# LABORATORY OF INFORMATION TECHNOLOGIES

In 2018, research on two topics of first priority, namely, "Information and Computing Infrastructure of JINR" and "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data", was conducted by the Laboratory of Information Technologies (LIT) in the scope of the JINR research field "Networks, Computing, Computational Physics". The LIT staff participated in research on 25 topics of the JINR Topical Plan within cooperation with other JINR Laboratories.

In 2018, the Multifunctional Information and Computing Complex (MICC) of JINR was replenished with a new high-performance component. The "Govorun" supercomputer, representing a heterogeneous computing platform containing computing components with nodes based on the processors Intel® Xeon® Scalable and Intel® XeonPhi™ 7290 as well as a component with computing accelerators GPU NVIDIA V100 (DGX-1), was successfully installed and put into operation, which would enable conducting resource-intensive, massively parallel calculations that require different types of computing architectures. The processor component of the "Govorun" supercomputer was implemented by the Russian JSC "RSC Technologies", a developer and integrator of the "full cycle" supercomputer solutions of new generation based on advanced liquid cooling as well as a number of its own innovative solutions.

The JINR MICC consisting of four key components — the grid infrastructure, the central computing complex, the computing cloud, and the HybriLIT high-performance platform, which includes the "Govorun" supercomputer, ensures the implementation of a whole range of competitive research conducted at the world level at JINR in experiments: MPD, BM@N, ALICE, ATLAS, CMS, NO$\nu$A, BESIII, STAR, COMPASS and others. The MICC includes the Tier-1 grid center which is the only one in the JINR Member States and one of the seven world data storage and processing centers of the CMS experiment (CERN) of such a high level. The JINR Tier-1 and Tier-2 grid centers are elements of the global grid infrastructure used in the WLCG project for processing data from the LHC experiments and other grid applications.

In 2018, employees of the Laboratory of Information Technologies published 251 scientific papers in refereed scientific journals, presented 103 reports at international and Russian conferences.

## JINR INFORMATION AND COMPUTING INFRASTRUCTURE

In 2018, work related to the development and maintenance of the reliable operation of the JINR network and information and computing infrastructure was continued. The main elements of this infrastructure are telecommunication channels, the JINR local area network (LAN), a multifunctional information and computing complex, and basic software including those based on cloud, grid and hybrid technologies combining the Institute information and computing resources into one environment available for all users.

In 2018, works on the creation of new tools to support MICC users' work in terms of developing and simplifying data access, providing users with convenient tools to access their home directories, remote access to shared data storages and software, convenient and unified authentication method and authorization, began. The systems common to all the MICC components, such as CVMFS for organizing access to shared software of user groups, EOS for distributed storage and access to data, were installed and put into operation. The volume of the system based on EOS is 3.74 PB. These systems will be used to store, process, analyze data, simulate the NICA experiments using the MICC resources, and to create a single EOS space at two JINR sites.

**JINR Telecommunication Data Links.** In 2018, reliable operation of the Dubna–Moscow high-speed communication channel was ensured. The external JINR channel was built on the DWDM (Dense Wave Division Multiplexing) technology and used one 100 Gbit/s lambda and two lambdas (two frequencies) of 10 Gbit/s each. According to the development plans, the modernization of the network infrastructure and external communication channels (data link) began. The configured DWDM equipment for the organization of an additional fiber-optic channel Dubna–Moscow with a capacity of 100 Gbit/s was installed at the MMTS-9 site in Moscow which would give a new direct channel to CERN. Thus, the external distributed network of JINR will be represented by the JINR–CERN direct channel (data link) and a backup channel passing through MMTS-9 in Moscow and Amsterdam ensuring the operation of LHCOPN (JINR–CERN) for connection between Tier-0 (CERN) and Tier-1 (JINR) and the external superimposed network LHCONE intended for the JINR Tier-2 center, direct channels for connection using RU-VRF technology with the collaboration of RUHEP research centers and networks Runnet, RASnet.

The distribution of incoming and outgoing traffics over JINR subdivisions in 2018 (exceeding 10 TB by incoming traffic) is presented in the table.

| Subdivision | Incoming, TB | Outgoing, TB |
|---|---|---|
| DLNP | 197.8 | 67.84 |
| VBLHEP | 161.99 | 77.77 |
| LIT | 87.55 | 22.91 |
| FLNP | 76.84 | 39.77 |
| Hotel and Restaurant Complex | 67.72 | 8.11 |
| FLNR | 67.09 | 11.49 |
| Remote access node | 50.01 | 5.21 |
| JINR Directorate | 41.33 | 28.24 |
| BLTP | 29.08 | 7.91 |
| Medical-Sanitary Unit 9 | 19.92 | 1.12 |
| Dubna State University | 17.69 | 20.02 |
| JSC “NPK Dedal” | 16.89 | 1.25 |
| Social Infrastructure Management Office | 11.99 | 1.06 |
| Procurement and Logistics Service | 11.63 | 10.35 |
| LRB | 10.65 | 3.47 |

In 2018, the total incoming traffic of JINR including general-purpose servers, Tier-1, Tier-2 and computing complex amounted to 18.62 PB. Traffic with scientific and educational networks accounting for 96.6% of the total is the main one.

**JINR Local Computing Network.** In 2018, work on the development and improvement of network components of the JINR IT-structure designed to increase its efficiency was continued. A new $4 \times 100$ Gbit/s connection project is being implemented between the DLNP and VBLHEP sites with double redundancy in order to improve the reliability of the optical backbone. The 100 Gbit/s equipment for the optical backbone of the JINR network and the MICC network infrastructure is at the testing and configuration stage. The Internet exchange node IX-GW of the JINR network, the VPN service, and the computing cluster of the network service were modernized. The Institute mail cluster mail.jinr.ru was transferred to the new hardware, new software, and new type of data storage. The basis of this platform is a disk cluster based on CEPH and a virtual cluster based on Proxmox (KVM). At present mail service mail.jinr.ru contains 2621 actual mailboxes. A plugin which would enable working from mobile devices was installed on webmail.jinr.ru. The SSO-login system (single authentication login) simplifying the user access to applications integrated into the system was put into operation. To date, services such as PIN, JINR Document Database, ADB2, SED have been integrated into the SSO system. More than 400 network infrastructure elements, 150 services, 20 000 counters are being continuously monitored. Approximately 48 thousand events indicating attacks on the JINR network were recorded. Each month about 250 notifications are sent to external providers about attacks on the network.

The JINR LAN contains 7629 network elements and 13 897 IP-addresses, 6910 network users, 2465 mail.jinr.ru service users, 1489 electronic library users, and 344 remote access service users.

**JINR Grid Environment.** The JINR grid infrastructure is represented by the Tier-1 center for the CMS experiment at the LHC and the Tier-2 center which supports a whole number of virtual organizations (VO), particularly, ALICE, ATLAS, CMS, LHCb, BES, BIOMED, COMPASS, MPD, NO$\nu$A, STAR and others.

