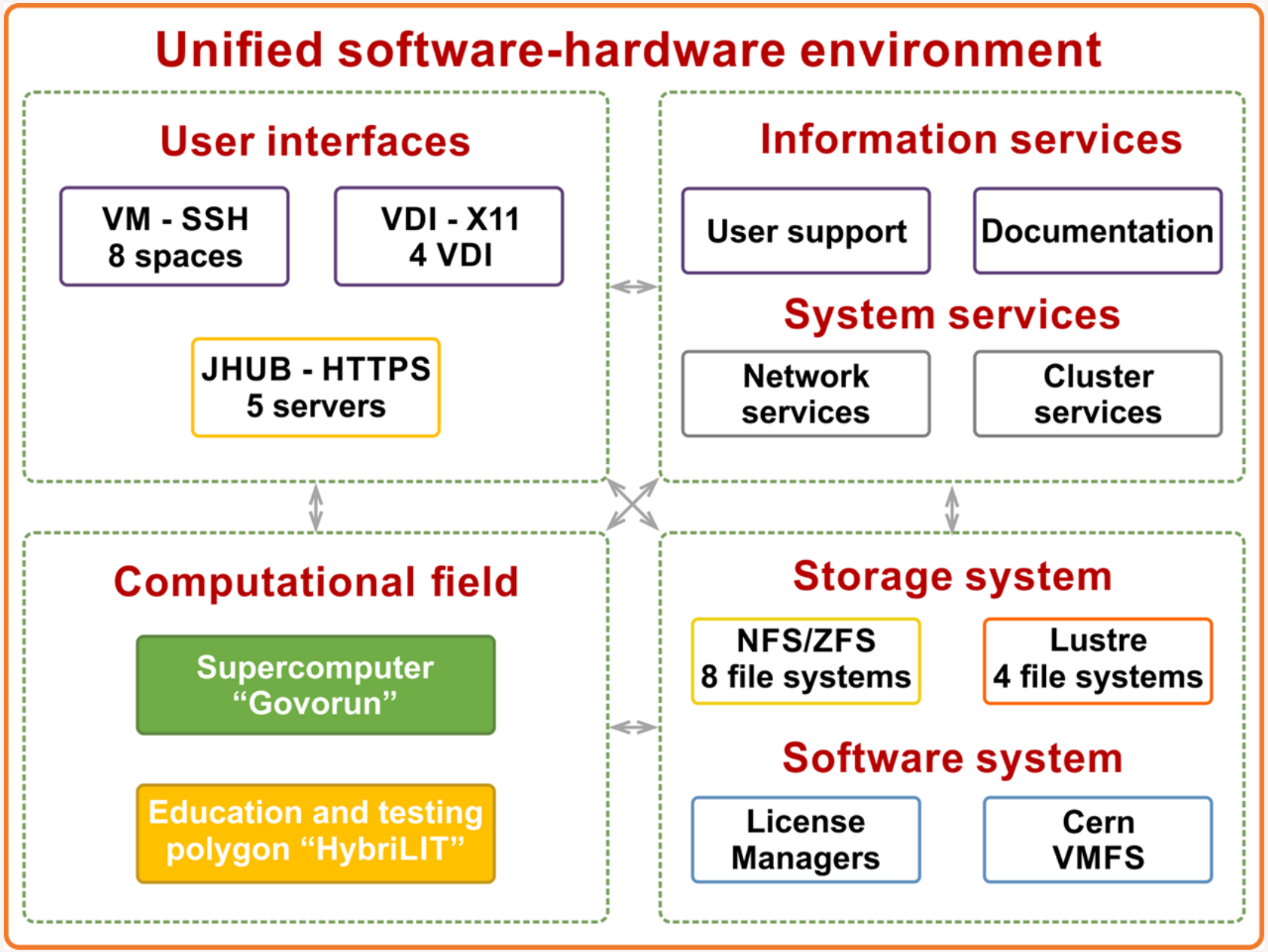
The Govorun supercomputer for JINR tasks

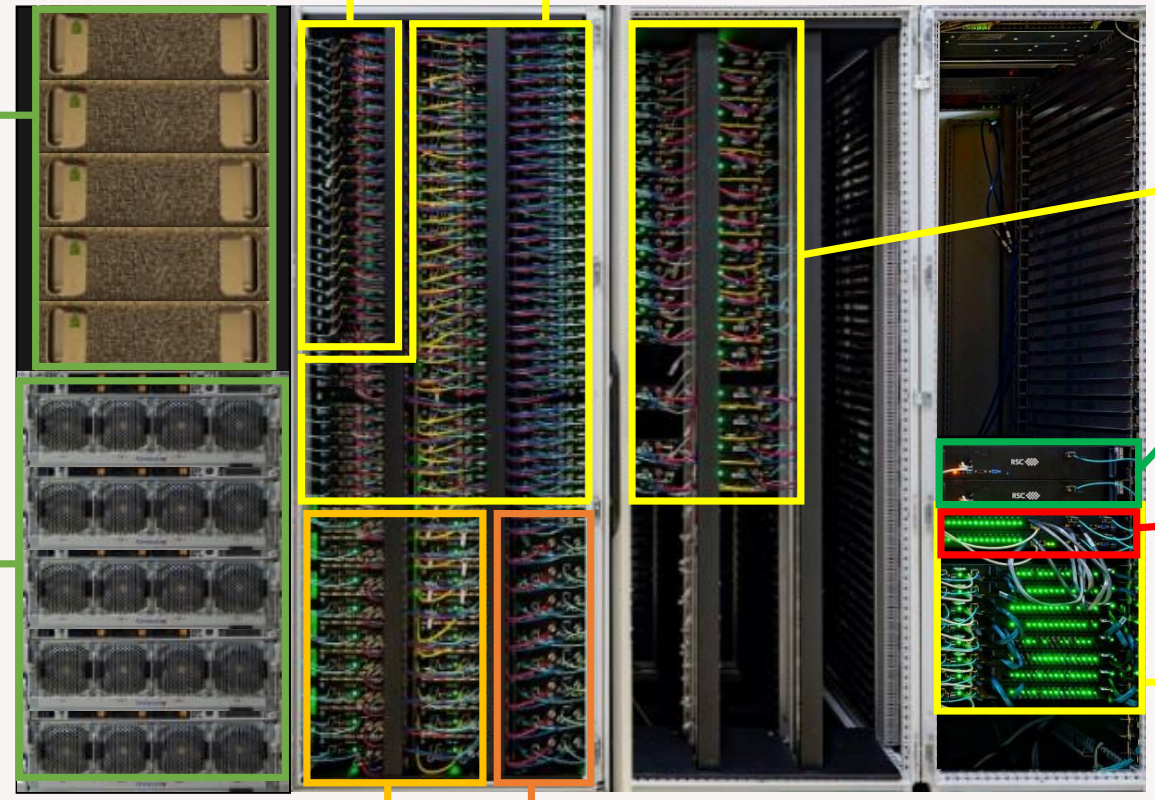
Zuev M.I. on behalf of a HybriLIT heterogeneous group

HybriLIT WORKSHOP 2025: Towards Efficient Scientific Computing
25-26 November 2025

Heterogeneous platform “HybriLIT”



The Govorun supercomputer. The current status



RSC Tornado nodes based on Intel Xeon Phi:
Intel Xeon Phi 7190 processors (72 cores)
Intel Server Board S7200AP
Intel SSD DC S3520 (SATA, M.2)
96GB DDR4 2400 GHz RAM
Intel Omni-Path 100 Gb/s adapter

21

80

RSC Tornado nodes based on Intel Xeon Scalable gen 3 (TDN511):
Intel Xeon Platinum 8268 processors (24 cores)
Intel Server Board S2600BP
Intel SSD DC S4510(SATA, M.2),
2x Intel SSD DC P4511 (NVMe, M.2) 2TB
192GB DDR4 2933 GHz RAM
Intel Omni-Path 100 Gb/s adapter

40

NVIDIA V100

32

16

NVIDIA H100

2x New servers +544 TF

40

NVIDIA A100

2x New servers +2 PB

10

Total capacity of Hierarchical Storage: 10.6 PB

Data IO rate: 300 Gb/s

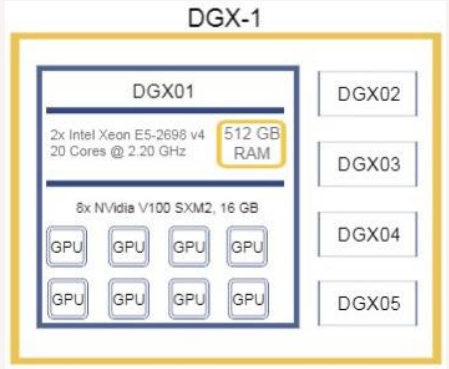
14

8

RSC Tornado nodes based on Intel Xeon Scalable gen 2 (TDN511S):
Intel Xeon Platinum 8280 processors (28 cores)
Intel Server Board S2600BP
Intel SSD DC S4510(SATA, M.2),
2x Intel SSD DC P4511 (NVMe, M.2) 2TB / 4x Intel (PMem) 450 GB
192GB DDR4 2933 GHz RAM
Intel Omni-Path 100 Gb/s adapter

The GPU-component of the Govorun supercomputer

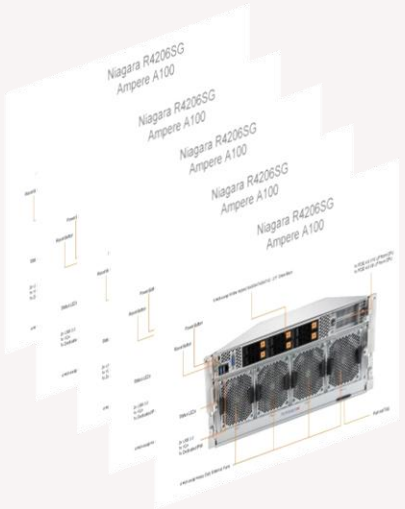
2017

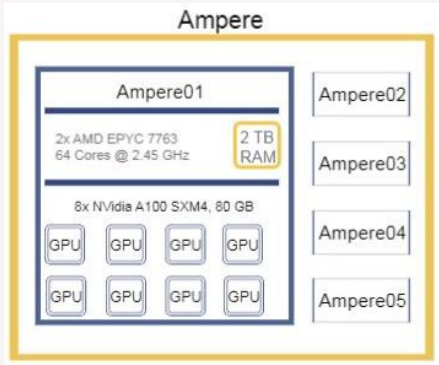


40 NVIDIA V100

+

2023





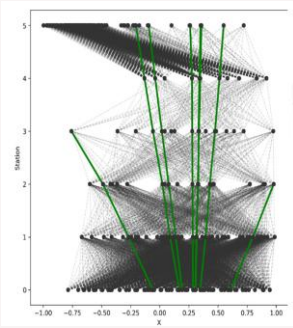
40 NVIDIA A100

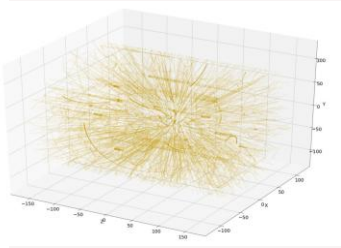
+

2025

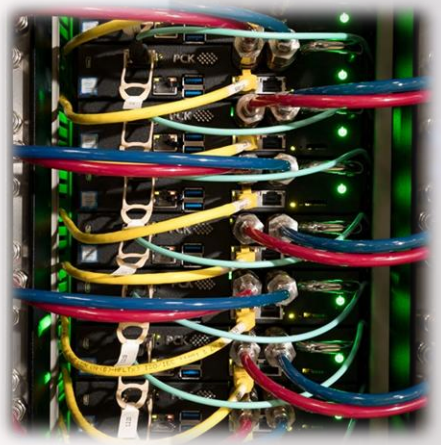
16 NVIDIA H100

The GPU-component gives a users of the supercomputer a possibility to use machine learning and deep learning algorithms for solving applied problems by neural network approach: process data from experiments at LRB in the frame of the Information System for radiation biology tasks; experimental data processing and analysis at the NICA accelerator complex and etc.





