# MESHCHERYAKOV LABORATORY of INFORMATION TECHNOLOGIES

The activity of the Meshcheryakov Laboratory of Information Technologies (MLIT) in 2023 was focused on ensuring the reliable functioning and growth of the JINR network, information and computing infrastructure (theme 05-6-1118-2014/2023 "Information and Computing Infrastructure of JINR"), 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 (theme 05-6-1119-2014/2023 "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data") on the basis of the JINR Multifunctional Information and Computing Complex (MICC). 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 2023, the MLIT staff published over 200 scientific papers, 5 monographs and more than 100 articles within international collaborations, presented over 150 reports at international and Russian conferences.

# MULTIFUNCTIONAL INFORMATION AND COMPUTING COMPLEX OF JINR

To attain the main objectives of JINR flagship projects, it is needed to ensure the high performance, reliability and availability in 24/7/365 mode of all components of the Multifunctional Information and Computing Complex (MICC) as a large research infrastructure project.

In 2023, work to modernize and enhance the performance of the hyperconverged Govorun supercomputer, distributed computing and data storage systems based on grid technologies and cloud computing was underway. The work was based on reliable engineering components and a state-of-theart network infrastructure with a bandwidth of up to  $4 \times 100$  Gbit/s.

In 2023, the active use of the MICC resources for JINR research and applied tasks continued. The HybriLIT platform, which includes the Govorun supercomputer and the education and testing polygon, was actively used to perform investigations within the JINR Topical Plan. The application of grid technologies based on the DIRAC Interware enabled to integrate not only the allocated computing resources of all MICC components, but also the clusters of the Member States' organizations. Such an approach made it possible for the first time at JINR to carry out a full cycle of processing experimental data obtained during the 8th run of the BM@N experiment, as well as to successfully perform simulation sessions for the MPD experiment. 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 and for 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.

#### JINR Network Infrastructure

The JINR local network infrastructure and telecommunication channels are the foundation for the JINR information and computing infrastructure, which is constantly developing, providing access to the computing resources and the data storage systems both within the Institute and in external scientific organizations cooperating with JINR.

In 2023, the JINR telecommunication channels functioned reliably. First of all, the reliable functioning of the Moscow backup channel with a bandwidth of 4 × 100 Gbit/s was ensured. To operate the Tier-1 grid site, one must be a full member of the LHCOPN network to communicate with Tier-0 (CERN) and other Tier-1 sites. This connection is provided by the 100 Gbit/s JINR–CERN direct channel and its 100 Gbit/s backup channel passing through Moscow and Amsterdam. JINR Tier-2 connectivity is ensured by the LHCONE external overlay network designed for Tier-2 grid sites. The RU-VRF technology is employed for communication with Russian institutes 3 October. Delegation of the NAS of the Republic of Kazakhstan (NAS RK), headed by President of the Board of NAS RK K. Zakarya on an excursion at the Laboratory during a visit to JINR



involved in processing data from the LHC. The National Research Computer Network of Russia (NIKS), created as a result of integration of the federal university computer network RUNNet (Russian UNiversity Network) and the network of organizations of the Russian Academy of Sciences RASNet (Russian Academy of Science Network), provides communication with scientific and educational organizations of the Russian Federation. The DWDM (Dense Wave Division Multiplexing) technology is used for data transfer via the external optical telecommunication channel.

The distribution of the incoming and outgoing traffics by the JINR subdivisions in 2023 (exceeding 25 TB by the incoming traffic) is shown in the Table.

Subdivision	Incoming traffic, TB	Outgoing traffic, TB
MLIT	639.8	519.5
HRC	459.46	75.97
VBLHEP	406.14	191.04
DLNP	253	111.8
FLNR	156.41	30.47
FLNP	155.12	48.98
Dubna State University	147.03	37.45
JINR Directorate	121.02	64.59
Remote Access Node	88.18	12.76
UC	52.73	9.84
BLTP	35.78	11.76
LRB	30.98	3.8
SIMO	30.4	4.55
CPED	29.59	2.08

The overall incoming traffic of JINR, including the general-purpose servers, Tier-1, Tier-2, the Govorun supercomputer and cloud computing, amounted to 41.45 PB in 2023, while the overall outgoing traffic reached 27.28 PB. The traffic with the scientific and educational networks, accounting for 96.21% of the total, is overwhelming.

The local area network (LAN) is based on the JINR backbone network with a bandwidth of  $2 \times 100$  Gbit/s and the distributed multinode cluster network between the DLNP and VBLHEP sites ( $4 \times 100$  Gbit/s).

The JINR Network Operation Centre (NOC) regularly updates software on 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 2023, over 1400 requests from JINR users regarding the network operation, email services, VPN, DNS, electronic libraries, WiFi, security, etc., were processed. The NOC IPDB database was modernized, namely, the search system was expanded, new registration tools were added. The general database contains 40 thousand elements (users and equipment). About 60 incidents with violations of JINR network security were processed, 25 local websites were checked for vulnerabilities, more than 30 servers and virtual machines of the NOC were supported, and over 800 network devices were monitored.

The JINR LAN comprises 12 803 network elements, 21 640 IP addresses in IPv4 format, 1385 IP addresses in IPv6 format, 5750 network users, 4554 @jinr.ru email addresses, 1165 users of electronic libraries, 854 users of the remote access service and 130 users of the EDUROAM service.

#### **MICC Engineering Infrastructure**

In 2023, 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 power supply system is provided by two transformers of 2500 kVA each, two diesel generator units of 1500 kVA, and a system of uninterruptible power supplies (8 × 300 kVA).

