LABORATORY OF INFORMATION TECHNOLOGIES

In 2020, the studies on two themes of first priority “Information and Computing Infrastructure of JINR” and “Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data” were carried out by the Laboratory of Information Technologies (LIT) within the direction “Networks, Computing, Computational Physics”. The LIT staff participated in research on 26 themes of the JINR Topical Plan as part of cooperation with the other JINR Laboratories. The LIT activity is aimed at developing the JINR network, information and computing infrastructure, mathematical support and software for research and production activities underway at the Institute and its Member States on the basis of the JINR Multifunctional Information and Computing Complex (MICC).

In 2020, the staff of the Laboratory of Information Technologies published over 170 scientific papers and presented more than 120 reports at Russian and international conferences.

INFORMATION AND COMPUTING INFRASTRUCTURE OF JINR

One of the major directions of the LIT activity in 2020 was the development of the JINR MICC [1] and provision of the reliable functioning of the JINR network infrastructure, which during the pandemic was subject to additional demands to accommodate remote work of all the JINR employees. The MICC development encompassed the continuation of extensive modernization of the MICC cooling and power supply systems, which started in 2019, modernization and development of the MICC computing resources and data storage systems, development of the IT infrastructure of the NICA megascience project, expansion of the performance of the grid components, i.e., Tier-1 and Tier-2, extension of the cloud component and creation of an integrated cloud environment for JINR experiments, enlargement of the HybriLIT heterogeneous computing platform, including the “Govorun” supercomputer.

JINR Telecommunication Channels. In 2020, the reliable functioning of the following JINR telecommunication channels was ensured: the Moscow–JINR redundant channel with a bandwidth of 3×100 Gbit/s; the JINR–CERN direct channel with a bandwidth of 100 Gbit/s and its 100 Gbit/s backup channel, which passes through MMTS-9 in Moscow and Amsterdam, ensuring the operation of the LHCOPN network for the connection between Tier-0 (CERN) and Tier-1 (JINR) and of the LHCONE external superimposed network designed for the JINR Tier-2 center; direct channels up to 100 Gbit/s for communication with the collaboration of RUHEP research centers and the Runnet and ReTN networks using the RU-VRF technology [2].

The distribution of the incoming and outgoing traffics by the JINR subdivisions in 2020 (exceeding 25 TB by the incoming traffic) is shown in the table.

Subdivision	Incoming, TB	Outgoing, TB
DLNP	425.84	271.81
VBLHEP	208.03	130.76
FLNP	97.70	130.15
LIT	93.26	87.99
Hotel and Restaurant Complex	87.04	27.71
Dubna State University	86.97	51.16
FLNR	81.98	70.52
Remote access node	63.91	10.89
JINR Directorate	56.09	90.55
University Centre	31.40	10.59
BLTP	24.39	27.85

The overall incoming traffic of JINR, including the general-purpose servers, Tier-1, Tier-2, the computing complex, the "Govorun" supercomputer and cloud computing, amounted to 29.91 PB in 2020, while the overall outgoing traffic reached 36.94 PB. The traffic with the scientific and educational networks, accounting for 97% of the total, is overwhelming.

JINR Local Area Network (LAN). In 2020, the fault-tolerant operation of the backbone of the Institute's local area network with a bandwidth of 2×100 Gbit/s and the distributed computing cluster network between the DLNP and VBLHEP sites with a capacity of 400 Gbit/s was ensured. To increase the reliability of the optical backbone network, double redundancy was provided.

The work on the development and improvement of the network components of the JINR IT infrastructure was in progress. The EOS distributed storage network and the network "Cloud Computing" were connected to the RU-VRF/LHCONE external network. The commissioning of the fourth module in the MICC hall and its equipping with computing resources were performed together with setting up and connecting central and rack switches.

Several systems (Cisco Meeting Server, BigBlueButton, Videomost, Zoom, etc.) were tested for video conferencing. For mass use, the Cisco Webex system was chosen, and 816 meetings were held in 2020 using it.

The modernization of the cluster of virtual services of the JINR network service was in progress. The NOC network service works with virtual machines that provide key services for the entire network infrastructure of JINR: DNS, DHCP, relays — intermediate mail servers, network database servers, the NOC web hosting server, as well as a number of third-party services for LIT and JINR University Centre.

The cluster consists of six compute nodes and two data storage systems. The data storage systems operate under the management of the ZFS file system. The cluster functions in a 24×365 mode. The architectural solution enables nonstop work during updates of both software and hardware components of the network cluster.

The functionality of the system for network traffic analysis was expanded with the help of new written scripts that can identify infected and hacked user computers. The support of the Wi-Fi eduroam network at LIT, the "Dubna" hotel, the House of International Meetings, the House of Scientists, and the UC hostel is provided. The status of 560 hosts, of more than 150 services and conditions is monitored in the network monitoring system. Several types of notifications, namely, e-mail messages and SMS alerts, are used.

JINR LAN comprises 8895 network elements and 16 884 IP-addresses, 7388 network users, 3192 users of mail.jinr.ru, 1419 users of electronic libraries, and 445 users of the remote access service.

MICC Engineering Infrastructure. In 2020, the work on the replacement and improvement of the MICC engineering infrastructure, designed to ensure a reliable, uninterrupted and fault-tolerant operation of information and computing systems and data storage resources, was in progress. The system of central uninterruptible and redundant power supply based on accumulator sources and diesel-generator units was put into operation for the MICC hall. The climate control system, involving a complex of interconnected equipment with different air and liquid cooling schemes, which creates a temperature regime for the MICC functioning in a 24×365 mode, was partially modernized.

JINR Grid Environment. The JINR grid infrastructure is represented by the Tier-1 center for the CMS experiment at the LHC and the Tier-2 center for processing data from the experiments ALICE, ATLAS, CMS, LHCb, BES, BIOMED, MPD, NOvA, STAR, ILC and others. Both JINR grid sites ensure 100% availability and reliability of services.

In 2020, the Tier-1 data processing system was increased to 13 376 cores, providing a performance of 203.569 kHS06. The storage system, comprising disk arrays and long-term storage of data on tapes, was expanded. The total usable capacity of disk servers was increased to 13.7 PB. In April, the commissioning of a new tape library IBM TS4500 with a total volu-

