MESHCHERYAKOV LABORATORY OF INFORMATION TECHNOLOGIES

An important component of the Laboratory's activity in 2021 was to ensure the reliable functioning and growth of the JINR network, information and computing infrastructure, as well as to develop mathematical support and software for the research and production activities of the Institute and its Member States on the basis of the JINR Multifunctional Information and Computing Complex (MICC). The research was carried out within two topics: "Information and Computing Infrastructure of JINR" and "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data".

In 2021, the staff of the Meshcheryakov Laboratory of Information Technologies (MLIT) published over 200 scientific papers and presented more than 150 reports at international and Russian conferences.

INFORMATION AND COMPUTING INFRASTRUCTURE OF JINR

The major information and computing resources of JINR are concentrated in the MICC [1], which can be considered as JINR's unique basic facility that plays a key role in studies asking for modern computing power and data storage systems. The uniqueness of the MICC is ensured by a combination of all state-of-the-art information technologies, namely, a network infrastructure with a bandwidth of 4×100 Gbit/s, distributed computing and data storage systems based on grid technologies and cloud computing, a hyperconvergent high-performance computing infrastructure with liquid cooling for supercomputer applications. The MICC is characterized by multifunctionality, high reliability and availability for calculations in 24/7 mode, scalability and high performance, a reliable data storage system, information security and an advanced software environment. The JINR computing infrastructure comprises an IT ecosystem for the experiments of the NICA megaproject (BM@N, MPD, SPD), which, thanks to grid technologies (DIRAC Interware), brings together the dedicated computing resources of all the MICC components: the Tier-1 grid site for the CMS experiment at the LHC; the Tier-2 grid site, which provides data processing for the experiments at the LHC, NICA, FAIR and other large-scale experiments, as well as support for users from the JINR Laboratories and Member States; the integrated cloud environment of the Member States devoted to support of users and experiments (NICA, ALICE, BESIII, NOvA, Baikal-GVD, JUNO, etc.); the HybriLIT platform, which includes the basic resource for high-performance computing, the "Govorun" supercomputer, and the training and testing polygon.

JINR Network Infrastructure. The network infrastructure is a fundamental component of the IT infrastructure of JINR and of the MICC. It provides access to the Internet, the computing resources and the data storage systems, as well as enables experimental data processing and computing. It is necessary to ensure the reliable and fault-tolerant operation of all the components of the network infrastructure: the external telecommunication channels, the JINR backbone network with a multi-node cluster structure and the MICC local area network.

In 2021, the reliable functioning of the following JINR telecommunication channels was ensured: the Moscow–JINR backup channel with a bandwidth of 3×100 Gbit/s, the 100 Gbit/s JINR–CERN direct channel together with its 100 Gbit/s backup channel, which passes through Moscow and Amsterdam and ensures the operation of the LHCOPN network for the connection between Tier-0 (CERN) and Tier-1 (JINR) and of the LHCONE external overlay network allocated to the JINR Tier-2 centre for communication with the RUHEP collaboration and the networks of the National Research Computer Network of Russia and RetN using RU-VRF technology. IPv6 routing was implemented for the Tier-1 and Tier-2 sites. In 2021, the Nortel DWDM equipment on the RSCC fiber-optic links route (Dubna, Radishchevo, Moscow) was replaced with the Infinera new equipment, which made it possible to broaden the bandwidth of all Dubna–Moscow channels.

The distribution of the incoming and outgoing traffics by the JINR subdivisions in 2021 (exceeding 25 TB by the incoming traffic) is shown in Table 1.

Table 1

Subdivision	Incoming traffic, TB	Outgoing traffic, TB
DLNP	941.9	158.27
MLIT	325.56	449.63
VBLHEP	280.18	160.98
Hotel and Restaurant Complex	171.74	33.52
Dubna State University	129.73	41.08
FLNR	108.59	48.07
FLNP	106.46	69.34
Remote Access Node	77.75	10.44
JINR Directorate	76.42	76.51
University Centre	29.83	6.35
BLTP	26.22	21.64

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 33.23 PB in 2021 (29.91 PB in 2020), while the overall outgoing traffic reached 35.86 PB (36.94 PB in 2020). The traffic with the scientific and educational networks, accounting for 97% of the total, is overwhelming.

The local area network (LAN) is based on the JINR backbone network with a bandwidth of 2×100 Gbit/s and the distributed multi-node cluster network between the DLNP and VBLHEP sites (4×100 Gbit/s). In 2021, the hardware and software of the Cisco C9500 routers of the JINR Laboratories (with 100 Gbit/s interfaces) were upgraded up to the latest version recommended by the vendor.

The MICC internal network has a Tier-1 segment built at the Brocade factory with a bandwidth of 80 Gbit/s. The network segments of the EOS data storage system, Tier-2, cloud computing and the "Govorun" supercomputer are built on Dell and Cisco hardware. The 10 Gbit/s and 100 Gbit/s ports are used to connect server components to the switches of the MICC network core built on Cisco Nexus 9504 and Nexus 9336C switches with an $N \times 100$ Gbit/s port bandwidth.

The internal network of the "Govorun" supercomputer consists of three main parts, namely, a communication and transport network, a control and monitoring network, and a task management network. The communication and transport network uses Intel OmniPath 100 Gbit/s technology. The network is built on a "thick tree" topology based on 48-port Intel OmniPath Edge 100 Series switches with full liquid cooling. The control and monitoring network enables the unification of all compute nodes and the control node into a single Fast Ethernet network. This network is built using Fast Ethernet HP 2530-48 switches. The task management network connects all compute nodes and the control node into a single Gigabit Ethernet network. The network is built using HPE Aruba 2530 48G switches.

In 2021, the central network virtual cluster of the JINR network service (NOC), which is built on top of the Proxmox VE (Virtual Environment) open source software under the GNU license, was modernized. This approach made it possible to use the NOC central cluster in 24/7 mode. It is noteworthy that the virtual machines operating in the central cluster serve all essential elements of the JINR network.

New software (Proxmox Mail Gateway) was introduced on the @jinr.ru email cluster; it significantly reduced the number of spams by training the system in spam filtering mechanisms.

Continuous availability monitoring and logging of logins to network sessions were added to the SSO system. The ability to edit LDAP entries for working in external services and the ability to register non-JINR staff members were added. The coverage of the eduroam WiFi network on the JINR territory was extended.

The JINR LAN comprises 8768 network elements and 17 602 IP addresses, 6377 network users, 6377 users of mail.jinr.ru, 1419 users of electronic libraries and 504 users of the remote access service.

MICC Engineering Infrastructure. In 2021, the work on the replacement and enhancement of the MICC engineering infrastructure, designed to ensure the reliable, uninterrupted and fault-tolerant operation of the information and computing systems and the data storage resources, was in progress.

