MESHCHERYAKOV LABORATORY of INFORMATION TECHNOLOGIES

Memorial cabinet of M. G. Meshcheryakov

The activity of the Meshcheryakov Laboratory of Information Technologies (MLIT) in 2022 was focused on ensuring the reliable functioning and growth of the JINR network, information and computing infrastructure, as well as on developing mathematical support and software for the research and production activities of the Institute and scientific centres of its Member States on the basis of the JINR Multifunctional Information and Computing Complex (MICC). The research was carried out within two themes: "Information and Computing Infrastructure of JINR" and "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data". A distinctive feature of ongoing research directions is close cooperation with all the Laboratories of the Institute, institutes of the JINR Member States and other countries.

In 2022, the next stage of modernization of the "Govorun" supercomputer took place. The performance of this high-performance system enhanced by 23.5% and reached 1.1 PFlops.

In 2022, the staff of the Meshcheryakov Laboratory of Information Technologies published over 250 scientific papers and 5 monographs, presented more than 100 reports at international and Russian conferences.

INFORMATION AND COMPUTING INFRASTRUCTURE OF JINR

The Multifunctional Information and Computing Complex, as JINR's large-scale strategic infrastructure project, successfully continued its operation in 2022 and played a decisive role in research asking for modern computing power and data storage systems. The uniqueness of the project is ensured by the use of the reliable engineering infrastructure and state-of-the-art information technologies in the MICC architecture, namely, networks with a bandwidth of up to 4 × 100 Gbit/s, distributed computing and data storage systems based on grid technologies and cloud computing, the hyperconverged "Govorun" supercomputer. Multifunctionality, availability for calculations in 24/7 mode, scalability and high performance, a reliable data storage system, information security and an advanced software environment are the major requirements that the MICC meets.

In 2022, the active use of the MICC resources for JINR's research and applied tasks continued. Due to grid technologies (DIRAC Interware), which brought together the dedicated computing resources of all the MICC components, simulation campaigns for the MPD experiment of the NICA complex were successfully held. The Tier-1 grid site for the CMS experiment at the LHC continued to be a leader among similar world sites. Tier-2/CICC provided 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 the Member States. The cloud environment of JINR and its Member States was mainly used for computing within the JINR neutrino programme. The HybriLIT platform, which includes the basic resource for high-performance computing, the "Govorun" supercomputer, and the education and testing polygon, was actively used by registered users.

JINR Network Infrastructure

The network infrastructure is a fundamental component of the IT infrastructure of JINR and of the MICC. This is an intricate complex of multifunctional network equipment and specialized software. It is the foundation for the JINR information and computing infrastructure, which was created and is constantly developing, providing access to the Internet, the computing resources and the data storage systems both within JINR and in external scientific organizations cooperating with JINR. The JINR network infrastructure consists of the following functional components: the external optical telecommunication data transmission channel JINR–Moscow, the backbone of the JINR local area network, the local area networks of the Institute's subdivisions.

In 2022, the reliable functioning of the following JINR telecommunication channels was ensured: the Moscow backup channel with a bandwidth of 4 × 100 Gbit/s, the 100 Gbit/s JINR–CERN direct channel and its 100 Gbit/s backup channel, which passes through Moscow and Amsterdam, ensuring the operation of the LHCOPN network for 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 [1]. The DWDM (Dense Wave Division Multiplexing) technology is used for data transmission via the external optical telecommunication channel.

The distribution of the incoming and outgoing traffics by the JINR subdivisions in 2022 (exceeding 25 TB by the incoming traffic) is shown in the Table. The traffic of the hotel and restaurant complex (HRC) increased significantly, which is related to the commissioning of a building on 2 Moskovskaya St. after repair, since it was equipped with a network infrastructure and 512 IP addresses.

Table

Subdivision	Incoming traffic, TB	Outgoing traffic, TB
VBLHEP	430.2	209.23
HRC	413.24	60.25
MLIT	330.76	204.99
DLNP	229.59	113.38
Dubna State University	139.03	39.38
FLNR	137.7	32.69
FLNP	137.05	42.05
JINR Directorate	96.16	53
Remote Access Node	84.88	11.84
UC	52.97	11.51
BLTP	35.57	15.96
LRB	29.49	4.53
SIMO	27.63	2.94

The overall incoming traffic of JINR, including the general-purpose servers, Tier-1, Tier-2, the "Govorun" supercomputer and cloud computing, amounted to 29.56 PB in 2022, while the overall outgoing traffic reached 34.19 PB. The traffic with the scientific and educational networks, accounting for 94.5% 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 2022, the modernization of the central network virtual cluster of the JINR Network Operation Centre (NOC), which was built on top of the Proxmox VE (Virtual Environment) open source software under the GNU license, was in progress. The NOC cluster ensures the operation of the NOC and JINR services, such as dns, dhcp, proxy, mail, webmail, maillist, ssl, database servers, virtual hosting, nmis monitoring, sshgate, centralized logging, sip telephony, etc.

The NOC regularly updates software on 15–20 servers (webmail.jinr.ru, indico.jinr.ru, mail.jinr.ru, maillist.jinr.ru, mx1.jinr.ru, mx2.jinr.ru, auth-1.jinr.ru (login.jinr.ru), auth-2.jinr.ru, etc.), which keeps the systems up to date.

In 2022, the jinr.int zone was registered, and the mail.jinr.ru mail server was adapted to work with the jinr.int zone.

The work on the improvement of the mail.jinr.ru service was systematically performed: a new hypervisor was prepared and put into operation, scripts were developed, a new adm-mail.jinr.ru server was created for the "cold" copy of mail.jinr.ru. Support for the mailing services (maillist.jinr.ru), "Personal Account", News, VPN, Edurom, Elibs, IPDB was carried out.

In 2022, about 1300 user requests were processed. Since March, an enhanced network protection regime has been provided. More than 80 incidents related to the hacking of the JINR network resources, copyright infringement, etc. were identified and processed. As part of cooperation with the third-party scientific organizations, VPN access to the network was provided for more than 110 users of the computing resources. A system for monitoring and tracking the status of over 770 network elements was ensured. The sshgate remote access service was put into operation. A mandatory check for vulnerabilities is performed for websites opened for access from the outside.