The climate control system of the grid components is built according to a mixed type and combines the raised floor supply of cold air with a forced exhaust of hot air by ventilation panels and the cooling of the cold corridor of the module with inter-row air conditioners. The total cooling supply consumption is 1400 kW.

In 2023, taking into account the need to expand the computing resources and the data storage systems, the enlargement of the server room by reconstructing the machine hall on the 4th floor of the MLIT building started.

The DCIM (Data Centre Infrastructure Management) system is utilized for controlling and accounting the MICC equipment.

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

In 2023, the successful operation of the JINR grid sites continued, and their on average 100% availability and reliability were ensured [1]. The creation of an accelerator complex at JINR within the NICA megascience project and experimental facilities on it entailed the extension of the functions of the JINR grid sites with the introduction of their resources in the system for modeling, processing and storing data from the BM@N, MPD and SPD experiments.

At present, the Tier-1 site provides:

 acquiring data of the CMS experiment from the Tier-0 site at CERN to the extent defined by an agreement with WLCG (Worldwide LHC Computing Grid);

archiving and responsible storage of initial experimental data transferred from Tier-0;

consistent and continuous data processing;

— additional processing (skimming) of raw data, RECO (reconstructed) data and AOD (analysis object data) data;

 data reprocessing and launch of production processing using new software or new calibration and alignment constants for the CMS detector parts;

access to AOD datasets to the Tier-1 and Tier-2 sites involved in CMS experiment data processing;

 — sending RECO and AOD datasets to other Tier-1/Tier-2/Tier-3 sites for their duplicate storage (replication) and physics analysis;

 obtaining modeled events and analyzing data written during the operation of the CMS experiment;
secure storage of modeled events;  obtaining modeled events and analyzing data for the experiments at NICA;

acquiring and processing experimental data from the BM@N experiment.

The functioning of the Tier-2 site ensures:

processing and analyzing data from all experiments at the LHC and providing resources to perform computing jobs to the participants of the experiments;

— acquiring modeled data and analyzing them for all virtual organizations registered in the Russian consortium RDIG (Russian Data Intensive Grid);

 acquiring modeled data and analyzing them for the experiments at NICA;

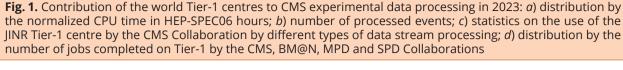
acquiring and processing experimental data from the BM@N experiment.

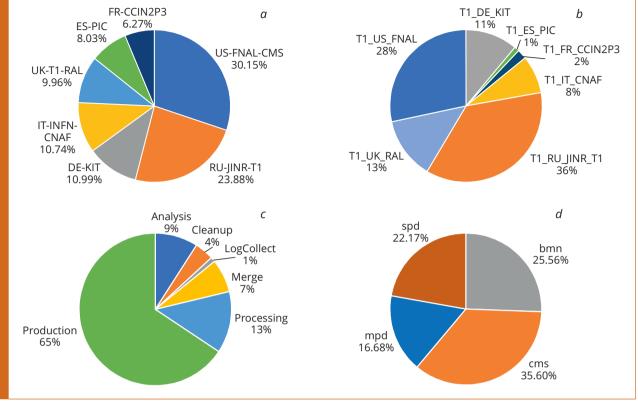
#### Tier-1 and Tier-2 Resources

The functioning of the computing resources of the JINR grid sites is provided by the SLURM (Simple Linux Utility for Resource Management) workload manager. To organize computing in the grid environment, the advanced resource connector (ARC), middleware for grid computing, is employed. It provides a common interface for transferring computing jobs to different distributed computing systems and can include grid infrastructures of varying sizes and complexity.

One of the uppermost elements of the JINR grid infrastructure, as well as the entire MICC, is the data storage system. This system is built on a hierarchical principle, and the level of storage depends on the duration of data storage and their volume. Computing cluster machines have limited disk space intended for storing the operating system (OS) itself, some additional utilities and temporary user files of a limited size. The AFS distributed global system is used to store and access user home directories and small volume software. The globally available system of maintenance and access to large software complexes of collaborations and user groups operates on the basis of the software developed at CERN, i.e., CVMFS. The dCache and EOS systems are utilized as the main data storage systems. These are systems for medium-term data storage. The latter should become the main data storage system in the MICC. EOS as a system for storing extremely large data amounts is optimal in terms of cost/storage capacity, supports multiple access protocols (POSIX when installed on the user computer, xroot and http for fast remote access) and is designed to provide high-speed data access thanks to parallel copying from many servers, etc.

With the start of sessions at the NICA complex, an intensive enlargement of long-term data storage systems on robotic tape libraries will be required. In addition to the tape robot for the CMS experiment on Tier-1, it is needed to create a long-term data storage for the experiments at the NICA complex, the neutrino programme and other user groups. This system is being created on top of the software





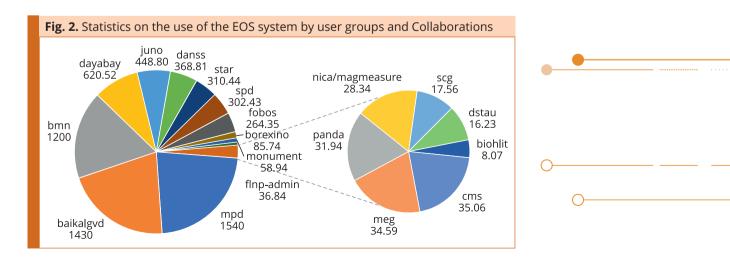
developed at CERN, i.e., CTA (CERN Tape Archive). It will be fully included in the MICC infrastructure. The major CTA component is EOS with the addition of an infrastructure for working with tape robots and manipulating the meta information of stored files. In 2023, EOSCTA was put into trial operation.