The Govorun supercomputer



CPU component

- **21x servers with Intel Xeon Phi**
  Intel Xeon Phi 7290 (72 cores @1.50 GHz), 96 GB RAM
- **76x servers with Intel Xeon Scalable Gen2 (RSC Tornado TDN511)**
  2x Intel Xeon Platinum 8268 (24 Cores @2.90 GHz), 192 GB RAM
- **32x servers with Intel Xeon Scalable Gen2 (RSC Tornado TDN511S)**
  2x Intel Xeon Platinum 8368Q (38 Cores @2.60 GHz), 2 TB RAM

Peak performance: 0.8 PFLOPS double precision

GPU component

- **5x servers with NVIDIA V100**
  2x Intel Xeon E5-2698 v4 (20 cores @2.20 GHz),
  8x NVIDIA V100 16 GB, 512 GB RAM
- **5x servers with NVIDIA A100**
  2x AMD EPYC 7763 (64 Cores @2.45 GHz),
  8x NVIDIA A100 80 GB, 2 TB RAM
- **2x servers with NVIDIA H100 (RSC Exastream AI)**
  2x Intel Xeon Platinum 8468 (48 Cores @2.1 GHz),
  8x NVIDIA H100 80 GB, 1 TB RAM

Peak performance: 58 PFLOPS half-precision

Storage system: 10.6 PB

Total peak performance

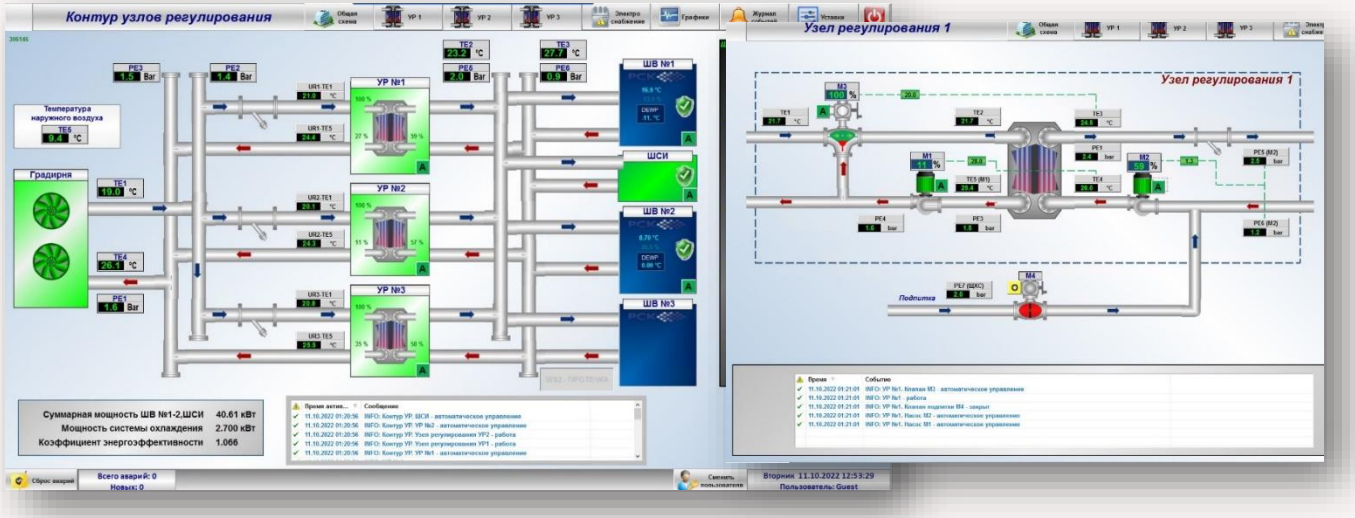
2.2 PFLOPS double precision
58 PFLOPS half precision

The Govorun supercomputer. Hot water cooling

PUE ~1,06

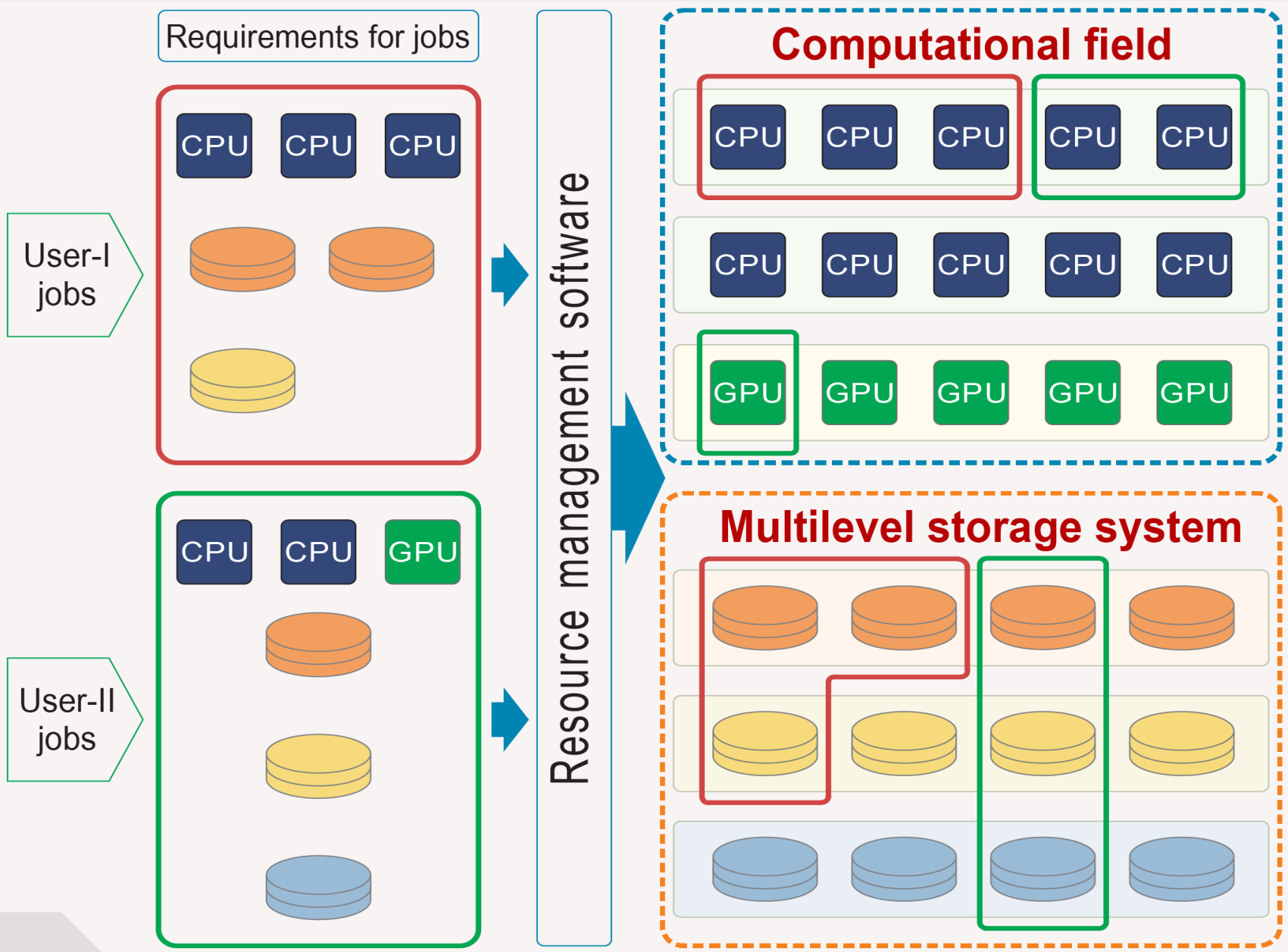
Power usage effectiveness

The supercomputer receives water cooled to a temperature of **45 °C**. Having passed through the entire circuit in the supercomputer, water heated to **50 °C** returns to the heat exchanger, where it is cooled, transferring thermal energy to the hydraulic circuit of the dry cooling tower.



The cooling system has a smooth performance adjustment, which allows you to increase or decrease the power of the cooling system in accordance with the actual load. This allows you to significantly reduce energy consumption at partial load.