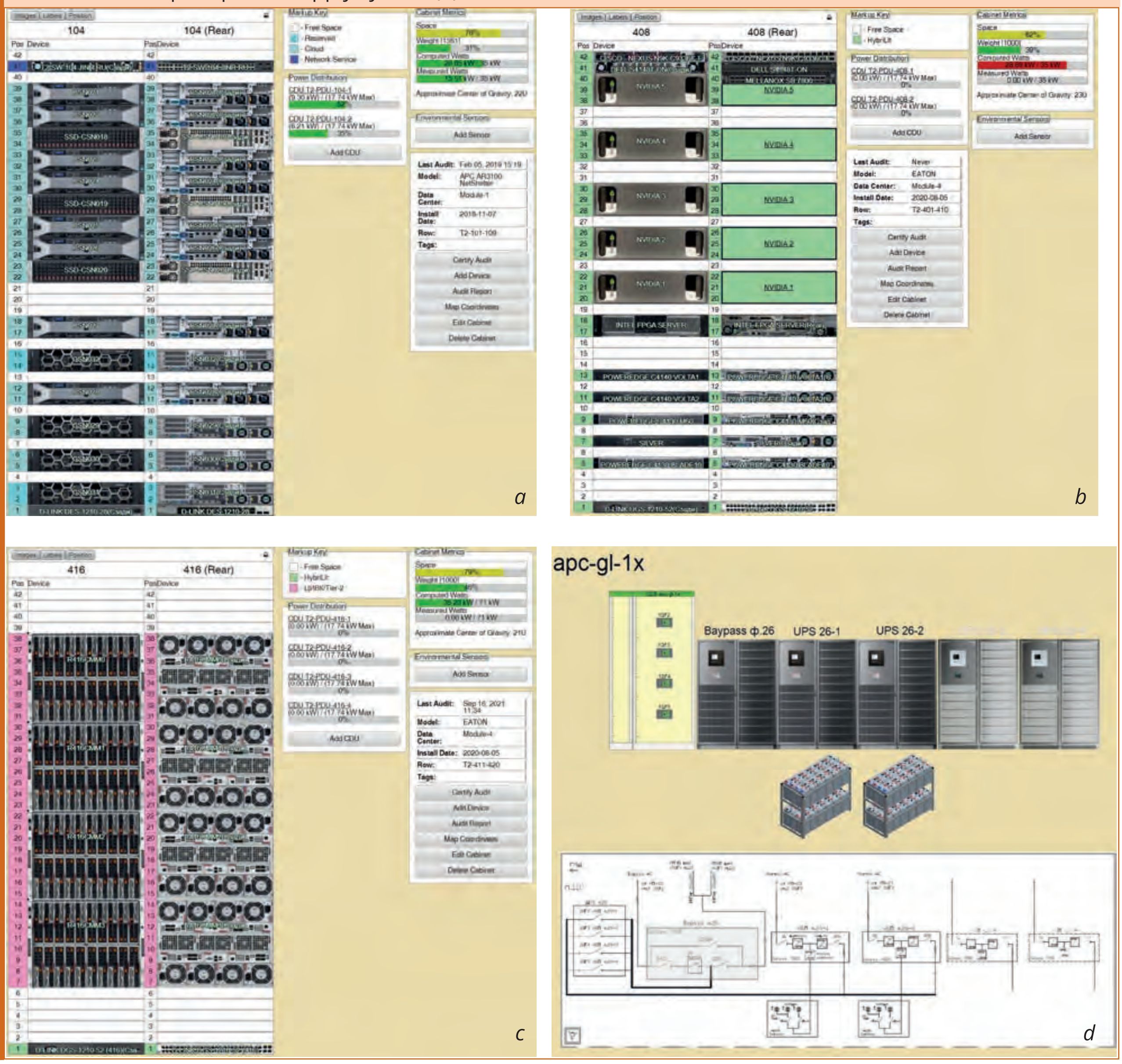
The JINR LAN comprises 9291 network elements and 18 044 IP addresses, 6355 network users, 4477 users of mail.jinr.ru, 1455 users of electronic libraries, 837 users of the remote access service and 111 users of the EDUROAM service.

MICC Engineering Infrastructure

In 2022, 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 with 2 MW power. 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. There are two diesel generator backups in operation to provide the computer centre with electricity in the case of disconnection from external power supply networks. All modules, except for the "Govorun" supercomputer, are air-cooled. The "Govorun" supercomputer is fully "hot" water-cooled, which allows for a power density of 100 kW per rack and PUE = 1.06.

Fig. 1. Examples of the equipment visualization system in racks 104 (*a*), 408 (*b*), and 416 (*c*) of the MICC hall and of the uninterrupted power supply system (*d*)



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

The DCIM (Data Centre Infrastructure Management) system is utilized for controlling and accounting the MICC equipment. This software allows one to visualize and control the MICC physical infrastructure on the basis of data on the equipment and its location entered in the DCIM database, to provide management and monitoring services. Figure 1 illustrates examples of equipment visualization.

JINR Grid Environment (Tier-1 and Tier-2 sites)

In 2022, the successful operation of the JINR grid sites continued, and on average 100% availability and reliability of services was ensured.

For many years, the Tier-1 resource centre was used only to perform jobs of the CMS experiment at the LHC within the participation of JINR and its Member States in this experiment. Since 2021, the introduction of the DIRAC platform has made it possible to utilize the allocated resources of this centre for simulation jobs of the MPD experiment of the NICA project. The amount of resources is regulated by requests from the MPD Collaboration. At present, Tier-1 contains 18 656 cores with a total performance of 297 135.18 HEP-SPEC06. The following software and compilers are used: CentOS Scientific Linux version 7.9, gcc (GCC) 4.8.5, gcc-11.2.1, gcc-c++-11.2.1, gcc-gfortran-11.2.1, C++ (g++ (GCC) 4.8.5, GNU Fortran (GCC) 4.8.5, dCache-6.2 for data storage, Enstore 6.3 for tape libraries and FTS. 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 complex and CMS experiments. Software for NICA is installed in the CVMFS using GitLab by users/software developers themselves.

In terms of performance, Tier-1 (RU_JINR_T1) is ranked first among Tier-1 world centres for the CMS experiment (Fig. 2, *a*). In 2022, more than 275 million events were processed, which accounts for 18% of the total number of processed events (Fig. 2, *b*) and 25% of the total CPU load of all Tier-1 centres for the CMS experiment.