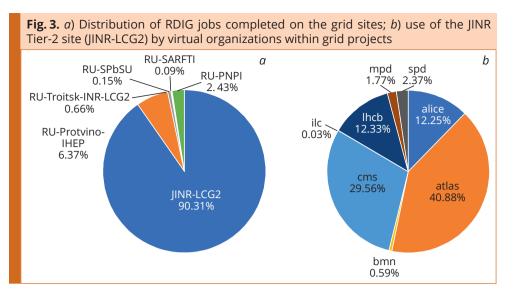
Currently, Tier-1 embraces 468 compute nodes (20 096 cores) with a performance of 323 820.54 HEP-SPEC06. The launch of jobs for CMS experiment data processing is carried out by 16 nuclear pilots, and all computing resources are available to them. Data storage is provided by the 12.4 PB dCache sys-

tem and the robotic tape storage with a capacity of 51.5 PB. The TS4500 robot runs the Enstore and dCache software. The TS3500 robot employs the EOSCTA system. To work with tapes, a 2.65 PB disk array is used to cache data.

In terms of performance, the JINR Tier-1 site is behind only the Tier-1 centre of Fermi National Accelerator Laboratory (USA) in the ranking of world Tier-1 sites that process data from the CMS experiment at the LHC (Fig. 1, a-c).

The JINR Tier-1 site is involved in performing jobs for the experiments at NICA (Fig. 1, *d*).





The Tier-2 site embraces 486 compute nodes (10 356 cores) with a total performance of 66 788.4 HEP-SPEC06. Data storage is provided by the 5.62 PB dCache system and EOS as a common distributed data storage system for all MICC users with a capacity of 23.3 PB (Fig. 2).

The JINR Tier-2 output is the highest in the Russian grid segment (Fig. 3).

#### **DIRAC** at JINR

At present, the DIRAC Interware (Distributed Infrastructure with Remote Agent Control) is the only system that integrates all MICC components. DIRAC acts as a middle layer between users and different computing resources, ensuring their efficient, transparent and reliable usage by providing a common interface to heterogeneous resources.

In 2023, DIRAC was employed to solve the tasks of Collaborations on all three experiments at the NICA accelerator complex, as well as on the Baikal-GVD neutrino telescope (Fig. 4).

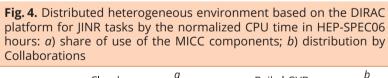
In 2023, for the first time at JINR, the complete processing of raw data from the 8th run of the

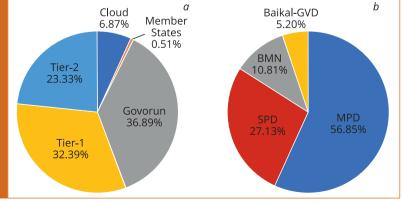
BM@N experiment was performed on the distributed heterogeneous computing infrastructure integrated using the DIRAC platform [2]. During the run, 430 TB of data was collected in the form of ~ 30 000 files. Throughout the year, after changes made to the BmnRoot package, which is used for data reconstruction, this procedure was applied to initial data reprocessing several times. In total, five large and seven small data reconstruction/generation sessions were completed within a year.

A prototype of a critical web application for an automated system that collects and processes data on the resources used at JINR and integrated into a unified infrastructure with the help of DIRAC was implemented. The application being developed provides valuable data for optimizing the operation of computing resources integrated in DIRAC [3].

#### **Cloud Infrastructure**

The JINR cloud is one of the MICC components, and its resources are utilized in the distributed information and computing environment (DICE) of the





JINR Member States [4]. The main users of cloud infrastructure resources in 2023 were collaborations of neutrino experiments and MLIT.

JINR cloud infrastructure servers run the CentOS 7.9.2009 operating system, the support period of which expires in the middle of 2024. In this regard, a number of works were performed to develop the procedure for transferring cloud servers and part of the services to another binary compatible distribution, for which AlmaLinux OS versions 8 and 9 were chosen (the specific version depends on the availability of this or that software for it). Work to update the cloud infrastructure configuration management service based on Foreman (from version 2.5.4 to version 3.8.0) and Puppet (from version 6 to version 7) software products was completed. The OS on this service was updated to AlmaLinux 8.9. Foreman templates and Puppet configuration files were enhanced for installation on AlmaLinux 9 OS cloud infrastructure nodes. For the same reasons, the OS is gradually being transferred to virtual machines (VMs) deployed in the cloud, including DLNP neutrino experiment VMs.

As part of expanding the range of cloud services provided, a service for publishing custom Docker containers in CernVM-FS [5] was developed and put into operation to ensure the possibility of their use in batch processing systems for the tasks of the neutrino platform, the NICA cluster, and all MICC components.

To meet the increasing needs of neutrino experiments for disk space for storing experimental data, the cloud storage capacity of the neutrino platform was increased from 1.5 to 3.1 PB of raw disk space through the purchase of new equipment.

Within the JINR DICE, on the basis of the resources of the JINR Member States' organizations, the following work was performed:

- update of the OpenNebula cloud platform software from version 6.4.0.1 to version 6.6.0 on the cloud of the Institute of Nuclear Physics of Uzbekistan;
- support and development of the cloud infrastructure at Khetagurov North Ossetian State University (Vladikavkaz) (network infrastructure, storage);
- addition of an interactive map that displays the geographic location of DICE participating organizations to the http://dice.jinr.ru web portal.

In 2023, 45 208 jobs were successfully completed on the DIRAC.JINR-CONDOR.ru resource (neutrino platform cloud resources available in the DICE), which corresponds to 325 056 CPU hours. All completed jobs were launched by the Baikal-GVD Collaboration.