The data processing system at the JINR CMS Tier-1 consists of 332 64-bit machines: $2 \times$ CPU, 6–16 cores/CPU forming altogether 6512 cores for batch processing and provides a performance of 96.43 kHS06. The storage system consists of disk arrays and long-term data storage on tapes and is supported by the dCache-3.2 and Enstore 4.2.2 software. The total usable capacity of disk servers is 8.3 PB, the IBM TS3500 tape robot is 11 PB. The Torque 4.2.10/Maui 3.3.2 software (custom build) is used as a resource manager and task scheduler. The PhEDEx software is used as a tool for management of the CMS data placement. The standard WLCG program stack is used for data processing: $2 \times$ CREAM, $4 \times$ ARGUS, BDII top, BDII site, APEL parsers, APEL publisher, EMI-UI, $220 \times$ EMI-WN + gLExec-wn, $4 \times$ FTS3, LFC, WMS, L&B, glite-proxyrenewal. The service support system provides the operation of a computing service, a data storage service, a grid service, a data transfer service (FTS — File Transfer System), a distributed computing management system (PBS — Portable Batch System), an information service (monitoring of services, servers, storage, data transmission, information sites).

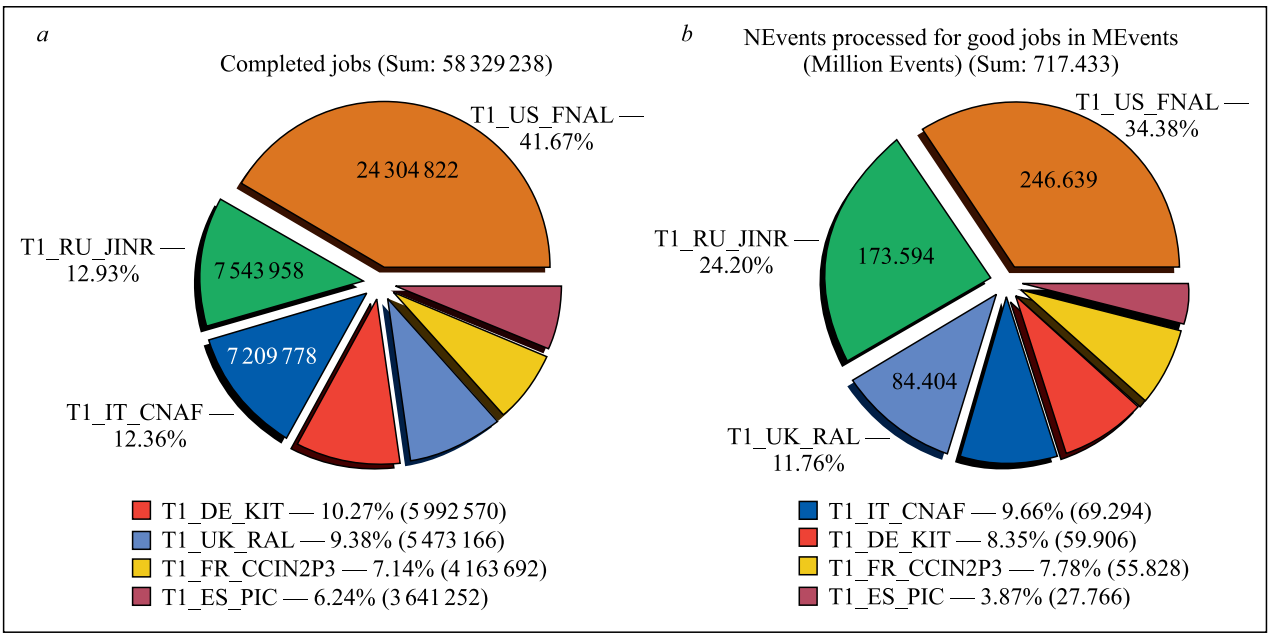


Fig. 1. The number of jobs (*a*) and events (*b*) processed for CMS by Tier-1 centers during 2018

The CMS Tier-1 center at JINR has demonstrated stable work through the entire period since its launch into full operation [1]. In 2018, 7 543 958 tasks were completed, 173 594 million events were processed which accounted for 24.2% of the total number of the CMS experiment events processed by all Tier-1 sites. Figure 1 demonstrates the contribution of the world first-level centers to the processing of CMS experimental data during 2018. The JINR site takes the second place in its performance among world CMS Tier-1 centers.

Figure 2 shows the number of events processed at the JINR CMS Tier-1 center in 2018 by different types of stream processing (reconstruction, modeling, reprocessing, analysis, etc.).

One of the main functions of the Tier-1 centers is to provide data exchange with all global sites operating on the CMS experiment and storage of raw experimental and simulated data. In 2018, the total data exchange with the tape robot was 12.3 PB (5.6 PB of new data). The disk storage was used more actively: the total amount of transferred data was 60.2 PB, of which 19.5 PB of new data. Figure 3 shows the statistics of the JINR CMS Tier-1 data exchange with other grid centers during 2018. The average data transfer rate for the JINR CMS Tier-1 is 400–520 MB/s.

The Tier-2 center at JINR provides data processing for all four experiments at the LHC (ALICE, ATLAS, CMS, LHCb) and apart from that supports a number of virtual organizations (VO) that are not members of the LHC (BES, BIOMED, COMPASS, MPD, NO$\nu$A STAR, ILC). The computing resources of the Tier-2 center consist of 4128 cores. The data storage system is installed in two versions of the software: two dCache

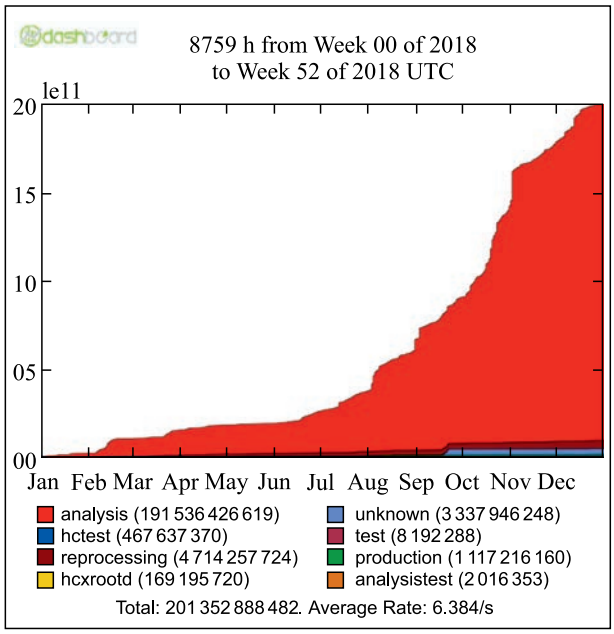


Fig. 2. Distribution of events processed at the JINR CMS Tier-1 center in 2018 by type of processing (reconstruction, simulation, reprocessing, analysis, etc.)

installations and two XROOTD installations. Figure 4 shows data on the use of the JINR Tier-2 site (JINR-LCG2) by VOs in the framework of grid projects in 2018.