Figure 2, *c* shows the statistics on the use of the JINR Tier-1 centre by the CMS experiment for different types of data stream processing (reconstruction, modeling, reprocessing, analysis, etc.). Figure 2, *d* il-

Fig. 2. Contribution of the world Tier-1 centres to CMS experimental data processing in 2022: *a*) distribution by the normalized CPU time in HEP-SPEC06 h; *b*) number of processed events; *c*) statistics on the use of the JINR Tier-1 centre by the CMS Collaboration by different types of data stream processing; *d*) distribution by the number of jobs completed on Tier-1 by the CMS, BM@N, MPD and SPD Collaborations

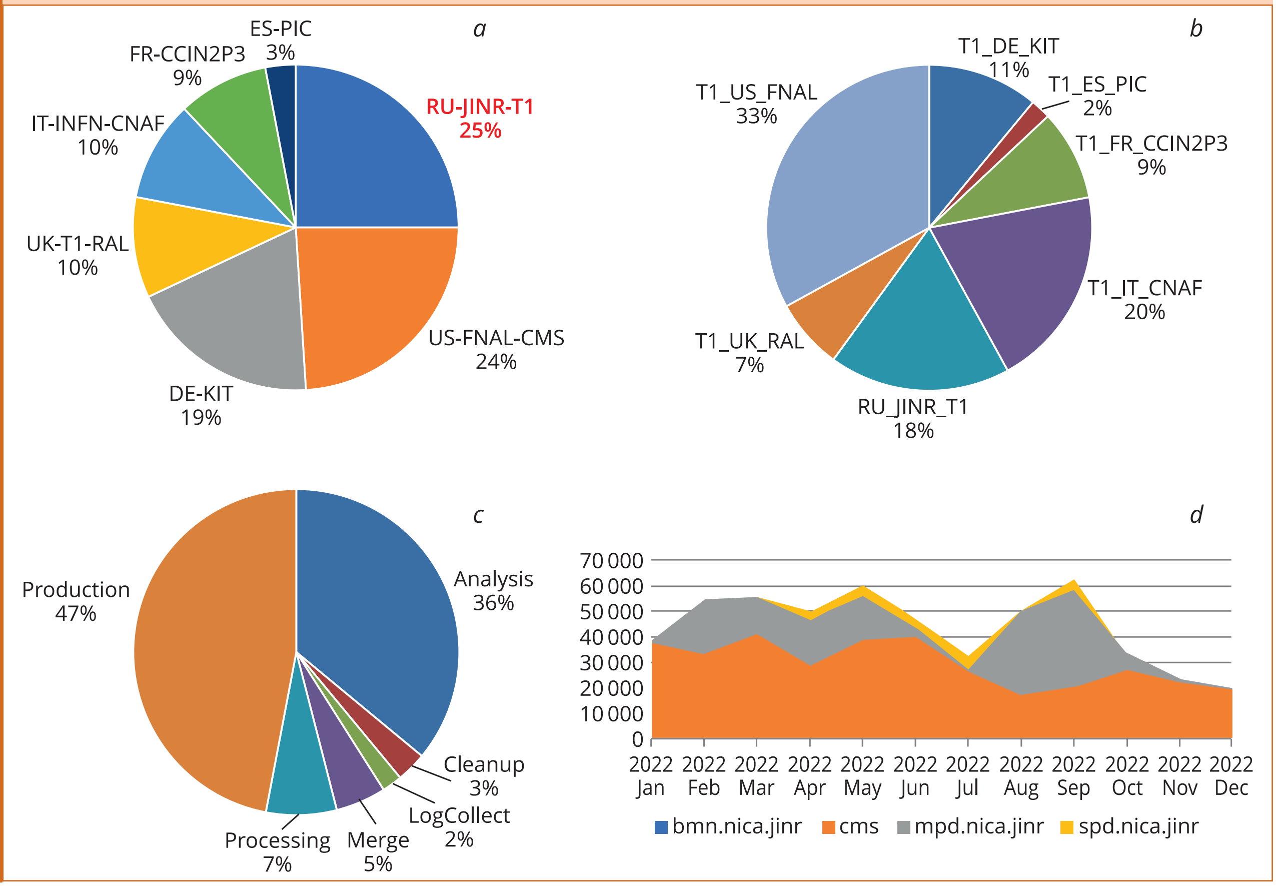
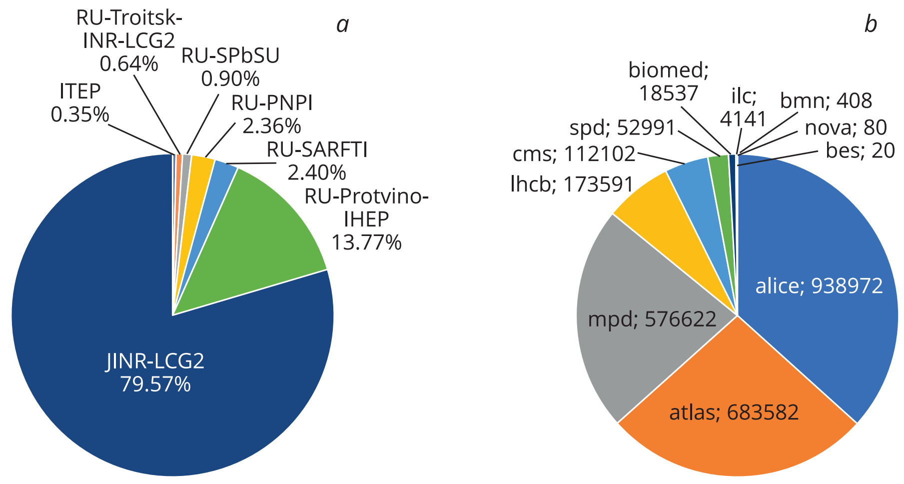


Fig. 3. *a*) Distribution of RDIG jobs completed on the grid sites; *b*) use of the JINR Tier-2 site (JINR-LCG2) by virtual organizations within grid projects



lustrates the distribution by the number of jobs performed on Tier-1 by the CMS, BM@N, MPD and SPD Collaborations in 2022.

The JINR Tier-2 output is the highest in the Russian Consortium RDIG (Russian Data Intensive Grid). 80% of the total CPU time in the RDIG is used for computing on this site. In 2022, the computing resources of the Tier-2 centre amounted to 9244 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 3, *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 2022 are shown in Fig. 3, *b*.

In 2022, the JINR subdivisions continued to use the EOS-based data storage system with a capacity of 17 PB. Figure 4 demonstrates the statistics on the use of the EOS system.

Cloud Infrastructure

Figure 5 provides information on the consumption of the cloud infrastructure resources in 2022: the main users are Collaborations of neutrino experiments and MLIT.