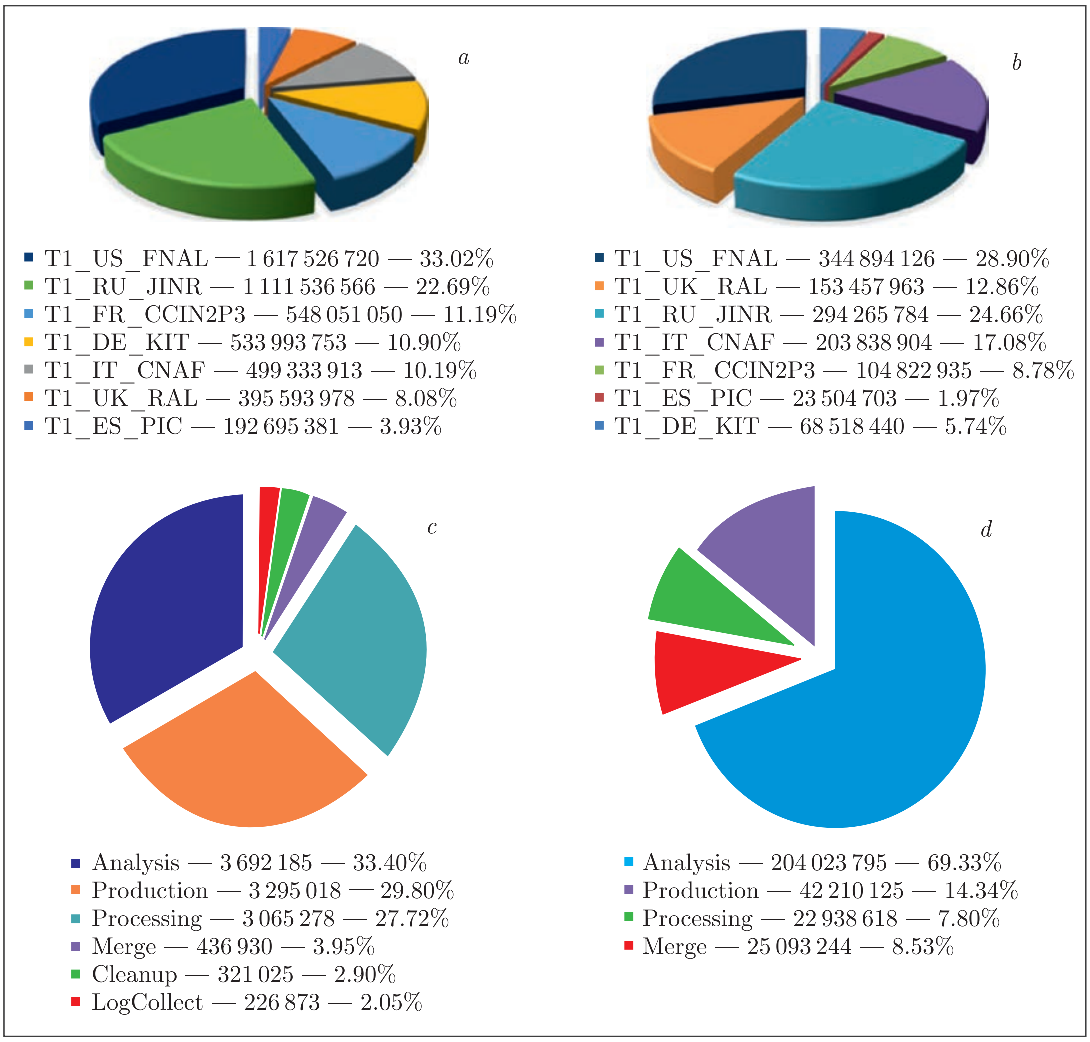

Fig. 1. Contribution of the world Tier-1 centers to CMS experimental data processing in 2020: *a*) distribution by the normalized CPU time in HS06 hours; *b*) number of processed events. Statistics on the use of the JINR Tier-1 center by the CMS experiment by different types of data stream processing in 2020: *c*) distribution of jobs; *d*) distribution of events by type of processing

me of 40 PB was completed. To date, the data long-term storage system consists of the IBM TS3500 and IBM TS4500 libraries and is focused on servicing the NICA and CMS experiments.

In terms of performance, Tier-1 (T1_RU_JINR) is ranked second among all the Tier-1 world centers for the CMS experiment (Fig. 1, *a*). In 2020, more than 294 million events were processed, which accounts for 25% of the total number of processed events (Fig. 1, *b*) and 23% of the total CPU load of all Tier-1 centers for the CMS experiment.

Figure 1, *c*, *d* shows the number of jobs and events processed at the JINR CMS Tier-1 center in 2020 by different types of data stream processing (reconstruction, modeling, reprocessing, analysis, etc.).

In 2020, at Tier-1 there happened a transition related, on the one hand, with the end of support of the software used for compute elements, i.e., CREAM-CE, the Torque batch processing system and the Maui scheduler, and, on the other hand, with the fact that the previous software and systems could not cope with the increased load and a large number of computing machines. To replace CREAM-CE, ARC-CE (Advanced Resource Connector-Computing Element) was chosen; it is widely used in WLCG (Worldwide LHC Computing Grid). SLURM, an open source, highly scalable, fault-tolerant cluster manager and job scheduler for large clusters, was selected as a resource manager. It enables flexible planning with priorities, fair distribution of resources between different users and optimization of the utilization of computing

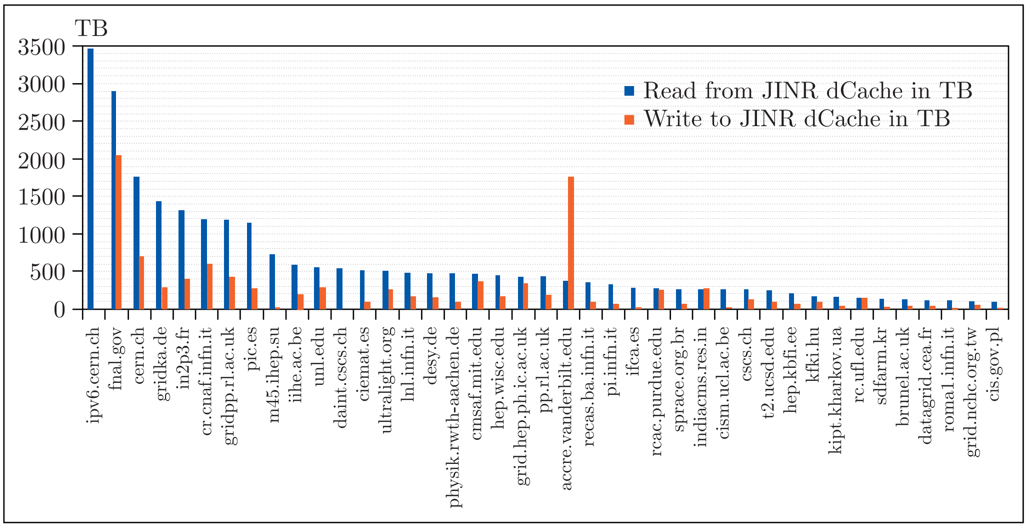

Fig. 2. Statistics on the exchange of JINR Tier-1 data with the world data processing centers of the WLCG infrastructure via the dCache-based data storage system: blue color — amount of data transferred from JINR Tier-1 to the other world Tier-1 and Tier-2 centers; red color — amount of transferred data from the world Tier-1 and Tier-2 centers to JINR Tier-1 for writing and processing