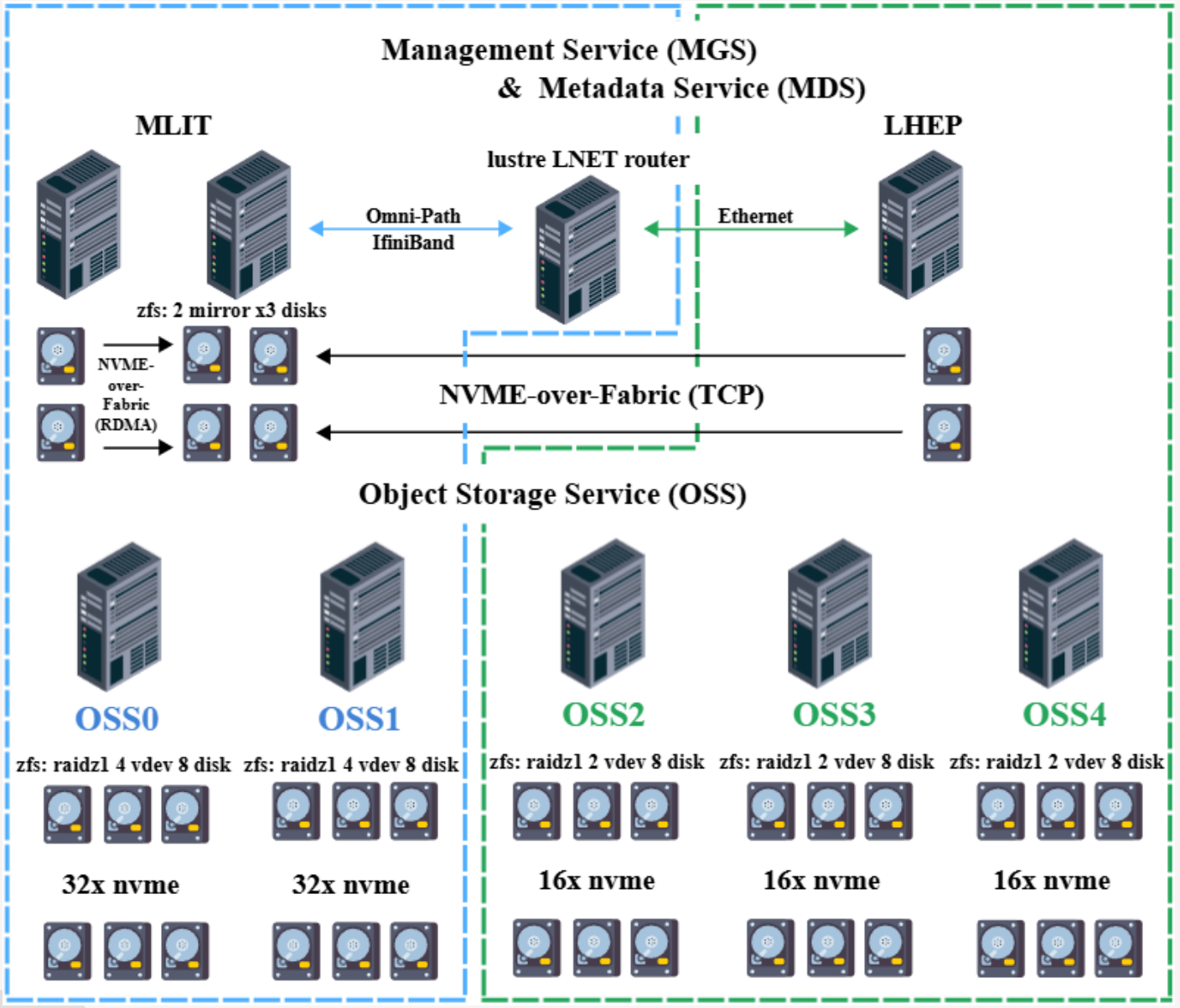
Orchestration and hyperconvergence



The Govorun supercomputer has unique properties for the flexibility of customizing the user's job. For his job the user can allocate the required number and type of computing nodes and the required volume and type of data storage systems.

This property enables the effective solution of different tasks, which makes the Govorun supercomputer a unique tool for research underway at JINR.

Lustre distributed parallel file system



The distributed parallel file system Lustre is deployed among the Govorun SC (MLIT) and the NCX cluster (LHEP). Lustre was created using two new RSC Tornado AFS servers.

Total capacity of Lustre is 2.1 PB

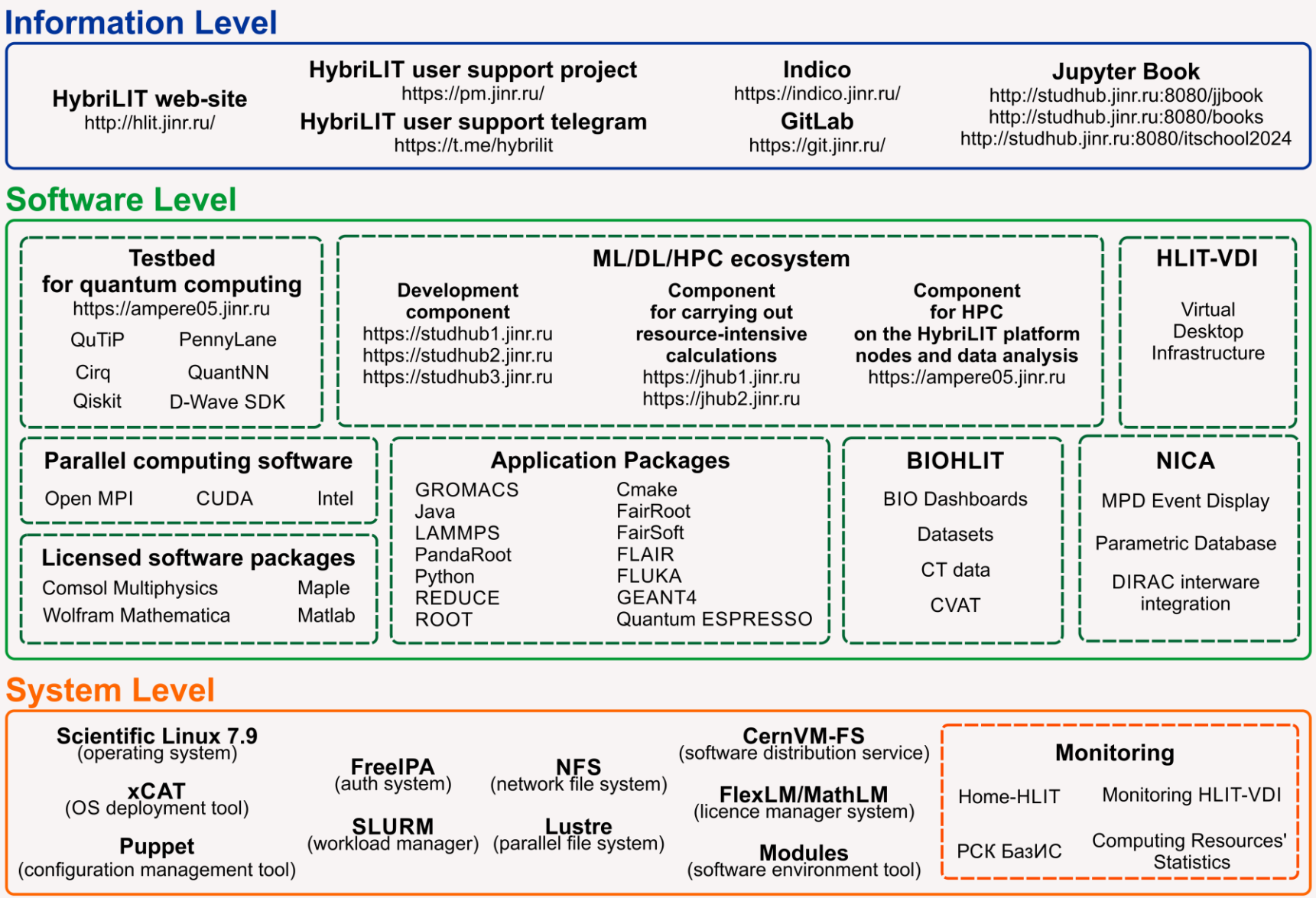
(Govorun – 1.5 PB, NCX – 0.6 PB)

Copied 200 TB of MPD Data

Maximum write speed 15 GB/s

- The ability to perform calculations on different computing resources without transferring data between clusters.
- High performance of computing tasks with intensive Input/Output operations on the data storage system.
- The user's ability to select a storage server (OSS), the number of data replicas, and the number of chunks to speed up work with the file.

Software and information environment of the Platform



Anikina A., Belyakov D., Bezhanyan T., Kirakosyan M., Kokorev A., Lyubimova M., Matveev M., Podgainy D., Rahmonova A., Shadmehri S., Streltsova O., Torosyan Sh., Vala M., Zuev M. Structure and Features of the Software and Information Environment of the HybriLIT Heterogeneous Platform. *27th International Conference «Distributed Computer and Communication Networks» (DCCN 2024), Moscow, Russia, September 23-27, 2024, Revised Selected Papers. Lecture Notes in Computer Science*, Vol. 15460, pp. 444-457 (2025).

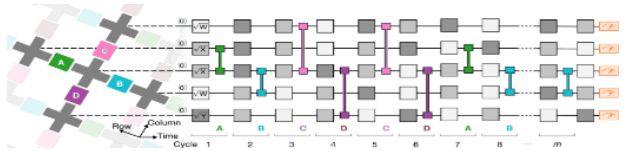
Capabilities of the HybriLIT heterogeneous computing platform

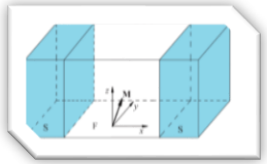
Processing and analysis of big data in high energy physics, nuclear physics and others

- Computing for NICA megascience project
- Calculations of radiobiology problems

High Performance Computing

- Calculations of Quantum Chromodynamics Problems on Lattice
- Modelling of systems based on Josephson junctions