**High-Performance Computing System.** The MICC allows users to perform calculations including parallel ones outside the grid environment. It is necessary for experiments such as NO$\nu$A, PANDA, BES, NICA/MPD and others, as well as for local users from

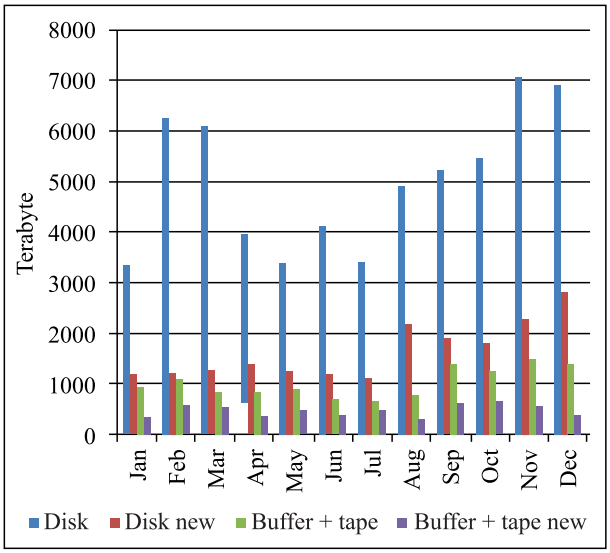


Fig. 3. Statistics of the JINR CMS Tier-1 data exchange with other grid centers during 2018: disk — all exchanges with the disk array (reading and recording); disk new — new data from the total volume (recording); buffer + tape — all exchanges with the tape robot (reading and recording); buffer + tape new — new data from the total volume transferred to the tape robot (recording)

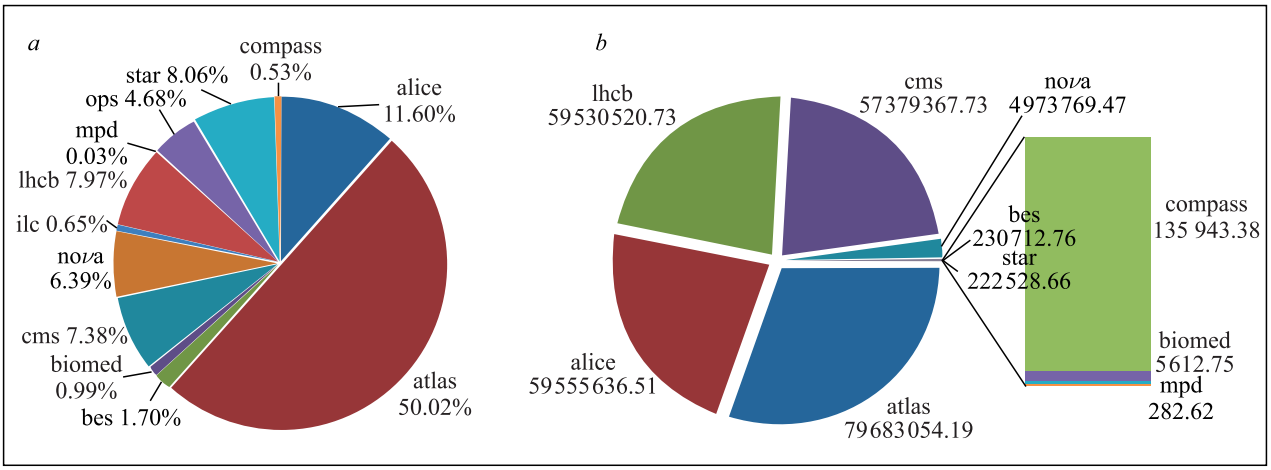


Fig. 4. The use of the JINR-LCG2 grid site at JINR by the virtual organizations of the global grid infrastructures: *a*) distribution by the number of jobs; *b*) distribution by the normalized CPU time in HS06 hours

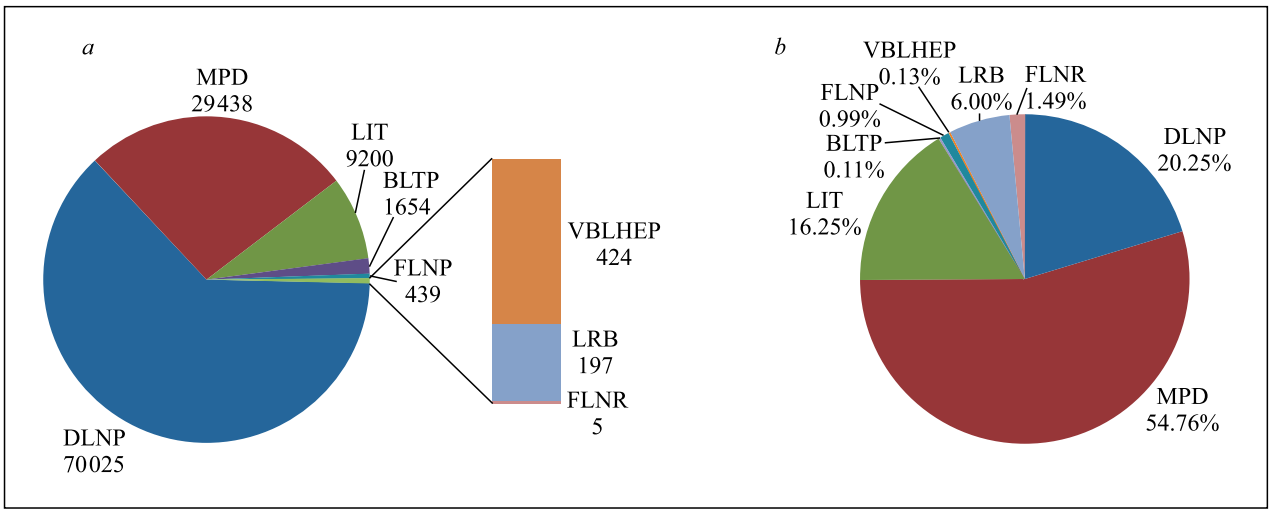


Fig. 5. Statistics of the use of the computing cluster by the JINR subdivisions and experiments without taking into account the users of the grid environment: *a*) distribution by the number of jobs; *b*) distribution by the normalized CPU time in HS06 hours

the JINR Laboratories. All computing resources are available to JINR users and users of the grid environment through a single system of batch processing of jobs. Figure 5 shows the time distribution of jobs performed on the computing cluster by the JINR Laboratories and user groups.

**Cloud Environment.** JINR takes part in a large number of research projects, in many of which computing resources are an important means for obtaining significant scientific results. In this connection the integration of the computing resources of the Institute Member States into a united information and computing environment is an important and urgent task, the solution of which would significantly speed up the research process. For effective use of local computing resources cloud infrastructures were or are being created in each of the organizations participating in their unification. In 2018, work on integrating the clouds of each of the partner organizations of the JINR Member States into a distributed platform based on the DIRAC software (Distributed Infrastructure with Remote Agent Control) was carried out [2]. Clouds of organizations integrated into the JINR distributed information and computing environment are shown in Fig. 6.

In 2018, the JINR cloud infrastructure resources were increased from 728 CPU cores and 3 TB of total RAM to 1572 CPU cores and 8 TB of total RAM. The main users of cloud infrastructure are DLNP, LIT and the NO$\nu$A experiment.

A service has been developed that provided JINR cloud users with the opportunity to gain access to computing resources through a problem-oriented web interface adapted to form a computing job using a specific application package or a set of them for work in a narrow area of research. The user of this service should only input the values for the parameters of his job and the address for downloading the results in the web interface [3]. The entire computing part will be performed on virtual machines (VM) of the JINR cloud infrastructure. The scheme and interrelations of the service components are presented in Fig. 7.