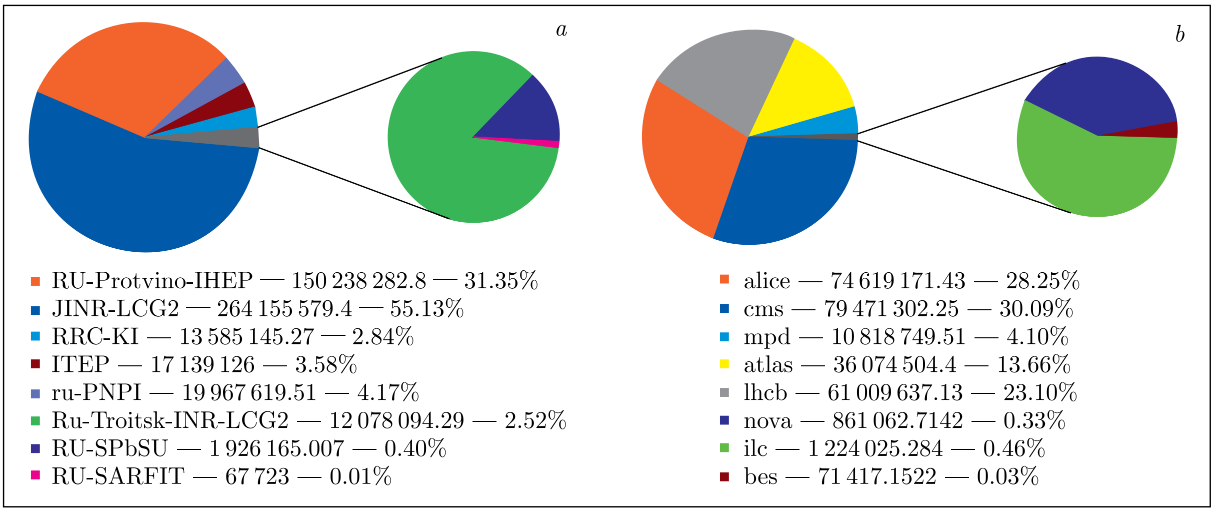

Fig. 3. Statistics of the JINR Tier-2 operation: *a*) distribution of the CPU time by the grid sites of the organizations being part of the Russian Consortium RDIG; *b*) use of the JINR Tier-2 site by virtual organizations of the global grid infrastructure (by the normalized CPU time in HS06 hours)

resources. SLURM is also used on the “Govorun” supercomputer.

One of the main functions of Tier-1 is to provide data exchange with all world sites operating for the CMS experiment and storage of raw experimental and simulated data. In 2020, the overall volume of data exchange with the dCache-based storage system, taking into account local exchanges, was 106 PB, of which 22 PB of new files were written. Figure 2 illustrates the statistics of data exchange of JINR CMS Tier-1 with the other grid centers with a volume of more than 100 TB for the outgoing traffic. 192 WLCG data processing centers for the LHC experiments downloaded 26 154.5 TB from the Tier-1 storage system, 130 of which transferred 10 655.7 TB of data for writing.

In 2020, the computing resources of the Tier-2 center were expanded to 7060 cores, which currently provides a performance of 100 kHS06. The total usable capacity of disk servers is 4763 TB for ATLAS, CMS and ALICE and 140 TB for other virtual organizations (VOs). The JINR Tier-2 site is the best in the Russian Consortium RDIG (Russian Data Intensive Grid). In 2020, 55% of the total CPU time spent on data processing and analysis using the RDIG resources were carried out at the JINR

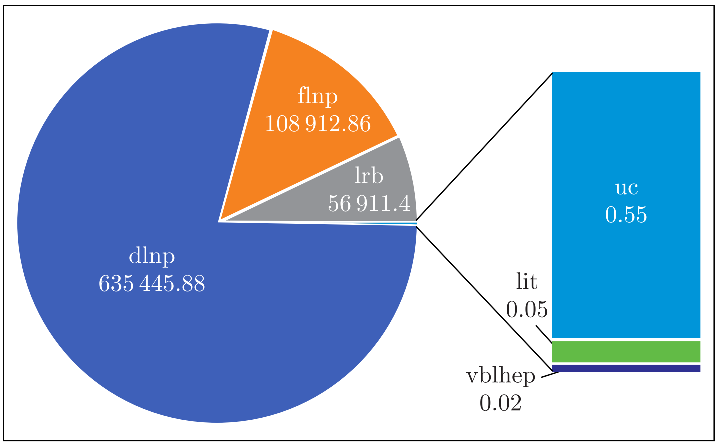

Fig. 4. Statistics on the use of the computing cluster: distribution by the CPU time in hours, normalized to 1000 Specint2000, by jobs performed on the local (not grid) computing cluster by the Institute's subdivisions and user groups

Tier-2 site (Fig. 3, *a*). The data on utilizing the JINR Tier-2 site by virtual organizations within grid projects in 2020 are shown in Fig. 3, *b*.

The MICC allows users to perform calculations outside the grid environment. It is necessary for some experiments and local users of the JINR Laboratories. JINR and grid users have access to all computing power via a unified batch processing system. The time distribution of jobs performed on the MICC computing cluster by the Institute's subdivisions and user groups is given in Fig. 4.

In 2020, the EOS-based data storage system was extended. At present, 7.12 PB of disk space is available for EOS users. Baikal-GVD, DANSS, FOBOS, JUNO, BM@N, MPD, SPD, PANDA are its major users.

The stable and efficient operation of Tier-1, Tier-2, storage systems and the required level of cluster cybersecurity were ensured by systematic updating of the firmware of the server components, the version of the operating system kernel and the firmware of the service modules of the IDRAC/IPMI servers.

Cloud Environment. In 2020, the resources of the cloud infrastructure were enlarged due to contributions of the NOvA experiment (480 CPU cores, 2.88 TB of RAM, 1.728 PB of disk space for ceph-based storage) and the commissioning of 2880 CPU cores with 46.08 TB of RAM purchased by the JUNO experiment. The total amount of the resources located in the JINR cloud infrastructure is 5000 CPU cores, 60 TB of RAM and 3.1 PB of raw disk space in ceph-storage. Figure 5 shows the information on the resource consumption of the cloud infrastructure in 2020.

The JINR cloud is one of the participants of the distributed information and computing environment (DICE) based on the resources of

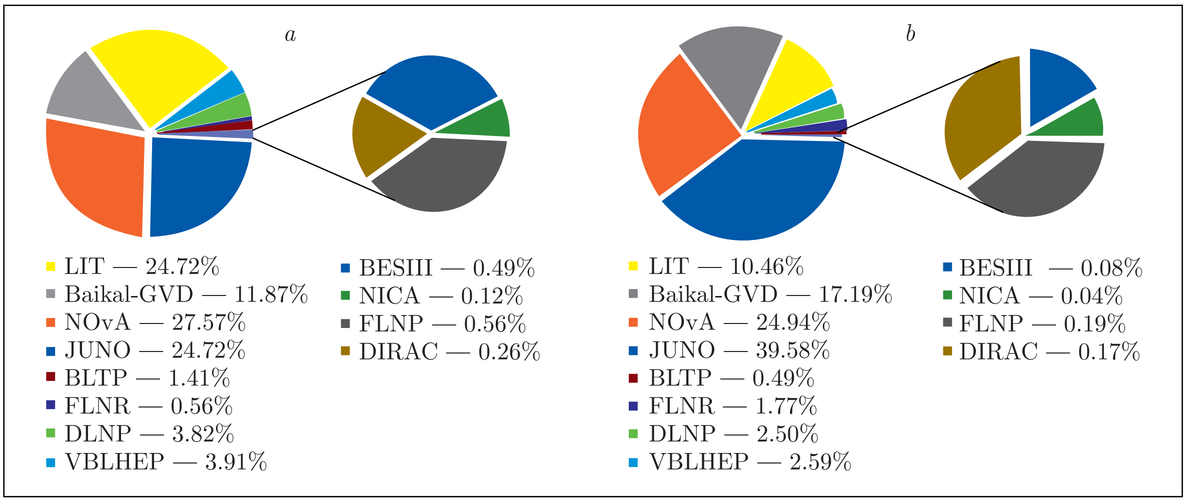

Fig. 5. Consumption of the resources of the JINR cloud infrastructure in 2020: *a*) CPU time, *b*) RAM usage

