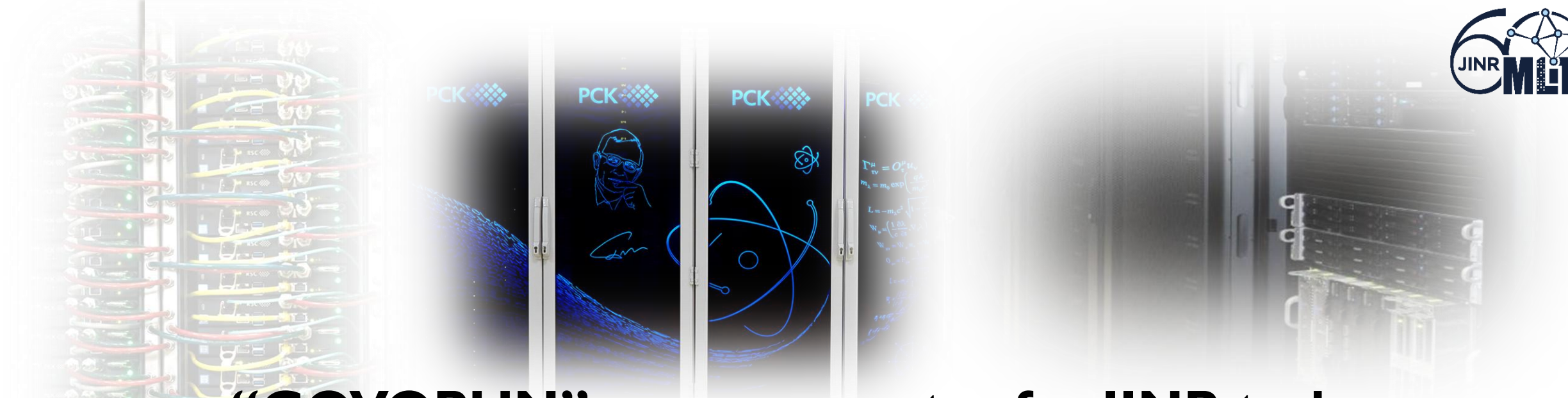


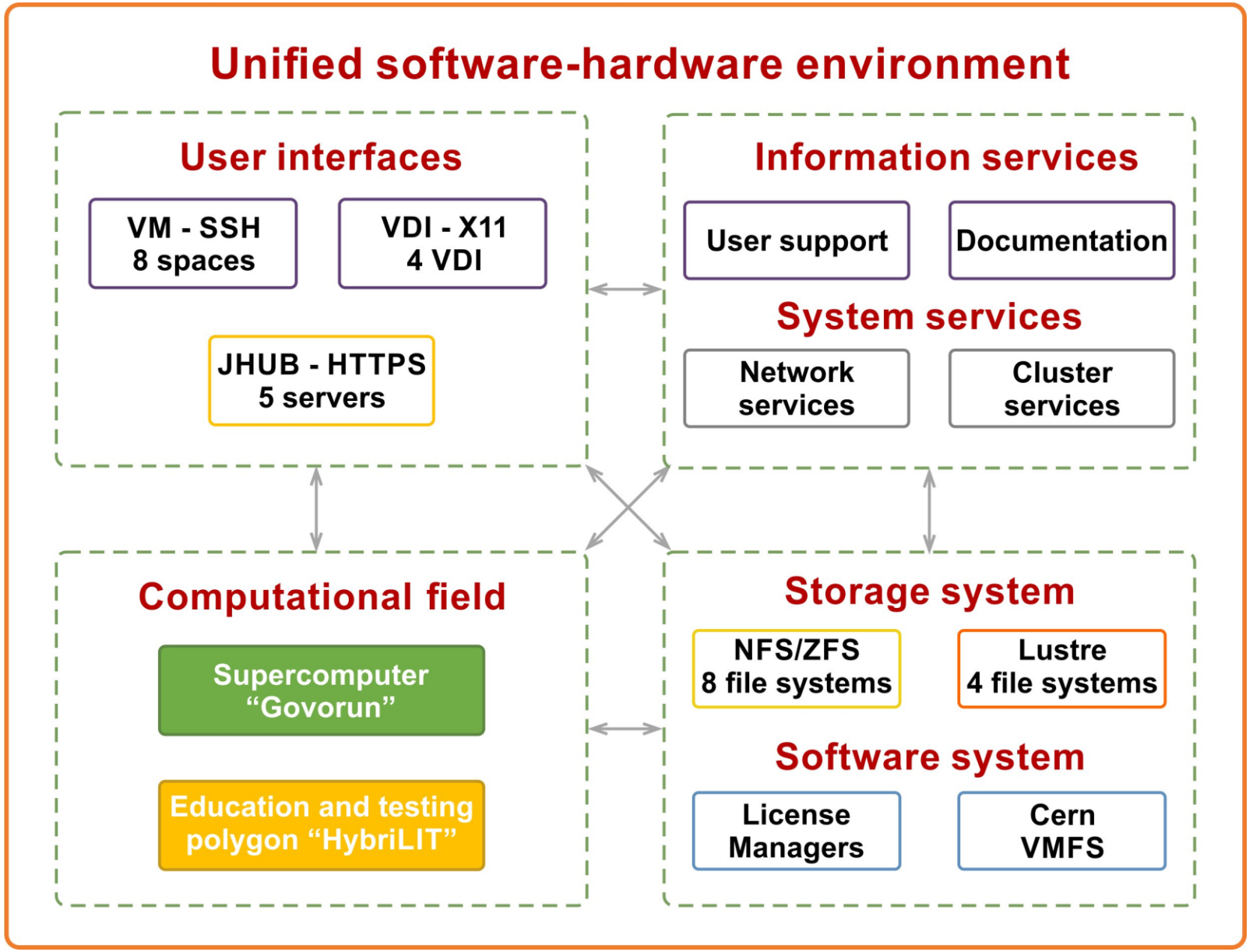
“GOVORUN” supercomputer for JINR tasks

D.V. Podgainy

Meshcheryakov Laboratory of Information Technologies

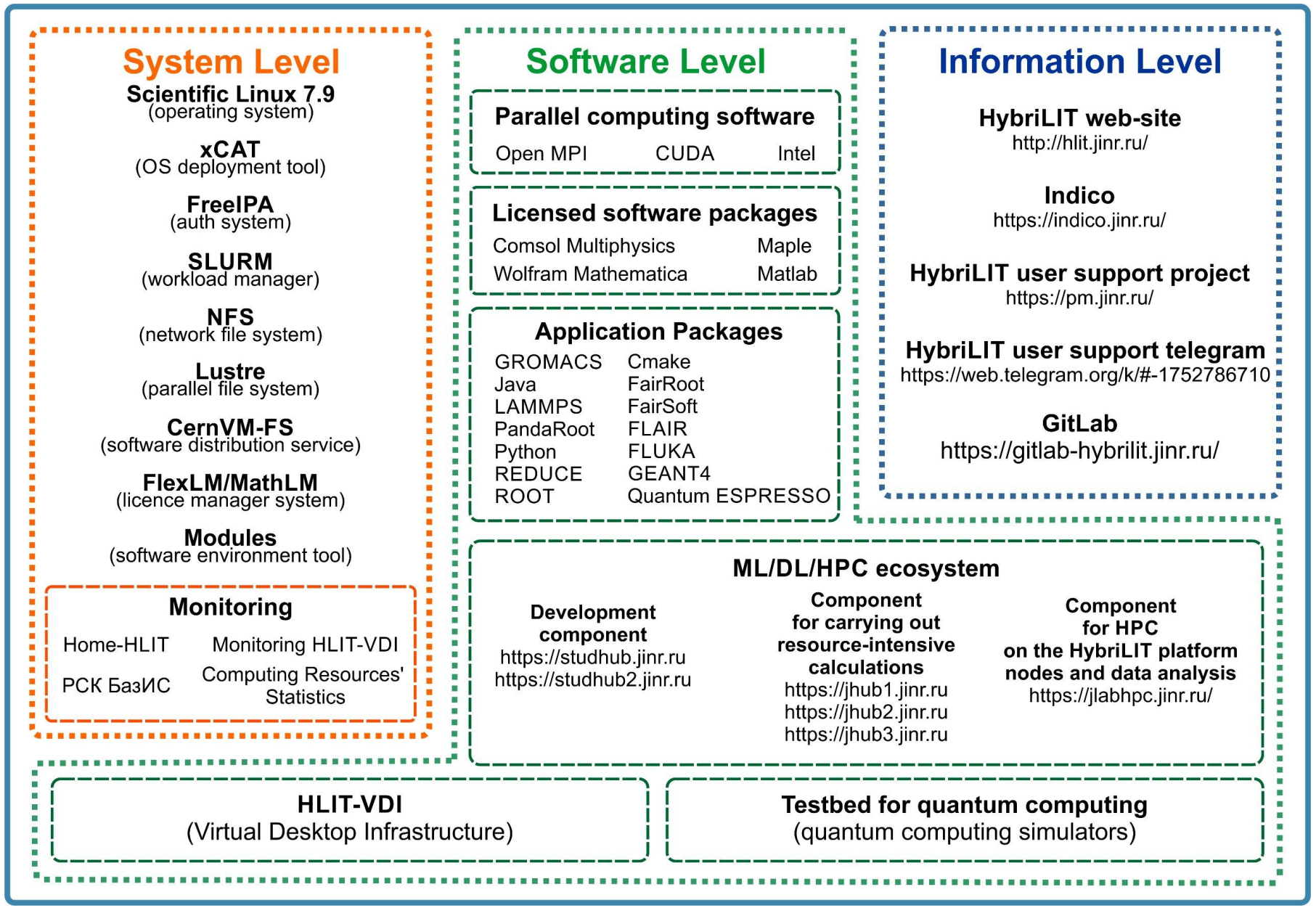
10th International Conference "Distributed Computing and Grid Technologies in Science and Education"
(GRID’2025) 7–11 July 2025