A prototype of a computing system to develop a distributed computing environment for the SPD experiment based on PanDA WFMS/WMS is being created in the JINR cloud. The FTS file transfer service and the Rucio data management service were deployed.

#### Heterogeneous Infrastructure

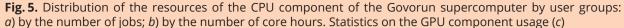
In 2023, the HybriLIT heterogeneous platform, which is a component of the JINR MICC, was actively developing. The next stage of modernization of the Govorun supercomputer, associated with the enhancement of the GPU component, took place. Five high-performance servers, each of which contains two AMD EPYC 7763 processors with 2 TB of RAM and eight NVIDIA A100 graphics accelerators with 40 GB of memory were introduced in the supercomputer. As a result, the total peak performance of the Govorun supercomputer reached 1.7 PFlops for double-precision operations (or 3.4 PFlops for single-precision operations), the total capacity of the hierarchical storage is 8.6 PB. The enhancement of the GPU component opened up new opportunities for lattice quantum chromodynamics computations, quantum computing using simulators, Big Data analytics, the development of algorithms based on a neural network approach for LRB experimental data analysis, data processing and analysis within the experiments at the NICA accelerator complex.

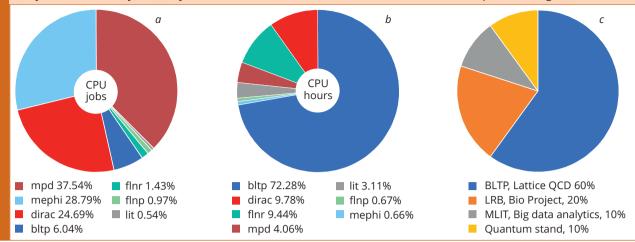
Within the task of creating a distributed data storage and processing system for the NICA project, a testing polygon was deployed. It comprises three Lustre distributed file systems and combines the Govorun supercomputer and the NCX computing cluster (VBLHEP). The Lustre distributed file system was built using disk resources and servers located on the MLIT and VBLHEP sites, and contains two disk pools, OST0 (server at MLIT) and OST1 (server at VBLHEP), integrated into one disk pool with the function of data mirroring between the OST0 and OST1 disk pools. This mechanism enables to write data to one pool and obtain a full copy of these data to the other pool, which significantly simplifies the procedure for transferring data from one computing resource to the other.

A quantum computing polygon with installed quantum computing simulators, namely, Cirq, Qiskit, PennyLane, was deployed on the resources of the ML/DL/HPC ecosystem of the HybriLIT platform. Expanding the polygon allows conducting research in the Jupyter environment, which makes it possible to visually work with quantum circuits and perform computations in the browser.

In 2023, there was made a transition to new software with the TurboVNC remote access client of the HLIT-VDI service, designed to organize user work in a graphical mode of access to software packages such as COMSOL, MAPLE, MATHEMATICA, MATLAB, etc. At the request of users, 113 software modules were installed and updated taking into account versioning.

The total number of Govorun supercomputer users is currently 312, of which 255 are JINR staff members, and 57 are from the Member States. Within 2023, all groups of Govorun supercomputer users completed 640 861 jobs on the CPU component, which corresponds to 16 million core hours, and 7808 jobs on the GPU component, which corresponds to 45 400 GPU hours. Figure 5 demonstrates





the distribution of the resources of the CPU component of the Govorun supercomputer by user groups. The average load of the CPU component was 96.4%, while the GPU component load was 91.2%.

#### Monitoring and Accounting System

The successful functioning of the MICC is ensured by the monitoring and accounting system, which must be up-to-date. For these purposes, it is planned to enhance the monitoring system by integrating local tracking systems for power supply systems (diesel generators, power distribution nodes, transformers and uninterruptible power supplies) into it and create an engineering infrastructure control centre (special information panels for visualizing all statuses of the MICC engineering infrastructure in a single access point). The transition to the project planning of the scientific activity and resource planning on user requests entails the elaboration of a special accounting system for the use of the MICC resources by each project/user. At present, such an accounting system is organized for user groups on the MICC grid infrastructure. The Grafana system is employed to visualize accounting data. In 2023, a new database for storing monitored equipment characteristics was put into operation in the LITMon monitoring system. The use of the InfluxDB2 database made it possible to optimize the process of transferring data to the Grafana visualization system and organize data replication to enhance the security of the storage system.

#### **Information Services**

In 2023, work on the Digital JINR platform was intensively performed. The testing, deployment and integration of software packages for services and the basic infrastructure of the Digital EcoSystem (DES) (planning and project management, electronic help desk, authorization, digital archives, scientific information management, etc.) were carried out; a software environment and documentation for the development of digital services and their integration were prepared. Within the development of the DES shell and services, two-way communication with the GLPI system (project maintenance) to process user requests was implemented; the integration of the electronic document management system (EDMS) and the geographic information service (GIS) to link repair and construction contracts and capital construction contracts to specific buildings or premises was completed; a built-in service "Forms" was elaborated; some functions of the EDMS, ADB2, Document Database, etc., were connected to the DES in the form of separate services.

As part of the development and maintenance of the "Dubna" EDMS, the EDMS core was significantly modernized: a subsystem for archival storage of completed documents in PDF was developed, a subsystem for defining access rights was upgraded; a system for protection against hacker attacks and unauthorized access was enhanced; the user interface was modernized, its design was updated, and its operation was accelerated; seven new types of documents (Correspondence of JSC STRABAG, Technical conditions for design, Technical solutions for design and construction work, etc.) were elaborated; a new module "Statistics" was developed; adaptation to the new accounting and financial policy for projects and activities was completed.

Within the development of information services in the cloud infrastructure, a service for planning events, newdle.jinr.ru, was deployed on top of the Newdle system (analog of the popular Doodle service), and the JINR SSO login was implemented in it.

