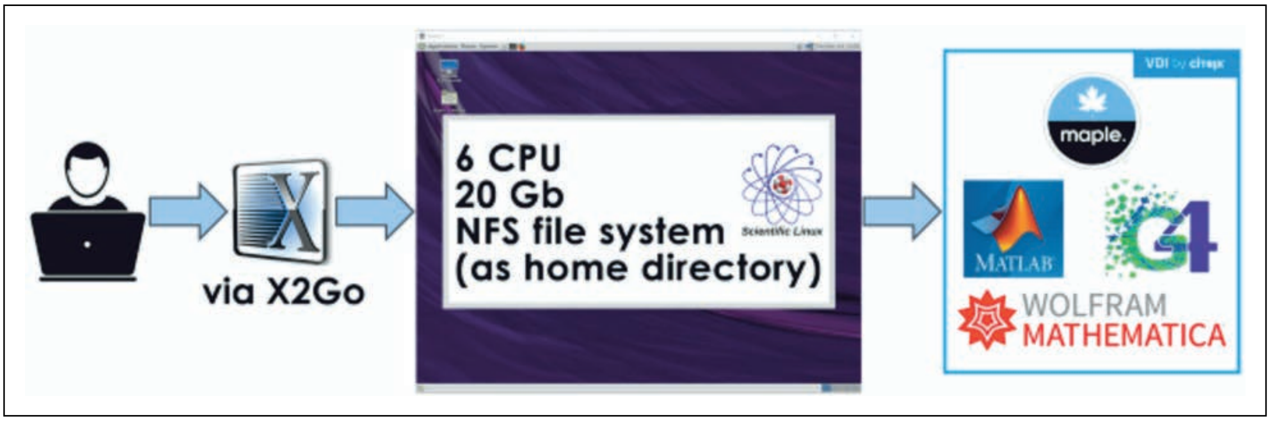

Fig. 8. A scheme of work with HLIT-VDI service

actively developing structure which includes state-of-the-art HPC computing architectures and possesses an advanced software and information environment, educational programs of advanced level are being developed. These programs allow students, postgraduates and young scientists to learn how to work on the present-day computing platforms and to study advanced IT technologies [6].

Information and Software Support. A specialized platform was designed at the Laboratory of Information Technologies. It is a set of interconnected cloud services and resources providing useful tools for management and processing of bio-monitoring data and allowing one to simplify and automate the stages of the monitoring beginning from the selection of places for sample collection and ending with the generation of the contaminant distribution maps and prediction of changes in the environment. The need to develop such a platform is caused by the need of automation of the control over the environment pollution, which is of great importance for the countries of Europe and Asia and overseen by a special Commission of the UN. The platform, using modern analytical, statistical, programs and organizational methods, allows one to improve the quality and speed of data processing, to expand the possibilities of interaction between the participants, to provide a framework for retrospective analysis as well as to arrange access to all available information which could give opportunity to strengthen forecasting of distributing the transboundary pollutions. Currently, the system contains information on more than 6000 sampling points in 40 regions across Europe and Asia. The program participants can go online to analyze data, to make comparisons with other regions, mapping contaminants and more. The platform can be used for other areas with a similar research process [7].

In 2017, the computer program SyMSim (Synthesis of Monitoring and SIMulation), developed for simulation of grid and cloud storage systems and data processing, was first used for modeling interprocessor communication when running HPC applications in the cloud on the basis of MPI implementation of the program calculation of the volt-ampere characteristics of long Josephson junctions. Comparison of the results obtained empirically and the results of simulations has shown that the simulation model correctly simulates the parallel computations performed with the help of the MPI technology and proved that for fast computing of this class tasks one should increase the network throughput simultaneously with increasing the number of processors. The results have demonstrated that the simulation software SyMSim can be successfully used to estimate the execution time of MPI algorithms in the cloud environment taking into account interprocessor connections [8]. For solving this problem, a service with a web user interface has been developed for modeling long Josephson junctions, the computations being performed on virtual machines dynamically created in the cloud and connected as work nodes of the batch system HTCondor. Also in 2017, software SyMSim was used to simulate a distributed data processing for the BM@N experiment as well as for an infrastructure optimization of the data centre in a joint project with IHEP (China).