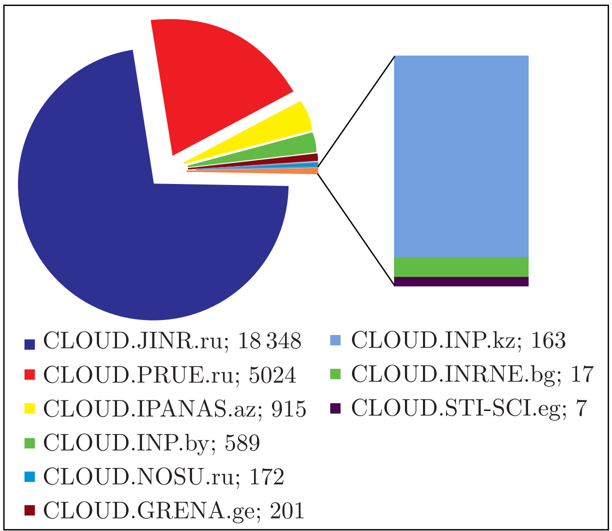

Fig. 6. Distribution of the number of successfully completed jobs by users of all VOs on the cloud resources of the JINR Member States' organizations in 2020

JINR and its Member States' organizations. In 2020, cloud infrastructures at North Ossetian State University, Sofia University "St. Kliment Ohridski" and the Institute for Nuclear Research and Nuclear Energy of the BAS were deployed and connected to the DICE. The deployment of cloud infrastructures at Georgian Technical University and the Egyptian National STI Network of the Academy of Scientific Research and Technology was started.

In 2020, the Baikal-GVD experiment joined the utilization of the DICE computing power. A pie chart with the number of jobs successfully performed in 2020 on the resources of all DICE participants by users of all virtual organizations is represented in Fig. 6.

In 2020, idle resources of the DICE were involved in research on the SARS-CoV-2 virus within the Folding@Home platform. Figure 7 illustrates a pie chart with the contribution of each of the DICE resource centres.

Heterogeneous Infrastructure. The heterogeneous infrastructure of the JINR MICC is represented by the HybriLIT component, which consists of the education and testing polygon and the "Govorun" supercomputer, managed by a unified software and information environment. In 2020, the development and implementation of an ecosystem for machine/deep learning and high-performance computing (ML/DL/HPC ecosystem) into this environment were completed; the ecosystem is actively used to create algorithms based on neural network approaches for solving applied tasks.

In 2020, up-to-date versions of more than 20 software packages, in particular, GSL (BLTP); FairSoft, FairRoot, PyROOT with add-ons for BmnRoot and MpdRoot, SMASH, Valgrind (NICA); ABINIT, Wien2k, Amber, AmberTools (FLNP); DIRAC, ELPA, FLUKA, LAMMPS (FLNR); FreeSurfer, FSL, MRIConvert, GROMACS (LRB); Expect, FORM, SMILEI (LIT), etc., were implemented into the HybriLIT environment and supported at the request of user groups.

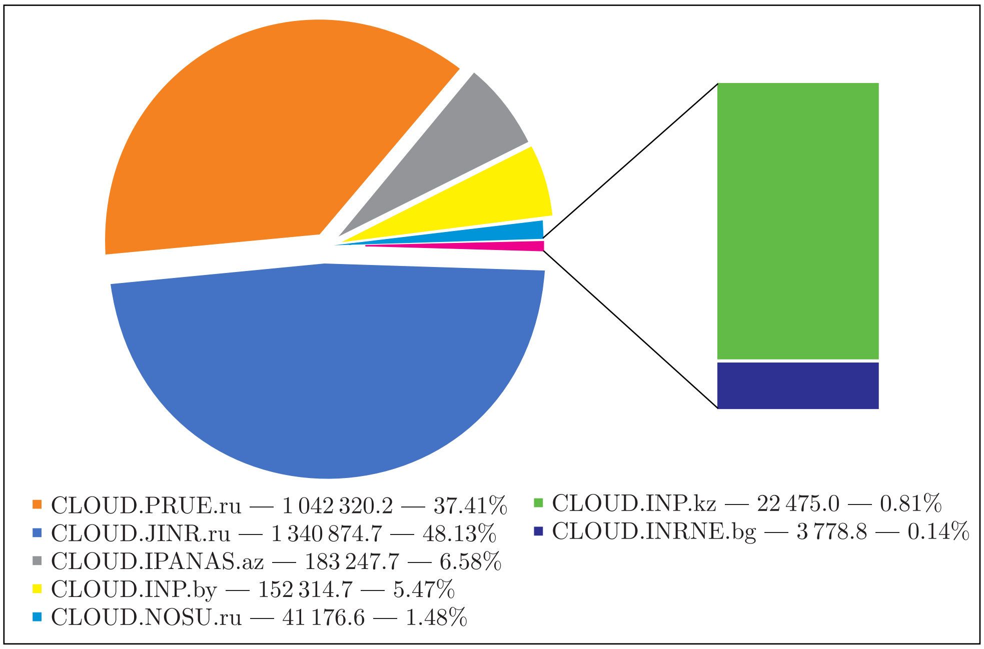

Fig. 7. Distribution of contributions of the DICE participants to the study of the SARS-CoV-2 virus via the Folding@Home platform in CPU HS06 hours

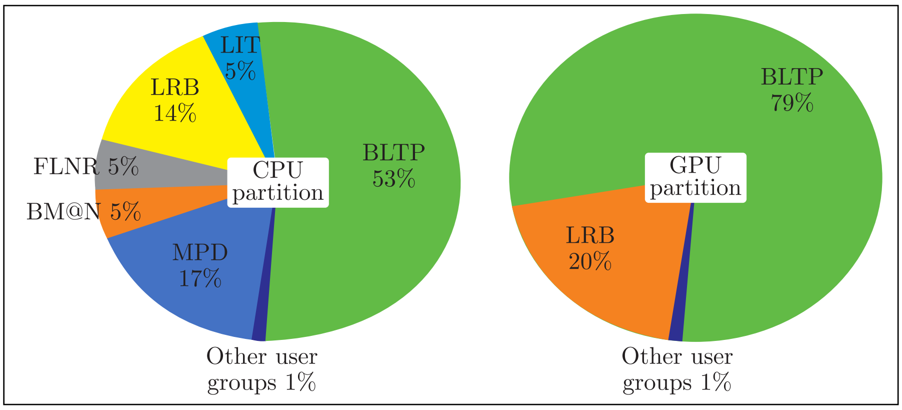

Fig. 8. Distribution of the resources of the “Govorun” supercomputer by user groups