MICC component: HybriLIT platform

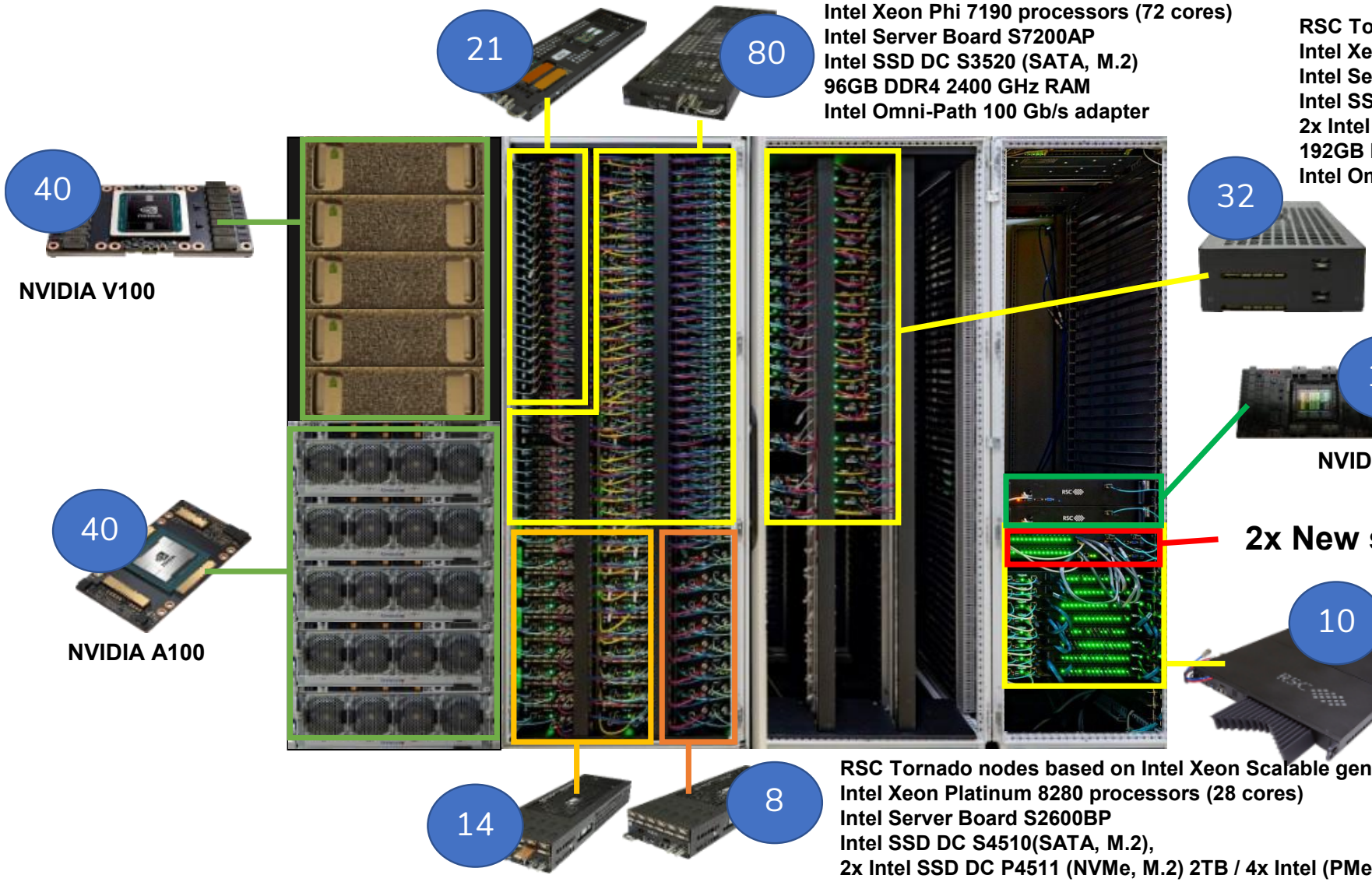


The unified software and information environment of the HybriLIT platform allows using the education and testing polygon, exploring the possibilities of novel computing architectures and IT-solutions, developimg and debuging applications, and carrying out compitations on the supercomputer.