During 2017, a traditional direction of LIT activity was the development and the support of the program library JINRLIB. The library was replenished with educational materials related to parallel programming technology and with two programs: PSD2SAS — a computer program to convert data of a position-sensitive detector of the small-angle neutron scattering spectrometer in case of isotropic scattering sample, authors A. G. Solovyov, S. A. Kutuzov, O. I. Ivankov, A. I. Kuklin, and IntroOMP — selection of training programs-examples on parallel programming technology OpenMP, authors M. V. Bashashin, T. F. Sapozhnikova, E. V. Zemlyanaya.

In 2017, the development of the unified system 1C 8.2 UPP was progressing as well as provision of the regular end-user support in the system. Also, regular work was continued on the creation and storage of electronic documents related to scientific and administrative activities of the Institute; in particular, the software of the JINR Document Server (JDS) was improved. It was developed as a repository of open access articles, pre-prints, collections of video lectures for young scientists and other materials that reflect the research activity underway at the Institute.

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

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

New calculation schemes and algorithms have been suggested for solving a parametric self-adjoint elliptic boundary-value problem with the Dirichlet and/or Neumann type boundary conditions in a 2D finite domain using a high-accuracy finite element method (FEM) with rectangular and triangular elements. The programs complexes implementing the algorithms calculate eigenvalues, surface eigenfunctions and their first derivatives with respect to the parameter and the potential matrix elements — the integrals of the products of surface eigenfunctions and/or their first derivatives with respect to the parameter which appear when reducing the multidimensional boundary-value problem to a one-dimensional one by means of the Kantorovich method. The efficiency of the proposed calculation schemes and algorithms is demonstrated in benchmark calculations of the 2D elliptic boundary-value problems describing quadrupole vibrations in a collective nuclear model [9].

The influence of the iterative parameter in the continuous analog of Newton's method (CANM) on the area and speed of convergence is under study. The proposed approach to the optimization of the process of convergence of the CANM is based on the use of a quadratic interpolation polynomial. Based on this approach, a mechanism was developed for control over the CANM convergence rate using as a control parameter the coefficient of changing a step of difference scheme for a numerical solving of the CANM differential equation. On the basis of the developed mechanism, a modification of the continuous analog of Newton's method has been proposed [10].

In order to obtain a more effective algorithm for calculation of characteristics for SDEs, it is proposed to use a representation of the probability density function (PDF) for solution of SDE by means of a functional integral and methods for approximate evaluation of the arising functional integrals. To represent PDF by means of functional integral, the Onsager–Machlup functionals technique is proposed to be used. In order to evaluate the arising functional integrals, a method is used which is based on distinguishing among all trajectories a classical trajectory for which the action takes an extreme value, and decomposition of the action with respect to the classical trajectory [11].

A model of quantum evolution has been constructed on the basis of combining methods of computational group theory and Monte Carlo simulation. The model is inspired by the quantum Zeno effect — the most convincing illustration of the role of observation in the dynamics of quantum systems. In the model under consideration, the trajectory of a quantum system is represented as a sequence of observations with unitary transitions between them. Time is assumed to be fundamentally discrete. From a mathematical viewpoint, the *observation* (*measurement*) is an orthogonal projection onto the subspace of a Hilbert space that is defined by the "measuring device". Statistics of the results of observations is described by the Gleason theorem (a special case of which is the Born rule). Standard quantum mechanics assumes a single deterministic unitary evolution of a quantum system in the time interval between observations. However, in accordance with the principle of least action, this single evolution appears as the dominant element in some set of "virtual" evolutions. A unitary transition between observations is interpreted as a kind of gauge connection, that is, a way of identifying indistinguishable entities at different instants of time (in discrete time it is impossible in principle to trace the individuality of indistinguishable objects in the process of their evolution), and it is assumed that all possible unitary transformations are involved in transitions between observations with weights corresponding to transition probabilities. This assumption is confirmed by the Monte Carlo simulation that demonstrates a sharp dominance of some of the evolutions over the others. This dominance grows rapidly with increasing size of the symmetry group of states and the dimension of the Hilbert space. The probability of a trajectory of a quantum system is calculated as a product of the probabilities of transitions between adjacent observations. The continuum limit of the (negative) logarithm of this product is an *action*. Thus, the principle of selection of the most probable trajectory turns into the principle of least action in the continuum limit [12].