The support and development of the website hosting infrastructure (www.jinr.ru, flnph.jinr.ru, flerovlab.jinr.ru, micc.jinr.ru, mpdroot.jinr.ru, etc.) were in progress. The support and development of the infrastructure of administrative servers (pin.jinr. ru, adb2.jinr.ru, sed.jinr.ru, etc.), the pm.jinr.ru service (automated project management system), and the disk.jinr.ru service (cloud storage service for JINR staff members) were provided. The work on the maintenance and modernization of central information servers, portals and databases for information support and software for the activities of MLIT (lit.jinr.ru) and JINR (www.info.jinr. ru, dissertations.jinr.ru, pepan.jinr.ru, etc.) was 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 IINR. In 2023, the design, development, implementation and maintenance of a user-friendly computing environment on the MLIT heterogeneous computing platform, which involves the HybriLIT cluster and the Govorun supercomputer, were of paramount importance. Highly needed and appreciated contributions were brought to the three-dimensional simulation asked by the NICA magnet validation, highest-level solutions of specific tasks within the BM@N, MPD and SPD experiments, the development of data processing system software for the Baikal-GVD experiment. The software development within the JINR contribution to the CMS and ATLAS Phase 3 experiments at CERN summarizes the best results produced within Theme 1119 for experimental data processing.

A summary of selected results is presented below.

A modern paradigm of test-driven development (TDD) to verify the MPD data reconstruction mechanism in the MPDRoot framework was implemented. Necessary changes to the codebase architecture, the diagnostic environment and data analysis are shown to enhance the potential for future developments of the reconstruction mechanism. The first results of a comparison of different modules are presented [6].

The first results within a study of the application of machine learning in the charged particle identification task in the MPD experiment were obtained [7]. A variation of the gradient boosting algorithm on decision trees, implemented in the CatBoost library, was used. A comparison of the algorithm with the n-sigma method, which is currently implemented in the MpdRoot software environment, evidenced the better capabilities of gradient boosting at small and large momentum values. The ongoing research was made possible thanks to the computing resources of the HybriLIT heterogeneous platform.

In 2023, the initial design and prototyping of the SPD online filter was completed. A workload management system [8], one of the key components of the online filter, was implemented. It comprises a server component responsible for data processing by generating and executing a sufficient number of jobs and an agent application that monitors and manages job execution on the compute node.

A data processing system for the Baikal-GVD experiment was developed and continues to be en-

hanced. It is characterized by simplicity, modularity and parallelism, corresponding to the physical properties of the neutrino telescope under construction. The modular architecture of the system enables to easily modify individual components, without compromising their integrity, and add new ones. The parallelism of the system consists of several levels. Firstly, the processing of individual clusters occurs in parallel on different virtual machines. Secondly, the processing of one cluster is performed in two sequential workflows: fast and offline processing. In both workflows, some jobs are also executed in parallel. The current state of the processing system has already made it possible to produce astrophysical results.

A web application that resolves the tasks of fitting data obtained on the small-angle neutron scattering spectrometer at the IBR-2 reactor and studying the shape and size of sample nanoparticles was developed [9]. The fitting process is parallelized using implicit multithreading and vectorization.

A new method for studying two-particle transverse momentum ( $P_{T}$ ) correlations in soft hadronic interactions was proposed [10]. It is shown that Monte Carlo models, namely, PYTHIA 6 and Geant4 FTF (FRITIOF), give different predictions for the correlations in proton–proton interactions. The correlations are connected with the Schwinger mechanism of particle production and can be studied in current and future high-energy physics experiments, in particular, at NICA.

The mutual cancellation of contributions from the channels of attraction and repulsion in the scalar interaction in a thermal pion gas at finite temperatures was investigated [11]. The pressure of the interacting pion gas was calculated using the Beth–Uhlenbeck approach to the relativistic virial expansion with Breit–Wigner phase shifts for  $\sigma$ - and  $\rho$ -meson resonances. The result of the investigation explains the absence of the  $\sigma$  meson in the hadronic resonance gas model at low temperatures and the need to take it into account in the statistical model of chemical freezeout in heavy-ion collisions.

The review paper [12] devoted to modeling the process of electron hydration based on the approach developed by the authors within the dynamic polaron model was presented. The mathematical formulations of problems and computational schemes were elaborated, complexes of problem-oriented programs were created using MPI parallel programming technology. The results of the numerical modeling and calculation of the observed physical characteristics of the electron hydration process under study were considered. The agreement of the obtained numerical results with the corresponding experimental data confirms the adequacy of the proposed approaches and the prospects for their further application and development.

The numerical simulation of experimental data accumulated at FLNP on the interaction of beta-amyloid peptide  $A\beta(25-35)$  with DPPC phospholipid membranes, which is devoted to the clarification of the role of beta-amyloid peptide ( $A\beta$ ) as a key factor in Alzheimer's disease, enabled to elucidate the dynamic properties of lipid membranes regulated by the addition of melatonin, cholesterol and beta-amyloid peptide [13].

Investigations on the analysis of pion-nucleus scattering data for a number of target nuclei based on a microscopic model of the pion-nucleus potential were performed [14]. It is shown that the developed approach provides an adequate description of experimental data on pion-nucleus scattering in the energy region of the pion-nucleon (3,3) resonance and enables the study of the influence of the nuclear medium on pion-nucleon scattering. The developed theoretical approach and the numerical study procedure were adapted to the case of proton-nucleus scattering.