MICC component: HybriLIT platform



“Govorun” supercomputer. The current status 2025



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

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

2x New servers +544 TF

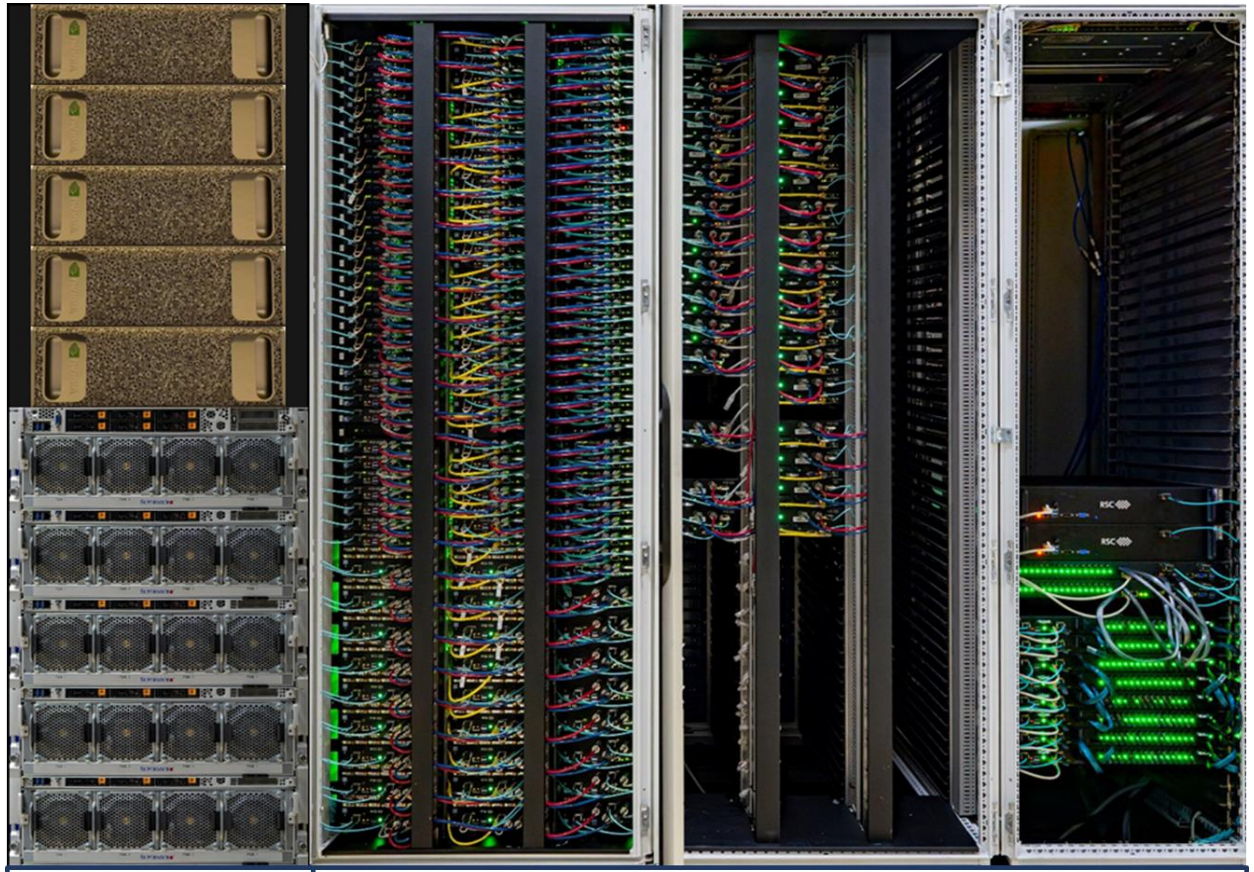
2x New servers +2 PB

Total capacity of Hierarchical Storage: **10.6 PB**

Data IO rate: **300 Gb/s**

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

"Govorun" supercomputer. The current status 2025



GPU-accelerators Air cooled	Hyperconverged CPU, GPU and Distributed Storage Nodes Water cooled

Current status:

CPU component

163 hyperconverged compute CPU nodes

8552 compute cores

Peak performance of the CPU component:

800 Tflops for Double-Precision computations

GPU component

96 GPU accelerators

Peak performance of the CPU component:

1,4 Pflops for Double-Precision computations

58 Pflops for Half-Precision computations

Total peak performance:

2.2 PFlops DP

58 PFlops HP

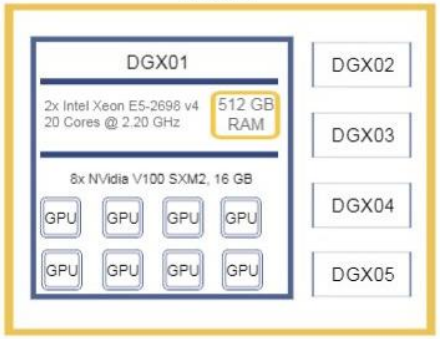
Total capacity of Hierarchical Storage: **10.6 PB**