In order to improve the quality of the muon track reconstruction in the CSC (Cathode Strip Chamber) of the muon system of the CMS experiment, a new algorithm has been developed [13]. A detailed comparative analysis was conducted to confirm the necessity of using the new algorithm as a basic algorithm of reconstruction in the CSC using the Monte Carlo [14] and experimental data. As compared to a standard algorithm, the multiplicity of track segments significantly reduces (Fig. 9, *a*). This increases the accuracy and reduces the execution time of reconstruction at the subsequent stages which require sorting all the built track segments. The efficiency of the standard algorithm decreases with increasing pseudorapidity, while for the new algorithm the efficiency remains at high ($\sim 95\%$) level for the entire range of pseudorapidity overlapped by CSC (Fig. 9, *b*). The accuracy of the reconstruction of azimuthal coordinate that provides a precision of the muon transverse momentum reconstruction has been significantly improved (Fig. 9, *c*, *d*), as clearly demonstrated by the example of high-energy muons (Fig. 9, *c*), where a standard deviation of the displayed distribution is more than three times smaller for the new algorithm as compared to the old one. The new algorithm for the track-segment reconstruction was implemented in the official software package CMS in July 2016, and since 2017 it has been used by default in the reconstruction of simulated and experimental data.

A fast and efficient algorithm has been designed for the reconstruction of muon tracks in decay $J/\psi \to \mu^+ + \mu^-$ registered by the MUCH detector of the CBM experiment. One of the key tasks of this experiment is to study the processes of birth of charmonium in high-energy nucleus–nucleus collisions. The registration of such decays as $J/\psi \to \mu^+ + \mu^-$ will be done in real time. The muon track recognition algorithm is based on the model of cellular automaton (CA) which is used successfully in a number of experiments in high energy physics. The CA model is good because it allows one to reduce the number of recursive operations on the in-