In 2020, to increase the efficiency of solving user tasks, as well as to expand the efficiency of the utilization of both computing and data storage resources on the “Govorun” supercomputer, an approach to their management, i.e., resource orchestration, was elaborated and implemented [3]. This notion means software disjunction of a compute node, i.e., the separation of compute nodes and data storage elements (SSDs) with their subsequent integration in accordance with the requirements of user jobs. Thus, the computing elements (CPU cores and graphics accelerators) and data storage elements (SSDs) form independent fields. Due to orchestration, the user can allocate for his job a required number and type of compute nodes (including graphics accelerators), as well as a required volume and type of data storage systems. After the job is completed, the compute nodes and storage elements are returned to their corresponding fields and are ready for the next use. This feature allows one to effectively solve user tasks of different types, enhance the confidentiality level of working with data, and avoid system errors that occur when crossing the resources for different user tasks.

Within 2020, 491 609 jobs were performed on all computing components by all user groups utilizing the resources of the “Govorun” supercomputer to solve tasks in the framework of 25 themes of the JINR Topical Plan. Most of the jobs (440 813) were carried out on the Cascade component, 45 411 and 5385 were performed on the KNL and DGX components, respectively. In total, in 2020, over 35 million core-hours were accumulated on the Cascade component. The average load on the computing components in 2020 was the following: Cascade — 95.7%, KNL — 89.3%, DGX — 94.1%.

The overall number of users of the “Govorun” supercomputer is currently 157, of which 118 are from the JINR Laboratories and 39 are from other organizations of the JINR Member States. Moreover, in 2020, 75 new users were registered. The distribution of the computing resources by user groups is shown in Fig. 8.

The main users of the CPU component of the supercomputer came from BLTP and the NICA megaproject, in total 75%. User groups from the other Laboratories utilize a quarter of the resources. At the same time, for the GPU component, about 80% of the resources of the “Govorun” supercomputer are used by BLTP and 20% — by LRB, which is related to the implementation of neural network approaches for the tasks of radiation biology.

In 2020, users of the platform published 65 scientific papers. The summary report is available at http://hlit.jinr.ru/users_publications/.

In 2020, the work on the development of the offline computer complex for data modeling, processing, analysis and storage within the NICA project, which was built on the basis of the JINR MICC as a distributed scalable hybrid cluster, allowing one to organize computing for the NICA project efficiently and without additional labor costs at the request of a different class of jobs and users, was in progress. The integration of distributed computing resources was essential in creating such an infrastructure. One of the middleware options is the DIRAC Interware, a product for integrating heterogeneous computing resources and data storage resources into a unified platform, based on the use of standard data access protocols (xRootD, GridFTP, etc.) and pilot jobs. At the end of 2020, all the MICC components, the clouds of the JINR Member States, as well as the cluster of the National Autonomous University of Mexico (UNAM, within cooperation on the MPD project) were integrated into DIRAC.

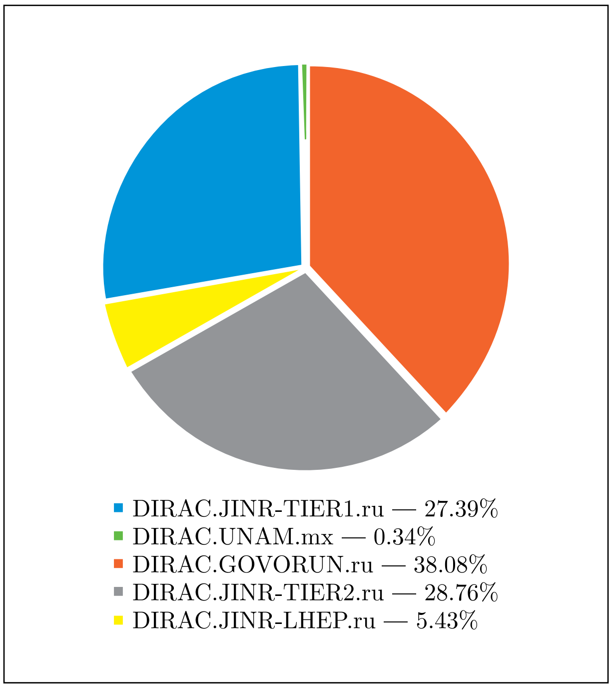

Fig. 9. Statistics on the normalized CPU time in HS06 hours used for simulation jobs within MPD on the DIRAC-based computing resources

Using the integration via DIRAC, it was possible to involve the largest amount of computing resources for centralized data generation with the Monte Carlo method for the MPD experiment. The "Govorun" supercomputer, the Tier-1/Tier-2 clusters, the NICA and UNAM clusters participated in the calculations. More than 500 000 jobs were successfully completed, and the amount of generated data exceeded 130 TB. All data is registered in the DIRAC file directory and stored in the EOS file system. Figure 9 illustrates the statistics on the normalized CPU time in HS06 hours used for simulation jobs within MPD on the DIRAC-based computing resources.

A software complex that enables the simulation of a distributed computing system for acquiring, storing and processing data from the BM@N experiment of the NICA project under different scenarios for launching jobs for the next run, which is planned to be held in 2021, was developed. The purpose of the modeling was the optimal distribution of the flows of primary data processing for the BM@N experiment to the compute nodes in order to minimize hardware downtime during job execution. Based on the simulation results, one can predict the load of the compute nodes and telecommunication channels.

Monitoring System. The developed integrated monitoring system of the MICC allows one to receive information from different components of the computing complex: the engineering infrastructure, networks, compute nodes, job launch systems, data storage elements and grid services, which guarantees a high level of reliability of the MICC. In 2020, the cloud infrastructure was connected to the common monitoring system. The Litmon monitoring system is modular and distributed. Thus, the addition of new nodes of the monitoring system entails the installation of a new node of the load distribution for the monitoring system. At present, the monitoring system comprises four servers [4]: the central control server litmon-01 and three load distribution nodes (Fig. 10).

A number of works on the development and current maintenance of the "Dubna" electronic document system (EDS) were completed. In particular, a module for maintaining the procurement plan was worked out, the ability to sign invoices for payment using an enhanced electronic signature was implemented, a subsystem for the automated formation of supply contracts on the basis of standard forms was developed, a module for monitoring, electronic archive storage and search for supply contracts was elaborated.

The work on the current maintenance and development of the APT EVM project management system for NICA was in progress. Specifically, the integration of Cost Book data with the procurement plan in EDS "Dubna" was implemented.

A new version of the CERN DB information system for registering business trips at CERN, managing accommodation and accounting financial expenses was developed and put into operation.

The ongoing maintenance and development of the following information systems upon users' requests were performed: HR LHEP, ADB2, PIN, ISS, Document Base and Electronic Photo Archive.