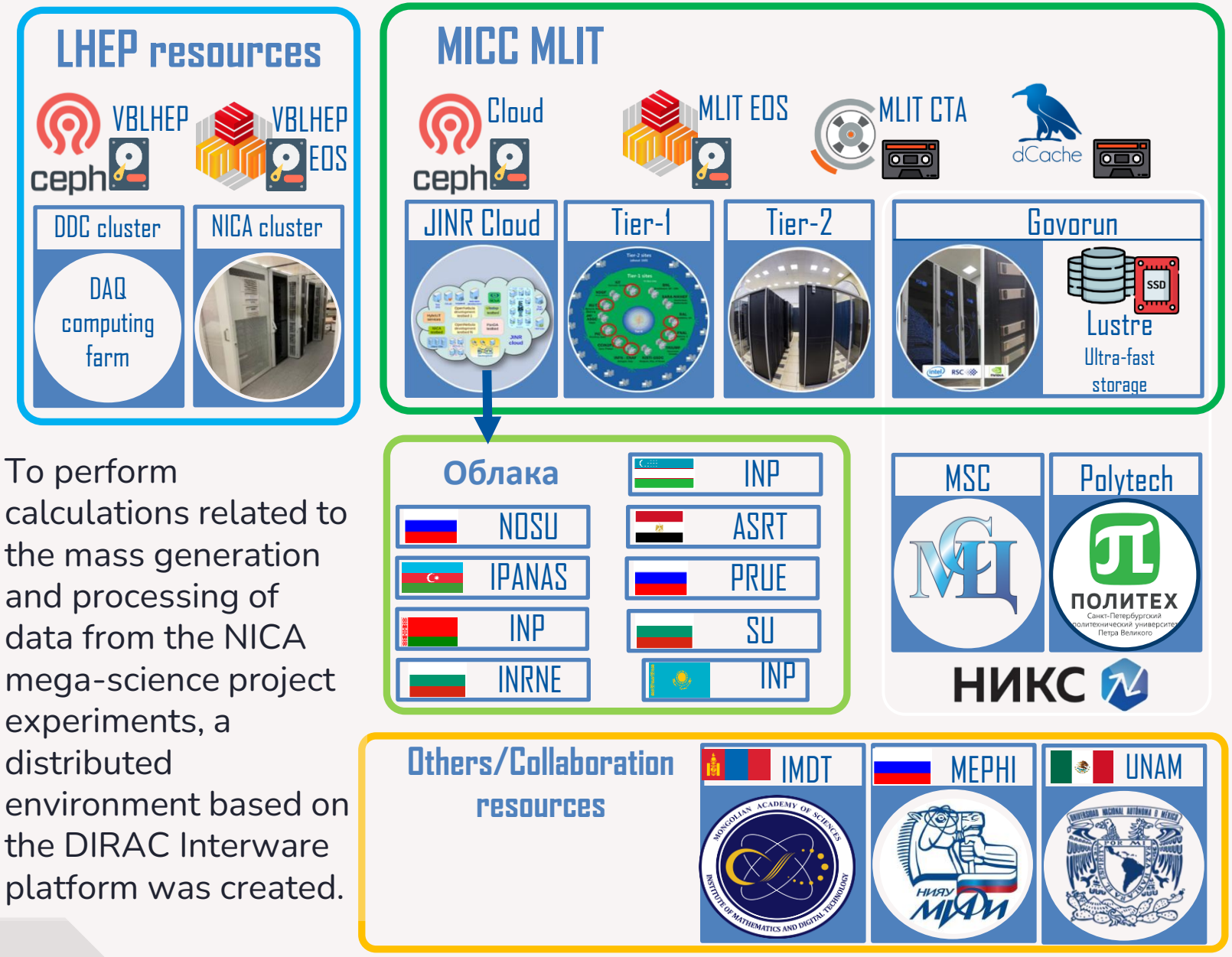




Development of algorithms

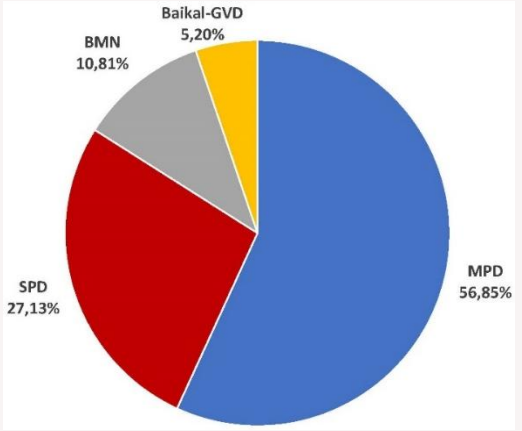
- Applying of methods of machine learning and deep learning for analysis of video and images
- Applying Computer Vision for analysis of video and images
- Applying quantum computing for nuclear physics

DIRAC-based distributed heterogeneous environment

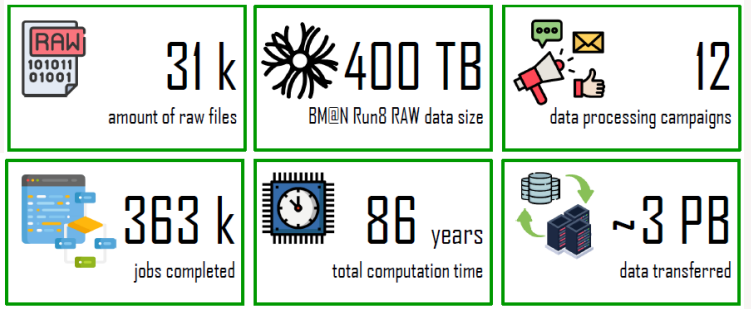


To perform calculations related to the mass generation and processing of data from the NICA mega-science project experiments, a distributed environment based on the DIRAC Interware platform was created.

Share of the use of different MICC components for MPD tasks: the Govorun SC resources are the most efficient for MPD tasks.

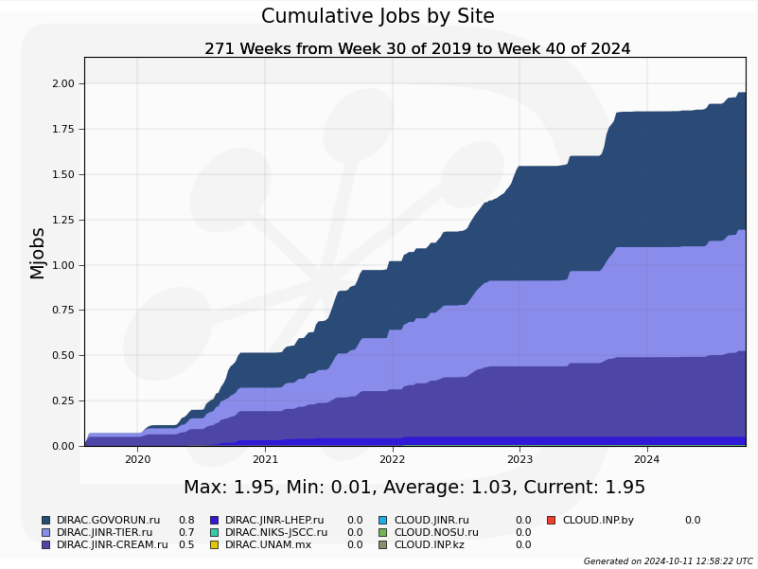


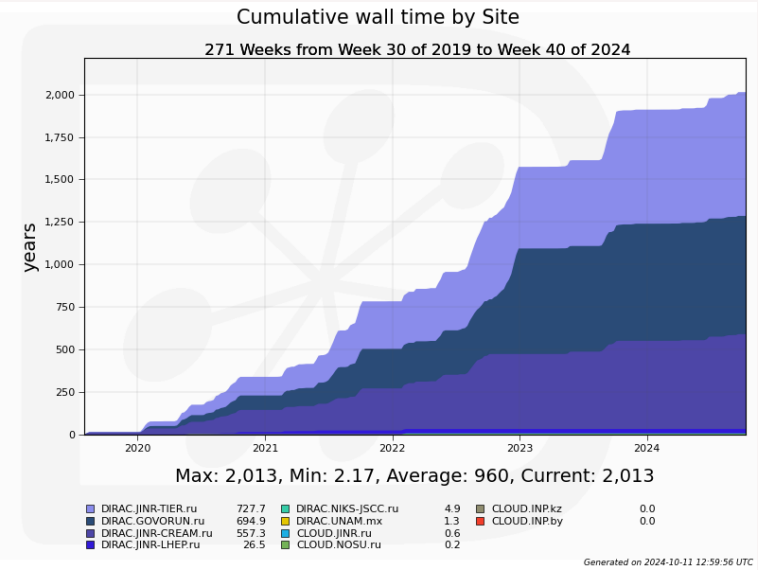
In 2023, for the first time at JINR, the complete processing of raw data from the 8th run of the BM@N experiment was performed on the distributed heterogeneous computing infrastructure integrated using the DIRAC platform.



Summary statistics of using the DIRAC platform for BM@N Run 8 data processing

Heterogeneous distributed computing environment for the MPD experiment





Available resources of the DIRAC platform for the MPD experiment:

- **The Govorun** supercomputer: up to **4,864** cores in the latest production
- **Tier1**: **1,500** cores
- **Tier2**: **1,000** cores
- **Clouds** (JINR and JINR Member States): **~500** cores
- **NICA offline cluster**: **1,000** cores (limit for users)
- **UNAM** (Mexico University): **100** cores
- National Research Computer Network of Russia (**NIKS**, now resources from SPBTU and JSCC): **672** cores.

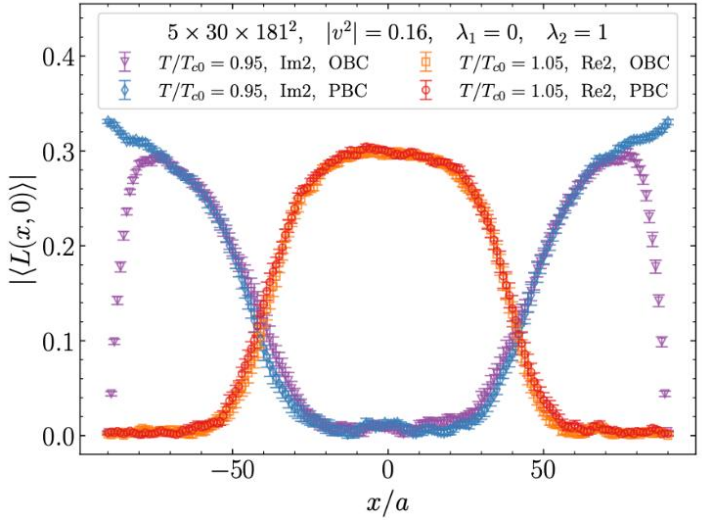
The mass production **storages** integrated into the Dirac File Catalog are **1.5 PB** in size.