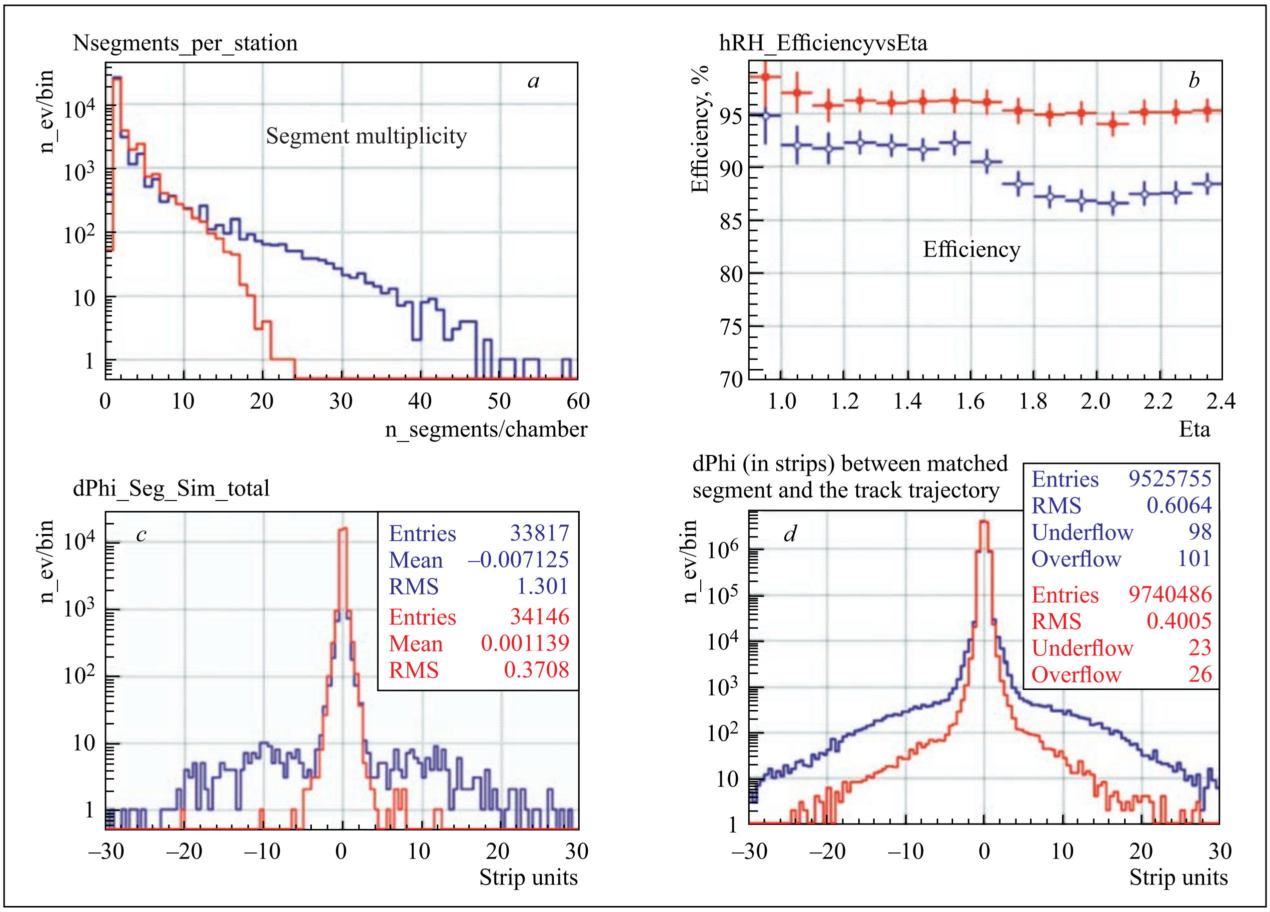

Fig. 9. Comparison of standard ST (blue) and new RU (red) algorithms for track-segment reconstruction: *a*) number of reconstructed track segments in the chamber for simulated muons with $P_t = 1$ TeV; *b*) dependence of the efficiency of the reconstruction upon pseudorapidity for simulated muons with $P_t = 1$ TeV; *c*) difference of azimuthal coordinates (in units of the strip width) of the track segment associated with the reconstructed muon, and the simulated muon with $P_t = 1$ TeV; *d*) difference of the azimuthal coordinates of a track segment associated with the muon and the reconstructed muon on experimental data of 2016

put data array and to perform most of the calculations locally. In this case, the CA elements ("cells") are segments of the broken line from which the approximation of the straight track is built. The track recognition algorithm includes three consecutive stages: calculation of average points; forming segments — the elements of the reconstructed tracks; connection of the segments and track reconstruction. The developed algorithm was included into the package CBMROOT as a dynamic link library under the name of Lx. This same library is also supplied with algorithms that implement a trigger to select decays $J/\psi \to \mu^+ + \mu^-$ and a set of methods for tuning the parameters of the algorithm on model data. In the future we plan to investigate a possibility of applying a similar approach for the selection of light vector mesons decaying in the muon channel [15].

The variation of the multiply differential cross section of the $(e, 2e)$ simple ionization of H_3^+, with the incident and ejection energy values, as well as the directions of the ejected and scattered electrons, is studied. The calculations have been performed in the framework of the perturbative first Born procedure, which has required the development of equilateral triangular three-centre bound and continuum state wave functions. The results explore the optimal conditions and the particularities of the triangular targets, such as the appearance of interference patterns in the variation of the fourfold differential cross section (FDCS) with the scattering angle for a fixed orientation of the molecule. The comparison between the results obtained by two H_3^+ ground wave functions, with and without a correlation term r_{12}, shows that the effect of correlation on the magnitude of the triple differential cross section is not large, but it produces some modification in the structure of the FDCS [16].

As examples of algorithmic construction of difference schemes for partial differential equations receiving their basic algebraic properties on a discrete level, new difference schemes have been constructed for Navier–Stokes equations and Korteweg–de Vries equation. These new schemes demonstrate a good numerical behavior [17].

The methods of obtaining functional equations for Feynman integrals on the basis of the algebraic relationships for propagators have been improved. The computations of the QCD contributions to the constant of renormalization of the mixed propagator of fermions are performed taking calibration into account [18].

A geometric description of the Maxwell equations in terms of stratified spaces has been obtained. Proposed were different variants of a permeability tensor and, correspondingly, different versions of geometrization of the Maxwell equations. In particular, the version of geometrization based on a quadratic metric leading to the Yang–Mills type equations should be noted. The developed formalism was applied to the problems of transformation optics and designing optical instruments and devices of a sub-wave range [19].

APPLIED RESEARCH

A fundamental possibility of predicting the daily energy consumption for the Moscow Region using artificial neural networks (ANN) has been demonstrated. Such factors as an optimally matched ANN architecture, an adequate structure of the sample at the input of the network, as well as originally built procedures for training and predicting the network, play an important role in the solution of this problem. The first three variables at the input of the ANN are responsible for the seasonal and periodic fluctuations in the energy consumption. Particularly noteworthy is the fourth variable which plays a role of a "tip" for the ANN which is taken either from filtered data (during the training phase of the network) or from predicted values calculated with the help of the "Caterpillar"-SSA package (at the network's testing phase). The fifth variable is the value taken from the original series (during the network training) or the value predicted for the day by the trained ANN (at the training stage). It is shown that thus formed input sample has allowed one to achieve a fast and effective training of the neural network and to provide an acceptable medium-term forecasting of the daily energy consumption for the Moscow Region [20].