In 2020, a personal account with the possibility of online payment for tenants of the Institute's housing stock was developed and put into operation. Together with the electronic document system, a system for processing invoices in an electronic form, for the signing of which an internal certification center was implemented, was created. In the personnel system, a subsystem for accounting electronic employment record books was created, and the system for special job assessment was completely revised.

The Institute's management reporting was improved; as part of the development of project management, a corresponding module, which al-

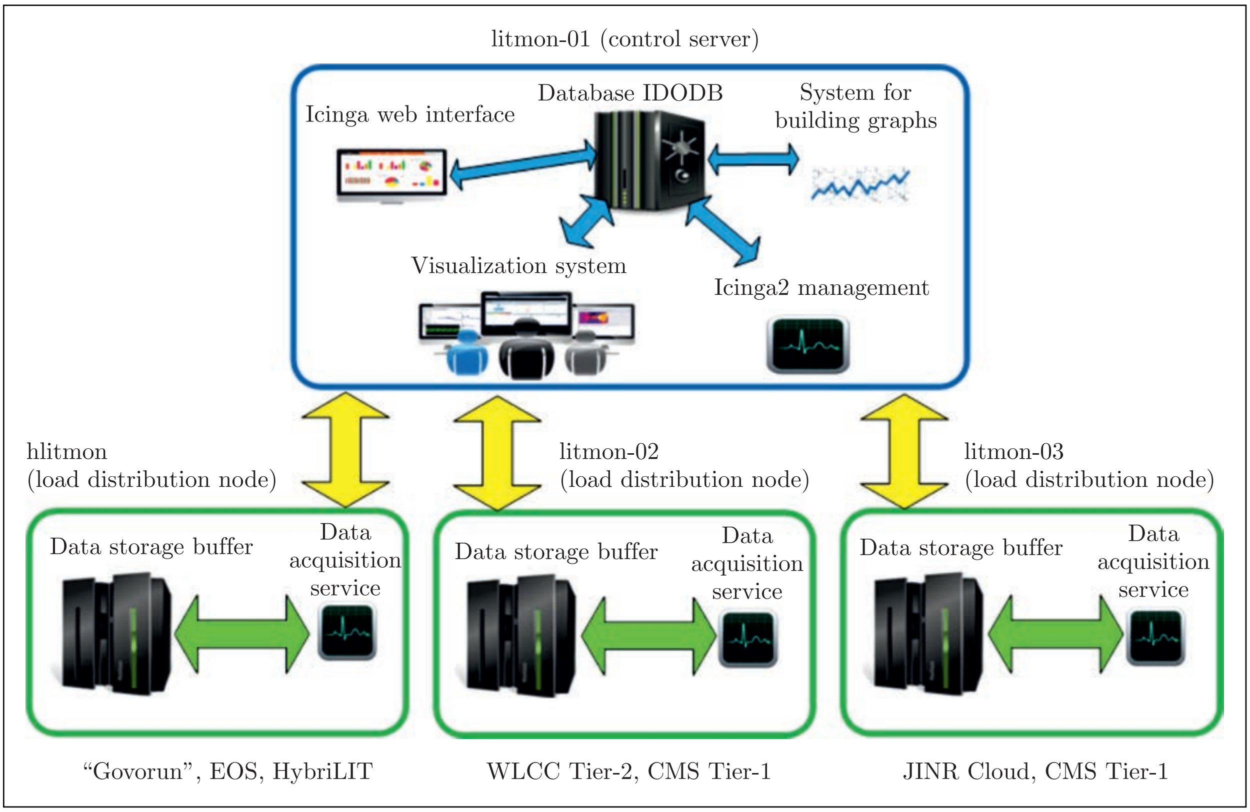

Fig. 10. Scheme of the Litmon monitoring system

lows one to track the work progress, to draw a Gantt chart and assign financial resources, was elaborated in the 1C program.

The ongoing training and support of users, as well as the maintenance and modernization of 1C programs, were carried out. The work on the creation of a system for accounting trip tickets to the "Dubna" Resort Hotel started; a new accounting methodology for the "Dubna" Resort Hotel was worked out and tested together with other services.

In 2020, the JINR Information System for Scientific Certification (ISSC) (https://dissertations.jinr.ru/) and the "Visit Centre" portal (https://visitcentre.jinr.ru/) were maintained. The modernization and support of the web site of the journals "Physics of Elementary Particles and Atomic Nuclei" (PEPAN) and "Physics of Elementary Particles and Atomic Nuclei, Letters" (PEPAN Letters) (http://pepan.jinr.ru) continued. The traditional development, creation and maintenance of web sites of conferences, symposia at the request of the Laboratories and other JINR subdivisions were in progress.

The maintenance of the following servers and systems of general use was conducted: the infrastructure of site hosting (www.jinr.ru, flnph.jinr.ru, flerovlab.jinr.ru, micc.jinr.ru, mpdroot.jinr.ru, etc.), the infrastructure of administrative servers (pin.jinr.ru, adb2.jinr.ru, sed.jinr.ru, etc.), the automated project management system (pm.jinr.ru) and the cloud storage service for the JINR staff (disk.jinr.ru).

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

One of the main activities of LIT is to provide mathematical, algorithmic and software support for experimental and theoretical research underway at JINR. A summary of prominent results is presented below.

A prototype of the platform for streaming analytics using Big Data technologies was deployed [5]. The platform was tested on the example of network traffic analysis in the distributed network.

Geometry and software models for different configurations of the inner tracker system of the BM@N experiment, which comprises the coordinate GEM, Forward Silicon and STS detectors, were developed. Algorithms for realistic simulations of the passage of charged particles through the sensitive planes of the tracker system detectors were implemented. The required characteristics of the gas mixture planned for use as a working medium in the gas-filled chambers of the GEM detector were calculated for future configurations in 2021–2022.

A software module for simulating data reconstruction in the drift chambers (DCH) of the BM@N experiment was elaborated. The required similarity of the process of reconstructing simulated and experimental data was obtained. The software was implemented in the BMNROOT software package. The DCH reconstruction chain was unified and automated for processing all types of data from the BM@N experiment.

Neural network models RDGraphNet and TrackNETv2, developed for the BM@N experiment with a fixed target, were successfully adapted for the cylindrical CGEM detector of the BESIII collider experiment (IHEP, Beijing). The training on simulated data and subsequent testing of the RDGraphNet model showed promising results, namely, 98% completeness and 86% accuracy, as well as 99% completeness and 77% accuracy for TrackNETv2 [6].

A further extension of the Monte Carlo generator of heavy-ion collisions DCM-SMM, which is used to simulate tens of millions of events for BM@N and MPD (NICA) on the HybriLIT cluster, was performed [7].

The impact of varying parameters in three GEANT4 hadronic physics models on the agreement with thin-target datasets was investigated, and using the Professor model tuning framework the correspondence to these datasets was described [8]. It was found that varying parameters produced a substantially improved agreement with some datasets; however, more degrees of freedom are required for full agreement.