The MICC computing facilities are hosted in one computing hall of 800 m^2 of floor space at the 2nd floor of the MLIT building. It currently consists of eight separate IT equipment modules (Fig. 1) with 2 MW power:

- Module 1 and Module 2: 22.55 m^2 of floor space each, 33 server racks and 20 kW per rack;
- Module Tier-1: 29.33 m^2 of floor space, 16 server racks and 35 kW per rack;
- Tape library space: 13 m^2 of floor space, two robotic tape libraries IBM TS3500 and IBM TS4500 with a total capacity of 50.6 PB;
- "Govorun" supercomputer: 1.97 m^2 of floor space, 4 racks and 100 kW per rack;

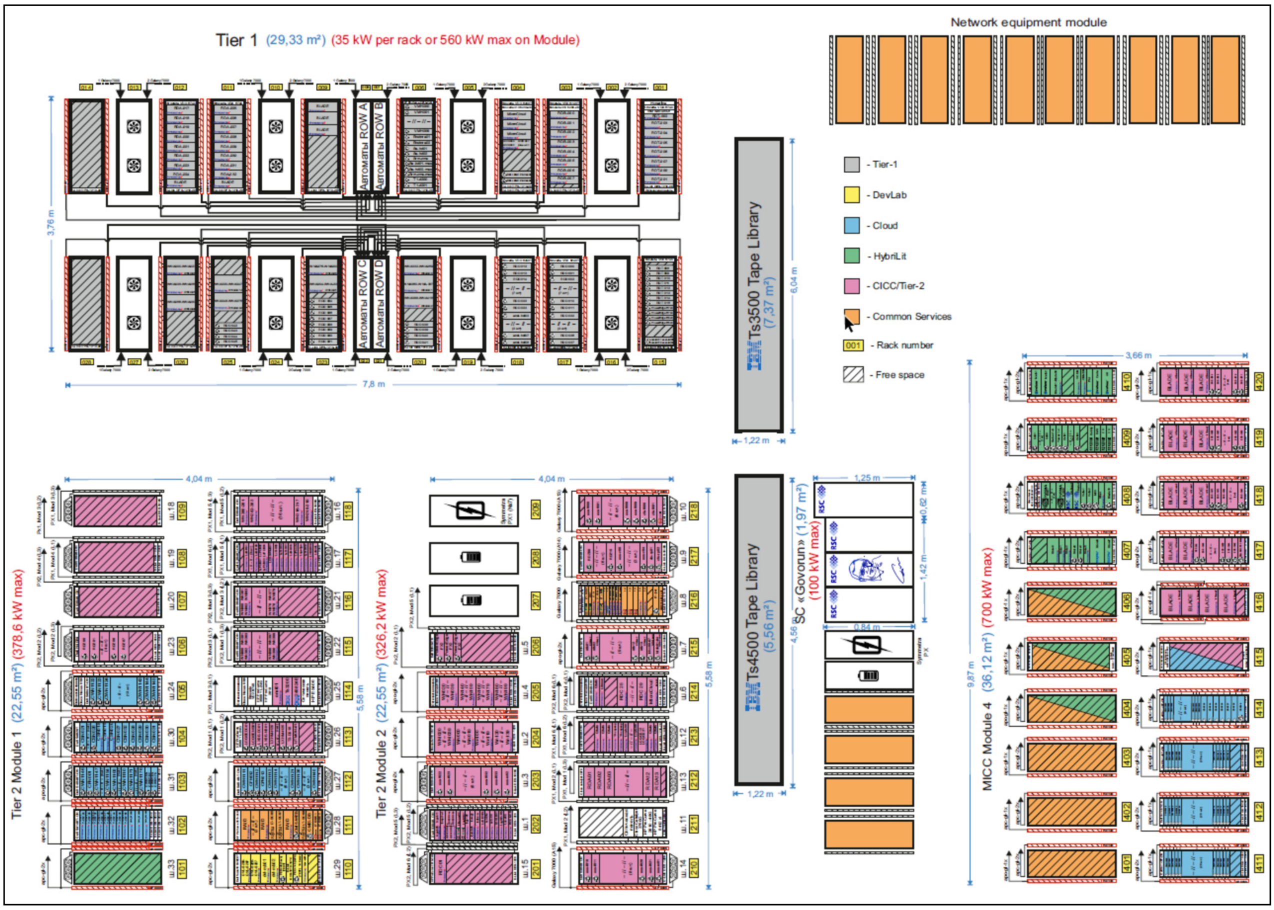

Fig. 1. Location of equipment in the MICC server hall

• Module that hosts critical services of the standard business computing type (administrative systems and databases, etc.);

• Module 4: 36.12 m^2 of floor space, 20 server racks and 35 kW per rack;

• Network equipment module that hosts the main network services for the MICC, JINR local and wide area networks.

All racks are UPS backed up with an autonomy of 10–15 min. Racks are equipped with intelligent (switched and metered) power distribution units, which enable the fine-grained monitoring of power consumption. In addition, there are two diesel generator backups for critical services.

Module Tier-1 and Module 4 are air-cooled with in-row racks arranged between server racks. Modules 1 and 2 are air-cooled, and the cold air is blown through large ducts underneath the false floor, where it diffuses into cold aisles through perforated floor tiles. The “Govorun” supercomputer is fully “hot” water-cooled, which allows for a power density of 100 kW per rack and PUE = 1.06.

All engineering equipment that provides both the guaranteed energy supply to the MICC and the cooling system is located at the first and basement floors of the building. Only chillers, dry coolers and diesel generators are located on the territory adjacent to the MLIT building.

The DCIM (Data Centre Infrastructure Management) system was put into operation for controlling and accounting the equipment of the MICC hall.

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

Since 2021, the Tier-1 resource centre has also been used to perform simulations for the MPD experiment of the NICA project. At present, there are 16 096 cores with a total performance of 253 135.18 HEP-SPEC06. The software and compilers used are CentOS Scientific Linux release 7.9, gcc (GCC) 4.4.7, C++ (g++ (GCC) 4.4.7), GNU Fortran (GCC) 4.4.7, dCache-5.2 for data storage, Enstore 6.3 for tape libraries and FTS. FairSoft, FairRoot and MPDRoot were installed to support the experiments of the NICA megaproject. The total usable capacity of disk servers is 14 PB, and that of tape libraries is 50.6 PB. The long-term data storage system based on the IBM TS4500 library is focused on servicing the NICA and CMS experiments.

In 2021, all resources of the JINR grid sites were migrated from CREAM-CE and Torgue-Maui to the Advanced Resource Connector Compute Element