Data IO rate: **300 Gb/s**

The GPU-component of the “Govorun” Supercomputer

2017

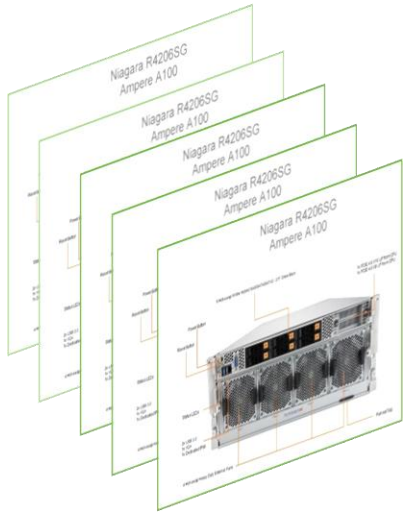
DGX-1



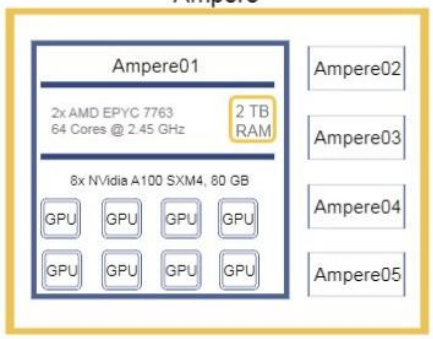
40 NVIDIA V100

+

2023



Ampere



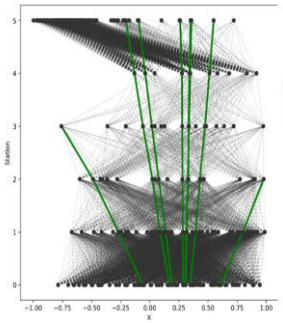
40 NVIDIA A100

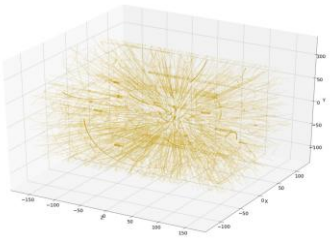
+

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 ect.



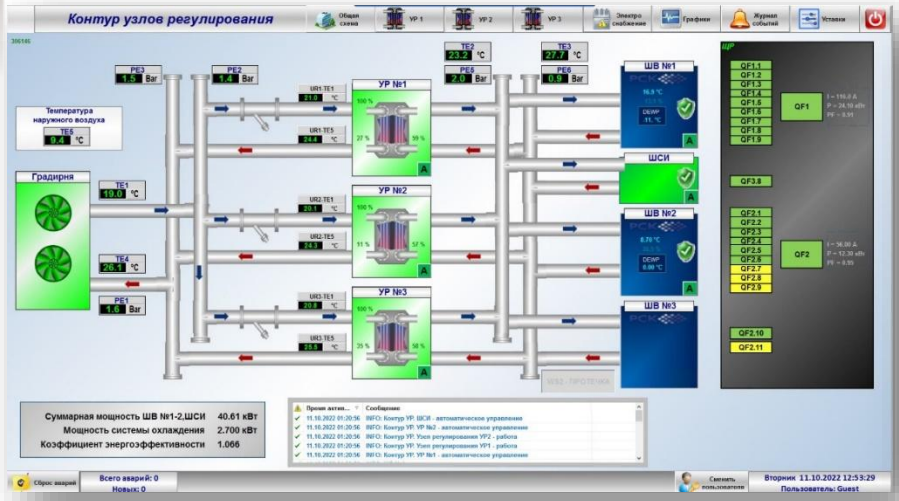


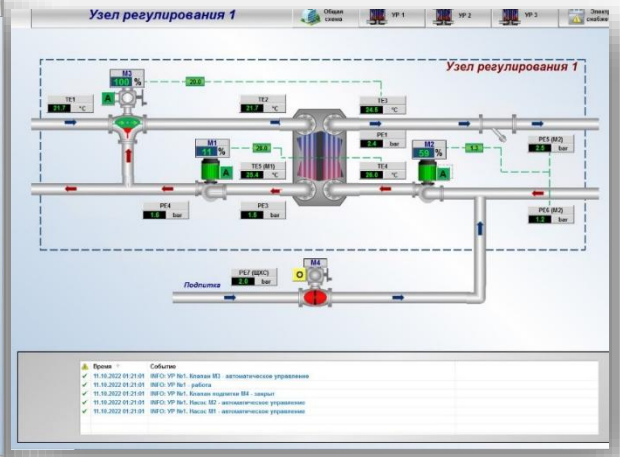
Supercomputer "Govorun". Hot water cooling.

PUE ~ 1,06

Power usage effectiveness

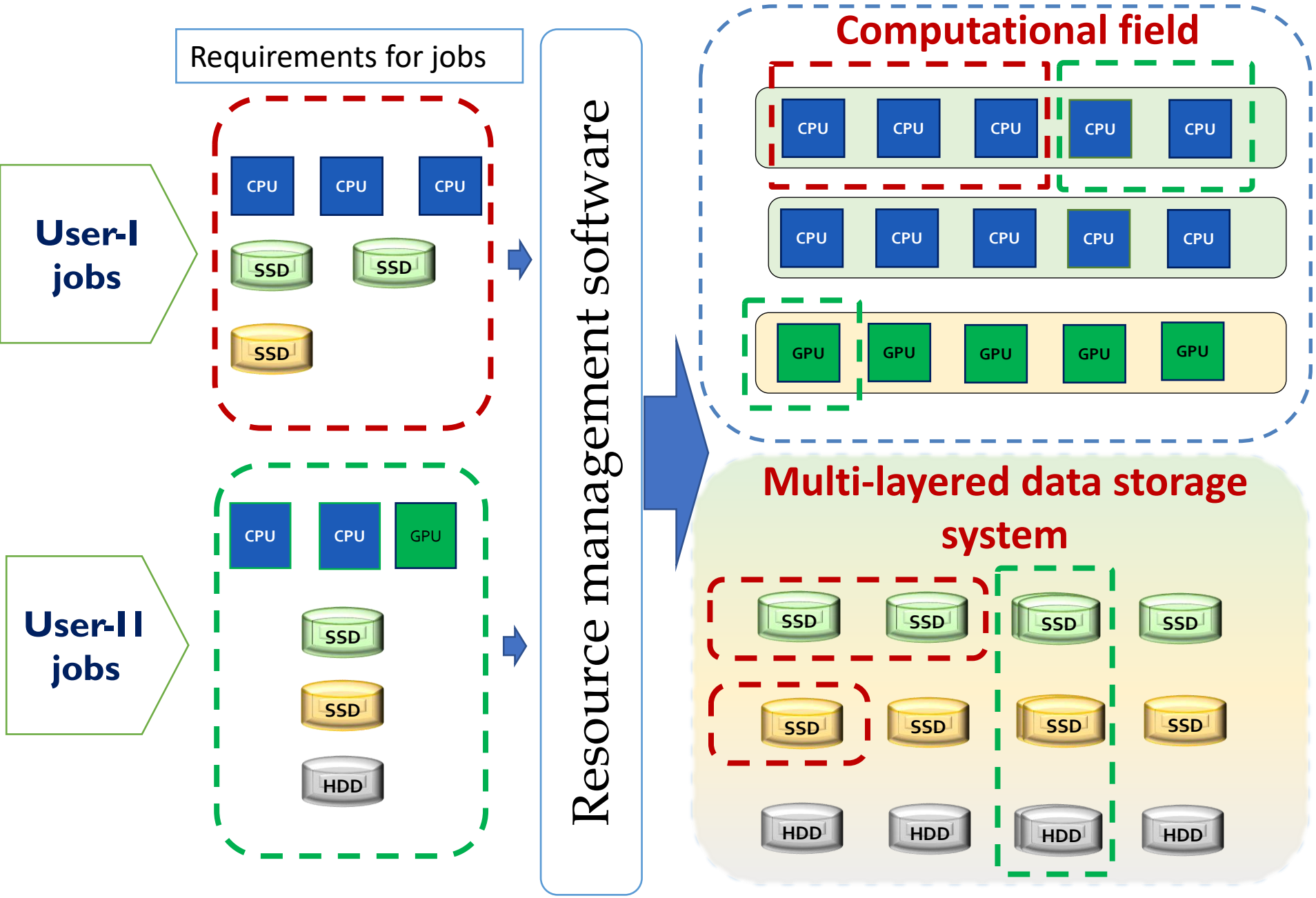
The supercomputer receives water cooled to a temperature of 45 degrees. Having passed through the entire circuit in the supercomputer, water heated to 50 degrees returns to the heat exchanger, where it is cooled, transferring thermal energy to the hydraulic circuit of the dry cooling tower.