In cooperation with the Plekhanov Russian University of Economics, an automated system for monitoring and predict matching of a compliance of higher vocational education with the needs of labor market has been developed. To create the system, a significant arsenal of methods and tools of Big Data Analytics and the experience gained in the projects on computing for the ATLAS and CMS experiments at CERN were used. The task, which lies in the mainstream of the so-called "digital economy", looks quite complicated so its solution requires new approaches and methods of data science, including methods of semantic analysis and machine learning. The constantly updated information database is generated using open sources. The developed system provides additional opportunities to reveal qualitative and quantitative interrelationships between education and labor market. It is aimed at a broad circle of users, including authorities and management of regions and municipalities; the management of universities, companies, and recruitment agencies, as well as graduates and university enrollees [21].

Simulations of structural changes on the nickel surface exposed to 100–700 MeV uranium ions have been performed. The dimensions of specific injuries have been obtained in dependence on the energy of irradiation at different points of time. It should be noted that when irradiating the metal sample by high-energy ions, the most energy is lost in the electron gas and then passed to the crystal lattice, but a certain amount of the energy is accumulated in the electron gas. Therefore, if choosing the initial conditions for the molecular dynamics simulation, this fact must be taken into account. The initial conditions (temperature profiles) can be varied in this case. In addition, the experimental data can be used to refine the initial conditions. In the framework of the conducted research, one can make the following two conclusions: the technique proposed is well suited to describe the structural changes in the surface layers of the material under irradiation and to obtain more accurate predictions on the structural changes; the use of experimental data is recommended as well as a better use of nonlinear dependence on the temperature of parameters of a thermal spike model [22].

INTERNATIONAL COOPERATION

The LIT specialists, in cooperation with their colleagues from the international CBM collaboration, develop the readout and data acquisition systems of the ring imaging Cherenkov detector (RICH), an integral component of the future Compressed Baryonic Matter (CBM) experiment at the Facility for Antiproton and Ion Research (FAIR) in Darmstadt, Germany. A detailed analysis of the readout and DAQ prototype has been conducted using the data gathered during the tests of the CBM RICH prototype in the beam conditions at CERN and using the results of the laboratory measurements performed by means of a specifically developed test stand. The readout and DAQ module prototype consists of a Hamamatsu H12700 MAPMT, PADIWA preamplifier-discriminator boards and a TDC-HUB board TRBv3. Calibration techniques were developed and implemented along with the DAQ and analysis code in the CbmRoot framework. Optimization of the readout module components has been performed which allows achievement of best timing characteristics in the high beam rate conditions, expected at CBM. The obtained sub-nanosecond time precision also allows one to directly measure the time profile of the additional wavelength-shifting films on top of the MAPMT windows and investigate their effect on timing of the full CBM RICH readout chain [23].

In cooperation with Bulgarian colleagues, LIT researchers developed a continuously atomic model (CAM) to simulate the interactions of high-energy heavy ions with condensed matter. The CAM is described by two different classes of equations, namely, continuous heat conduction equations of the thermal spike model and by equations of motion of material points of the molecular dynamics method. The use of high-performance systems for the continuous–atomistic modeling requires the development of new computational schemes and parallel algorithms. To study the CAM, a computational scheme and algorithms with the ability of their using in multiprocessor systems have been developed. The efficiency of the numerical scheme and the parallel algorithms is investigated [24].

In cooperation with colleagues from South Africa and USA, a recipe for the stable PT-symmetric extension of the Dirac equation has been proposed. The P- and T-breaking terms account for the gain and loss of energy in the system. The recipe has been used to formulate three PT-symmetric spinor models with cubic nonlinearity. Of these, the PT-symmetric extensions of the Thirring and Gross–Neveu models were shown to possess infinitely and finitely many conserved quantities, respectively. The PT-symmetric extension of the third, novel, spinor system has no conservation laws at all. Despite this dramatic difference in the integrability and conservation properties, all the three PT-symmetric models were shown to have exact soliton solutions. Numerical analysis indicates that all these solitons are stable — regardless of the soliton's frequency and the value of the PT-extension parameter. The persistence under the P- and T-breaking perturbations, as well as the all-inclusive stability, highlights a remarkable sturdiness of spinor solitons in two dimensions. The structural stability of spinor solitons with respect to the perturbations that violate P- and T-symmetry, as well as stability to perturbations of initial data, points to a fundamental nature of the particle like objects in the theories described by a nonlinear Dirac equation [25].