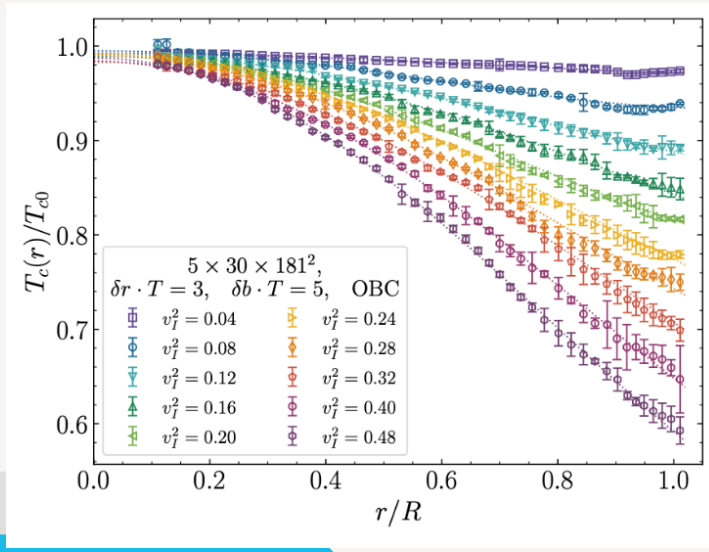
The Govorun supercomputer for QCD tasks

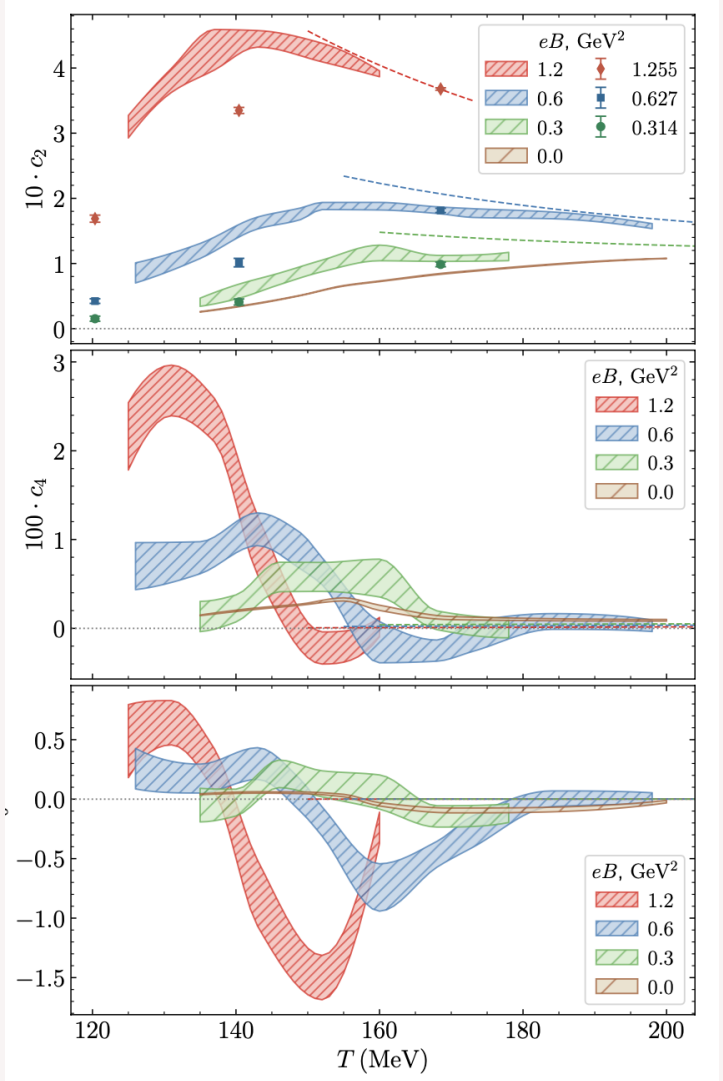
MLIT, BLTP

The resources of the Govorun supercomputer were used to perform calculations in the following areas:

- Finding the equation of state of quark-gluon plasma in the presence of an external magnetic field and non-zero chemical potential;
- Studying the effect of rotation on the properties of gluon plasma.







The results are published in the articles:

[1] Braguta V., Chernodub M., Kudrov I., Roenko A., Sychev D. *Moment of inertia and supervortical temperature of gluon plasma.* PoS LATTICE2023, 181 (2024), arXiv:2311.03947 [hep-lat].

[2] Braguta V., Chernodub M., Roenko A., Sychev D. *Negative moment of inertia and rotational instability of gluon plasma.* Phys. Lett. B 852, 138604 (2024), arXiv:2303.03147 [hep-lat].

[3] Braguta V., Chernodub M., Kudrov I., Roenko A., Sychev D. *Negactive Barnett effect, negative moment of inertia of the gluon plasma, and thermal evaporation of the chromomagnetic condensate.* Phys. Rev. D 110, 014511 (2024), arXiv:2310.16036 [hep-ph].

[4] Braguta V., Chernodub M., Roenko A. *New mixed inhomogeneous phase in vortical gluon plasma: First-principle results from rotating SU(3) lattice gauge theory.* Phys. Lett. B 855, 138783 (2024), arXiv:2312.13994 [hep-lat].

[5] Astrakhantsev N., Braguta V., Kotov A., Roenko A. *QCD equation of state at nonzero baryon density in an external magnetic field.* Phys. Rev. D 109, 094511 (2024), arXiv:2403.07783 [hep-lat].

The Govorun supercomputer for nuclear physics tasks

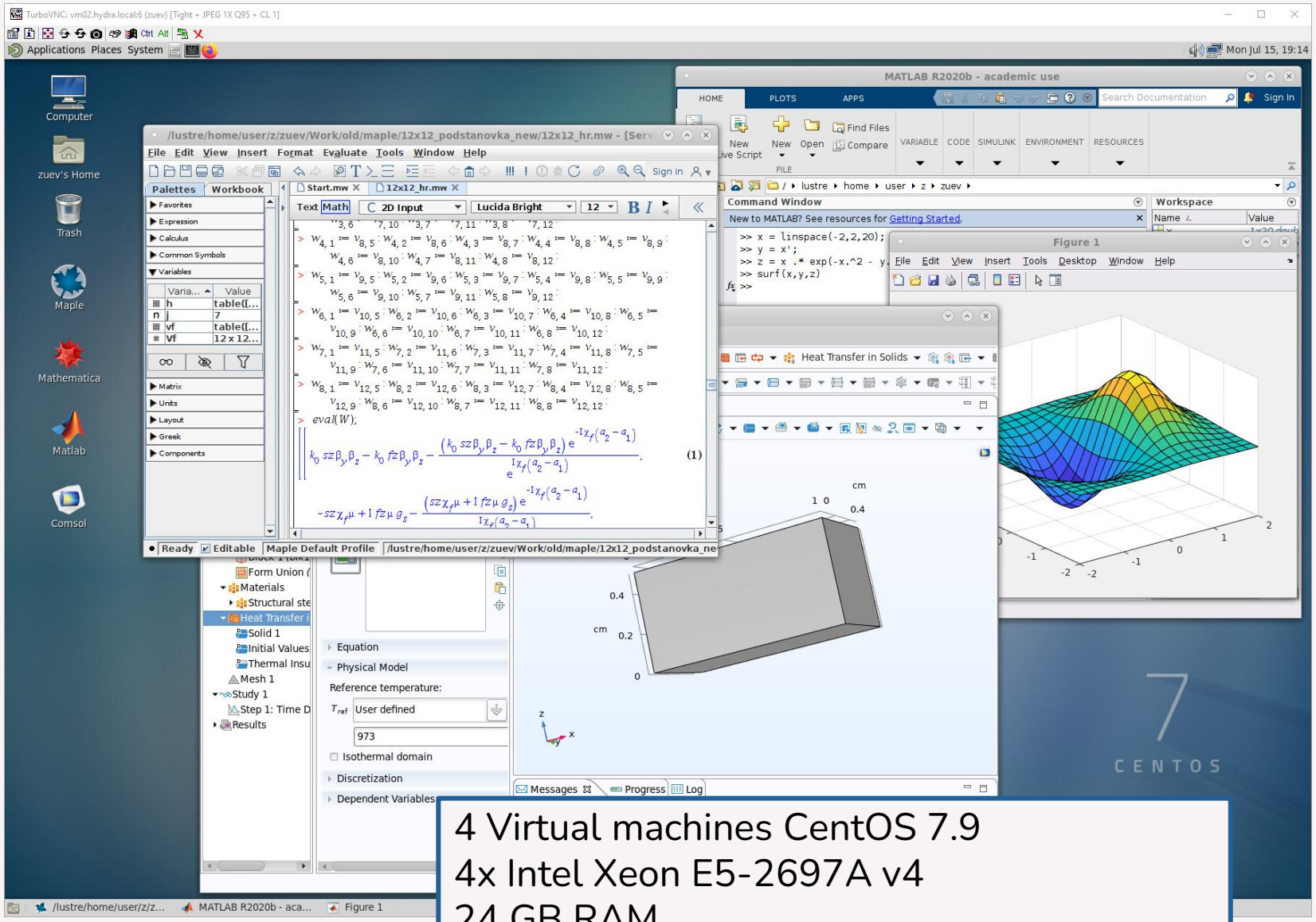
- Study of the structure of light exotic, heavy and superheavy nuclei and reactions with them.
- Simulations and data processing for the experiments with exotic nuclei
- Relativistic molecular and periodic quantum-chemical calculation of superheavy elements and their compounds
- Study of changes in the Periodic Law in the region of extremely heavy elements. Study of the electronic structure of elements at the end of the 7th and beginning of the 8th periods.
- Study of radiation safety of heavy ion accelerators at FLNR JINR using Monte Carlo simulation
- Modeling the radiation environment of the DC-140 accelerator complex using the FLUKA software package
- Modeling the kinetics of excitation and relaxation of dielectrics irradiated by fast heavy ions

For calculations of electronic properties of superheavy elements. an on-demand computing system was created. It containing **380 physical cores** (760 logical cores) and **80 TB** file storage managed by the NFS file system. Intensive calculations were carried out on this system using AMS, DIRAC, KANTBP, etc. software. During the past year, over **11,800 tasks** were solved, on which over **3,800,000 core hours** were spent.

The results are presented in the next publications:

1. A.A. Kotov, Y.S. Kozhedub, D.A. Glazov, M. Ilias, V. Pershina, V.M. Shabaev // ChemPhysChem. 2023. **24**. C. E202200680;
2. A. Ryzhkov, V. Pershina, M. Ilias, V. Shabaev // Phys. Chem. Chem. Phys. 2023. **25**. C. 15362;
3. I. M. Savelyev, M. Y. Kaygorodov, Y. S. Kozhedub, A. V. Malyshev, I. I. Tupitsyn, and V. M. Shabaev // Phys. Rev. A **107**, 042803;
4. V.A. Zaytsev, M.E. Groshev, I.A. Maltsev, A.V. Durova, V.M. Shabaev // Int. J. Quant. Chem. 2023. C. e27232.

HLIT-VDI Remote Desktop



4 Virtual machines CentOS 7.9
4x Intel Xeon E5-2697A v4
24 GB RAM
Nvidia Tesla M60, 8 GB

Users have the opportunity to work with mathematical and physical software (Matlab, Mathematica, Maple, COMSOL, Geant4, ROOT) through a graphical user interface (GUI).