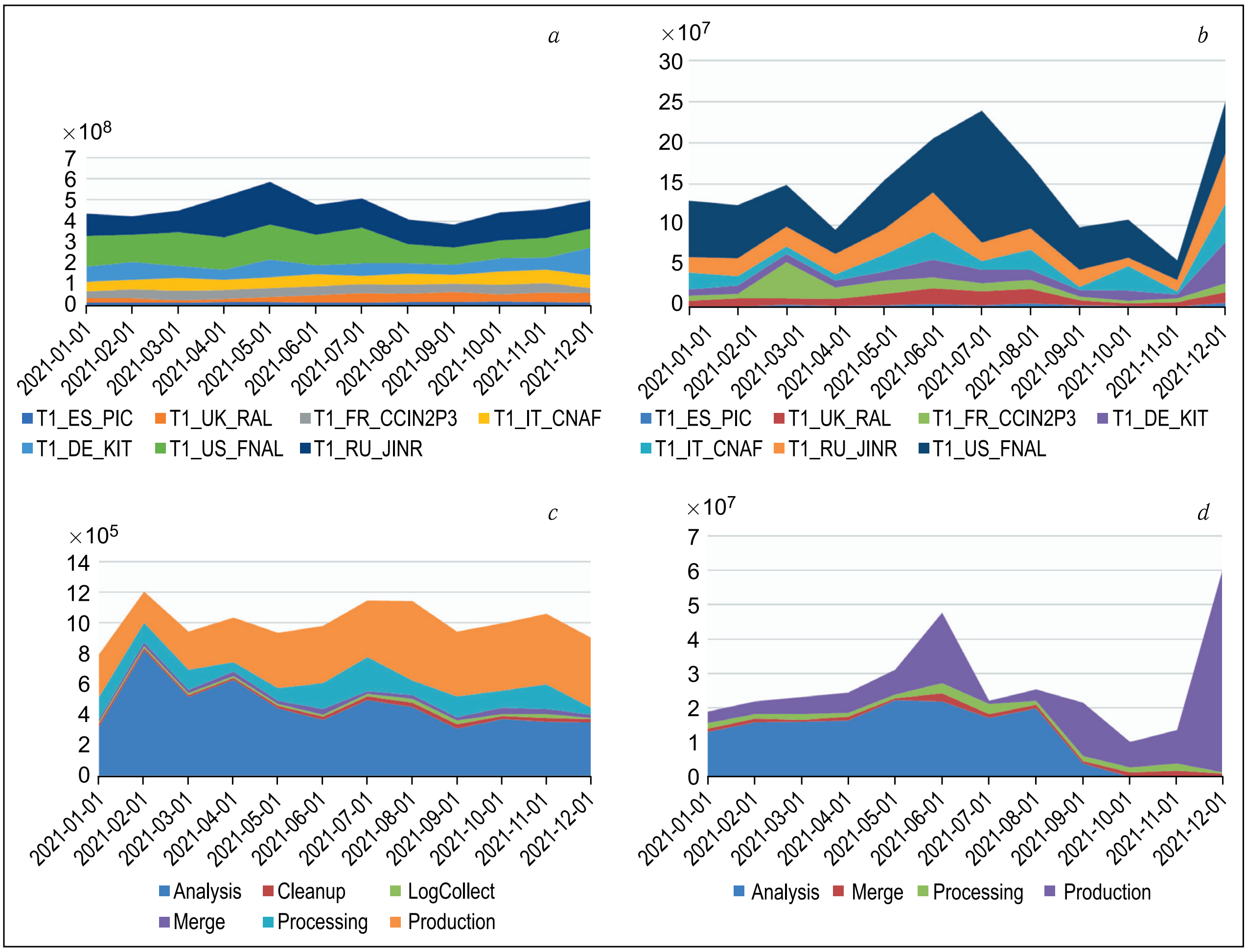

Fig. 2. Contribution of the world Tier-1 centres to CMS experimental data processing in 2021: *a*) distribution by the normalized CPU time in HEP-SPEC06 hours; *b*) number of processed events. Statistics on the use of the JINR Tier-1 centre by the CMS experiment by different types of data stream processing in 2021: *c*) distribution of jobs; *d*) distribution of events by the type of processing

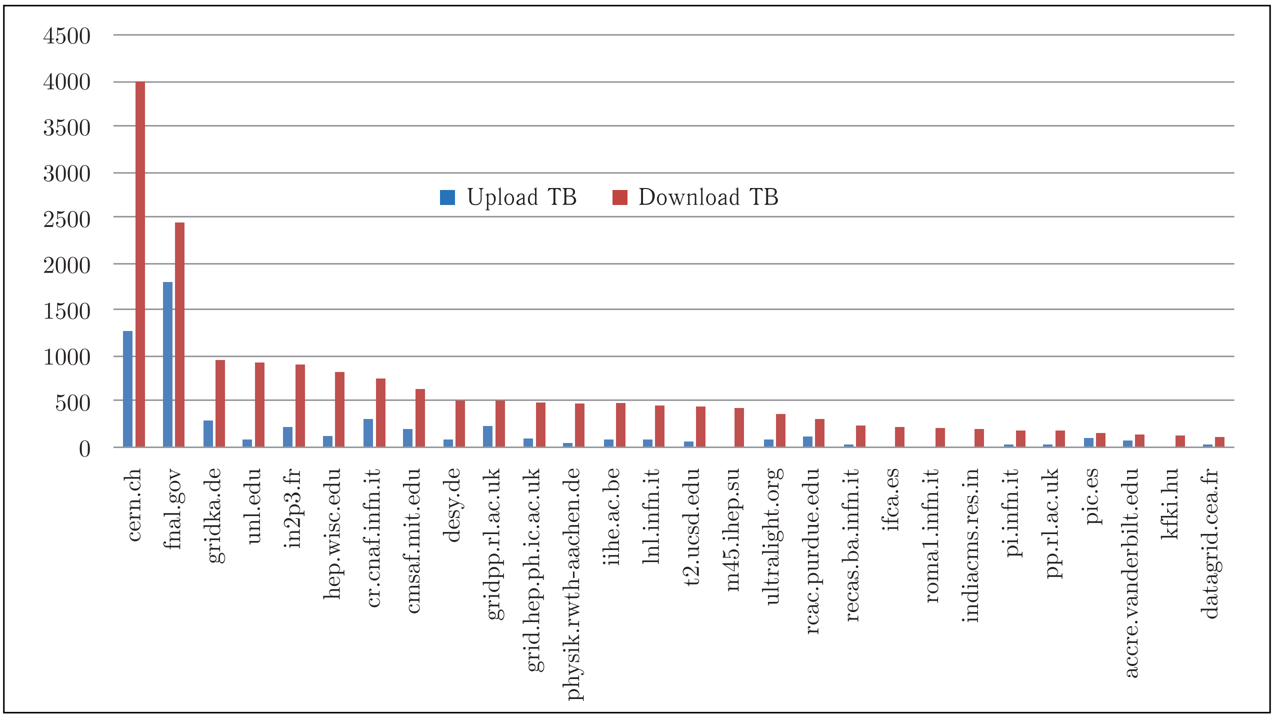

Fig. 3. Statistics on JINR Tier-1 data exchange with the world data processing centres of the WLCG infrastructure via the dCache-based data storage system

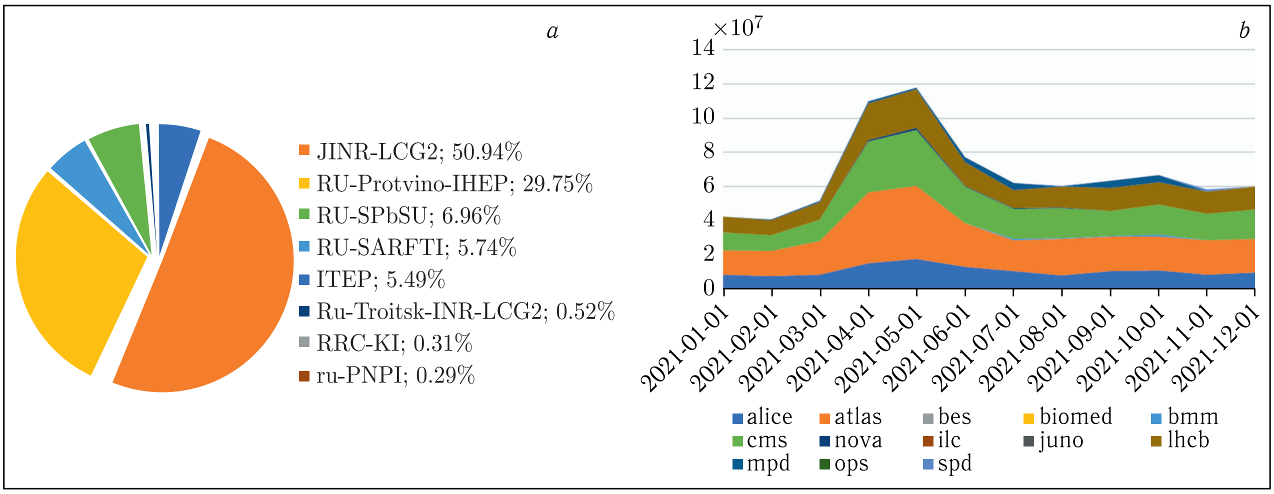

Fig. 4. Statistics of the JINR Tier-2 operation: *a*) distribution of the number of jobs by the web sites of the organizations being part of the Russian Consortium RDIG; *b*) use of the JINR Tier-2 site by virtual organizations of the global grid infrastructure (by the normalized CPU time in HEP-SPEC06 hours)

(ARC-CE) and the SLURM resource manager (adapted to kerberos and AFS), which is also used on the "Govorun" supercomputer.