A method of increasing the efficiency of using cloud resources was developed [4], which was based on the idea of dynamic redistribution of VMs on physical equipment. A two-rank strategy of VM distribution through cloud infrastructure nodes was implemented, that would allow minimizing the amount of idle resources of cloud infrastructure and the impact of congestion at the same time.

**Heterogeneous Infrastructure.** In 2018, the JINR MICC was replenished with a new high-performance component — the "Govorun" supercomputer [5]. It is a natural development of the HybriLIT heterogeneous platform and has led to a significant increase in the performance of both the CPU and GPU components of the platform. The supercomputer GPU component includes 5 NVIDIA DGX-1 servers. Each server has 8 GPU NVIDIA Tesla V100 based on the latest NVIDIA Volta architecture. In addition, one NVIDIA DGX-1 server has 40 960 CUDA cores which are equivalent to 800 high-performance CPUs in their computing power. DGX-1 uses a whole number of new technologies including NVLink 2.0 bus with a capacity of up to 300 Gbit/s.

The new supercomputer includes a high-density and energy-efficient solution "RSC Tornado" with direct liquid cooling developed by specialists of the Russian group of RSC companies. New universal computing cabinets "RSC Tornado" with a record energy density and a system of precision liquid cooling balanced for

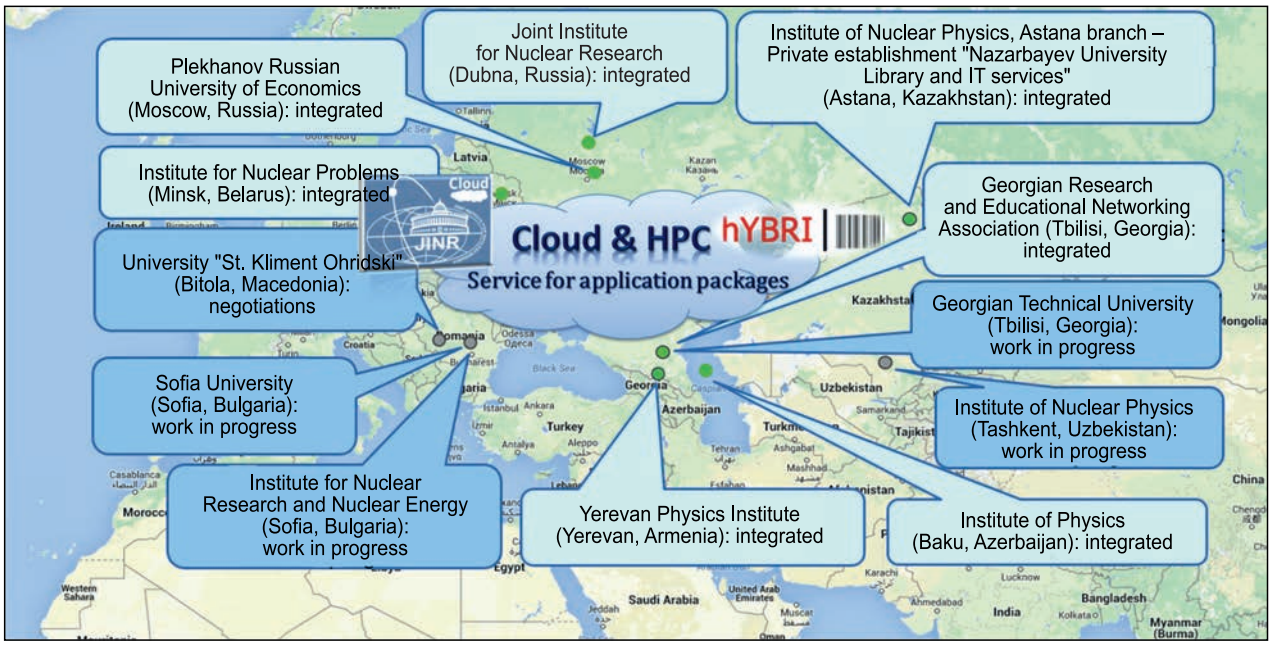


Fig. 6. Clouds of organizations integrated into the JINR distributed information and computing environment

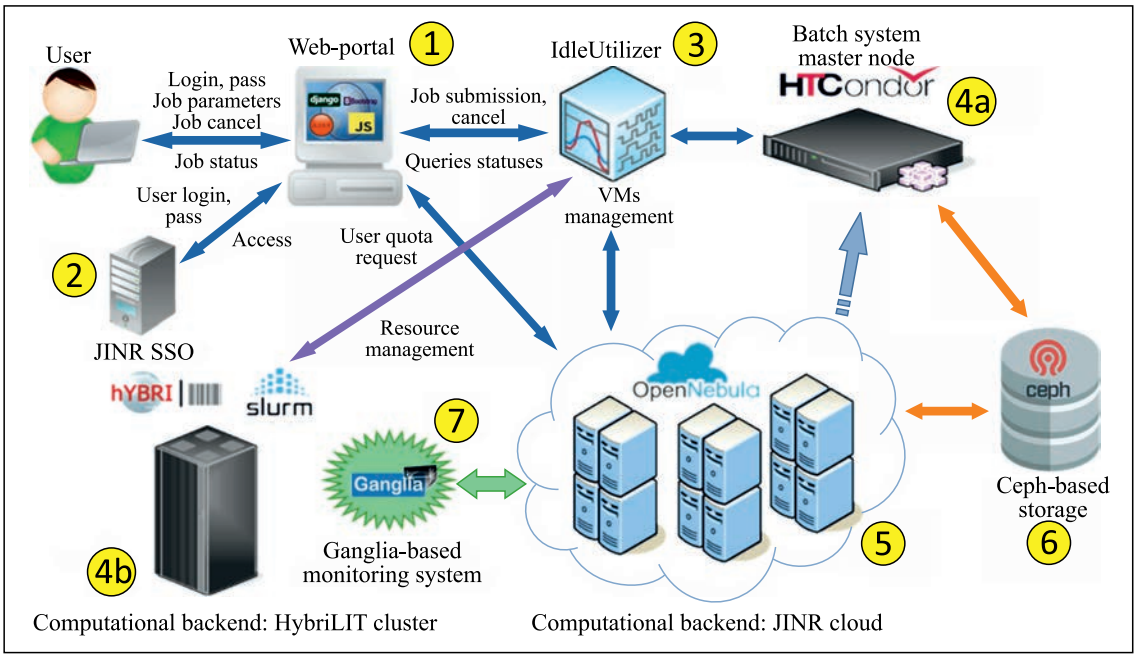


Fig. 7. The scheme of the service for providing users with access to computing resources through a problem-oriented web interface

constant work with a high-temperature coolant (up to $+63\,^{\circ}\mathrm{C}$ at the entrance to the computer cabinet) were installed at LIT. The work in the "hot water" mode for the given solution allowed one to apply the year-round free-cooling mode ($24 \times 7 \times 365$) using only dry-cooling towers operating at an ambient temperature of up to $+50\,^{\circ}\mathrm{C}$ and also completely get rid of the freon circuit and chillers. As a result, the average annual PUE of the system reflecting the level of energy efficiency is less than 1.03. Thus, cooling consumes less than 3% of all consumed electricity which is an outstanding result for the HPC industry.