MATLAB

Maple™

COMSOL MULTIPHYSICS®

G4

ROOT
Data Analysis Framework

ML/DL/HPC Ecosystem of the HybriLIT Heterogeneous Platform

Component for educational purposes (without GPUs)

For teaching students
https://studhub1.jinr.ru

For conducting workshops within the framework of JINR scientific events
https://studhub2.jinr.ru
https://studhub3.jinr.ru

Component for carrying out resource-intensive computations (with GPUs)

https://jhub1.jinr.ru
https://jhub2.jinr.ru

HPC component for scientific projects (with installed specialized libraries)

BioProject services
https://cell.jinr.ru
http://mostlit.jinr.ru
http://bio-dashboards.jinr.ru/morris

Jupyter Books infrastructure
http://studhub.jinr.ru:8080/jjbook
http://studhub.jinr.ru:8080/books
http://studhub.jinr.ru:8080/itschool2024

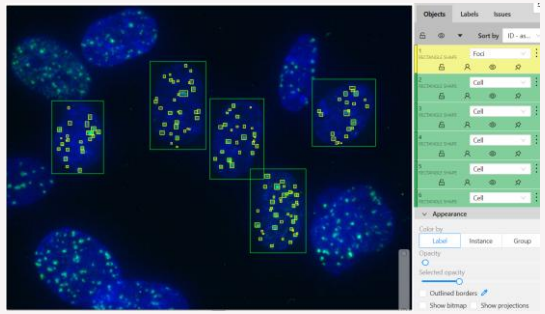
CVAT services
http://159.93.36.88:8080
http://159.93.36.67:8080

A polygon for visualization of brain CT data
hlit-th-ct.jinr.ru

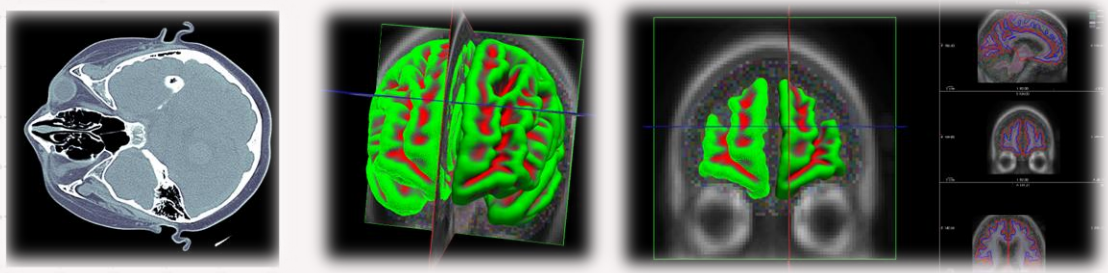
A polygon for quantum computing
https://ampere05.jinr.ru

Scientific Projects

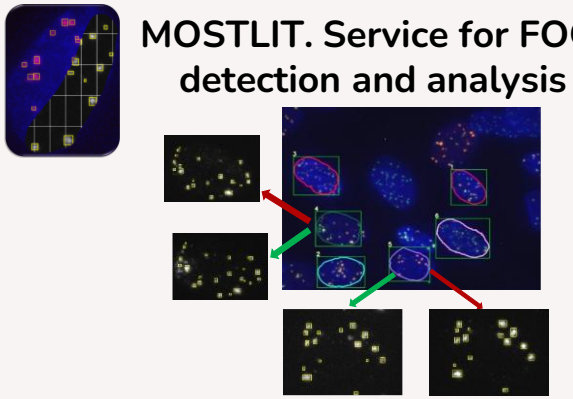
CVAT. Image & Video Data Annotation Platform



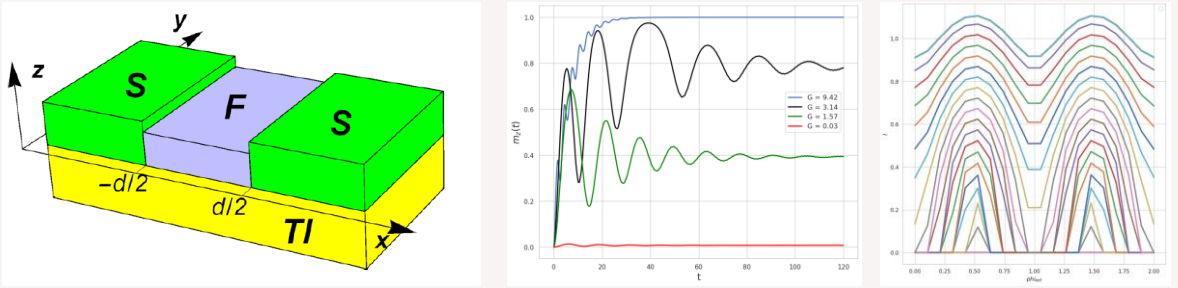
A polygon for visualization of brain CT and MRI/fMRI data



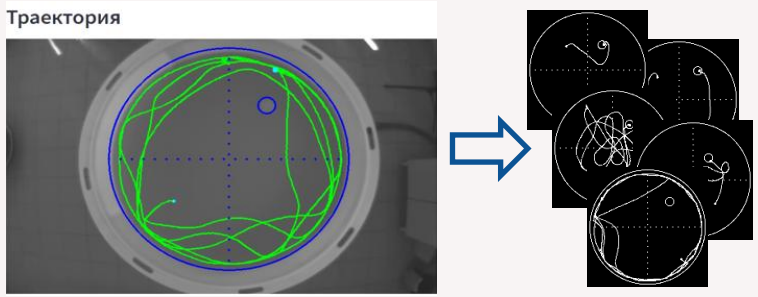
MOSTLIT. Service for FOCI detection and analysis



Research of systems based on Josephson junctions



Web service for “Morris Water Maze” behavioral test



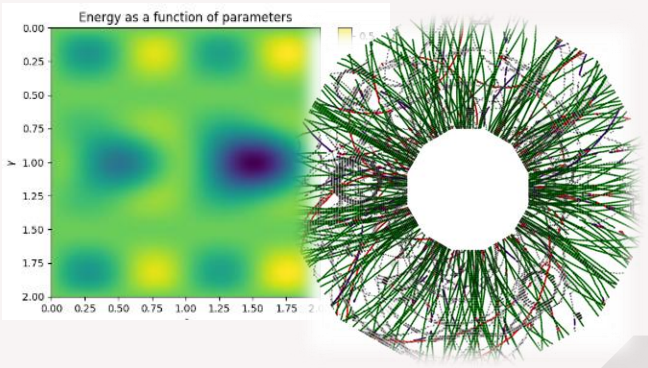
A polygon for quantum computing

Cirq

cuQuantum

PENNYLANE

Qiskit



A polygon for quantum computing

While quantum computers are not available for widespread use, various simulators of quantum computing on classical computers are being developed.
These are libraries on various programming languages or frameworks that allow to create, transform, optimize and effectively simulate quantum circuits. Thus, they allow user to completely control the behavior of a quantum system.

The work is organized in two modes:

- **using task scheduler (in SLURM queue mode)**

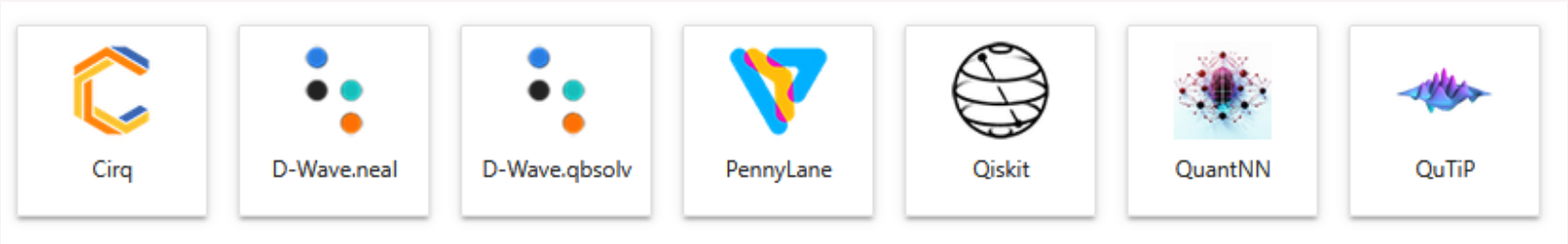
  The main advantages:

  - the ability to perform multi-node computations using MPI technology;
  - the use of resources of the entire Platform.

- **in interactive mode via web-browser**

  The main advantages:

  - the ability to visually develop algorithms, visualize quantum circuits;
  - available Python language materials can significantly speed up research.

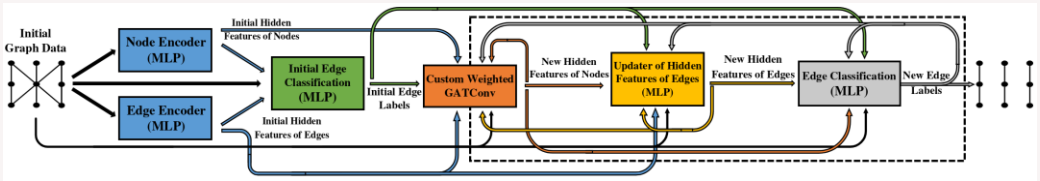


Server specifications: 2x AMD EPYC 7763 (64 Cores @2.45 GHz), 2 TB RAM, 8x NVIDIA Tesla A100 80 GB

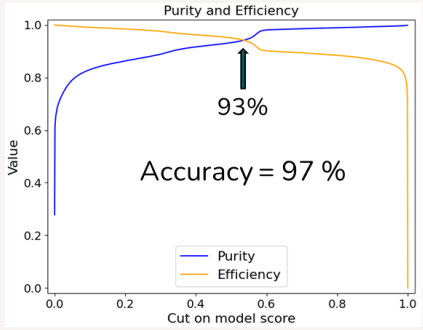
Using the GNN for particle track reconstruction in the MPD of the NICA

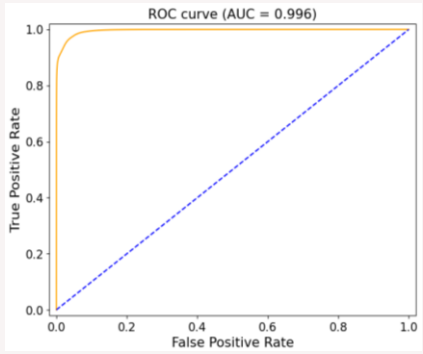
Dr. Yauheni Talochka, Prof. Gennady Ososkov, Dr. Nikolay Voytishin

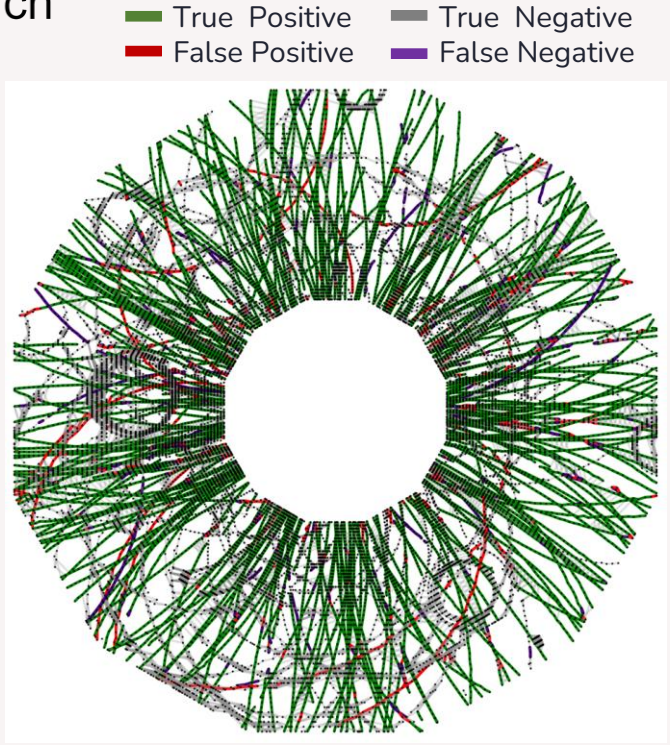
The main goal is the development of a Graph Neural Network for particle track reconstruction in the MPD of the NICA.