In terms of performance, Tier-1 (T1_RU_JINR) is ranked first among the Tier-1 world centres for the CMS experiment (Fig. 2, *a*). In 2021, more than 321 million events were processed, which accounts for 18% of the total number of processed events (Fig. 2, *b*) and 29% of the total CPU load of all Tier-1 centres for the CMS experiment.

Figure 2, *c*, *d* shows the number of jobs and events processed at the JINR CMS Tier-1 centre in 2021 by different types of data stream processing (reconstruction, modeling, reprocessing, analysis, etc.).

The main functions of Tier-1 are to provide data exchange with all world sites operating for the CMS experiment and storage of raw experimental and simulated data. In 2021, the overall volume of data exchange between the 210 sites of the WLCG global network for processing data of the experiments at the LHC with the dCache-based storage system at JINR amounted to more than 30.5 PB, of which 24 PB of data were read and 6.5 PB of new files were written. Figure 3 illustrates the statistics of data exchange of JINR Tier-1 with other grid centres with a volume of over 100 TB for the outgoing traffic.

The JINR Tier-2 output is the highest in the Russian Consortium RDIG (Russian Data Intensive Grid). Over 83% of the total CPU time in the RDIG used for computing is provided by JINR Tier-2. In 2021, the computing resources of the Tier-2 centre were expanded to 9272 cores, which currently provides a performance of 149 938.7 HEP-SPEC06. The total usable capacity of disk servers is 4763 TB for ATLAS, CMS and ALICE and 140 TB for other virtual organizations.

Figure 4, *a* presents the distribution of jobs performed on the RDIG grid sites. The data on utilizing the JINR Tier-2 site (JINR–LCG2) by virtual organizations within grid projects in 2021 are shown in Figure 4, *b*.

The MICC allows users to perform calculations outside the grid environment. This is necessary for some experiments and local users of the JINR Laboratories. JINR and grid users have access to all the computing power via a single batch processing system.

In 2021, the EOS-based data storage system was extended to 16.7 PB. Figure 5 demonstrates the statistics on the use of the EOS system.

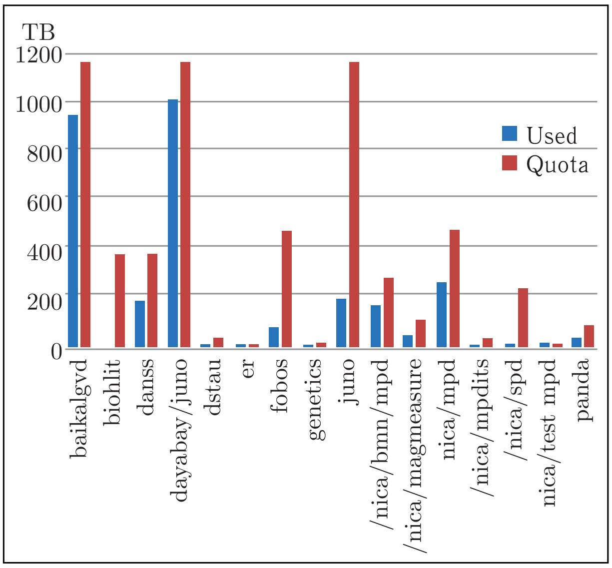

Fig. 5. Use of storage resources in the EOS system by user groups and JINR's experiments

To ensure the guaranteed and stable operation of the infrastructure under constant load conditions, centralized and timely software maintenance and the rapid introduction of new compute nodes are required. As a solution to this problem, the Lifecycle Management Service (LMS) was created; its purpose is to automate the process related to software maintenance and the commissioning of new computing resources [2].

Cloud Environment. 2021 was mainly devoted to the optimization of JINR cloud computing. Besides the general-purpose ceph-based storage with a total raw capacity of 1.1 PB, two new storage elements were deployed: the first is devoted to NOvA experiment needs only, and the second is an SSD-based ceph storage for a set of production services and users with high demands in terms of disk I/O. The main parameters of all these cloud storage systems are listed in Table 2.

A fairly wide set of software was used for JINR cloud servers and for the monitoring of some of its services (Nagios, InfluxDB time series database (TSDB), Prometheus TSDB, etc.). node_exporters were deployed on all cloud servers to provide Prometheus with servers state data. Alerting is implemented at the Prometheus level. Grafana is used for data visualization.

JINR cloud management is done along the "Infrastructure-as-a-Code" (IaC) approach, where host provisioning and management are performed via configuration files. The Foreman and Puppet software are used for this purpose.

Table 2. Characteristics of the cloud storage elements

Storage element	Disk type	Consumers	Ceph version	Raw capacity, PB	Replication	Connectivity
Regular cloud storage	HDD	All	14.2.21	1.1	3 ×	2 × 10 GBase-T
NOvA storage	HDD	NOvA	15.2.11	1.5	3 ×	2 × 10 GBase-T
Fast cloud storage	SSD	High disk I/O demands	15.2.13	0.419	3 ×	4 × 10 GBase-T + 2 × 100 Gbps –

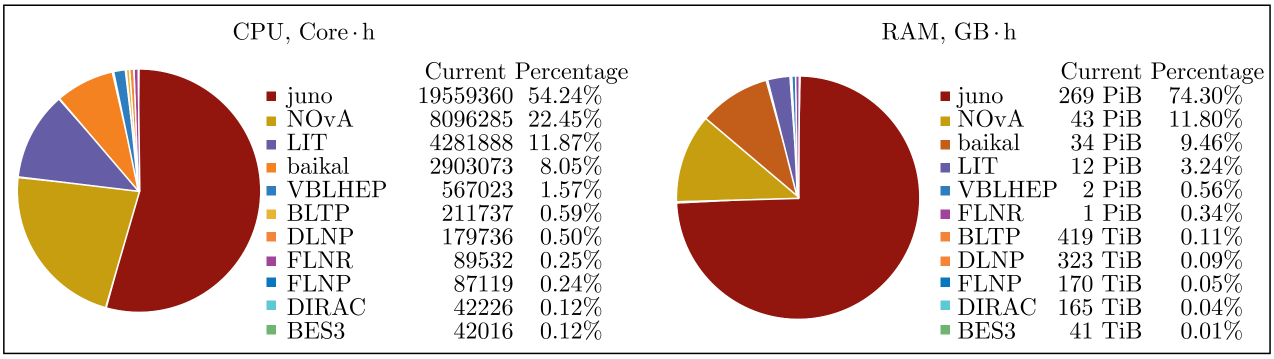

Fig. 6. Use of cloud computing by JINR's experiments and subdivisions

Figure 6 provides information on the use of the cloud infrastructure resources in 2021.

The JINR cloud is part of the distributed information and computing environment (DICE) based on the resources of JINR and its Member States' organizations [3, 4]. The amount of JINR cloud resources contributed to the DICE varies depending on its load.

In 2021, the cloud of the Egyptian National STI Network of the Academy of Scientific Research and Technology was put into operation and integrated into the DICE. At present, the Plekhanov Russian University of Economics (Russia), the North Ossetian State University (Russia), the Astana branch of the Institute of Nuclear Physics (Kazakhstan), the Institute of Physics of the National Academy of Sciences of Azerbaijan, the Egyptian National STI Network of the Academy of Scientific Research and Technology, the Institute for Nuclear Research and Nuclear Energy (Bulgaria), Sofia University "St. Kliment Ohridski", the Scientific Research Institute for Nuclear Problems of the Belarusian State University are fully integrated into the DICE, and the Institute of Nuclear Physics (Uzbekistan) and the Georgian Technical University are in the progress of integration.