In 2022, the work on the development and support of the computing platform for neutrino experiments was underway. Due to the termination of support for the GSI authentication and the transition of the DUNE and NOvA experiments to an authenti-

Fig. 4. Statistics on the use of the EOS system by user groups and Collaborations

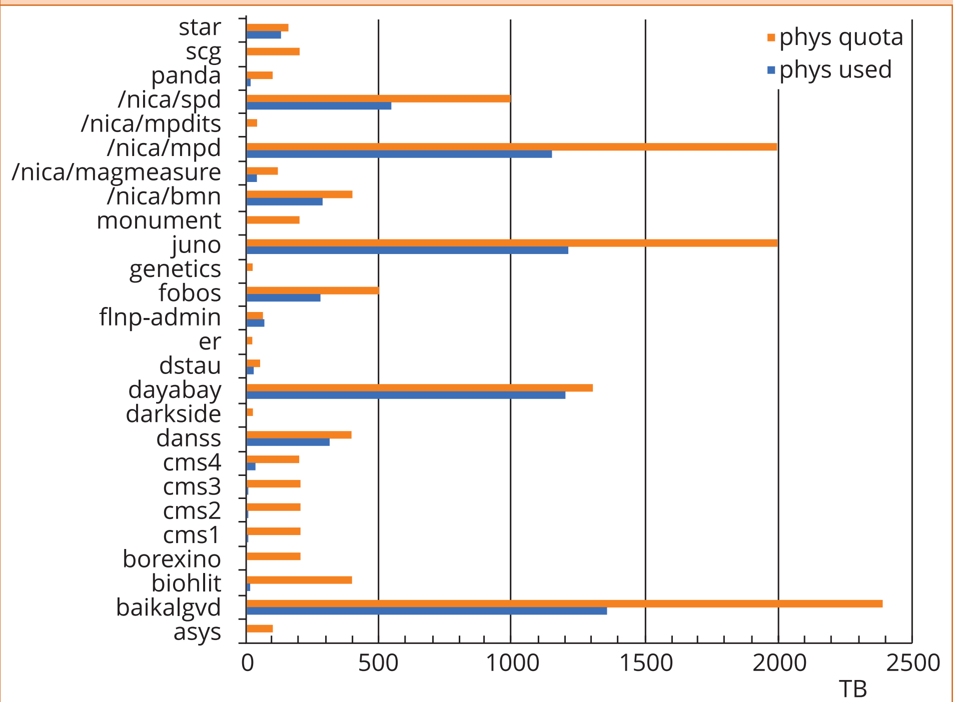
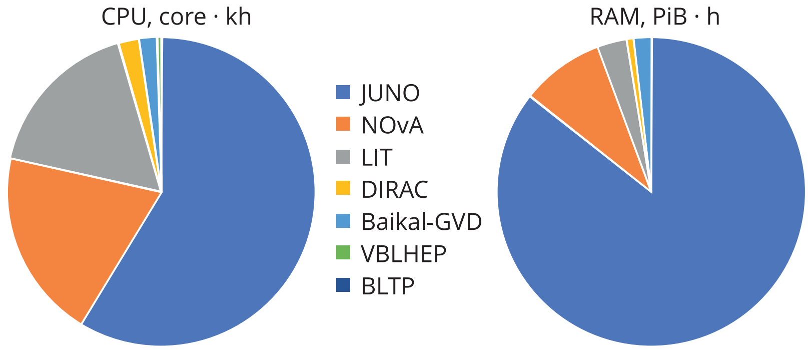


Fig. 5. Use of cloud computing by Collaborations and JINR's subdivisions



data completely independently of FermiLab infrastructure tools.

About 60 TB of data from the Borexino experiment was copied from the CNAF data centre (Italy) to the EOS storage at JINR. A fairly new approach together with the IAM (Identity and Access Management) service was used to authenticate and authorize the user under whom the data was copied.

The http:/dice.jinr.ru web portal with information about the participants of the Distributed Information and Computing Environment (JINR DICE), which combines the JINR cloud and cloud infrastructures of the JINR Member States, and about conducted training events on work at the JINR DICE was put into operation. Most of the jobs in the JINR DICE in 2022 were performed on the neutrino computing platform (DIRAC.JINR-CONDOR.ru) (Fig. 6). The main consumer of the JINR DICE resources in 2022 was the Baikal-GVD Collaboration (96%).

In addition, a number of auxiliary cloud services for different JINR scientific experiments were deployed on top of the JINR cloud: several documentation storage systems for experiments and user groups (ad-docs.jinr.ru for the VBLHEP Accelerator Department, spd-docs.jinr.ru and bmn-docs.jinr.ru for the SPD and BM@N experiments, respectively, baikal-docs.jinr.ru for the Baikal-GVD experiment, as well as neutrino-docdb.jinr.ru for joint use by the participants of the JINR neutrino programme; the first version of the ad-operations.jinr.ru electronic journaling system was realized and implemented for the VBLHEP Accelerator Department).

cation system using tokens, the HTCondor cluster of the cloud neutrino platform was updated to version 9.0, in which support for authentication by JSON web tokens (i.e., JWT) was implemented. For the DUNE experiment, the StashCache caching data storage with a total volume of 1 TB was deployed and connected to the Open Science Data Federation (OSDF).

At the request of the JUNO Collaboration, an exporter of data both on the current load in the batch cluster of the neutrino platform to use this data by the experiment in order to optimize the distribution of computing jobs in the JUNO global grid infrastructure and on the EOS storage used by the experiment and the load of JINR network channels was developed.

In the jupyter.jinr.ru interactive computing service, at the request of users, instead of a set of different images with different software, one universal image based on Datascience Notebook from the Jupyter Docker Stacks set, including all the basic software and modified environment necessary for the correct operation of the ROOT software, was prepared for data analysis.

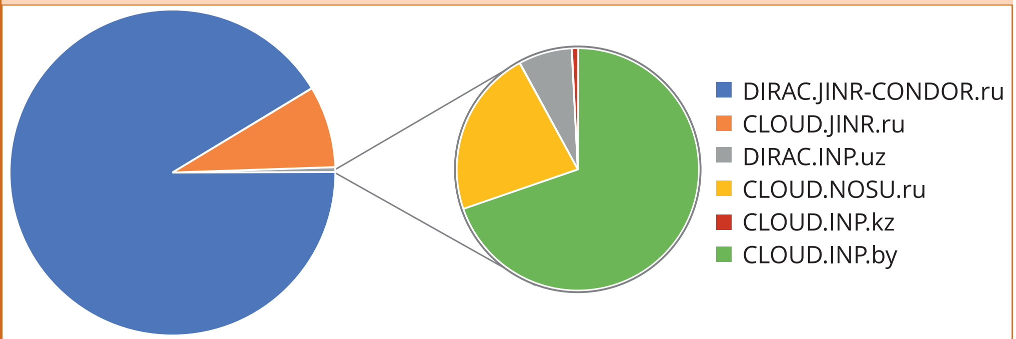
A server with the NVIDIA A100 Ampere 40 GB graphics card was purchased and put into operation for neutrino computing platform users involved in the development of machine learning algorithms, as well as using the corresponding application software.