The computing nodes were based on Intel server products: the most powerful 72-core server processors Intel® XeonPhi™7290, processors of Intel® Xeon® Scalable (models Intel® Xeon® Gold 6154 and the latest high-speed solid-state disks Intel® SSD DC P4511 with NVMe interface and a capacity of 1 TB). For high-speed data transfer between computing nodes, the supercomputer uses an advanced switching technology Intel® Omni-Path providing the speed of non-blocking switching up to 100 Gbit/s based on 48-port switches Intel® Omni-Path Edge Switch 100 Series with 100% liquid cooling that ensures a high efficiency of the cooling system in the "hot water" mode and the lowest total cost of ownership of the system. The use of Intel® Omni-Path Architecture allows not only matching the current needs of resource-intensive user applications but also providing the necessary network bandwidth for the future.

Peak supercomputer performance is 1 PFlops for single-precision operations and 500 TFlops for double-precision operations.

At present, the supercomputer is used to solve problems that require massively parallel calculations in various fields of nuclear physics and high energy physics, particularly, in lattice quantum chromodynamics to study the properties of hadronic matter at high-energy density and baryon charge and in the presence of supramaximal electromagnetic fields. It is also applied for mathematical modeling of interactions of antiprotons with protons and nuclei using DPM, FTF and UrQMD + SMM generators developed at JINR and being of interest for the NICA/MPD experiment, for modeling the dynamics of collisions of relativistic heavy ions, as well as for solving applied problems such as calculating Josephson junctions, modeling the dynamics of many-particle Boson systems in magnetic optical traps, calculating corrections for the matrix element in the first Born approximation in case of a direct ionization of a helium atom by a fast proton taking into account different models of the final state and others.

The average load on computing components is the following: the component based on Intel® Xeon® Scalable is 80.58% (maximum 89%); the component based on Intel® XeonPhi™ is 38.41% (maximum 74%); the component with GPU computing accelerators is 73.58% (maximum 100%). In total, over the period of operation all the groups performing calculations on the supercomputer completed over 66 000 tasks on all computing components.

**Monitoring System.** To ensure reliable operability of the MICC in the 24/7 mode, it is extremely important to monitor all components at three levels: hardware, network and service. Different components of

the MICC require a different approach to monitoring, and one can hardly find a single monitoring system capable of satisfying all the requirements and at the same time remaining flexible for changes. A multilevel monitoring system of the MICC was created, and at present it is being expanded using different technologies such as Nagios, Icinga2, Grafana as well as systems developed at LIT. Grafana as a visualization tool is currently used only in the JINR computing cloud, but can be accepted for other components. The monitoring of the Tier-1 services, monitoring of the HybriLIT heterogeneous cluster and the "Govorun" supercomputer were specially developed at LIT.

In 2018, work on refining the software package for modeling distributed data storage and processing systems (SyMSim) with the aim of using it to improve the topology of the computer network and the performance of the data center of the Institute of High Energy Physics of the Chinese Academy of Sciences was carried out. Parameters from the database of the computing infrastructure of the Institute as well as some data from the BESIII experiment were used as input data for simulation. The first simulation results showed that the proposed approach allowed making an optimal choice of the network topology increasing its performance and saving resources [6].

In the framework of the creation of a system for storing and processing data from the BM@N and MPD experiments included in the NICA complex, a new macro-modeling scheme was developed and implemented. This program uses a probabilistic approach to assess various equipment configurations which would determine the probabilities of loss of information arriving from the detectors for each of these configurations. This probability would not exceed the specified limit and the price would be minimal, selected taking into account economic factors. The program was tested on the calculations of the efficiency of the data acquisition and storage system of the BM@N experiment from price investments in the system of the disk memory of the intermediate data storage [7].

A set of interconnected cloud services and tools for managing and processing data of biomonitoring were developed; these tools allow one to simplify and automate the stages of monitoring starting from selecting sites for collecting samples and ending with generating maps of pollution distribution and predicting environmental changes. This is the first solution in Russia and Europe that allows all specialists involved in the biological monitoring network to get access to the data on environmental pollution. In 2018, the development of the architecture and technologies of the portal moss.jinr.ru was continued (Fig. 8). The ability to compare the concentrations of heavy metals in samples of different years in the form of diagrams as well as statistical calculations was added. The module for comparison of concentrations in countries and regions was optimized. The module for calculating geo-indexes was improved — now it is possible to set the level of background pollution. The possibility of creating pollution maps by users of the platform was expanded and the ability to import data into Google Earth was added. Maps and statistical calculations for the atlas 2015–2016 were formed. An alpha-version of a mobile application for

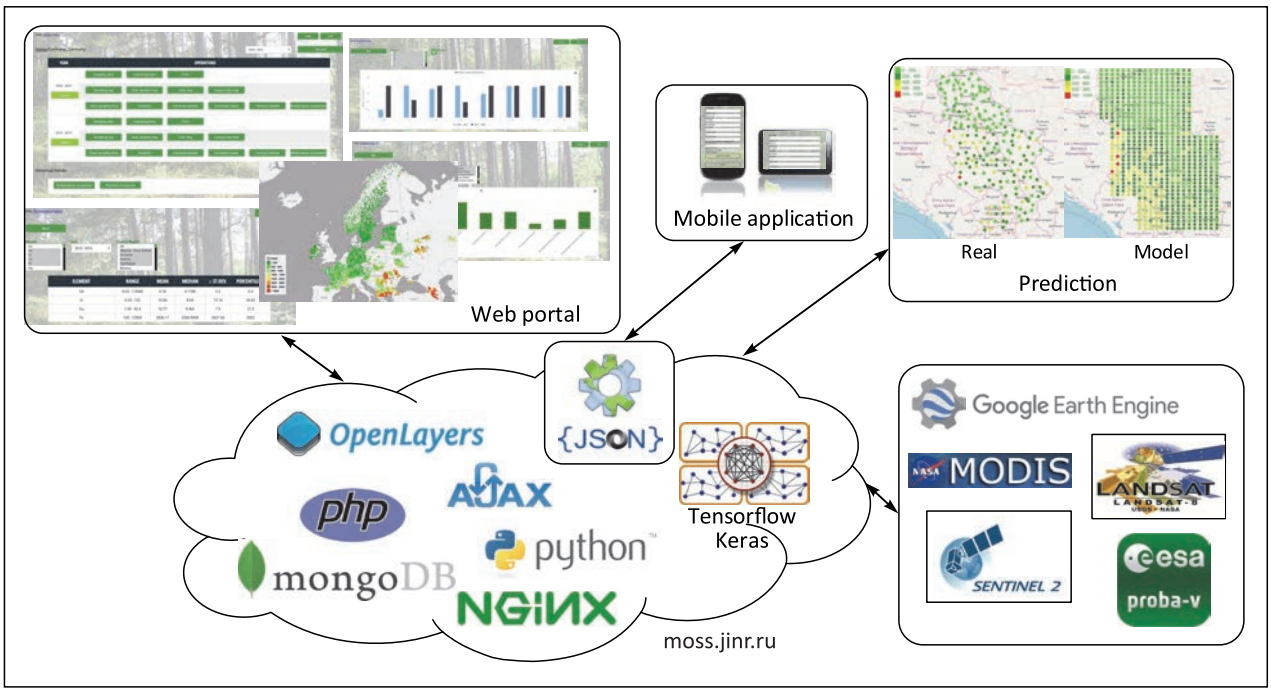


Fig. 8. Architecture and technologies of the portal moss.jinr.ru

registering data on sampling sites and uploading them to the platform was developed. The application will reduce the number of errors when filling out forms and provide the potential to verify the correctness of the definition of moss type by the participants through the use of machine learning methods.