A test server for the new version of the EventIndex system being developed was created as part of the project development to prepare the ATLAS experiment for RUN3. Services for calculating the matrix of intersection of trigger chains were implemented. The creation of a new Event Picking Service within the ATLAS EventIndex project was started. The operational monitoring system of the TDAQ system was adapted for the new versions of the Grafana product. The data visualization service for the network traffic monitoring system in ATLAS (NETIS) was modernized.

The magnetic field modeling involved: intense research concerning three-dimensional computer simulation of magnetic systems in the framework of the NICA project for the validation of the magnetic field uniformity in the working areas of new physical magnets, as well as the improvement of design tools for new medical cyclotrons, computed on the "Govorun" supercomputer.

In 2020, the JINRLIB library was supplemented with programs developed by the LIT specialists for general use: EORP 2020, a program for computing closed equilibrium orbits (http://wwwinfo.jinr.ru/programs/jinrlib/eorp/index.html); Split, a parallel implementation of the numerical solution of a system of algebraic equations with a tridiagonal matrix using the partition algorithm and MPI technology (http://wwwinfo.jinr.ru/programs/jinrlib/split/index.html); SIR-model, the simplest epidemic process model (http://wwwinfo.jinr.ru/programs/jinrlib/sir-model/index.html). The SAS program, devoted to primary processing of small-angle scattering spectra (http://wwwinfo.jinr.ru/programs/jinrlib/sas/index.html), was updated.

In cooperation with the Joint Institute of High Temperatures of RAS, a model that describes the passage of a multicomponent gas-condensate mixture through a porous medium in the depletion mode was formulated [9]. A quantitative agreement of the numerical results with experimental data on the dynamics of hydrocarbon recovery depending on pressure was obtained. The parallel implementation of the algorithm enables a 6-fold acceleration of computations on the HybriLIT cluster.

The influence of the inelastic channel and the choice of a model for the distribution density of nucleons in ^{12,14}Be nuclei on the agreement with experimental data was investigated [10]. For the density of ^{12,14}Be nuclei in the form of the symmetrized Fermi function, parameters that improve the agreement of $^{12,14}\mathrm{Be} + {}^{12}\mathrm{C}$ differential scattering cross sections with experimental data were obtained. The calculations were performed on the HybriLIT cluster.

A hybrid MPI + OpenMP model for parallelizing the multiple precision Taylor series method was proposed, implemented and tested [11]. With the help of this model, a trajectory for the Lorenz attractor was calculated in a rather long time interval [0, 7000].

To study strongly interacting nuclear matter, in particular, in neutron star nuclei, the extended sigma–omega model was investigated by means of the Bayesian analysis method. The most probable values of the physical parameters of the model were found using state-of-the-art multimessenger astronomical observations [12].

The Lagrange problem of finding all approximate solutions of the three-body problem on the plane, for which the distances between the bodies remain constant, was formulated. Two theorems that reduce the problem to the study of the midpoint scheme properties for a system of coupled oscillators were proved [13]. It was shown that in the case when the bodies formed a regular triangle the approximate solution inherited the periodicity property of the exact Lagrange solution.

The problem of the quantum-mechanical description of the near-barrier fusion of heavy nuclei, which occurs at a strong coupling of their relative motion to surface vibrations, was analyzed [14]. To this end, an efficient finite element method was proposed for the numerical solution of a system of coupled Schrödinger equations with boundary conditions corresponding to total absorption. It was found that the experimental data could be reproduced with a Woods–Saxon potential, without introducing repulsive cores. It was shown that the fusion cross sections at deep sub-barrier energies were sensitive to the potential pocket profile.

The interaction of pulsed ion beams with metal targets was modeled by the molecular dynamics method [15]. A numerical study of the dependence of the dynamics of thermal and structural processes in irradiated targets when changing the size and inhomogeneities of the structure was performed using the averaged values of the parameters of ion beams.

The basic parameters and wave functions determining the structure and properties of light nuclei with $A = 6$ (^{6}Li and ^{6}He) in the $\alpha + NN$ cluster model, which takes into account dibaryon resonances in the nucleon–nucleon interaction, were obtained [16].

An original three-center wave function was constructed by means of the irreducible representations of the D_{3h} point group, which characterizes the symmetry of the planar equilateral triangular H_3^+ molecule [17]. The results of this work and the implementation of computational methods pave the way for further studies of complex three-center systems.

Numerical simulation of laser ablation of the material under the action of ultrashort laser pulses was performed. The dependence of the maximum temperature on the sample surface and the thickness of the ablation layer on the radiation dose of the incident laser pulse was obtained. Numerical calculations were carried out using the finite difference method [18].

A method of ultrafast polarization switching in ferroelectrics was proposed and numerically studied using the self-acceleration effect of the polarization dynamics through a feedback field [19].

A new algorithm for representing polynomials in problems of computing involutive and Gröbner bases of systems of nonlinear polynomial equations was proposed [20]. The new approach enables the delegation of some parts of this computational task to GPUs, which opens up new opportunities for solving more complex problems.

The parameters on a conjugacy class in the Lie group $SL(n)$ and the parameters on a coadjoint orbit in the space $sl^*(n)$ dual to the Lie algebra $sl(n)$ were found. In this way the trivialization problems for the foliations of the $SL(n)$ group and the space $sl^*(n)$ were solved [21].

Three-loop computations of the renormalization group function γm, which determines the behavior of the effective mass of fermions in gauge theories, were carried out [22]. Dimensional regularization and the ‘t Hooft minimal subtraction scheme were used. The values of the anomalous dimensions of fermions for quantum chromodynamics and electrodynamics were obtained.

A new universal symbolic-numerical algorithm, which was implemented as the first version of $O(5) \times SU(1,1)$ in Wolfram Mathematica for computing the orthonormal basis of the Bohr–Mottelson collective model and which can be implemented in any computer algebra system, was elaborated [23]. This kind of basis is widely used to calculate the spectra and electromagnetic transitions in solid, molecular and nuclear physics.

Algorithms for algorithmic verification of linearizability for nonlinear (ordinary) differential equations were developed. The first algorithm is based on the construction of the Lie point symmetry algebra and calculation of the derived algebra; the second algorithm uses the differential Thomas decomposition and allows one not only to verify linearizability but also to generate a system of nonlinear partial differential equations that determine the point transformation and the coefficients of the linearized equation [24].

In the framework of constructive quantum mechanics, the problem of the emergence of geometry from entanglement in composite quantum systems was investigated. It was shown that the second Rényi entanglement entropy could be useful when applying polynomial computer algebra to model metric structures in quantum systems with geometry [25].

Using the negative property of the Wigner function, a global indicator of nonclassicality of the state space of an N-level quantum system in the Hilbert–Schmidt distribution was introduced, and its value for $N \to \infty$ was given [26].

The dependence of the global indicator of classicality on the geometry of the space of quantum states for a whole family of representations of Wigner quasiprobability distributions was investigated using the example of the Hilbert–Schmidt, Bures and Bogoliubov–Kubo–Mori ensembles of qubits and qutrits [27].

The robustness of entanglement in two qubits with maximally entangled mixed states was studied under quantum decoherence channels [28].