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 on the “Govorun” supercomputer

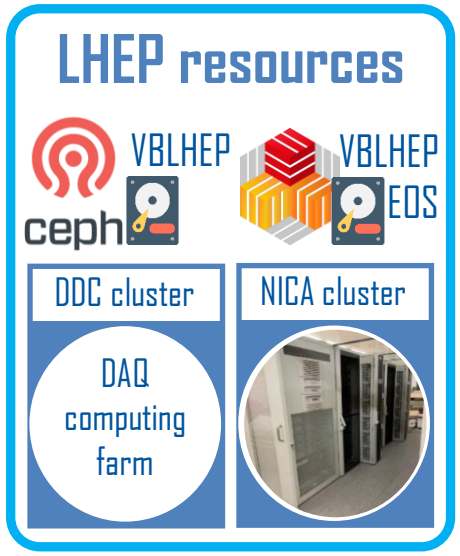


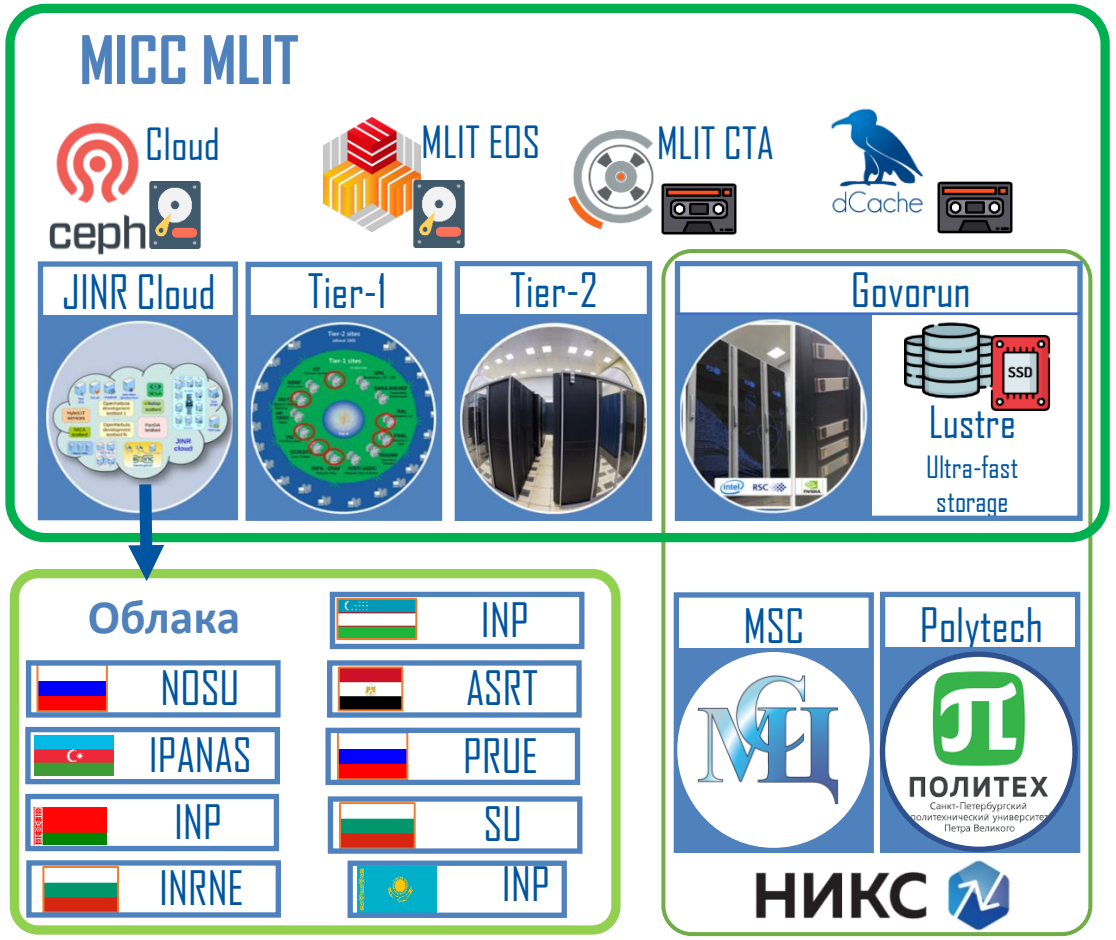
The “Govorun” supercomputer has unique properties for the flexibility of customizing the user’s job.

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.

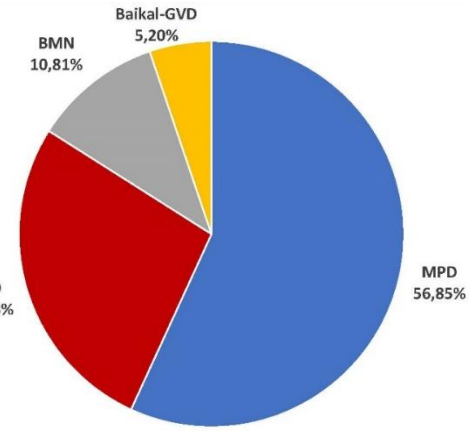
DIRAC-based distributed heterogeneous environment



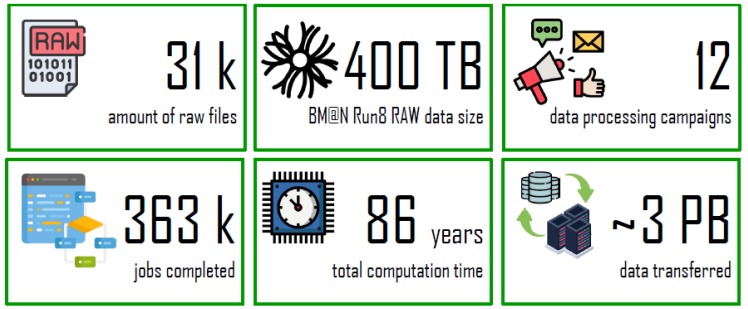


To perform calculations related to the mass generation and processing of data from the NICA mega-science project experiments, a distributed environment based on the DIRAC Interware platform was created.