In the framework of the project with RFBR, methods and tools for using high-performance computing infrastructures and software applications for processing textual and graphical information about plant diseases to minimize losses in agriculture were developed [8]. A platform architecture (Fig. 9) for identifying plant diseases using modern software and organizational technologies was proposed. A web site of the project (http://pdd.jinr.ru/) was implemented. A special model of a deep convolutional network with a Siamese architecture allowing one to evade the problem of a small sample was developed. The recognition accuracy on the test sample of images was more than 95%.

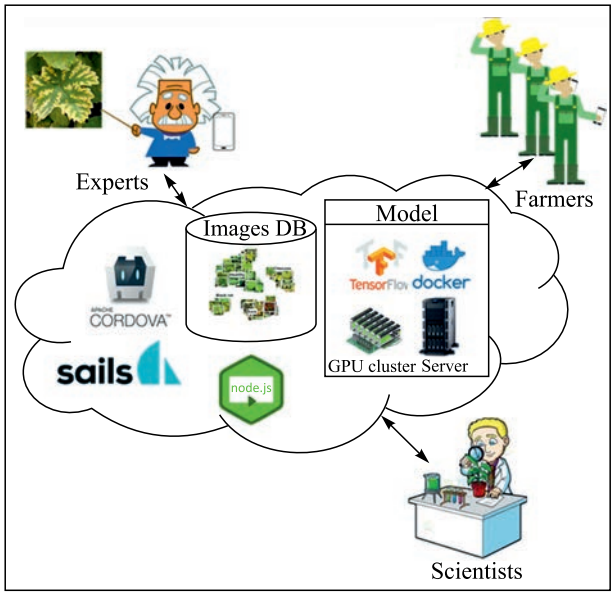


Fig. 9. Platform architecture

Works on the further development of the APT EVM project management system for NICA were completed: a consolidated report "NICA — Disbursement of Funds" with the possibility of detailing was developed. It would allow quickly controlling the information on project financing as well as forecasting expenses for the current year based on expert estimation. A module for accounting payments under contracts was developed, other current works for forming references and reports were completed, the system was maintained.

As part of the task for the further development of "1C Manufacturing Enterprise Management", a module for the purchase of computer equipment was created. The module for forming regulated reports of self-supporting units was improved. In the first half of 2018, the programs "1C: ERP Enterprise Management 2" and "1C: SPM Salary and Personnel Management" were purchased, now they are being set up, and employees of the 1C group are being trained to use the given products. On the basis of the program "1C: Retail" cash registers were launched at the "Nauka" stadium and the Athlete's House.

In the framework of the development of the "Dubna" electronic document system (EDS), ten new documents were developed and put into operation and eight were prepared for commissioning. Three specialized reports on monitoring the status and timing of documents' passage in the system were developed (Fig. 10). A version of the "Dubna" EDS adapted for mobile devices was developed and put into operation. The following works on the improvement of the system part of the "Dubna" EDS were carried out: user authentication through the JINR SSO unified authentication system was implemented and put into operation; complete refactoring of the means of assigning and verifying user access rights to documents for more flexible management of access rights was carried out; tools for automating the creation of a new type of document, its form and patterns of agreement routes were developed. When developing the "Dubna" EDS, open technologies and software, such as Java Servlet, Apache Tomcat, WALT, MySQL, JQuery, Linux, were used. Rapid and effective development of the system was achieved because of the use of the Agile software development principles.

The development of the JINR Document Server information services is being carried out under the JOIN2 project (Just anOther INvenio INstance) aimed at bringing together the partner organizations for the development of the Invenio software platform taking into account their specifics. The project partners are libraries of research centers and universities in Germany. To date, a collection of authoritative records of the Organization, Division and Personnel was deployed on the test server jds-join2. Data for forming a directory of grants with the participation of JINR were collected. Web forms with extended functionality were introduced into the data entry module which would allow automatic metadata import into publications from external bibliographic databases by a number of identifiers such as DOI, arXiv, InsWoS.

In 2018, the state registration certificate of the computer program "Software Complex of Intellectual Scheduling and Adaptive Self-Organization of Virtual Computing Resources" was received. N. A. Balashov, A. V. Baranov, I. S. Kadochnikov, V. V. Korenkov, N. A. Kutovsky, I. S. Pelevanyuk are the authors. The software complex is designed to optimize the consumption of computing resources in cloud infrastructures and can be used by cloud providers in infrastructures built on the IaaS model on the OpenNebula platform. The complex includes the VM strategy of planning based on VM and server rankings, API for interacting with the

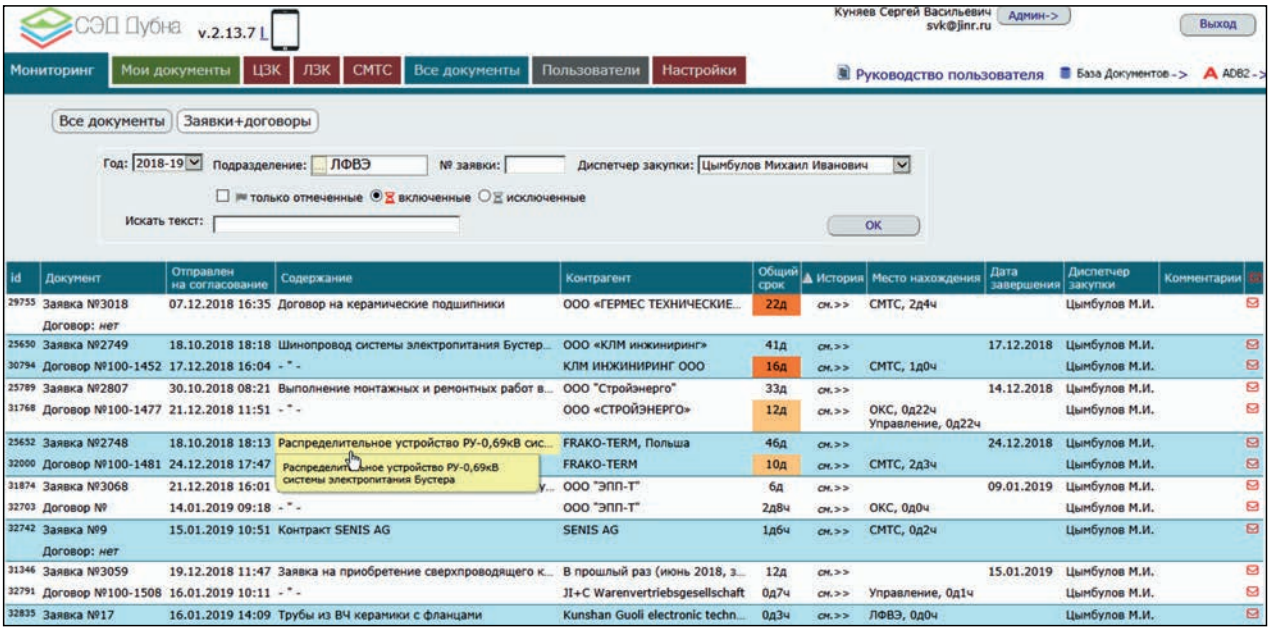


Fig. 10. Specialized report of monitoring the status of purchase requisitions and supply contracts

OpenNebula platform, an administrative web interface, net-snmp extensions and corresponding polling modules for Icinga 2 which allow collecting information on the current use of VM resources based on KVM as well as OpenVZ containers.