The total number of jobs performed by the most active JINR DICE clouds is shown in Fig. 7.

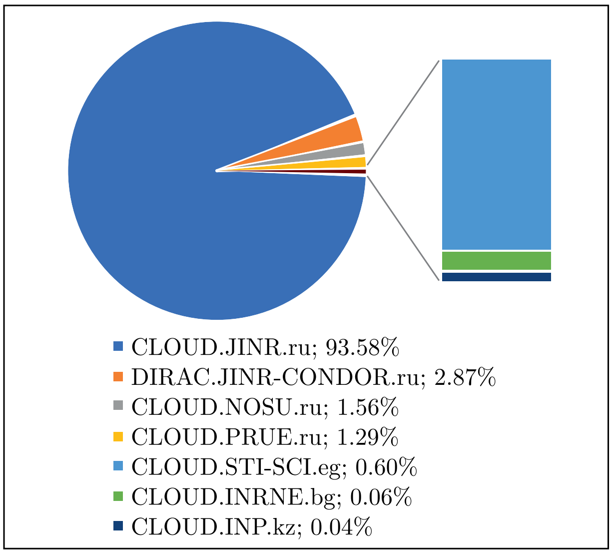

Fig. 7. Distribution of jobs completed in the JINR DICE in 2021

Similar to the previous year, idle resources of the JINR DICE were involved in research on the SARS-CoV-2 virus within the Folding@Home platform. Figure 8 illustrates the contribution of each of the DICE resource centres to this undertaking.

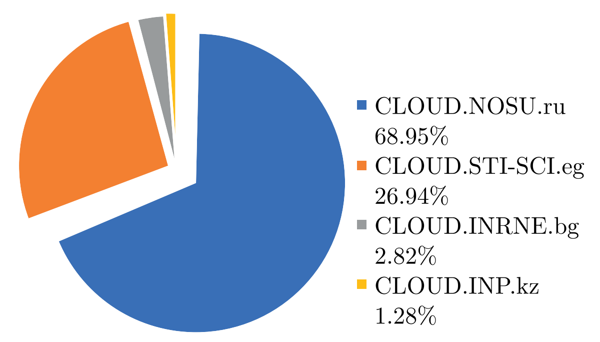

Fig. 8. Distribution of contributions of the DICE participants to the study of the SARS-CoV-2 virus via the Folding@Home platform

Heterogeneous Infrastructure. The JINR MICC heterogeneous infrastructure is represented by the HybriLIT platform, which involves the education and testing polygon and the "Govorun" supercomputer, driven by a common software and information environment. In 2021, an Information and Computing System (ICS) was developed on the platform at a very rapid rate to solve tasks related to the calculations of electron shells of superheavy elements. The ICS encompasses the computing resources of the "Govorun" supercomputer and a set of IT solutions and software required for modeling electron shells. The created system enables the solution of tasks of different types, with distinct requirements for both the amount of computing resources and the amount of data and the requested speed of access to them. The ICS itself is based on the on-demand computing system created on the "Govorun" supercomputer, which contains 288 physical cores (576 logical cores) and a 7 TB file storage managed by the NFS file system. Intensive computing using the AMS and DIRAC software was carried out on this system to calculate the electronic properties of superheavy elements.

Another important direction associated with the ICS enhancement is the development of quantum algorithms implemented on quantum computing simulators. For this purpose, a number of quantum simulators, capable of working on different computing architectures, were implemented in the ICS.

To work with Big Data, including for the NICA megaproject, a hierarchical data processing and storage system with a software-defined architecture was developed and implemented on the "Govorun" supercomputer [5]. According to the speed of accessing data, the system is divided into layers that are available for the user's choice. The fastest layer of the hierarchical system is based on the latest DAOS (Distributed Asynchronous Object Storage) technology. DAOS was deployed on eight nodes of the "Govorun" supercomputer and demonstrated a high read/write speed, ranking 16th in the "10 node challenge" nomination in the current edition of the IO500 list (https://io500.org/list/isc21/ten). Great prospects for the use of this technology are associated with its application to the NICA project at all stages of its work, from experimental data acquisition to final physics analysis (Fig. 9).

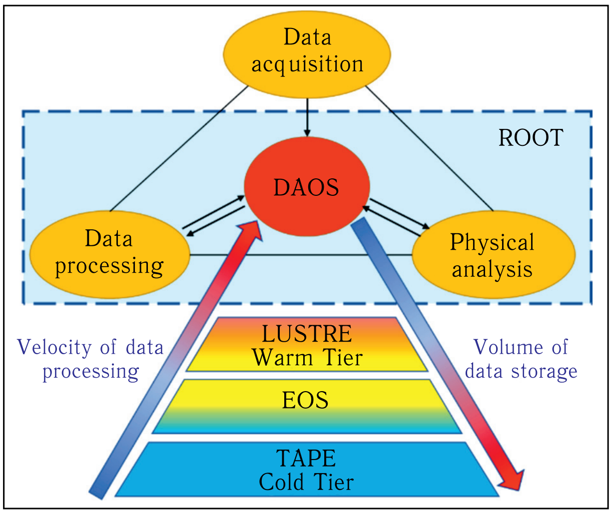

Fig. 9. Planned use of DAOS technology for the NICA project

The use of DAOS for the NICA project will enable the storage and read of multidimensional data structures of TB size in a single address space. Moreover, the DAOS technology looks promising in applications to other types of tasks related to Big Data. These are primarily ML/DL tasks and quantum computing [6, 7].

In 2021, latest versions of more than 20 software packages, in particular, Quantum Espresso (BLTP); JAM, current versions of FairSoft and FairRoot with add-ons for BmnRoot and MPDRoot (NICA); AMS, FLUKA, FLAIR (FLNR); ORCA (DLNP); MAGMA, ViennaCL, Tesseract (MLIT), etc., were implemented in the HybriLIT environment and supported at the request of user groups.

The total number of registered users of the "Govorun" supercomputer is currently 517, of which 322 are JINR staff members and 195 are from the Member States.

In 2021, the overall usage of the resources of the "Govorun" supercomputer amounted to 551 016 jobs, which corresponds to 40 million core hours, and to 56 763 jobs on the GPU component, which corresponds to 18 158 GPU hours. The average load of the CPU component was 96.1%, while the GPU load was 92.3%.

In 2021, HybriLIT platform users published 38 papers, 11 of them in Q1 and 4 in Q2, including an article published by the BM@N collaboration in *Nature Physics* (*BM@N Collab.* Unperturbed Inverse Kinematics Nucleon Knockout Measurements with a 48 GeV/c Carbon Beam // Nature Phys. 2021. V. 17. P. 693–699).

Integration of Computing Resources. A significant feature of the created infrastructure is the integration of the distributed computing resources. For three years now, the integration of the heterogeneous distributed computing resources on the basis of the DIRAC Interware platform has been functioning at JINR. The DIRAC Interware is a product for combining heterogeneous computing and storage resources into a single platform; it is based on the use of standard data access protocols (xRootD, GridFTP, etc.) and pilot jobs. By the end of 2021, all the MICC components, the clouds of the JINR Member States, the NICA cluster, as well as the cluster of the National Autonomous University of Mexico (NAUM, within the cooperation on the MPD project), were integrated into DIRAC. During the reporting year, new clouds of the Member States were added. Figure 10 displays the contribution of all the organizations integrated on the DIRAC platform to data processing.