A modification of the thermal peak model (TPM) based on a system of two coupled hyperbolic heat conduction equations was proposed [15]. The action of the laser in the electron gas was taken into account through the source function, which was chosen in the form of a double femtosecond laser pulse. In the hyperbolic TPM, in contrast to the parabolic TPM, there are additional parameters that characterize the relaxation times of the heat flux in the electron gas and the crystal lattice. A numerical study of the solutions of the parabolic and hyperbolic equations of the TPM for the same physical parameters and a comparative analysis of the results obtained were carried out.

An original approach and an algorithm in the Maple system for solving the scattering problem in the single-channel approximation of the close-coupling method of the optical model, described by a second-order ordinary differential equation with a complex-valued potential and regular boundary conditions, were developed [16]. The efficiency of the proposed approach is shown by numerically solving the scattering problem and calculating the reference fusion cross section and metastable states for a pair of heavy ions  $^{16}O + ^{144}Sm$  in the single-channel approximation of the close-coupling method.

Numerical simulations were carried out on a microscopic statistical model of a superfluid quantum solid, where regions of disorder, such as dislocation networks or grain boundaries, can coexist within the crystal lattice [17]. This model gives the opportunity to answer the question which real quantum crystals can exhibit the property of superfluidity and which cannot.

Using specific input validation procedures, a recursive algorithm for the automatic adaptive quadrature of one-dimensional Riemann integrals based on the Bayesian inference was developed to provide stable and reliable automatic solutions at critical stages of the solution path [18]. The Bayesian predictor-corrector algorithm provides an automatic solution to the integrand function conditioning at the ends of a subrange decision tree root. The new subrange partition strategy enables the highest accuracy available output under cancellation by subtraction.

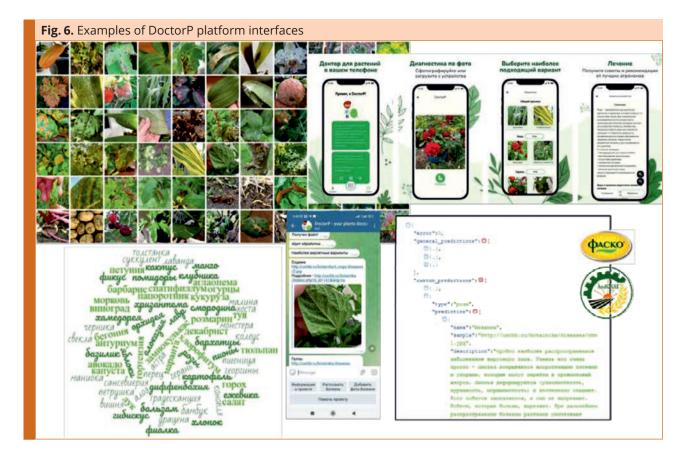
The functional reduction method for Feynman integrals, developed at MLIT, was employed to calculate one-loop integrals corresponding to diagrams with four external lines [19]. The integrals that emerge in the calculations of radiative corrections to the amplitudes of light scattering by light, photon splitting in an external field and the Delbruck scattering were considered. For an arbitrary value of the space dimension *d*, new analytical results were produced for master integrals. For d = 4, compact expressions are given in terms of dilogarithms.

The interrelation between classicality/quantumness and symmetry of states was addressed within the phase-space formulation of finite-dimensional quantum systems [20]. It was found that the quantum states ordered with respect to their "symmetry" also exhibited the ordering with respect to their "classicality": the larger the symmetry, the more classical the quantum states are.

## APPLIED RESEARCH

The design of embedded intelligent control systems based on fuzzy logic, neural networks, genetic and quantum algorithms for the task of nitrogen pressure stabilization in the cryogenic system of the test stand of the JINR VBLHEP magnet factory was completed. The efficiency of the system functioning was demonstrated experimentally [21].

Within the BIOHLIT joint project (MLIT and LRB), an algorithm for tracking a laboratory animal in the "Morris Water Maze" behavioral test was developed on the basis of computer vision methods. A web service prototype for the "Morris Water Maze", which enables to monitor the correctness of the generated trajectory on video and form a dataset in different representations, and a web service prototype for the "Open Field" behavioral test, the functionality of which allows one to resolve the laboratory animal tracking task, build a heat map, count the sectors covered and provide the user with summary analytics, were elaborated.



In 2023, within a joint project between MLIT and BLTP, the development of a service for modeling systems based on Josephson junctions was in progress. The service was supplemented with materials for modeling the Josephson junction dynamics under the influence of external radiation using the example of a superconductor-insulator-superconductor type transition [22]. Algorithms to calculate the current-voltage characteristic (CVC) of a Josephson junction under the influence of external radiation and find the Shapiro step width on the CVC curve were developed using Python in the Jupyter Book environment. A parallel algorithm to compute the dependence of the Shapiro step width on the external radiation amplitude was implemented, and the efficiency of the parallel implementation was demonstrated.

A platform and a mobile application (DoctorP) (Fig. 6) for detecting plant diseases and pests are being developed at MLIT [23]. Both a general model capable of detecting 68 disease classes and specialized models for 29 ornamental and agricultural crops are available. In 2023, the platform processed

over 70 000 user requests. To obtain a prediction and treatment recommendations from experienced agronomists, one just needs to send a photo showing the problem. The platform can be accessed by third-party applications and services. Garden Retail Service (formerly Fasko) and the Andijan Institute of Agriculture and Agrotechnology (Uzbekistan) have already took advantage of this opportunity.

A software complex for creating digital twins of distributed data acquisition, storage and processing centres (DDCs) was developed and registered in the Register of Russian Computer Programs [24]. The uniqueness of this program is that the digital twins created with its help effectively monitor the DDC functioning in terms of data flows and related tasks. A DDC digital twin is a virtual copy of a data centre that demonstrates how it operates under any possible scenario. A successful verification of the simulation program was performed using the example of the operation of the computing infrastructure of the BM@N experiment at the NICA accelerator complex during the 8th physics run in 2023.