Traditional work on the maintenance and development of the JINRLIB program library continued. The library included the DFM-POTM/DFM-POTM_MPI software package which implemented the construction of a nucleus–nucleus optical potential of elastic scattering based on the double folding model and included the DFM-POTM sequential version and the DFM-POTM_MPI parallel version written in C++ and developed with the use of MPI technology (authors are K. V. Lukyanov, E. V. Zemlyanaya, M. V. Bashashin; http://wwwfofo.jinr.ru/programs/jinrlib/dfm-potm/index.html).

In 2018, works on maintenance and development of the functionality of the services rendered to the users of the "Visit Center" portal providing online support for the implementation of the JINR visitors reception process (https://visitcentre.jinr.ru/) and the modernization of the JINR journals' web portal "Physics of Elementary Particles and Atomic Nuclei" (PEPAN) and "Letters to PEPAN" (http://pepan.jinr.ru/) were carried out. Traditionally the development, creation and maintenance of websites of conferences, symposia at the request of Laboratories and other JINR departments were carried out (ECPM-2018, http://ecpm2018.jinr.ru; EXON-2018, http://exon2018.jinr.ru). Hosting with the transfer of all the information of past conferences (from 2006 to 2017) to create the site of the international conference "Mathematical Modeling and Computational Physics" (MMCP-2019) (http://mmcp.jinr.ru) was organized.

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

One of the main activities of LIT is to provide mathematical, algorithmic and software support for experimental and theoretical studies conducted at JINR. Below there is a breif report on some results.

Two different algorithms based on deep neural networks for the reconstruction of elementary particle tracks in the processing of experimental information from the GEM tracking detector in the BM@N experiment at the NICA collider were developed and implemented. The first algorithm using deep recurrent networks showed an efficiency of 98% on the carbon–carbon collisions modeled by the Geant4 program. The second algorithm based on the original generalization of the convolutional neural network showed high efficiency and speed of work on model events without a magnetic field [9].

New probabilities of the birth of strange quark–antiquark and diquark–antiquark pairs were proposed

and introduced into the FTF model of the Geant4 package. A good agreement between calculations using the improved version of the FTF model and experimental data from the NA61/SHINE collaboration on the production of $K$-mesons, antiprotons and Lambda-hyperons into proton–proton, proton–carbon and pi-meson–carbon interactions at different initial energies was obtained. In the framework of the improved FTF model, the kinematic characteristics of Lambda-hyperons and $K$-mesons produced in antiproton–proton interactions were calculated and compared with experimental data at different momentum values of incident antiprotons. A good agreement between experimental data and calculations using the FTF model with new probabilities and rotating quark–gluon strings was achieved. The applicability of the FTF model for the development of the physical program of the Panda Phase0 and Panda Phase1 experiments was shown [10].

The reactions $p$, $d$, He, C + C, Ta, and C + Ne, Cu at momentum of 4.2, 4.5, and 10 GeV/s per nucleon were modeled using the UrQMD model supplemented by the Statistical Multifragmentation Model (SMM). Azimuthal correlations of pions and protons produced in the listed reactions were calculated and compared with the experimental data obtained at VBLHEP on the SKM-200-GIBS and Propane Bubble Chamber installations. A good agreement between calculations using UrQMD + SMM and experimental data was achieved [11].

For the NICA/SPD experiment elastic $pp$ and $\bar{p}p$ interactions were simulated in the scope of a unified systematization of experimental data (USESD) in a wide range of initial energies from 100 MeV to several TeV. Inelastic proton–proton interactions were simulated using FTF at different incident proton energies, and the applicability of the USESD and FTF models for the NICA/SPD experiment was justified [12].

The method of separated form factors (SFF) is an effective method for studying the structure of polydisperse systems of phospholipid vesicles based on the analysis of small-angle scattering data. In this approach the basic parameters of the vesicular system are determined by minimizing the discrepancy between the experimental data of the small-angle scattering intensity and the results of SFF calculations. The minimization procedure is based on the generalized method of the least squares implemented in the FUMILI program of the JINRLIB library. The efficiency of parallel implementation was tested on the HybriLIT cluster using the parallel MPI version of this program — PFUMILI. It was shown that the acceleration of calculations was 6–9 times depending on the number of experimental points. The assessment of the structural parameters of the vesicles of the phospholipid transport system was made on the basis of the numerical analysis of small-angle neutron scattering data obtained on the YuMO small-angle spectrometer at the Frank Laboratory of Neutron Physics [13].

Based on the hybrid model of a microscopic optical potential using three models of $^{12,14}$Be nuclei density, calculations of the observed physical characteristics of the scattering of these nuclei during the interaction of these nuclei with a carbon and proton target were carried out. A good agreement with the experimental data on the scattering of $^{12,14}\mathrm{Be} + p$ at an energy of 700 MeV was obtained. It was shown that adequate reproduction of the differential scattering cross sections of $^{12,14}\mathrm{Be} + ^{12}\mathrm{C}$ at an energy of 56 MeV/nucleon required consideration of the contribution of inelastic channels. The momentum distributions of $^{8}$B breakup fragments in the reactions of this nucleus with other nuclei and the total cross sections for the reactions of $^{6}$He and $^{8,9}$Li with other nuclei in a wide range of atomic masses and energies were calculated on the basis of the microscopic approach [14].

A parallel version of the program for calculating the nucleus–nucleus potential of double folding based on the OpenMP technology was developed. The calculations performed on the HybriLIT cluster confirm the efficiency of the developed parallel program comparable to the previously developed MPI implementation [15].

The stability of solutions of the third family for hybrid compact stars with a quark core corresponding to the emergence of high-mass twins with respect to the softening of the phase transition using a design imitating the effects of "pasta" structures in the mixed phase was investigated. A parameterized class of hybrid models of the equation of state based on the relativistic mean-field model was considered for both hadronic and quark phases of matter. The effect of the construction of phase transition with a mixed phase consists in the appearance of additional pressure near the critical point belonging to the coexistence of the hadronic and quark phases of matter. The value of the relative additional pressure of about 6%, at which the solution corresponding to the third family of compact stars disappeared, was found. It was shown that at least the heavier star from the registered merger of a pair of neutron stars GW170817 could be a member of the third family of hybrid stars [16].

Within the framework of the continuous atomistic model which consisted of a combination of the thermal peak model and the molecular dynamics method, an approach was developed on the basis of which processes in a nickel target were irradiated with uranium ions of a 700-MeV energy. To solve the equations of the continuous-atomistic model, a software package was developed, the calculations were carried out on the HybriLIT heterogeneous platform [17].