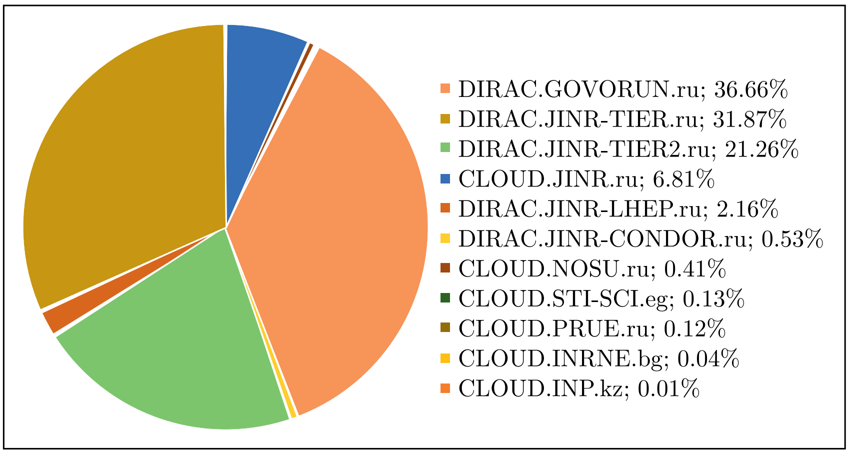

Fig. 10. Contribution of all the organizations integrated on the DIRAC platform to data processing

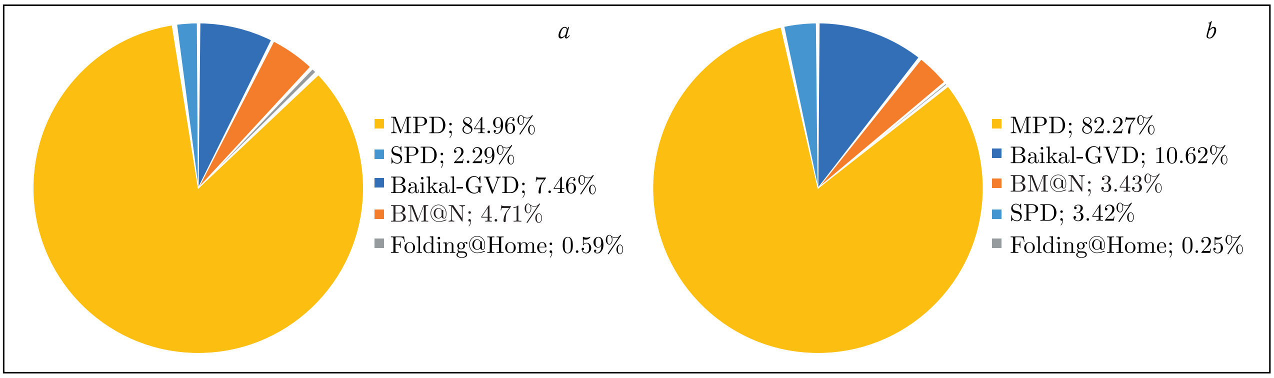

Fig. 11. Use of resources integrated into DIRAC by main users: *a*) consumed computing resources in HEP-SPEC06 hours; *b*) by the number of jobs

A total of 614 000 jobs (+30% compared to 2020) was completed during the year under review. The average time of job completion amounted to 7.6 h. The overall amount of consumed computing resources was 86 million HEP-SPEC06 hours (+65% compared to 2020). The first physics jobs of the BM@N and SPD experiments were launched. For the time being, the distributed infrastructure is used by the following experiments: MPD, Baikal-GVD, BM@N, and SPD (Fig. 11).

Thanks to the integration via DIRAC, it became possible to use the largest amount of computing resources for centralized data generation by the Monte Carlo method for the MPD experiment. The "Govorun" supercomputer, the Tier-1/Tier-2 clusters and the NICA cluster participated in computing. Over 505 000 jobs were successfully completed. All data are registered in the DIRAC file directory and stored in the EOS system.

To simplify the access of MPD collaboration members to the computing resources, a special application was developed; it enables the description of the data generation job in physical terms, i.e., collision energy, type of the generator used, target and beam material [8]. The developed application was integrated into the web interface of the DIRAC platform at JINR and can be accessed by all MPD users.

Monitoring System. The developed integrated monitoring system of the MICC allows receiving information from different components of the computing complex: the engineering infrastructure, the network, the compute nodes, the job launch systems, the data storage elements, the grid services, which guarantees a high level of MICC reliability. In 2021, a new accounting system [9] was introduced to the Litmon monitoring system; it allows the collection of statistical data on the use of resources by user jobs (for any time interval), namely, the astronomical job execution time and CPU time in HEP-SPEC06 hours, the number of jobs and efficiency of using the computing cluster. The system enables accounting for resources and their use within the distributed data processing system.

Information Services. In 2021, the Electronic Document System (EDS) "Advance Reports" was developed and put into operation; it is designed for electronic recording in the JINR Accounting Department to receive prepayment and report on business trips and household expenses. The system enables preliminary loading of the required data to accelerate the work of the Accounting Department and generates a number of financial reports.

A number of works on the development and current maintenance of the "Dubna" EDS were completed. In particular, new documents "Instruction" and "Request" with the possibility of automatic control of deadlines, the document "Strabag (KS-2, KS-3, invoice)", "SEDNPSS archive" for storing the technical documentation of the Scientific and Engineering Department of Nuclotron Power Supply Systems of VBLHEP were introduced. A number of works on the adaptation of the "Dubna" EDS to accommodate the changes in the organization of the procurement procedures at JINR were carried out.

The ongoing maintenance and on-demand development of the APT EVM information systems for NICA, CERNDB, ISSC, HR LHEP, ADB2, PIN, ISS, Document Base and Electronic Photo Archive were performed.

In 2021, the work on enhancing and applying the WALT (Web Application Lego Toolkit) platform, which is a template-oriented platform designed for developing web applications of different complexity, was in progress. In contrast to many other platforms that are "magic black boxes", the WALT underlying idea is to provide transparent, extensible and modifiable tools to solve specific tasks arising in the development of web applications. The WALT platform is used to develop JINR's corporate web applications such as ADB2, PIN, NICA EVM, EDS, etc. [10].

In 2021, to improve the quality of accounting the publication activity of JINR staff members, the work on the development and introduction into trial operation of the information system of the institutional repository of scientific publications based on the JOIN2 software platform (JINR Document Server — publications.jinr.ru) was in progress. To achieve this goal, the work to organize a single subsystem for entering bibliographic metadata into the JINR Document Server and JINR Personal INformation (PIN) systems is underway.

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

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

In 2021, within the optimization of the characteristics of the superconducting magnets of the NICA project, the three-dimensional modeling of the collider's quadrupole magnet, the vertical output dipole magnet and the final focus lens was performed. The forces acting on the superconducting winding of the solenoid for the SPD experiment, as well as the level of the magnetic field in the detector area of the BM@N facility, were investigated.

A comparative analysis of the efficiency of numerical calculations of magnetostatic fields was carried out by the finite element method (FEM) in the COMSOL Multiphysics® environment in terms of magnetic vector and total scalar potentials for modeling accelerator magnets [11]. Computations were illustrated by the model of a dipole magnet designed to form a magnetic field in the SC200 isochronous cyclotron. The numerical effectiveness of both methods was analyzed in terms of the relevant FEM parameters, accounting for the cost of computing resources. In particular, it was shown that the use of the scalar potential as compared to its vector counterpart substantially reduced the number of degrees of freedom, the use of computer memory and the computational time for a similar relative error.

Modeling in the drift chambers of the BM@N experiment was fine-tuned for all types of data acquired during runs in 2018 to more accurately identify the resulting particles. It was shown that the modeling completely agreed with the experimental data. Reconstruction efficiencies were obtained for all types of data and particles [12].