PyTorch / Libtorch







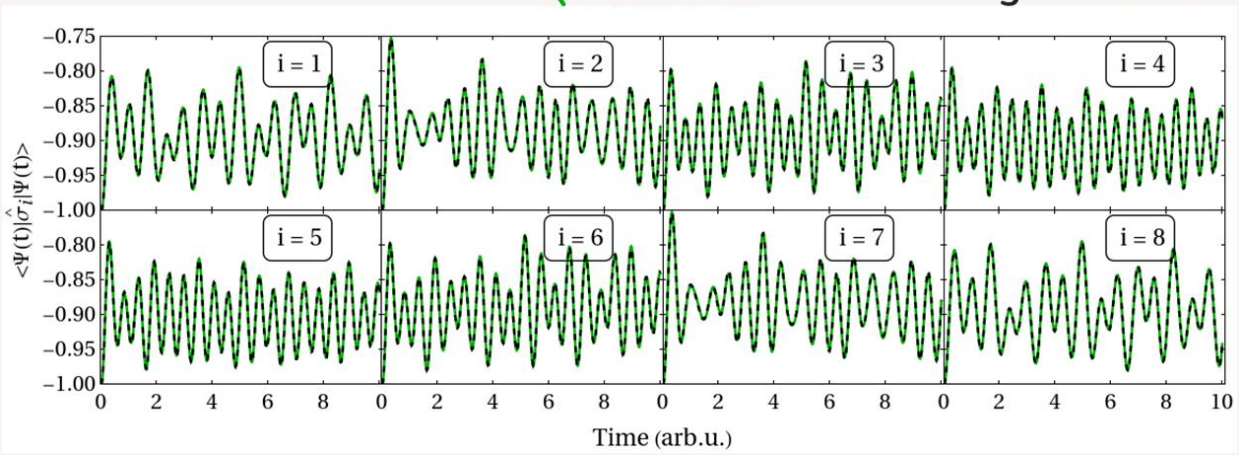
Talochka Y., Ososkov G., Voytishin N. Graph Neural Network with Attention and Two-Stage Aggregation for Particle Track Reconstruction in the TPC MPD of the NICA accelerator complex. *Computing and Software for Big Science* (accepted for publication).

Tensor Networks for Efficient Quantum Computing

Dr. Yauheni Talochka, Dr. Arsen Khvedelidze ,
Prof. Gennady Ososkov , Dr. Iurie Palii , Dr. Nikolay Voytishin

cuQuantum + JINR MLIT = CUDA-based QTensorNet

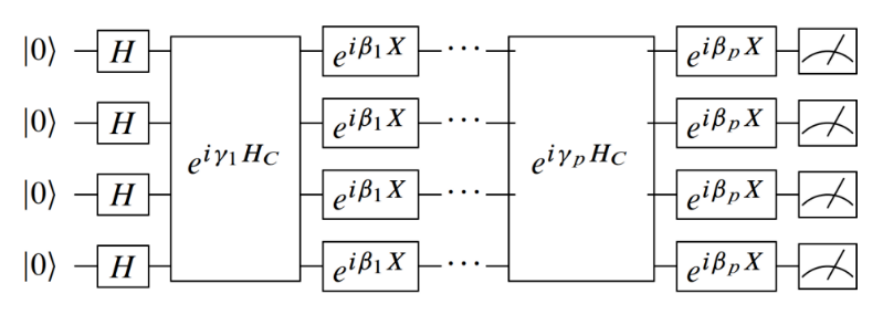
QTensorNet allows you to reduce the number of parameters of a tensor of rank *N* ($d^N \rightarrow Nd\chi_{max}^k$) by constructing a tensor network (single-hierarchy-level TN) with an arbitrary graph using singular value decomposition (SVD) with a given accuracy.



Searching for the state with the lowest energy in the Ising model with a longitudinal magnetic field using the quantum approximation optimization algorithm (QAOA)

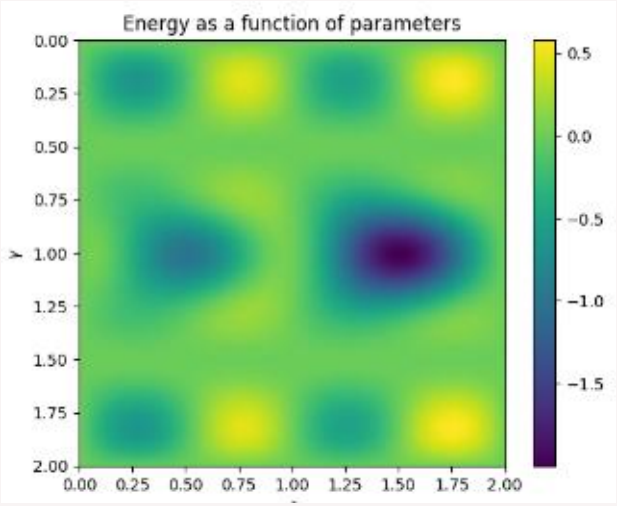
Dr. Yury Palii, Dr. Alla Bogolubskaya, Dr. Denis Yanovich

The solution to the problem is to find a pair of parameters γ, β, at which the energy value $E(\gamma, \beta)$ will be minimal.



A quantum circuit to the variation ansatz of QAOA

$$|\psi(\gamma,\beta)\rangle = \underbrace{U(\beta_p, B)U(\gamma_p, \mathcal{H})}_{p} \ldots \underbrace{U(\beta_1, B)U(\gamma_1, \mathcal{H})}_{1} H^{\otimes n}|0\rangle^{\otimes n}$$



Coincidence of state vector search and sampling search

The optimized **qsim simulator** integrated into Cirq is written in C++ and uses SIMD instructions for vectorization, OpenMP for CPU calculations, and CUDA for GPU calculations.
During the computations, the task on the **3x3x3** lattice took up **~1 TB RAM CPU** and **~1.5 GB RAM GPU**.

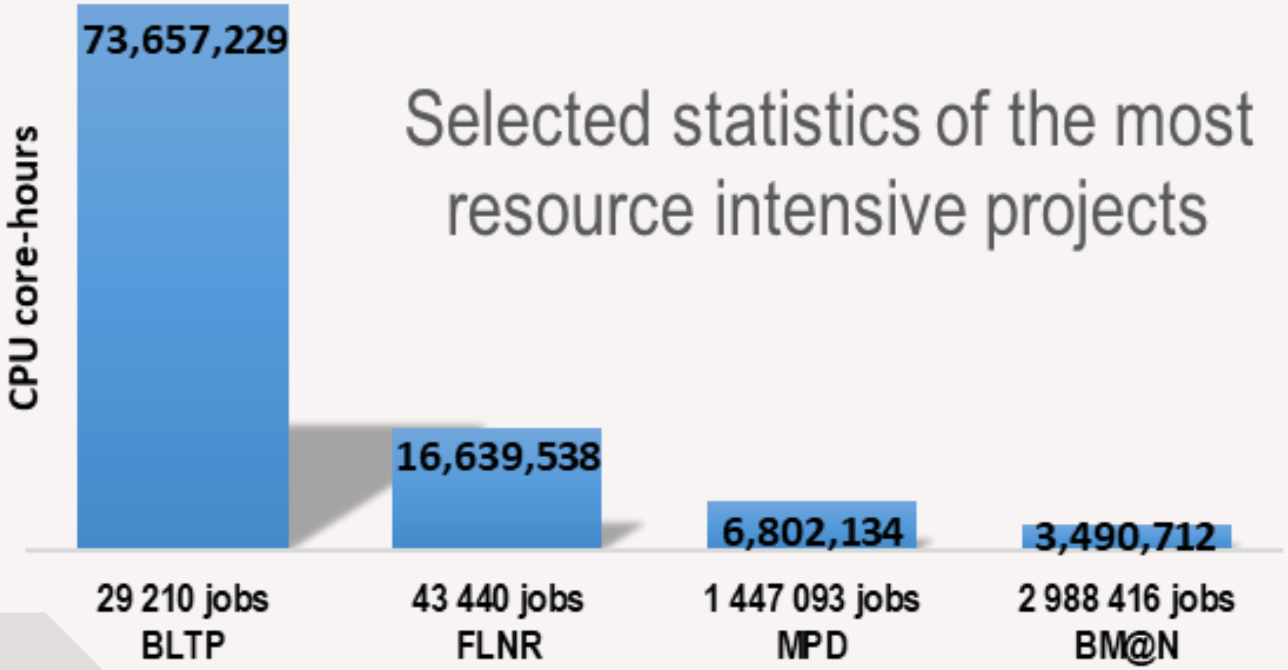
Ising Model 3x3x3 lattice 27 qubits	**AMD EPYC 7763, 128 threads**	**Intel Xeon Platinum 8368Q, 128 threads**	**NVIDIA A100, cuStateVec**
Computation time	3 h 20 min	3 h 10 min	**14 min 35 sec**

Palii Yu., Belyakov D., Bogolubskaya A., Zuev M., Yanovich D.. Simulation of the QAOA Algorithm at the JINR Quantum Testbed. *Phys. Part. Nuclei* **56**, 989-993 (2025).
Palii Yu., Bogolubskaya A., Yanovich D. Quantum Approximation Optimization Algorithm for the Ising Model in an External Magnetic Field. *Phys. Part. Nuclei* **55**, 600-602 (2024).