A new method for constructing fully symmetric multidimensional Gaussian quadratures on a simplex was developed. The main idea of the method is to replace the coordinates of nodes with their symmetric combinations obtained by the Vieta theorem, which simplifies the system of nonlinear algebraic equations. The construction of the required systems of equations is performed analytically using the original author's

algorithm implemented in the Maple system. Up to the sixth order the given systems are solved using the built-in Polynomial System procedure that implements the Gröbner basis technique, while the systems of higher order are solved using the developed symbolic-numerical algorithm based on numerical methods for solving a system of nonlinear algebraic equations implemented in the Maple–Fortran environment. The obtained quadrature formulas are used to solve self-adjoint elliptic boundary-value problems in the $d$-dimensional polyhedral finite region by the finite element method of high order of accuracy [18].

The problem of describing an $N$-level quantum system in terms of quasiprobability distributions was considered. The classification of the Wigner quasiprobability distributions on the phase space realized in the form of a symplectic flag manifold was studied. The Wigner quasiprobability distribution is constructed in the form of a dual convolution of the density matrix and the Stratonovich–Weyl kernels [19]. It was shown that the moduli space of the Stratonovich–Weyl nucleus was given by the intersection of the orbit space of the connected action of the $SU(N)$ group and a single $(N-2)$-dimensional sphere. The general approach is illustrated by a detailed description of the module space of 2-, 3-, and 4-dimensional systems.

A new algorithm for decomposing the irreducible components of the permutation representations of finite groups over zero characteristic fields was proposed. The algorithm is based on the fact that the components of an invariant scalar product in invariant subspaces are projection operators into these subspaces which makes it possible to reduce the problem to solving systems of quadratic equations. In the zero characteristic the proposed algorithm significantly exceeds the most well-known algorithm in the computing group theory called MeatAxe. The current implementation of the algorithm allows splitting representations of dimensions to hundreds of thousands [20].

The TDDS software package (Thomas Decomposition of Differential Systems) in the Maple symbolic computation language intended for algebraic analysis of systems of nonlinear partial differential equations is included in the Computer Physics Communications program library and the latest version of Maple (Maple 2018) [21].

A Bayesian automatic adaptive quadrature solution for numerical integration was proposed which took into account three main factors: refining the automatic adaptive m-panel scheme by using quadrature sums adapted to the scales of the length of the integration domain; quick assessment of the problem complexity; the use of a weaker accuracy of the two possible ones (specifications of input accuracy and internal properties of the integral function). Consideration of the above factors allows one to achieve the highest possible accuracy of the solution with the minimum possible computation time [22].

## APPLIED RESEARCH

In the course of research conducted together with FLNP in the framework of the international program on monitoring and forecasting air pollution in Europe and Asia (UNECE International Cooperative Program (ICP) Vegetation), a cloud platform was developed in the JINR cloud service for managing monitoring data. To ensure reliable storage, analysis, processing and collective use of monitoring data, modern methods of program management, statistics and machine learning were used, which also allowed using satellite imagery data to predict air pollution with heavy metals in some European regions. With the help of the developed models, the air pollution by Sb in Norway and by Mn in Serbia was successfully predicted [23]. At present the system contains information on more than 6000 sampling sites in 40 regions of various countries in Europe and Asia.

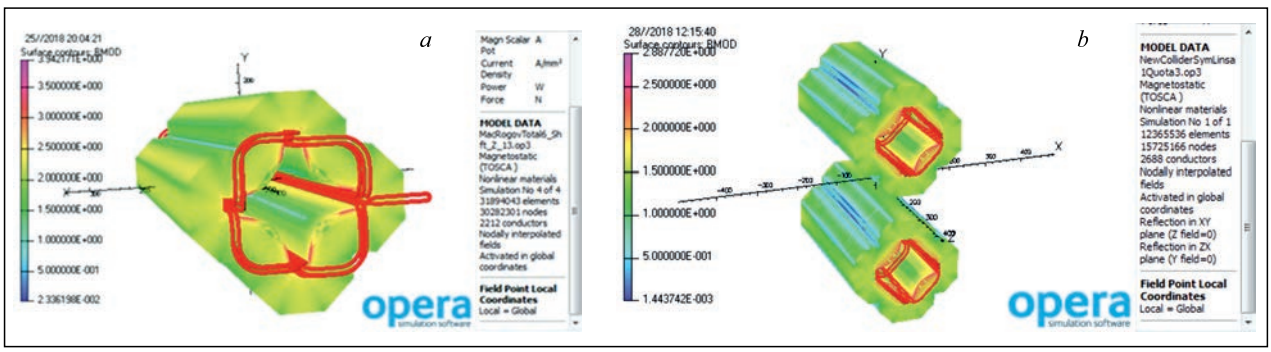


Fig. 11. *a*) 3D model of quadrupole magnet of the SIS100 (FAIR, GSI); *b*) 3D model of quadrupole magnet of the NICA collider

The method of volume integral equations of magnetostatics with a linear approximation of magnetization was applied for three-dimensional modeling of the magnet system of the CBM experiment (FAIR, GSI, Darmstadt) and the quadrupole magnet of the NICA collider. This method allows narrowing the solution of the problem of finding unknowns to the region filled with magnetic material. During simulation the symmetry of the magnetic field, which reduced the number of unknowns by eight times in the case of the SIS100 magnet of the CBM experiment and by sixteen times for the quadrupole magnet of the NICA collider, was taken into account. The influence of the deviation of magnet parameters on the quality of the field distribution in the working area of the magnet was also studied. The simulation results are presented in Fig. 11 [24].

The method of medium-term forecasting of daily passenger traffic volumes in the Moscow Metro was developed. It includes three prediction options: 1) based on artificial neural networks (ANN); 2) using a singular-spectral analysis implemented in the "Gusenica"-SSA package; 3) when using both ANN and the "Gusenica"-SSA approach. The developed methods and algorithms allow the medium-term forecasting of passenger traffic in the Moscow Metro with acceptable accuracy [25].

## INTERNATIONAL COOPERATION

In collaboration with colleagues from Bulgaria, Slovakia and Japan, a numerical analysis of the phase dynamics of the stack of long Josephson junctions was carried out taking into account inductive and capacitive coupling between neighboring Josephson junctions. The influence of the model parameters on the structure of the current–voltage characteristic, the radiation power and the dynamics of the fluxons in individual Josephson junctions inside the stack was studied. The coexistence of a charge traveling wave with fluxon states was demonstrated. The given state can be considered as a new collective excitation in the system of coupled Josephson junctions. It was shown that the observed collective excitation led to a decrease in the radiation power from the system [26].

In collaboration with University of Prešov, Slovakia, algorithms and software for the numerical simulation of the interaction of water and porous materials were developed and implemented. The relevance of these studies is due to the fact that the physical characteristics of porous materials significantly depend on water saturation and affect the strength, protective and other properties of these materials. One of the most common types of pores in natural and artificial building materials are the so-called blind half-closed pores, or pores of the bag type. A three-dimensional model of this type of pores was developed. This model was used to simulate the interaction of water vapor and individual pores using a hybrid method that combined the molecular dynamics method and the method based on the use of the diffusion equation. Special studies to determine the dependences between different implementations of thermostats and the preservation of thermodynamic and statistical characteristics of the water vapor – pore system were carried out. Two types of evolution of the water vapor – pore system, pore drying and wetting, were investigated. A complete study of the properties of the diffusion coefficient, diffusion velocity, and other diffusion parameters of the water vapor – pore system was also carried out [27].

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