An algorithm for quantum teleportation of two-qubit maximally entangled Bell states on different five-qubit processors was implemented. To reduce arising errors, several modifications of the original teleportation protocol were proposed. The comparison of the dynamics of the results of measuring the output probabilities, performed on the IBM Q Yorktown processor, demonstrates significant progress in improving the characteristics of IBM's quantum hardware [29].

APPLIED RESEARCH

Two tasks of image recognition were considered: plant disease detection on 25 classes of five different crops (grape, cotton, wheat, cucumbers and corn — a total of 935 images) and moss species identification (5 types, 599 images). A neural network architecture based on a Siamese network with a triplet loss function and MobileNetV2 as a base network was proposed. The given model showed impressive results in accuracy for both tasks. The average accuracy for plant disease detection amounted to over 98.1%, and 97.6% for moss species classification [30]. The results illustrate a huge potential of this approach when solving the tasks of image recognition in a small training sample.

In 2020, an information system (IS) for the tasks of radiation biology was developed within a joint project of LIT and LRB using the ML/DL/HPC ecosystem of the HybriLIT platform (Fig. 11). The IS is aimed at storing experimental data and analyzing changes in the central nervous system of mammals on the basis of molecular, pathomorphological and behavioral changes in the mammalian brain when exposed

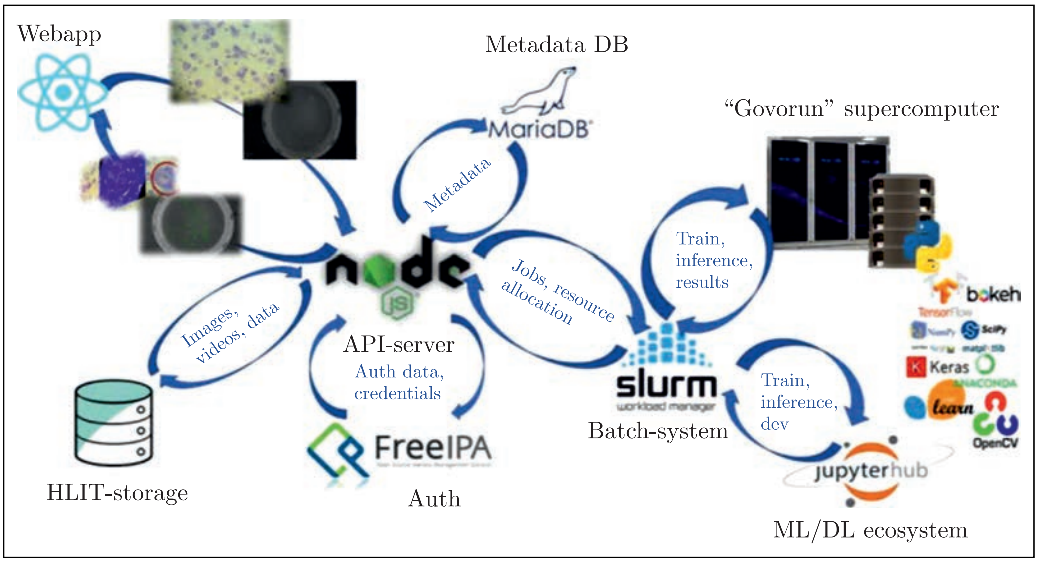

Fig. 11. Architecture of the information system

to ionizing radiation and other factors. Algorithms for experimental data processing based on machine and deep learning were implemented into the developed system. The IS comprises reliable modern means of authentication and hierarchical delimitation of access to data, a data storage system, as well as components for convenient work and visualization of data analysis results [31].

A Geometry Information System (GIS), which is configurable during deployment, was developed for use in all experiments of the NICA project. The general object model and architecture of the Geometry Database (DB) were designed. The GIS comprises central (PostgreSQL-based) and local (SQLite replica) Geometry Databases. The central DB is available on the Apache web server and provides all the functions required for detector geometry management. The local DB, being part of the software for the NICA experiments on the basis of the ROOT environment, is used primarily for loading the detector geometry in the jobs of modeling, reconstruction and physical data analysis. Application programming and web interfaces common for all NICA experiments were elaborated.

INTERNATIONAL COOPERATION

In 2020, within the cooperation agreement between JINR and DESY in collaboration with the partners of the JOIN^2 (Just anOther INvenio Instance) project (https://join2-wiki.gsi.de/cgi-bin/view), the work on the development of the JINR Document Server information system based on the JOIN^2 software platform (https://lt-jds-join2.jinr.ru/) was in progress. Bibliographic records were downloaded and verified, and authority records, namely, Topical Plan, Personalities, Subdivisions, Experiments, Grants, were downloaded and updated. This makes it possible to link publications with relevant funding sources, experiments with JINR's participation, etc. User authorization based on the Single Sign-On technology was implemented for the JINR staff [32].

An international research group, including scientists from LIT (O. Chuluunbaatar) and BLTP (Yu. V. Popov), conducted a kinematically complete experimental measurement of the characteristics of Compton scattering at free atoms using the highly efficient method of COLd Target Recoil Ion Momentum Spectroscopy (COLTRIMS). A theoretical description of this phenomenon is based on the calculations performed on the "Govorun" supercomputer [33].

In collaboration with colleagues from Poland, the "horn" effect in the K^+/π^+ ratio at a collision energy of ~ 8 GeV was studied within a $2+1$ flavor PNJL model. In parallel, to interpret the behavior of bound states in a dense and hot medium, the mean-field approximation (Breit–Wigner) and the Beth–Uhlenbeck approach were considered [34]. It was shown that the best agreement with the experimental data was obtained when the non-equilibrium chemical potential was involved in the calculations, and the absence of a critical end point in the phase diagram had no critical effect on the position and magnitude of the "horn".

EDUCATIONAL PROGRAM ON THE EDUCATION AND TESTING POLYGON

An important aspect of the activity that involves the resources of the HybriLIT platform is the educational direction related to conducting both training courses for JINR employees and practical classes for students of Dubna State University, Tver State University and other universities. In 2020, tutorials and master classes were remotely held for students from the Czech Republic and Armenia.

In 2020, tutorials and practical classes were held on the HybriLIT platform for more than 1000 students within the following courses: "Architecture of Computing Systems", "Technologies of High-Performance Computing", "Modern Methods of Analyzing Complex Systems", "Machine Learning and Data Mining", "Languages and Technologies of Data Analysis", "Mathematical Apparatus and Tools for Data Analysis" — using the ML/DL/HPC ecosystem, which allows students to master state-of-the-art technologies for developing parallel algorithms on novel computing hybrid architectures and tools (libraries and frameworks) for the tasks of machine and deep learning [35]. The platform resources were also actively used to train IT specialists within the International School of Information Technologies "Data Science" [36], whose students are engaged in real scientific projects of JINR (the results are presented in a collection of scientific and project activity reports: http://itschool.jinr.ru/other/Reports_ITSchool_eng.pdf). In 2020, three PhD theses and more than 15 Master's and Bachelor's theses were prepared using the resources of the HybriLIT platform.

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