Share of the use of different MICC components for MPD tasks: the SC "Govorun" 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.



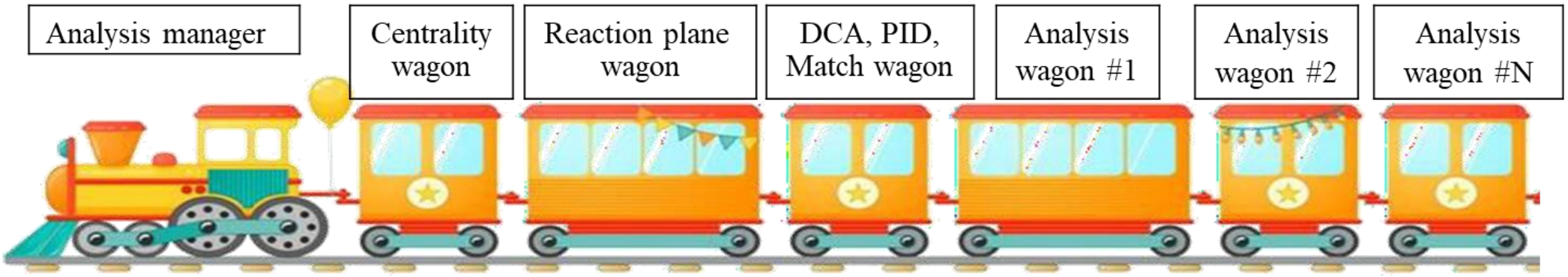
Summary statistics of using the DIRAC platform for BM@N Run 8 data processing

Heterogeneous distributed computing environment for the MPD experiment

❖ **Centralized Analysis Framework for access and analysis of data:**

- consistent approaches and results across collaboration, easier storage and sharing of codes and methods
- reduced number of input/output operations for disks and databases, easier data storage on tapes

❖ **Analysis manager reads event into memory and calls wagons one-by-one to modify and/or analyze data:**

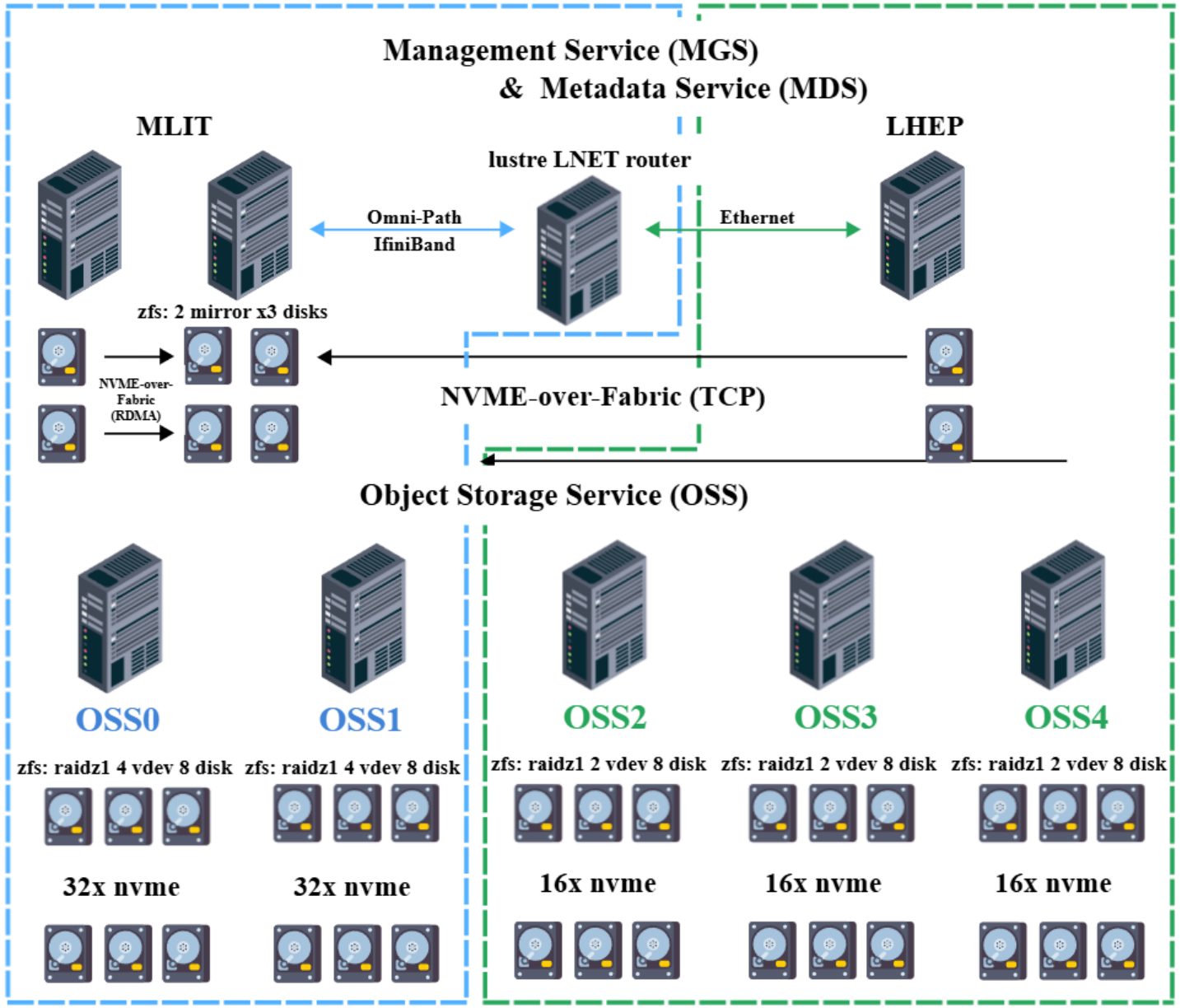


❖ **The first runs of analysis under this scheme took place in September 2023. Since then, "regular flights" have been carried out at the request of the physical data analysis groups of the MPD collaboration.**

❖ **12 productions of physical analysis of simulated data already done.**

- A typical analysis train run requires 2000 to 2500 cores and up to 20 GB of RAM per core.
- The train requires ~12 hours (at SC "Govorun") to process 50 million events for 10-15 train carriages.
- **1 150 000 000** simulated events were processed through the analysis trains.