In the JINR cloud storage, an additional local replica of modeled and real data sets in the Near and Far Detectors of the NOvA experiment was created to perform the oscillation analysis of the experimental

Heterogeneous Infrastructure

Resource-intensive massively parallel computing and work with Big Data are provided by the JINR MICC heterogeneous infrastructure represented by the HybriLIT platform, which involves the education and testing polygon, the ML/DL/HPC ecosystem [2] and the "Govorun" supercomputer, driven by a common software and information environment. The "Govorun" supercomputer is the key computing part of the HybriLIT platform and has an innovative

Fig. 6. Distribution of the number of jobs completed in the JINR DICE by participants



Yu. N. Migal (CJSC "RSC Technologies") speaks about the current stage of the modernization of the "Govorun" supercomputer

hyperconverged software-defined architecture with unique properties for customization flexibility for the user's task. The "Govorun" supercomputer comprises a GPU component, a CPU component, and a hierarchical data processing and storage system.

In November, the next stage of modernization of the "Govorun" supercomputer, which is associated with the expansion of the CPU component, implemented as part of a hyperconvergent approach to building a computing complex, underlying the "Govorun" supercomputer, took place. As a result of the modernization, the CPU component was extended to 32 hyperconverged compute nodes. Each node contains two Intel Xeon Platinum 8368Q processors (frequency 2.6 GHz, 38 cores, cache 57 MB, TDP 270 W), eight DDR4 RAM modules (256 GB), eight Intel Optane DC Persistent Memory modules (2 TB), four EDSFF E1.S NVMe SSDs (16 TB) and an M.2 NVMe SSD with a capacity of 128 GB. In addition, each node is equipped with two 100 Gbit/s Intel Omni-Path adapters (Fig. 7).

As a result of the modernization of the CPU component, the performance of the "Govorun" supercomputer increased by 239 TFlops, and the volume of the hierarchical data processing and storage system of the "Govorun" supercomputer was enlarged by 1.6 PB for the "very hot data" DAOS layer and by 8 PB for the "warm data" layer. Consequently, the performance of the "Govorun" supercomputer enhanced by 23.5% and reached 1.1 PFlops, and the total capacity of the hierarchical storage increased to 8.6 PB.

The hyperconvergence of new compute nodes already enabled their use for data mass genera-

Fig. 7. Location of new nodes of the "Govorun" supercomputer

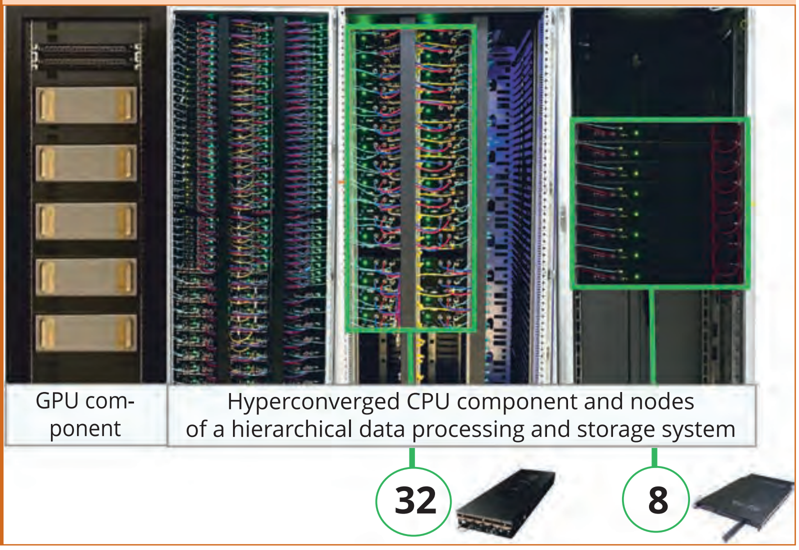
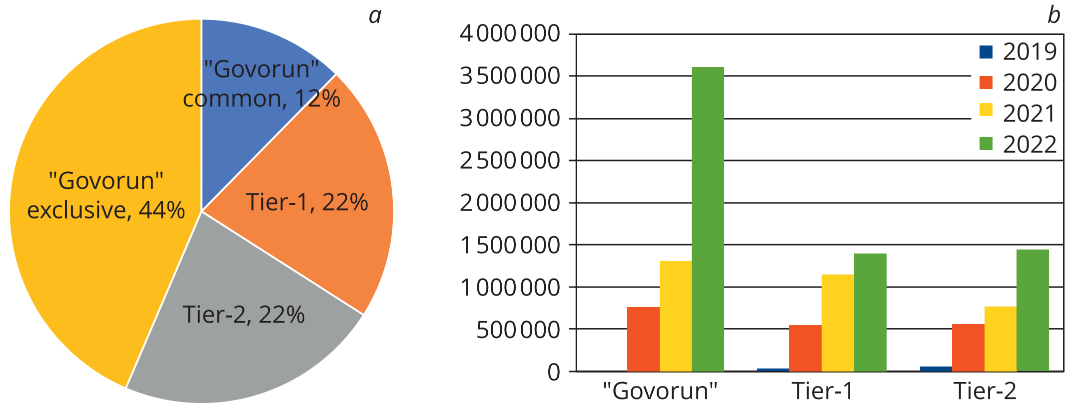


Fig. 8. DIRAC-based distributed heterogeneous environment for MPD tasks: *a*) share of use of different MICC components in 2022; *b*) increase in the share of the MICC computing resources in normalized CPU HEP-SPEC06 days



tion and reconstruction tasks within the NICA MPD experiment. It is noteworthy that for a number of MPD tasks, there was a need for a large amount of RAM, which is satisfied by new nodes. The computing resources and the hierarchical data processing and storage system of the "Govorun" supercomputer were integrated into a DIRAC-based distributed heterogeneous environment that includes the resources of JINR and its Member States. The experience of using different computing resources of JINR and other MPD Collaboration institutes has shown that at present, the use of the "Govorun" supercomputer resources is the most efficient (Fig. 8).

Figure 8, *a* shows the diagram of the use of different MICC components in the DIRAC-based distributed heterogeneous environment for MPD jobs. At the same time, the share of those jobs that can only be calculated on the "Govorun" supercomputer was about 44% in 2022, and the total contribution of the "Govorun" supercomputer resources to event mass generation and reconstruction for the MPD experiment was about 56%. Figure 8, *b* illustrates the increase in the share of the MICC computing resources in the heterogeneous environment for MPD jobs. The sharp increase in the share of the "Govorun" supercomputer is related to the modernization carried out in 2022. Thus, over 50 million events were generated on the new nodes.

The above-mentioned modernization of the "Govorun" supercomputer will make it possible to speed up studies in the field of lattice quantum chromodynamics, to qualitatively increase the efficiency of modeling the dynamics of relativistic heavy-ion collisions, to carry out calculations of the radiation safety of JINR experimental facilities and to enhance the efficiency of solving applied tasks. The modernized "Govorun" supercomputer makes it possible not only to perform computing, but also to use the supercomputer as a research polygon for developing software–hardware and IT solutions for JINR tasks.

The total number of users of the "Govorun" supercomputer is currently 323, of which 242 are JINR staff members, and 81 are from the Member States.