## INTERNATIONAL COOPERATION

The first in the Republic of Kazakhstan and 11th JINR cloud computing cluster was introduced in the JINR distributed information and computing environment. Staff members of scientific institutes and universities of Kazakhstan will be able to use the resources of the INP cloud cluster within their own research and as part of cooperation with JINR, participating in the NICA and Baikal-GVD megascience projects. The cluster, included in the DICE of JINR and the JINR Member States' organizations, allows



accessing a larger number of hardware resources than in the case of using the INP cloud only locally, which opens up opportunities for scientists to produce scientific results in a shorter time.

As part of the collaborative programme with the University of Cape Town (RSA), a study of the structure and properties of spherically symmetrical, time-periodic, spatially localized objects of a finite radius in the  $\phi^4$  model depending on the size of the radius and the frequency of oscillations was carried out at MLIT [25]. A parallel version of the Matlab script developed to enhance the performance of computations of Floquet multipliers enabled to reduce the computation time by more than 10 times. The computations were performed on the HybriLIT platform and using the Govorun supercomputer.

With the active participation of MLIT specialists, a catalog of events of the ATLAS experiment (LHC),



20 October. JINR Autumn School of Information Technologies. Winners of the Parallel Computing Hackathon



EventIndex, was created and is dynamically developing [26]. MLIT specialists were actively involved in the modernization of the system: the monitoring system was significantly enhanced; the transition to the Grafana platform was made; a new service for the automatic search and collection of events (Event Picking Service) was created, which made it possible to collect events for the second stage of the analysis of the production of *W* gauge boson pairs during the interaction of two photons (" $\gamma\gamma \rightarrow WW$ ") with the least amount of manual labor.

Within the JINR–Bulgaria Collaboration, periodic approximate solutions to the three-body problem were resolved with high accuracy [27]. Investigations were performed on the Govorun supercomputer and the Nestum cluster (Sofia, Bulgaria). A high-precision database of 462 choreographic orbits, including 397 new ones, was established.

# EDUCATIONAL PROGRAMME ON THE EDUCATION AND TESTING POLYGON

In 2023, the education and testing polygon of the HybriLIT platform was actively used for conducting semester-long training courses and within schools and workshops. On the basis of the polygon, training courses were held within the JINR Autumn School of Information Technologies, the Workshop "Modern Information Technologies in Biology and Medicine", the V International Summer School of Young Scientists "Computer Technologies for Scientific and Applied Tasks" (NOSU), the XVI International Internship for Young Scientists from the CIS Countries, in which 210 students participated. To conduct offsite training courses and seminars at Dubna State University, the HybriLIT mobile cluster was deployed. It is noteworthy that semester-long training courses in the IT disciplines "Architecture and Technologies of High-Performance Systems", "Parallel Distributed Computing", "Languages and Technologies of Data Analysis", "High-Performance Computing Technologies", "Mathematical Computing Software", held at Dubna State University and Tver State University, were attended by 310 students. In addition, five Bachelor's and seven Master's theses were prepared on the basis of the HybriLIT platform.

### REFERENCES

 Baginyan A., Balandin A., Dolbilov A., Golunov A., Gromova N., Kashunin I., Korenkov V., Mitsyn V., Pelevanyuk I., Shmatov S., Strizh T., Trofimov V., Vorontsov A., Voytishin N. JINR Grid Infrastructure: Status and Plans // Proc. of the 10th Intern. Conf. "Distributed Computing and Grid Technologies in Science and Education" (GRID'2023), Dubna, July 3–7, 2023; Phys. Part. Nucl. 2024. V. 55, No. 3. P. 355–359.

2. *Gertsenberger K., Pelevanyuk I.* BM@N Run 8 Data Production on a Distributed Infrastructure with DIRAC // Proc. of the XXVII Intern. Sci. Conf. of Young Scientists and Specialists (AYSS-2023); Phys. Part. Nucl. Lett. (submitted).