CONFERENCES, MEETINGS

On 3–7 July, LIT hosted the ninth international conference "Mathematical Modeling and Computational Physics" (MMCP'2017). The conference was devoted to the 60th anniversary of the foundation of the Joint Institute for Nuclear Research. Co-organizers of the conference were LIT, IFIN-HH (Bucharest, Romania), Technical University (Košice, Slovakia), Institute of Experimental Physics of the Slovak Academy of Sciences (Košice, Slovakia), and Pavol Jozef Šafárik University in Košice (Slovakia). The conference was sponsored by the Intel Company. The chairman of the conference was LIT Director V. V. Korenkov, and co-chairmen of the Organizing Committee were G. Adam (LIT JINR, IFIN-HH) and M. Hnatič (JINR Laboratory of Theoretical Physics, Institute of Experimental Physics of SAS and P. J. Šafárik University).

Scientific topics of the conference covered a wide range of issues, including distributed and parallel computing and tools for scientific computing; mathematical methods and application software for modeling complex physical and engineering systems; bioinformatics and computational biophysics; physical processes simulations and related computational methods; computer algebra and quantum computing with applications.

The conference was attended by over 250 scientists and specialists from various scientific centres of Romania, Bulgaria, Germany, Lithuania, Finland, France, Slovakia, USA, Mongolia, Canada and a large number of Russian research centres and universities such as NRC "Kurchatov Institute", IMPB RAS, ITAM SB RAS, St. Petersburg State University, Novosibirsk State University, PFUR and others.

In total, 212 reports (31 plenary, 158 oral and 23 poster ones) were presented at the conference.

A conference-school "Mathematical Modeling for the NICA Project" was organized in the framework of the MMCP conference under the support of the JINR Directorate. The school programme included lectures and practical classes as well as master classes.

The tutorials were conducted on the basis of the heterogeneous cluster HibryLIT under the support of the Heterogeneous Computing Team at LIT.

The conference-school was attended by 54 young scientists and specialists of JINR, students of the University “Dubna”, Moscow Engineering Physics Institute, MSU, St. Petersburg State University, Tver State University, PFUR, KazNU al-Farabi (Kazakhstan) and others.

On 25–29 September, the town of Budva, Montenegro, hosted the XXVI International Symposium on Nuclear Electronics and Computing (NEC’2017). The symposium has been traditionally held by JINR since 1963, and for the ninth time JINR and CERN became its organizers. Co-chairmen of the symposium were LIT Director V. V. Korenkov (from JINR) and Dr. Ian Bird (from CERN). The symposium was attended by more than 120 leading specialists in the field of modern computer and network technologies, distributed computing and nuclear electronics from 14 countries: Belarus, Moldova, Bulgaria, Great Britain, Germany, Russia, USA, France, Czech Republic, Slovakia, Italy, China, Netherlands, and Switzerland. The scientific programme of the symposium covered a wide range of issues and included the following sections: detector and nuclear electronics; triggering, data acquisition and control systems; machine learning and big data analytics; grid technologies and cloud computing; computing for large-scale accelerator facilities (LHC, FAIR, NICA, SKA, PIC, XFEL, ELI, etc.); non-relational databases and heterogeneous repositories; research data infrastructure, computations with hybrid systems (CPU, GPU, coprocessors) as well as a traditional topic of the symposium related to innovative IT education. Within the symposium, a BigPanDA Technical Interchange Meeting was held. The symposium was organized under the sponsorship of the companies Niagara Computers, JET Infosystems, Dell-EMC and IBS Platformix.

In total, 89 reports (36 plenary and 53 sectional ones) were heard. At the educational section, 10 reports were delivered.

For the fourth time the International School on Modern Information Technology for Students and Postgraduates was organized within the symposium. This school was devoted to heterogeneous distributed computing infrastructures.

The school was attended by leading scientists from Russia, UK, USA, Italy, as well as by employees from JINR, NRC KI, CERN and DESY.

The school-conference was attended by 32 senior students, as well as by masters and postgraduates majoring in information technology from the leading Russian universities (National Research Nuclear University MEPhI, St. Petersburg State University, University “Dubna”, Ryazan State Radio-Engineering University, Magnitogorsk State Technical University, Peoples’ Friendship University of Russia, and Tomsk Polytechnic University.

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