Lustre distributed parallel file system for NICA



The distributed parallel file system Lustre is deployed among the SC"Govorun" (MLIT) and the cluster NCX (LHEP).

Lustre was created using two new RSC Tornado AFS servers.

Total capacity of Lustre is 3 PB

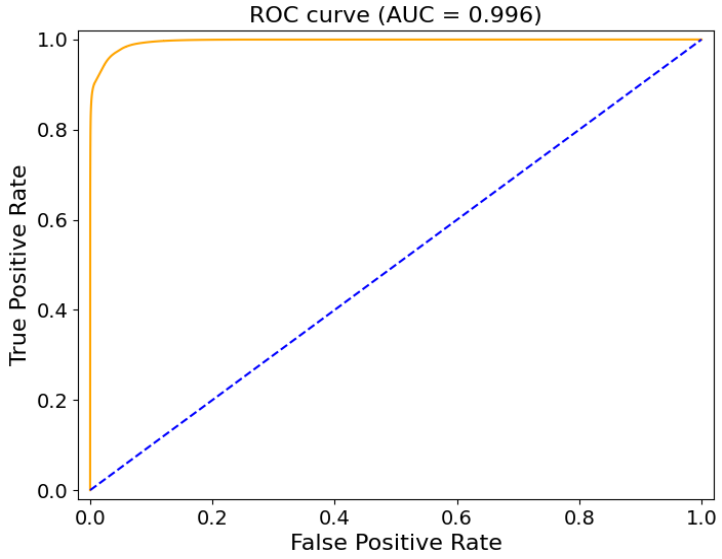
(SC “Govorun”- 2 PB, NCX – 1 PB)

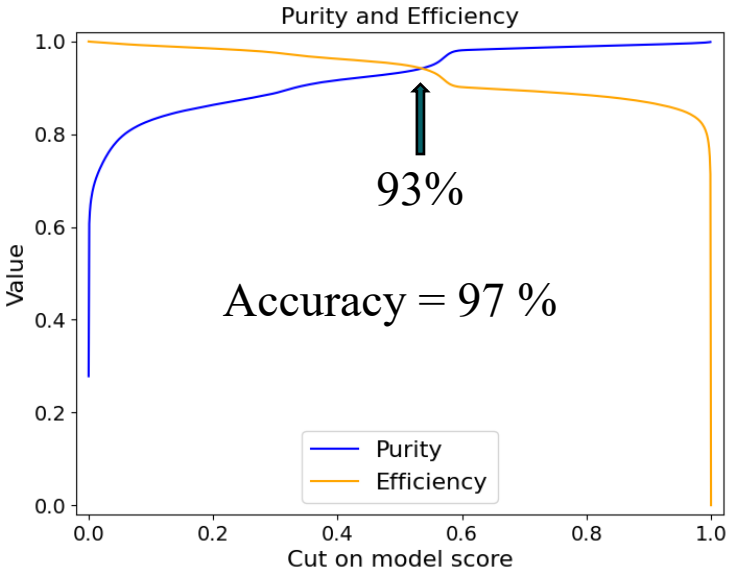
Copied 200 TB of MPD Data

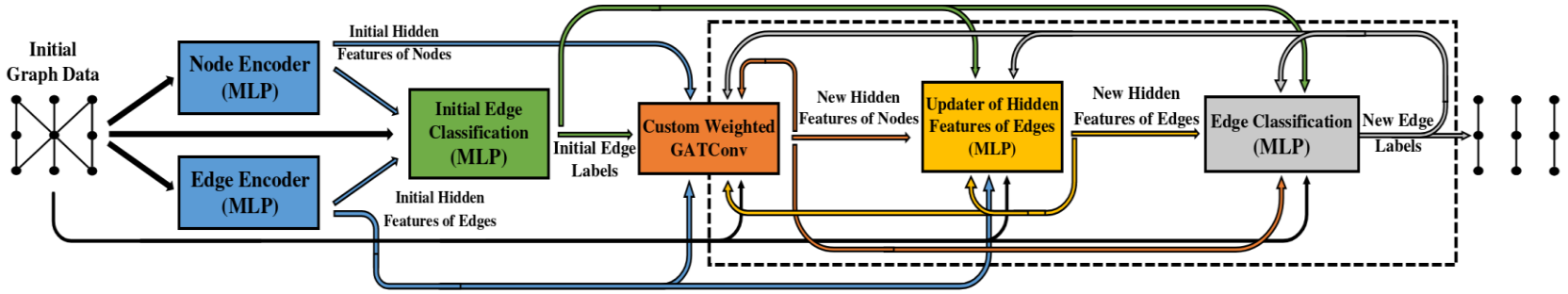
Maximum write speed 15 GB/s

- 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.

Training results of the Graph Neural Network for particle track reconstruction in the MPD of the NICA





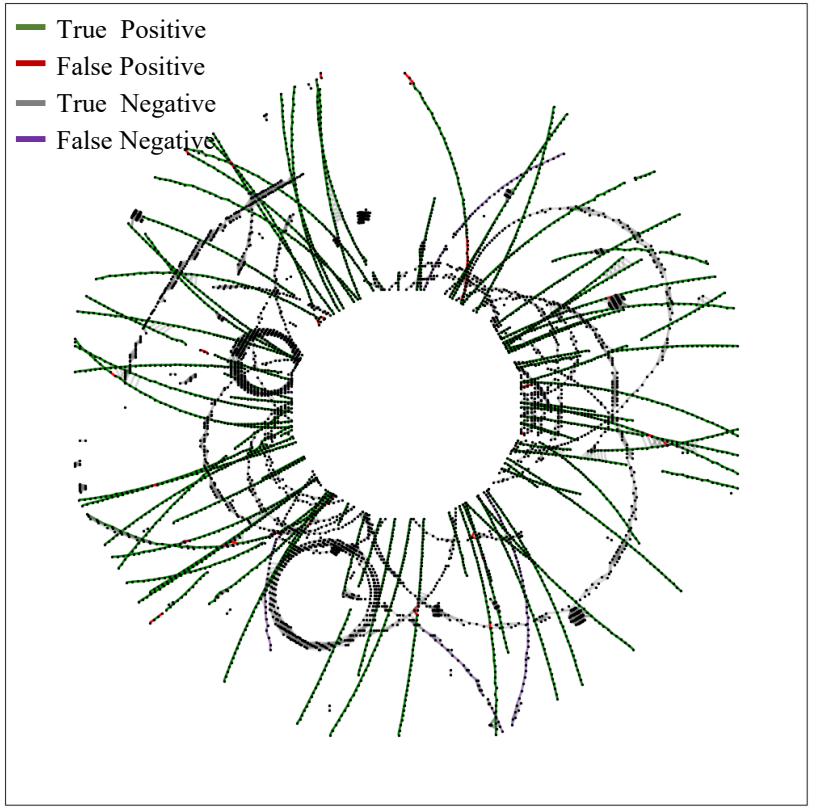


The main goal is the development of a Graph Neural Network for particle track reconstruction in the MPD of the NICA.