The geometric and software models of the tracking detectors (GEM, Forward Silicon and CSC) of the BM@N experiment were developed [13]. Algorithms for realistic Monte Carlo simulation and the reconstruction of the spatial coordinates of the points for passing charged particles through the detectors' planes were implemented.

The studies on the development of algorithms based on Deep Neural Networks for the reconstruction of elementary particle tracks in the BM@N, SPD and BESIII experiments were in progress. Algorithms of local tracking TrackNETv2 and of global tracking RDGraphNet and LOOT were enhanced [14–16]. All developed models of Deep Neural Networks were successfully implemented in the Ariadne library, i.e., a library for particle tracking using deep learning methods, being developed by the authors.

An event metadata system [17] was developed for the experiments of the NICA project; it represents a database that contains summary data on particle collision events and links to their storage location in a distributed storage, providing a quick search and selection of the required set of events according to the stored metadata for their further processing and physics analysis. It comprises an event metadata base, a web service for viewing metadata and selecting events, a software interface for automated recording of new metadata during event processing and a required events query according to specified criteria for physics analysis in the experiment software. The event metadata system was integrated with the condition database, which is also being developed by MLIT specialists.

Modeling that describes the structure of hadrons within the strongly correlated quark model was performed. It was shown how the properties of mesons and baryons could be modified in a dense nuclear medium, namely, nucleons were converted into delta isobars, hyperons and their excitations, and mesons were produced predominantly via vector resonances. Moreover, the properties of vector mesons, consisting of light quarks, changed drastically. The decay width increased, and the mass value decreased [18]. In-medium modifications, especially in the energy range of the NICA megascience project, can result in such observed effects as the enhancement of strangeness, "horn-effect", and enhancement of dilepton invariant mass spectra at 0.2–0.7 GeV.

The previously developed method for constructing a phase transition in nuclear matter under extreme conditions, which are formed in the nuclei of neutron stars, was systematically studied and applied [19]. The construction enabled one to model the equations of the state of nuclear matter, which admits a phase transition, even in cases when there is no phase equilibrium point in a physically justified region of densities. The applicability of this construction and its restrictions were demonstrated.

An algorithm for delimiting overlapping signals from two charged particles in the CSC (Cathode Strip Chambers) detector of the CMS experiment was developed. The reconstruction for the CSC chambers of special geometry ME1/1, developed and assembled at JINR, was tuned for problem areas [20]. The developed algorithms resulted in a more accurate and high-quality reconstruction of hits and segments in the CMS muon system and in the ME1/1 chambers, in particular. The authors' code was implemented into the official CMS software and will be used by default starting from Run 3 data taking.

As part of the software development for Run 3 of the ATLAS experiment, the Resource Manager component was upgraded in accordance with new security rules [21]. A new EventPicking service was developed for the ATLAS EventIndex project; it automates the procedure for finding event location using EventIndex and sending jobs to PANDA to receive the requested events [22]. The service was used for the second stage of the analysis of $\gamma\gamma \rightarrow WW$ events. The work on converting data from the old format to CREST and improving the corresponding tools was in progress.

Jointly with physicists of FLNR JINR, a computer model of the fine structure found on the basis of experiments with the transuranium element, californium, was developed [23]. To test the hypothesis that the found structure objectively exists and is not a noise artifact, a deep convolutional neural network was applied as a binary classifier. The preliminary results of using the developed neuroclassifier underlined the prospects of the proposed approach.

Air pollution dispersion modeling on the basis of the Land Use Regression (LUR) model was performed. Testing was carried out in the Tritia region. Two sets of air pollution factors, i.e., emission data and dispersion model results, were considered. Neural network-based regression was compared with linear regression. Neural network-based regression demonstrated significantly better results. It proved to have a positive impact on the quality of LUR models, since it better reflects the overall non-linear behavior of pollution dispersion [24].

A triplet loss function was successfully used to significantly improve the accuracy of vegetation recognition tasks [25]. The first task was plant disease detection on 20 classes of five crops (grape, cotton, wheat, cucumbers, corn). The second task was the identification of moss species (5 classes). In both tasks, self-collected image databases were used. A Siamese network with a triplet loss function and MobileNetV2 as a base network showed an accuracy of 97.8% for plant disease detection and 97.6% for moss species classification.

In 2021, the JINRLIB library was replenished with a program developed by MLIT specialists: RK4-MPI, a parallel implementation of the numeral solution of the Cauchy problem by the fourth-order Runge–Kutta method using MPI technology (http://wwwinfo.jinr.ru/programs/jinrlib/rk4-mpi/indexe.html).

In cooperation with FLNP, using the separated form factor method, an analysis of Small-Angle Neutron Scattering (SANS) spectra, measured on the YuMO small-angle spectrometer on polydisperse populations of single-layer vesicles of the phospholipid transport nanosystem and the Indolip nanodrug in heavy water at three concentrations, was carried out. The basic structural parameters of these vesicular systems, obtained by the computer analysis of the SANS spectra, generally agreed with the corresponding results of Small-Angle X-Ray Scattering (SAXS) data processing. At the same time, the SANS method turned out to be less sensitive in comparison with SAXS in terms of the detailed account of the structural features of the bilayer of the vesicle envelope [26].

The molecular dynamics method was used to study samples of copper, iron and nickel with the structure of real crystals with specified defects such as pores, irradiated by copper nanoclusters with an energy of 1–100 eV/atom [27]. Modeling and testing were carried out using a modified LAMMPS package installed on the HybriLIT cluster. The effect of shock waves on the defective structures of the pore type in the target was investigated within numerical modeling. Threshold irradiation energies of copper nanoclusters, which changed the structure of the defect in the targets, were obtained. The results showed a greater resistance of pore-type defects in an iron target to the impact of a shock wave in comparison with the samples of copper and nickel.

New efficient algorithms for calculating the normalized Mott scattering differential cross section of relativistic electrons by the Coulomb potential, as well as for calculating the total Mott–Bloch correction to the Bethe formula for heavy-ion ionization energy losses based on the proposed representation of the Mott exact cross section in terms of Mott partial amplitudes, were developed and implemented numerically [28]. The inapplicability of the known approximate methods for calculating the cross section of heavy elements and the advantage of the developed method for calculating the normalized Mott cross section in the region of high and medium electron energies were demonstrated.

The relativistic ground state energies of two-centre problems for the Dirac equation were calculated with an accuracy of 8–9 digits at an internuclear distance of $2/Z$ up to $Z = 121$ [29]. Slater-type orbitals (up to the orbital $g_{9/2}$, the maximum number of basis functions is 62) and the minimax method were used in the calculations. The major advantage of the minimax method is that the kinetic balance conditions are not necessary to exclude the false solutions, thereby significantly increasing the convergence rate in the number of basis functions.

A method that enables the extrapolation of asymptotic series to finite values of the coupling parameters, and even to their infinite limits, was proposed [30]. The method is based on the use of self-similar factor approximants, which allow for the extrapolation of function values to arbitrary values of the coupling parameters, knowing only the expansions of these functions in small coupling parameters. The efficiency of the method was illustrated with several problems of quantum field theory.

The spectrum of vibrational-rotational bound, metastable states and scattering states of the beryllium dimer in the ground $X^1\Sigma_g^+$ state was calculated [31]. The problem was solved using the authors' KANTBP 5M software package, which implements Newton's method and the high-accuracy finite element method. The spectrum of rotational-vibrational metastable states of the beryllium dimer with complex energy eigenvalues was obtained for the first time. The presented approach, implemented in the form of a software package, provides a useful tool for studying weakly bound states with eigenenergies close to the dissociation threshold and processes of the near-surface diffusion of diatomic molecules.