In 2022, the overall usage of the resources of the "Govorun" supercomputer amounted to 555 079 jobs, which corresponds to 40 million core hours, and to 455 jobs on the GPU component, which corresponds to 32 890 GPU hours. The average load of the CPU component was 96.2%, while the GPU load was 91.4%.

Monitoring System

Within the development of the resource management system for the Tier-1 and Tier-2 grid sites, a new accounting system [3] was created at JINR. It enabled to significantly expand the functionality of the original system, as well as to reduce the time of obtaining statistical data due to the creation of automatic data processing by the visualization system. The implemented approach provides the statistical data display directly from SLURM (Simple Linux Utility for Resource Management) and allows accounting for the resources and their use both within the distributed data processing system and locally. The visualization system yielded a powerful tool for analyzing and compiling different reports and presentations. The accounting system was integrated into the general MICC monitoring system, i.e., LITMon, which made it possible to organize a single entry point and combine disparate accountings into a unified structure.

Information Services

In 2022, a number of works on the development and current maintenance of the "Dubna" Electronic Document Management System (EDMS) were completed. For the further development and optimization of electronic document management, the EDMS software was configured for the process of coordinating technical specifications and design assignments for the development of design and/or working documentation for all capital investment objects of the Institute, for the document management of accounts and acts of work performed under budget items 18 "Design works" and 19 "Construction of buildings and technological systems", for the document management of accounts and acts of work performed KS-2, KS-3 under budget item 14, paragraphs a, b, etc. A number of works on the adaptation of the "Dubna" EDMS to accommodate the changes in the organization of 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.

The maintenance of a number of the JINR Directorate's sites and programs for accounting for international scientific and technical cooperation (ISTC), etc. was in progress. Certificates of registration of a computer program were received for a number of programs.

In 2022, the work on the creation of the Digital JINR platform started. Its main purpose is to provide a unified environment for the creation and development of digital services, their integration with each other and the analysis of information on all aspects of JINR's activities. The Digital EcoSystem will encompass a wide range of services, from resources for users of basic facilities to handling business trips, vouchers, ordering certificates, etc. The major groups of services are administrative (the area of responsibility of JINR Development of Digital Services Department) and scientific. At present, a prototype of the Digital EcoSystem single access point (https://eco.jinr.ru), a number of network services, a telephone directory and some others were implemented. Access to the system is based on the JINR Single Sign-On (SSO) authentication service.

The work on the maintenance and modernization of central information servers, portals and databases for the information maintenance and software for the activities of MLIT (lit.jinr.ru) and JINR (wwwinfo.jinr.ru, dissertations.jinr.ru, pepan.jinr.ru, etc.) was underway.

The License Management System (LMS, soft-lit.jinr.ru) was put into trial operation. The main purpose of creating the LMS is to automate the management, acquisition, maintenance and use of licensed software products. The LMS comprises the Network Licensing System (NLS), databases and a web interface. The NLS, as one of the main components, implements the automatic granting and issuance of network licenses. The LMS web interface was implemented in the "Dubna" EDMS development environment using the LegoToolkit web application.

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.

To optimize the characteristics of the magnetic system of the CBM experiment (GSI, Darmstadt), the three-dimensional modeling of the protective screen of RICH photodetectors was carried out [4]. For the BM@N magnetic system, the distribution of the field in the magnet working area was analyzed.

The numerical modeling of smooth-irregular liquid-crystal waveguide structures (4-cyano-40-pentylbiphenyl or 5cb) under the action of an external field was performed [5], which made it possible to investigate the inhomogeneous nonstationary regions that arise in this case. It was shown that when the external repetitively pulsed electric field was turned on, the attenuation and size of the inhomogeneities decreased.

It was proposed to replace the Runge–Kutta scheme in numerical calculations of the current-voltage characteristics of long Josephson junctions by an "explicit" second-order scheme [6]. A numerical-analytical algorithm for estimating round-off errors was developed. Their boundedness over the entire calculation interval when using the proposed scheme was proved. The calculations were carried out on the "Govorun" supercomputer with the REDUCE system.

The pion–nucleus scattering data for a number of target nuclei were analyzed on the basis of a microscopic model of the pion–nucleus potential [7]. The obtained numerical results of the elastic scattering cross section $\pi^{\pm} + {}^{40}$Ca at energies of 116, 163 and 241 MeV confirmed the earlier conclusions about the influence of the nuclear medium on the parameters of the pion–nucleus scattering amplitude.

To study the pion damping width (lifetime) of elementary particles, an algorithm for the calculation of multidimensional collision integrals based on the Monte Carlo method was developed [8]. The algorithm was applied to calculate the pion damping width in hot nuclear matter, which is typical of heavy-nucleus collision processes. The calculations were performed on the HybriLIT heterogeneous cluster. To optimize the computation time, parallel computing based on OpenMP and CUDA technologies was used.

The automation of the assembly, configuration and installation of software (DevOps) for the development and use of MPDRoot was implemented [9]. Typical MPDRoot DevOps operations that used to be cumbersome and time-consuming were reduced to just a few commands, accompanied by a short deployment guide, which greatly minimized the potential for errors on the end user and developer side. The main advantage of the current implementation is its wide compatibility and full modularity that makes it easier to maintain, upgrade and identify the source of potential problems in the future.

The software models of the track detectors of the BM@N experiment were upgraded and further optimized for the current configuration of the experimental facility (autumn run 2022) [10]. An electrostatic field map was calculated for the current configuration of the GEM detector to enhance the quality of the detailed simulation of processes inside triple gas electron multipliers.

Data reconstruction algorithms were fine-tuned for the SRC configuration at the BM@N facility during the spring run of 2022.

Algorithms based on deep neural networks were developed for event reconstruction on the time interval of the SPD facility under high-luminosity conditions. The TrackNET recurrent neural network, optimized for work on the "Govorun" supercomputer, was enhanced [11]. The data processing performance of up to 2000 events per second with an efficiency of up to 97% and a false track rate of 5% was achieved.

As part of the work on creating a configuration information system [12] for the experiments of the NICA project, a configuration manager, namely, a C++ class library for working with the DDS API, exchanging data with the database and processing REST requests, was developed. The work to transfer the configuration information system to trial operation is underway.

The development of track reconstruction algorithms and methods for estimating the operating parameters of new HGCal detector cassettes of the CMS experiment in a test module on cosmic muons started [13]. The detailed modeling of the test setup with the determination of the optimal dimensions of the trigger and sensitive planes for the subsequent testing of new detectors was performed.

Application of the HIJING, EPOS 1.99, UrQMD and Geant4 FTF models for the analysis of experimental data by the NA61/SHINE Collaboration was considered. It is shown that the Geant4 FTF model describes well the data on π-meson rapidity distributions in ^{40}Ar + ^{45}Sc interactions at $\sqrt{s_{NN}}$ = 5.2 and 6.1 GeV [14].