- Champish D., Ilina A., Pelevanyuk I. System for Analysis of the Performance of Scientific Jobs in Distributed Systems // Proc. of the 10th Intern. Conf. "Distributed Computing and Grid Technologies in Science and Education" (GRID'2023), Dubna, July 3–7, 2023; Phys. Part. Nucl. 2024. V. 55, No. 3.
- Balashov N., Kuprikov I., Kutovskiy N., Makhalkin A., Mazhitova Ye., Pelevanyuk I., Semenov R., Shpotya D. Changes and Challenges at the JINR and Its Member States Cloud Infrastructures // Proc. of the 10th Intern. Conf. "Distributed Computing and Grid Technologies in Science and Education" (GRID'2023), Dubna, July 3–7, 2023; Phys. Part. Nucl. 2024. V. 55, No. 3. P. 366–370.
- Balashov N. JINR Container Distribution Service // Proc. of the 10th Intern. Conf. "Distributed Computing and Grid Technologies in Science and Education" (GRID'2023), Dubna, July 3–7, 2023; Phys. Part. Nucl. 2024. V. 55, No. 3.
- Busa J., Jr, Bychkov A., Hnatic S., Krylov A., Krylov V., Rogachevsky O. MPD Data Lab: Towards the Modern Data Analysis Framework for the MPD Experiment // Proc. of the 25th Intern. Baldin Seminar on High Energy Physics Problems "Relativistic Nuclear Physics & Quantum Chromodynamics", Dubna, Sept. 18–23, 2023; Phys. Part. Nucl. (submitted).
- Papoyan V., Aparin A., Ayriyan A., Grigorian H., Korobitsin A., Mudrokh A. Machine Learning Application for Particle Identification in MPD // Phys. Part. Nucl. 2023. V. 86, No. 5. P. 869–873.
- Greben N., Romanychev L., Oleynik D., Degtyarev A. SPD On-line Filter: Workload Management System and Pilot Agent // Proc. of the 10th Intern. Conf. "Distributed Computing and Grid Technologies in Science and Education" (GRID'2023), Dubna, July 3–7, 2023; Phys. Part. Nucl. 2024. V. 55, No. 3. P. 612–614.
- Soloviev A. G., Solovieva T. M., Kuklin A. I., Balashoyu M. Development of a Web Application for Fitting Data from a Small-Angle Neutron Scattering Spectrometer // Parallel Computing Technologies (PCT'2023). Short articles and poster descriptions. Chelyabinsk: SUSU Publ. Center. 2023. P. 206–214 (in Russian).
- Galoyan A., Ribon A., Uzhinsky V. Towards Study of Two-Particle PT Correlations in Hadronic Interactions at NICA // MPDI Phys. 2023. V. 5, No. 3. P. 823–831.
- 11. *Blaschke D., Friesen A., Kalinovsky Yu.* Cancellation of the Sigma Mode in the Thermal Pion Gas by Quark Pauli Blocking // Symmetry. 2023. V. 15, No. 3. P. 711.
- Lakhno V. D., Amirkhanov I. V., Volokhova A. V., Zemlyanaya E. V., Puzynin I. V., Puzynina T. P., Rikhvitskii V. S., Bashashin M. V. Dynamic Model of the Polaron for Studying Electron Hydration // Phys. Part. Nucl. 2023. V. 54. P. 869–883.
- 13. *Kurakin S., Badreeva D., Dushanov E., Shutikov A., Efimov S., Timerova A., Kučerka N.* Arrangement of Lipid Vesicles and Bicelle-Like Structures Formed in the

Presence of Aβ (25–35) Peptide // BBA — Biomembranes. 2024. V. 1866, No. 1. P. 184237.

- Lukyanov V. K., Zemlyanaya E. V., Lukyanov K. V., Abdul-Magead I. Theoretical Analysis of Pion–Nucleus Scattering at Energies of the (3,3) Pion–Nucleon Resonance // Phys. Part. Nucl. 2023. V. 54. P. 734–755.
- Amirkhanov I. V., Sarkhadov I., Tukhliev Z. K. Numerical Results of Thermal Processes Occurring in Materials under the Action of Femtosecond Laser Pulses. JINR Preprint P11-2023-52. Dubna, 2023. J. Surf. Invest.: X-Ray, Synchrotron Neutron Techn. (accepted) (in Russian).
- Gusev A. A., Chuluunbaatar O., Derbov V. L., Nazmitdinov R. G., Vinitsky S. I., Wen P. W., Lin C. J., Jia H. M., Hai L. L. Symbolic-Numerical Algorithm for Solving the Problem of Heavy Ion Collisions in an Optical Model with a Complex Potential // Lect. Not. Comput. Sci. 2023. V. 14139. P. 128–140.
- 17. Yukalov V. I., Yukalova E. P. Statistical Model of a Superfluid Solid // Phys. Lett. A. 2023. V. 457. 128559-9.
- Adam G., Adam S. The Pivotal Role of Input Validation for Robust and Reliable Bayesian Automatic Adaptive Quadrature // 2023 Intern. Conf. on Advanced Sci. Comput. (ICASC), Cluj-Napoca, Romania, 2023. P. 1–6; doi: 10.1109/ICASC58845.2023.10328030.
- Tarasov O. V. Calculation of One-Loop Integrals for Four-Photon Amplitudes by Functional Reduction Method // Phys. Part. Nucl. Lett. 2023. V. 20, No. 3. P. 287–291.
- 20. *Khvedelidze A., Torosyan A.* On the Hierarchy of Classicality and Symmetry of Quantum States // Zapiski Nauch. Seminarov POMI. 2023. V. 528. P. 238–260.
- 21. Zrelov P. V., Nikiforov D. N., Reshetnikov A. G., Ulyanov S. V. Quantum Intelligent Control of Nitrogen Pressure in a Cryogenic Facility of Magnet Plant Test Bench // Phys. Part. Nucl. (submitted).
- 22. Rahmonov I. R., Rahmonova A. R., Streltsova O. I., Zuev M. I. Python Toolkit for the Simulation of the Josephson Junction Dynamics under the Influence of External Radiation. http://studhub.jinr.ru:8080/ jjbook
- 23. *Uzhinskiy A.* Advanced Technologies and Artificial Intelligence in Agriculture // Appl. Math. 2023. V. 3, No. 4. P. 799–813.
- 24. *Korenkov V. V., Priakhina D. I., Trofimov V. V.* Software Complex for Creating Digital Twins of Distributed Data Acquisition, Storage and Processing Centers // Register of Russian Computer Programs. 2023. No. 2023667305 (in Russian).
- 25. Alexeeva N. V., Barashenkov I. V., Bogolubskaya A. A., Zemlyanaya E. V. Understanding Oscillons: Standing Waves in a Ball // Phys. Rev. D. 2023. V. 107. 076023.
- 26. *Barberis D., Aleksandrov I., Alexandrov E. et al.* The ATLAS EventIndex: A BigData Catalogue for All ATLAS Experiment Events // Comput. Software Big Science. 2023. V. 7, No. 2. P. 1–21.
- Hristov I., Hristova R., Puzynin I., Puzynina T., Sharipov Z., Tukhliev Z. A Database of High Precision Trivial Choreographies for the Planar Three-Body Problem // Lect. Not. Comput. Sci. 2023. V. 13858. P. 171–180.