The studies on the analysis of the quantum information resource of a finite-dimensional quantum system using the method of quasidistributions in the phase space were in progress [32]. Measures of quantumness were introduced; they made it possible to quantitatively describe the degree of difference between quantum states and the corresponding classical analog. Based on the property of negativity of the corresponding Wigner quasidistribution, an indicator of quantumness of basic functions, qubits, and qutrits was calculated for different metrics (Hilbert–Schmidt, Bures and Bogoliubov–Kubo–Mori) given on the space of quantum states.

APPLIED RESEARCH

Based on the integration of the supercomputers of JINR, of the Interdepartmental Supercomputer Centre of the Russian Academy of Sciences and of Peter the Great St. Petersburg Polytechnic University, a scalable research infrastructure of a new level was created. Such an infrastructure is in demand for the tasks of the NICA megascience project; to date, 3000 event generation and reconstruction tasks were launched on it for the MPD experiment. As a result, about 3 million events were generated and reconstructed. The obtained data were transferred to Dubna for further processing and physics analysis.

A prototype of the "MLIT Information and Analytical System for Maintaining Licenses" (IAL, http://soft-lit.jinr.ru) was developed. The IAL main task is the automation of the management, purchase, maintenance and use of licensed software products (LSP), asked by the need to both plan and optimize the purchase of licensed software and the necessity of controlling the compliance with the rules of the licensing policy. The system database contains all the information on the purchased licenses, on the basis of which the user's personal account (PA) is formed. The PA stores data about licenses owned by

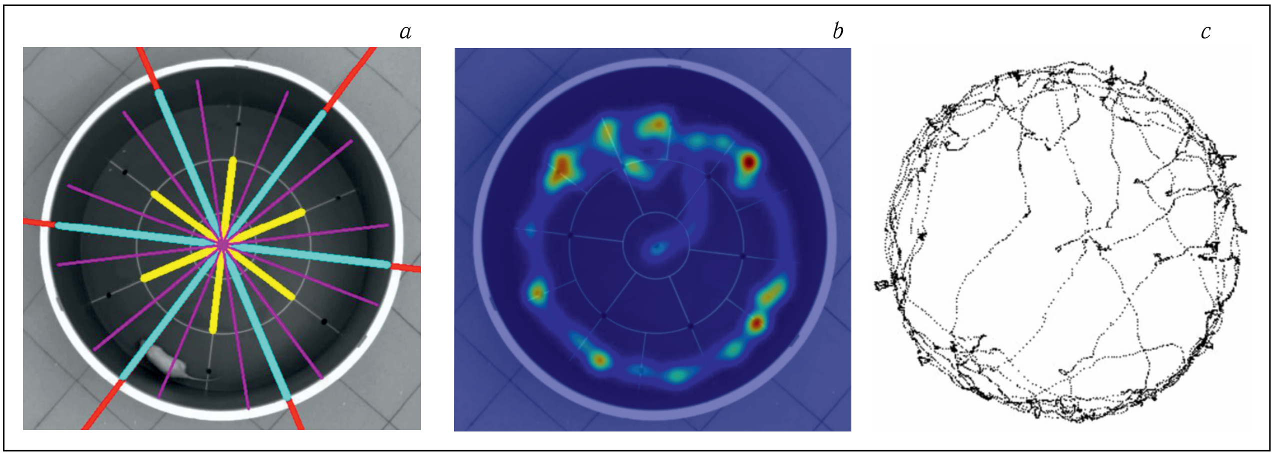

Fig. 12. *a*) Automated marking and refinement of the sector centres of the experimental setup "Open Field"; *b*) heat map of the movements of a laboratory animal in the experimental setup; *c*) frame-by-frame trajectory of the animal's movements

the user. The Administrator/Auditor PA is designed for LSP management and monitoring. Login to the IAL is made through the SSO-JINR user authentication system. The web interface is implemented in the WALT development environment.

Within the joint project of MLIT and LRB, new achievements in the development of the BIO-HLIT Information System (IS) for the tasks of radiation biology (https://bio.jinr.ru/) were obtained. The algorithmic block of the IS is based on the methods of machine and deep learning, as well as of computer vision. In 2021, algorithms for the automated marking and tracking of the behavior of a laboratory animal with the construction of a high-quality movement trajectory and accurate marking of the experimental setup were developed (Fig. 12). Components for visualizing the results of data analysis were elaborated [33].

INTERNATIONAL COOPERATION

In collaboration with BLTP and Cairo University, the cross sections for elastic scattering of charged π mesons by ^{28}Si, ^{40}Ca, ^{58}Ni, ^{208}Pb nuclei in the energy range from 130 to 290 MeV were calculated [34]. The calculations were carried out within two models of microscopic optical potential (OP), namely, the folding model and the local modified Kisslinger type OP. The cross sections of pion–nucleon scattering were obtained by the numerical solution of the Klein–Gordon equation. For both OP models, good agreement with the experimental data was obtained. By fitting the elementary $\pi^{\pm}N$ amplitude parameters in the folding OP to the $\pi^{\pm}A$ scattering experimental data, the effect of the nuclear medium on the mechanism of pion–nucleon scattering was investigated.

The successful cooperation involving MLIT, BLTP, and China Institute of Atomic Energy resulted in a new theoretical approach to the coupled channel method, stable computational schemes, algorithms, and a new modified programme KANTBP 3.1, which implements the finite element method of high-order accuracy [35]. The upgraded version of the programme was used to calculate the fusion cross sections of heavy ions ^{12}C + ^{12}C, ^{64}Ni + ^{64}Ni, ^{64}Ni + ^{100}Mo, ^{28}Si + ^{64}Ni, ^{36}S + ^{48}Ca. The results of calculating the fusion cross sections of heavy ions and the astrophysical S factor are in good agreement with the available experimental data.

Within a joint grant between JINR and Romania, a prototype of the IFA Database system for managing research programmes was developed. The system will be a major tool for the organization of competitive funding for studies in Romania. The prototype of the IFA Database system is implemented on top of the WALT platform, being developed by MLIT specialists, and currently comprises the following modules: registration and login of different users, grant application, administrator panel, registration and validation of organizations in the system.

EDUCATIONAL PROGRAMME ON THE EDUCATION AND TESTING POLYGON

In 2021, training courses and practical classes on "High-Performance Computing and Supercomputer Technologies" and "Machine Learning and Data Mining" were held on the HybriLIT platform. 780 students of Dubna State University and more than 300 students and postgraduates from other universities and JINR's Member States are registered on the training and testing polygon. In 2021, nine master's and bachelor's theses were prepared using the resources of the HybriLIT platform.

The programme of the International School of Information Technologies "Data Science", whose students are engaged in real scientific projects of JINR, is underway. The results of graduates are presented in a collection of scientific and project activity reports: http://itschool.jinr.ru/discipline.html#science-project.

In 2021, the workshop "Distributed Computing and Data Science", within which students attended the training course "Distributed Computing, Machine and Deep Learning for Solving Applied Tasks", and the 3rd IT School for Young Scientists "Modern IT Technologies for Solving Scientific Tasks", in which over 60 students and teachers from universities of the South of Russia (North Ossetia, Kabardino-Balkaria, Chechnya) and from the Tibilov South Ossetian State University participated, were held at the North Ossetian State University. Lectures on JINR's scientific projects, on information technologies and solutions for scientific tasks being developed at JINR were delivered; master classes and training courses on distributed computing, virtualization and cloud technologies, machine and deep learning algorithms for analyzing data of a complex structure were conducted.

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