A series of computational experiments using a number of quantum simulators, such as QuEST, Qiskit, CuQuantum, and the Circ quantum circuit generator, capable of operating on different computing architectures, were performed on the "Govorun" supercomputer [15]. It was shown that the dimension of the state vector grew exponentially with an increase in the number of qubits, and the possibilities for simulating quantum algorithms on the "Govorun" supercomputer (configuration before its modification) were limited to 38 qubits on a CPU, to 31 qubits on one GPU and 34 qubits on eight GPUs [16].

In 2022, the JINRLIB library (http://wwwinfo.jinr.ru/programs/jinrlib/) was replenished with the following programs developed by MLIT specialists: INQSIM, a program for converting PI-type fully symmetric quadrature rules on 2-,...,6-simplexes from compact to expanded forms; FITTER_WEB, a program for fitting experimental data obtained on a small-angle neutron scattering spectrometer, implemented as a web application.

The KANTBP 3.1 program for calculating the energy values, reflection and transmission matrices, and the corresponding wave functions in the adiabatic coupled-channel approach was developed and published in the CPC Program Library [17]. The theoretical cross sections obtained with the KANTBP 3.1 program describe well the experimental data for different heavy-ion fusion and fission reactions.

The momentum distributions of the nucleus and electrons were investigated in the case of the double Compton ionization of a helium atom at a photon energy of 40 keV [18]. It was established that the doubly charged ion momentum distribution was very close to the Compton profile of the nucleus in the ground state of the helium atom, while the momentum distribution of the singly charged ion gave a precise image of the electron Compton profile. The theoretical foundation of the new method is given in [19].

The Bayesian two-rule automatic adaptive quadrature (B2AAQ) of one-dimensional Riemann integrals is critically driven by the *a priori* input provided by the user. Conditions that enable a straightforward elementary input of problem parameters and result in either a single subrange decision tree or a forest of subrange decision trees were defined. This secures the increase of the B2AAQ robustness, reliability and efficiency, together with a significant expansion of its scope, beyond that of the QUADPACK package, which is the core of the computational integration chapters of the major computer libraries worldwide [20].

The numerical study of the fast regulation of the magnetization direction in magnetic nanomaterials, such as magnetic nanomolecules and nanoclusters, was performed [21]. The method can find application in the creation of memory devices and other spintronic appliances.

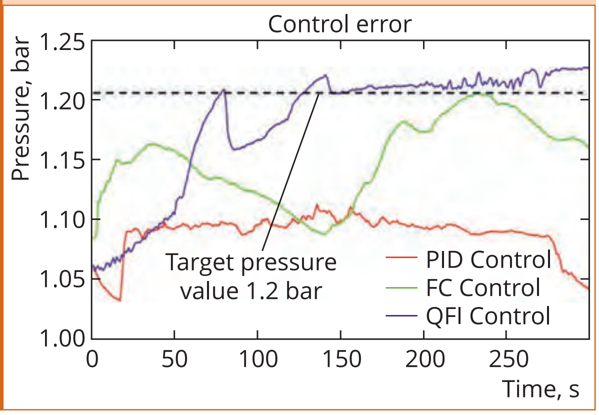
A mathematical model of multifractal dynamics has been proposed to be used to describe the COVID-19 pandemic. The calculated parameters of the model accurately determine the parameters of the trend and the large jump in daily diseases. The fractal dimensions of various segments of daily incidence in the world and variations in the main reproduction number of COVID-19 were calculated [22].

The Q_3 indicator of classicality of quantum states with different symmetries of a three-level quantum system [23], defined as the probability of finding a state with a positive Wigner function within a unitary-invariant ensemble of random states in the Hilbert–Schmidt, Bures and Bogolyubov–Kubo–Mori metrics, was analyzed. As a result of calculations of Q_3 indicators in all metrics, a regularity was revealed: the states with a higher symmetry were more classical.

A software and hardware platform was developed on the basis of quantum fuzzy controllers embedded into the control loop to control the pressure and flow of liquid nitrogen of superconducting magnets of the cryogenic system of the NICA accelerator complex [24]. The quantum controller demonstrated the highest speed in achieving the target value, low overshoot and accuracy of achieving the control goal compared to other types of controllers (Fig. 9, blue curve). The design of quantum fuzzy controllers is based on quantum information technologies and is performed using the QSCIT (Quantum Soft Computational Intelligence Toolkit) software toolkit developed by MLIT specialists.

Within the ML/DL/HPC ecosystem [2], using the example of solving a specific problem to investigate the dynamics of magnetization in a Josephson φ_0 junction, a methodology for developing software modules, which enable not only to carry out calculations, but also to visualize the results of the study and to accompany them with the necessary formulas and explanations, was presented (Fig. 10). A parallel implementation of the algorithm for performing computing for different values of the model parameters based on the Joblib Python library and modules with the integration of the Matlab code into Jupyter Notebook, which make it possible to effectively carry out applied computations for image analysis, were developed.

Fig. 9. Controlling the process of achieving the given level of nitrogen pressure by different types of regulators in cooling mode (blue curve — quantum controller, green — fuzzy controller, red — PID controller)



Within the joint project of MLIT and LRB, the development of the information system for radiation biology tasks on top of the ML/DL/HPC ecosystem was in progress: a module to study the behavioral patterns of small laboratory animals exposed to radiation was developed. The module enables the automation of the analysis of video data obtained when testing rodents in different test systems, one of which is the Open Field. The setup has a form of round arena with chequered-marked sectors and holes. An approach to marking the arena on the basis of determining key points within a neural network approach was proposed [25]. Three neural network models, namely, a simple convolutional model and two models based on the VGG16 and Xception architectures, which were trained using the transfer learning technique, were considered. The neural network architectures showed comparable results, however, the best accuracy was provided by an approach based on the simple convolutional model. The further development of the approach involves expanding the dataset for training and the set of key points to enhance the accuracy of labeling.