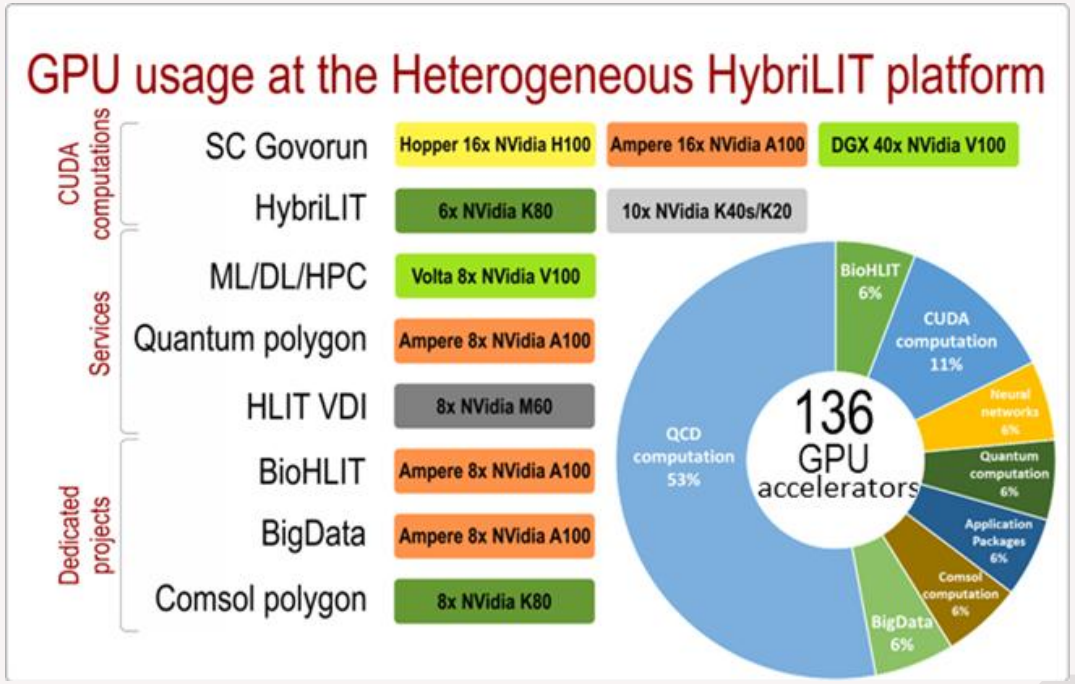
Using of the Govorun supercomputer

The resources of the Govorun SC are used by scientific groups from all the Laboratories of the Institute. **The projects that mostly intensive use the CPU resources of the Govorun SC:**

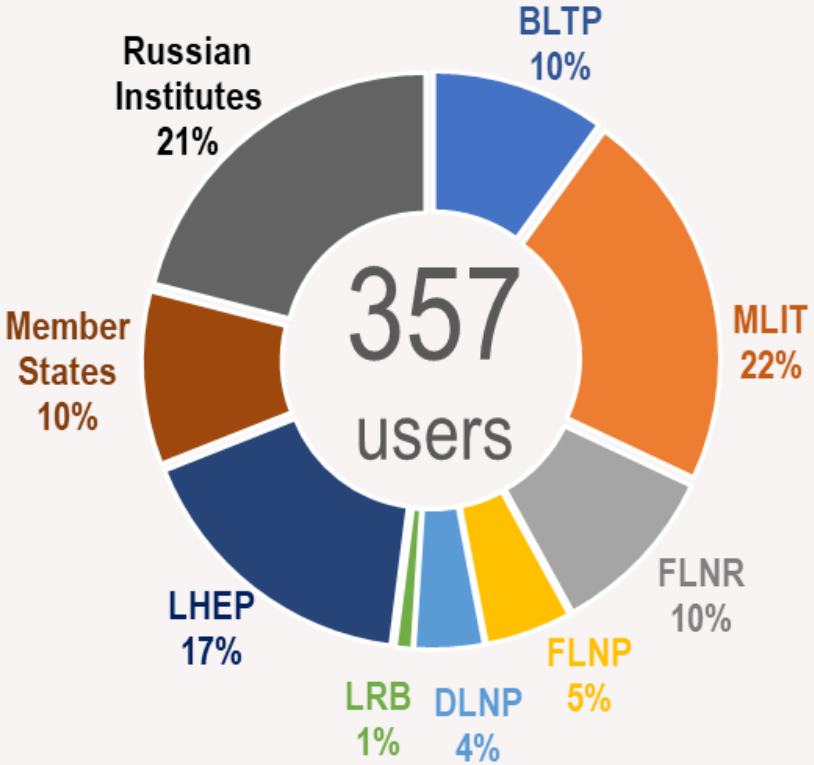
- calculations of lattice quantum chromodynamics.
- computations of the properties of atoms of superheavy elements
- NICA megaproject,



The Govorun SC users completed **13.94 M jobs** what corresponds to the **111.87 M core-hours**.
The average load of the CPU component was 97.2%
The average load of the GPU component:
DGX load was 99.2%, Ampere load was 87,7%.

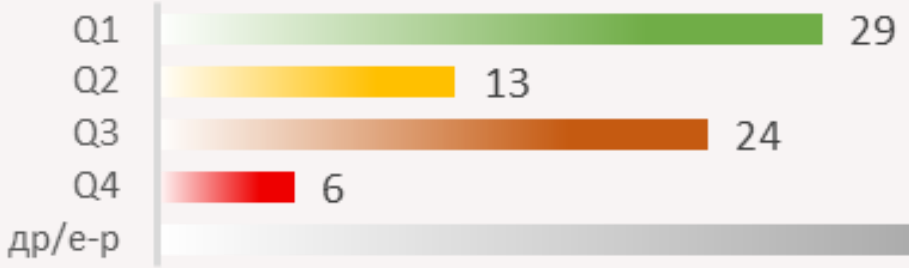


Publications



For all the time, users of the heterogeneous HybriLIT platform published articles in various fields:

- physics of elementary particles and the atomic nucleus,
- high energy physics,- biophysics and chemistry,
- neural network approach, methods and algorithms of machine learning and deep learning (ML/DL), etc.



2024-2025 years

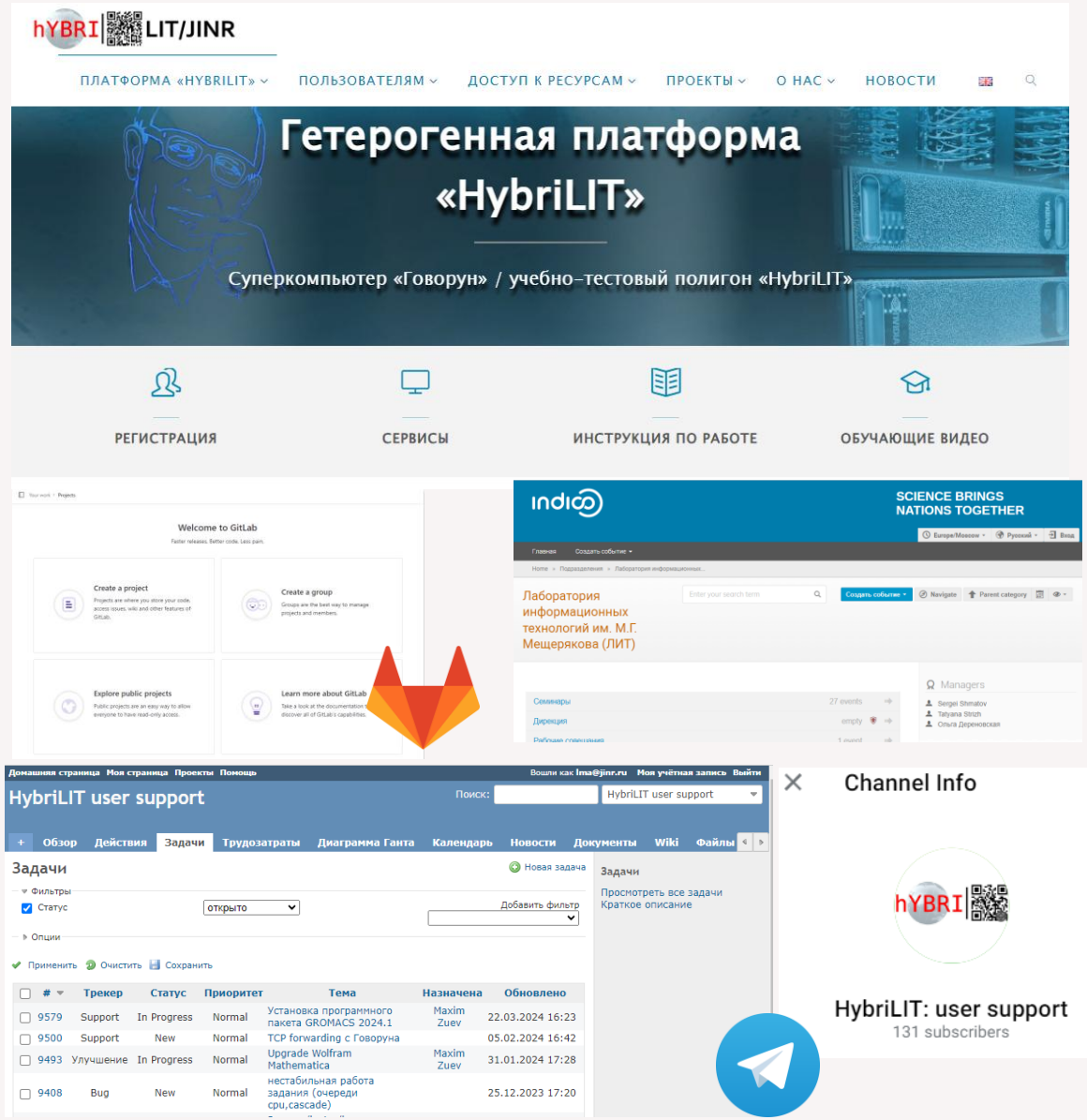
110

articles

Research results obtained using the supercomputer resources since 2018 are presented in **509** publications. Two of them were prepared in Nature Physics:

- M. Kircher ... , O. Chuluunbaatar et al. Kinematically complete experimental study of Compton scattering at helium atoms near the threshold. Vol. 16. № 4. Pp. 756-760
- BM@N Collaboration. Unperturbed inverse kinematics nucleon knockout measurements with a 48 GeV/c carbon beam. Vol. 17. Pp. 693-699

Information level



- **The website** provides a detailed description of the platform: hardware and software structure, characteristics of computing resources, and examples for working with installed application software
- **GitLab** collaborative development service provides the opportunity for the users of the platform to jointly develop application software and work with their own Git repositories.
- The **Indico** software platform is used to support the organization of conferences, seminars and meetings, including in a hybrid format.
- HybriLIT team provides user support and resolves issues related to the work process on the platform via **JINR Project Management Service**.
- A streaming channel **HybriLIT user support** on the **Telegram social network** is being used to promptly inform users