Fig. 10. Scheme of software modules for studying systems with Josephson junctions

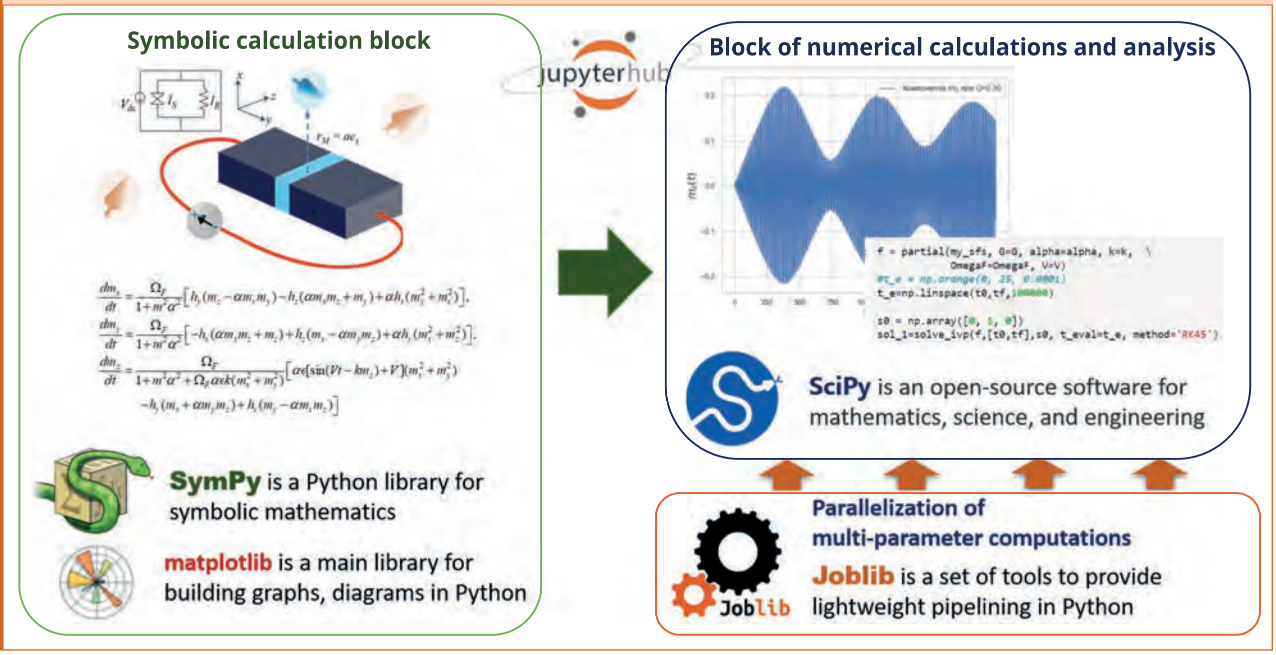
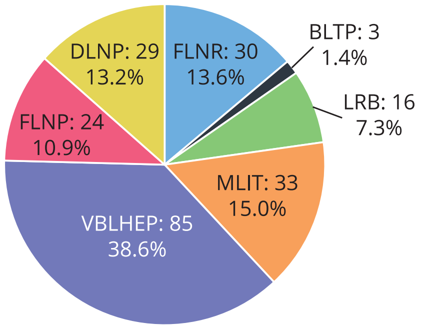


Fig. 11. Distribution of the number of excursions in 2022 by the Laboratories



The research performed jointly with FLNP within the UNECE ICP Vegetation international programme for monitoring and forecasting air pollution processes in Europe and Asia was underway. The possibility of using the Earth remote sensing data together with machine learning methods for predicting air pollution by heavy metals was investigated [26]. The average accuracy of the models exceeded 89%. Models of pollution by aluminum, iron, and antimony in the central region of Russia were constructed.

A service for planning and accounting for excursions to JINR (https://jinrex.jinr.ru) was developed together with the UC. The main functions of the service are as follows: saving information on excursions, excursion coordination, demonstration of the workload of visiting points, collecting analytics and demonstration of statistics. To date, over 100 people related to conducting excursions were registered in the system. In 2022, 220 excursions were held at JINR (Fig. 11).

INTERNATIONAL COOPERATION

In 2022, the cloud of the Institute of Nuclear Physics of the Academy of Sciences of Uzbekistan was put into operation and integrated into the JINR DICE. The server and network hardware for the cloud infrastructure of the Institute of Nuclear Physics (Almaty, Kazakhstan) was purchased and supplied. The work on putting the hardware into operation and expanding the cloud capacity of this organization is underway. At present, Plekhanov Russian University of Economics, the North Ossetian State University (Russia), the Institute of Nuclear Physics (Kazakhstan), the Institute of Physics of the National Academy of Sciences of Azerbaijan, the Institute for Nuclear Research and Nuclear Energy (Bulgaria), Sophia University “St. Kliment Ohridski” (Bulgaria), the Scientific Research Institute for Nuclear Problems of the Belarusian State University, the Institute of Nuclear Physics (Uzbekistan), the Egyptian National STI Network of the Academy of Scientific Research and Technology were fully integrated into the JINR DICE, and the Georgian Technical University is in the progress of integration.

The computing cluster of the Institute of Mathematics and Digital Technologies of the Mongolian Academy of Sciences (IMDT MAS) was integrated into the heterogeneous distributed environment based

Tashkent, 8 October. Launch of a cloud computing cluster created with the assistance of JINR at the Institute of Nuclear Physics of the Academy of Sciences of Uzbekistan

on the DIRAC platform. This makes it possible to utilize available cluster resources in computing for the NICA megascience project.

In 2022, the implementation of the joint project of LRB, MLIT and research centres of the University of Belgrade "Computer Identification, Characterization and Modeling of Histological Data" started within the Cooperation Agreement between JINR and the Ministry of Education, Science and Technological Development of the Republic of Serbia. In April, a workshop "Computational Biology and Physics" (https://indico-hlit.jinr.ru/event/310/) was held. The participants discussed a number of topical issues in neuroradiobiology and radiology, as well as technological and information tools for automating relevant studies and data processing. To implement the project, the BIOHLIT-Serbia web portal (https://it4bio.jinr.ru/) was deployed. The resources of the HybriLIT heterogeneous platform are actively used to solve the computational tasks of the project.

EDUCATIONAL PROGRAMME ON THE EDUCATION AND TESTING POLYGON

In 2022, the resources of the HybriLIT platform were actively used for educational purposes. This direction is connected both with training courses for JINR staff members and practical classes for students of Dubna State University, Tver State University, etc.

In 2022, practical classes on "Architecture of Computer Systems", "High-Performance Computing Technologies", "Modern Methods for Analyzing Complex Systems", "Machine Learning and Data Mining", "Languages and Technologies for Data Analysis", "Mathematical Apparatus and Tools for Data Analysis" were held using the resources of the education and testing polygon and the ML/DL/HPC ecosystem for more than 800 students, which enabled them to master state-of-the-art technologies for developing parallel algorithms on novel computing hybrid architectures and tools (libraries and frameworks) for machine and deep learning tasks [27].

The resources of the platform were also actively used during the first JINR Autumn School of Information Technologies, which was held on 14–19 November at MLIT. School participants attended training courses on topical issues in the field of distributed and high-performance computing, machine learning and artificial intelligence, mathematical modeling, modern methods and technologies for data processing and analysis.

In 2022, one PhD, eight Master's and four Bachelor's theses were prepared using the resources of the HybriLIT platform.

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