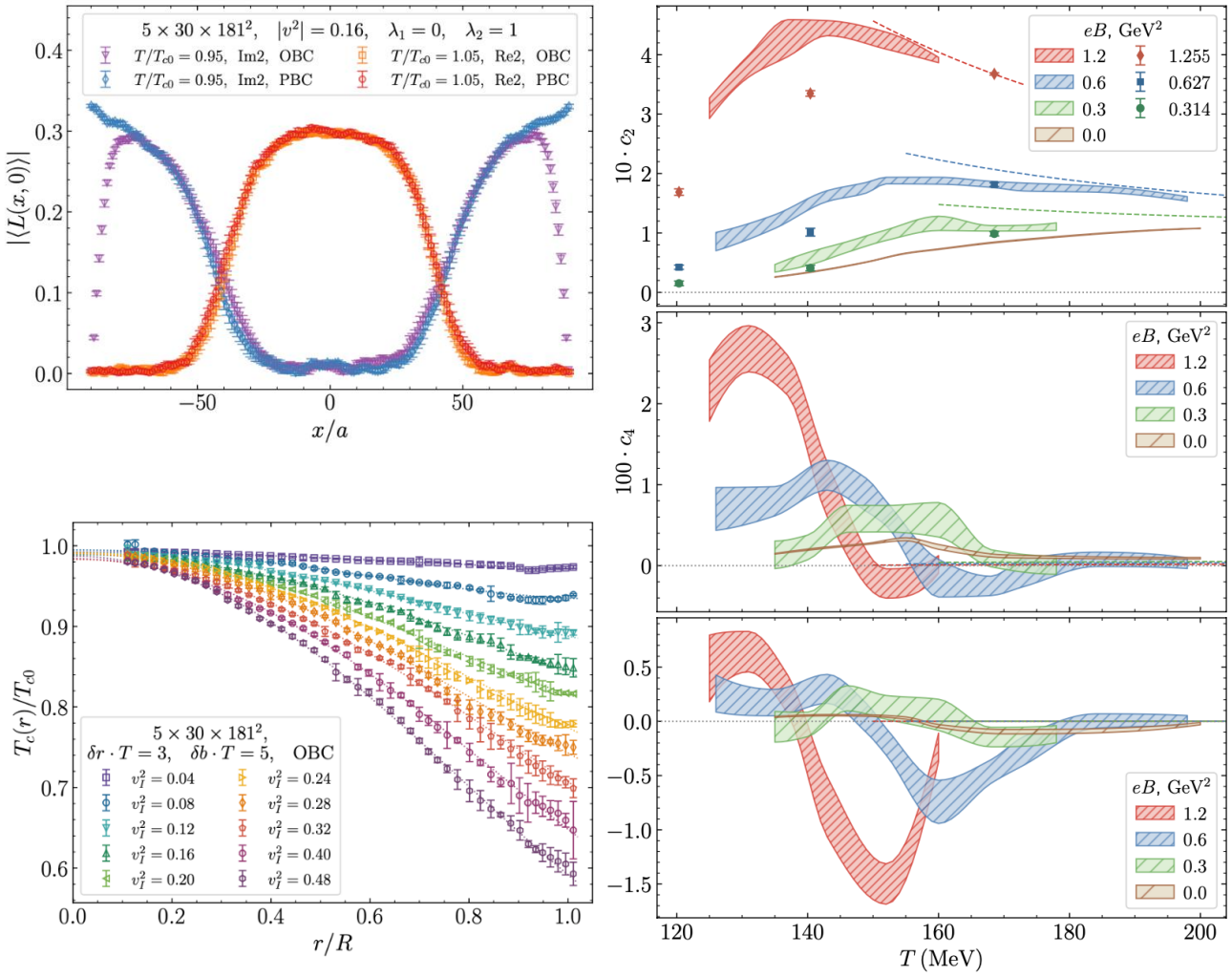
The work was carried out by Dr. Yauheni Talochka under strict guidance of Prof. Gennady Ososkov and Dr. Nikolay Voytishin.

The model was trained using an NVIDIA A100-SXM4-80GB

- Batch size = 1
- Epoch number = 100
- Event number = 1000
- GPU RAM usage ~ 50 GB
- Training time ~ 4 h



“Govorun” supercomputer for QCD tasks



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] Victor V. Braguta, Maxim N. Chernodub, Ilya E. Kudrov, Artem A. Roenko, and Dmitrii A. Sychev, “Moment of inertia and supervortical temperature of gluon plasma,” PoS LATTICE2023, 181 (2024), arXiv:2311.03947 [hep-lat].

[2] Victor V. Braguta, Maxim N. Chernodub, Artem A. Roenko, and Dmitrii A. Sychev, “Negative moment of inertia and rotational instability of gluon plasma,” Phys. Lett. B 852, 138604 (2024), arXiv:2303.03147 [hep-lat].

[3] Victor V. Braguta, Maxim N. Chernodub, Ilya E. Kudrov, Artem A. Roenko, and Dmitrii A. Sychev, “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] Victor V. Braguta, Maxim N. Chernodub, and Artem A. Roenko, “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] N. Astrakhantsev, V. V. Braguta, A. Yu. Kotov, and A. A. Roenko, “QCD equation of state at nonzero baryon density in an external magnetic field,” Phys. Rev. D 109, 094511 (2024), arXiv:2403.07783 [hep-lat].

“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) Kotov A. A., Kozhedub Y. S., Glazov D. A., Ilias M., Pershina V., Shabaev V. M. // ChemPhysChem. 2023. No 24. C. E202200680;
2) Ryzhkov A., Pershina V., Ilias M. and Shabaev V. // Phys. Chem. Chem. Phys.2023. No 25. C. 15362;
3) Savelyev I. M., Kaygorodov M. Y., Kozhedub Y. S., Malyshev A. V., Tupitsyn I.I., Shabaev V. M. // Phys. Rev. A. 2023. No 107. C. 042803;
4) Zaytsev V. A., Groshev M. E., Maltsev I. A., Durova A. V., Shabaev V. M. //Int. J. Quant. Chem. 2023. C. e27232.

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)

BioHlit project
https://cell.jinr.ru
http://mostlit.jinr.ru
http://bio-dashboards.jinr.ru/morris

CVAT cervices
http://159.93.36.88:8080
http://159.93.36.67:8080

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

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

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

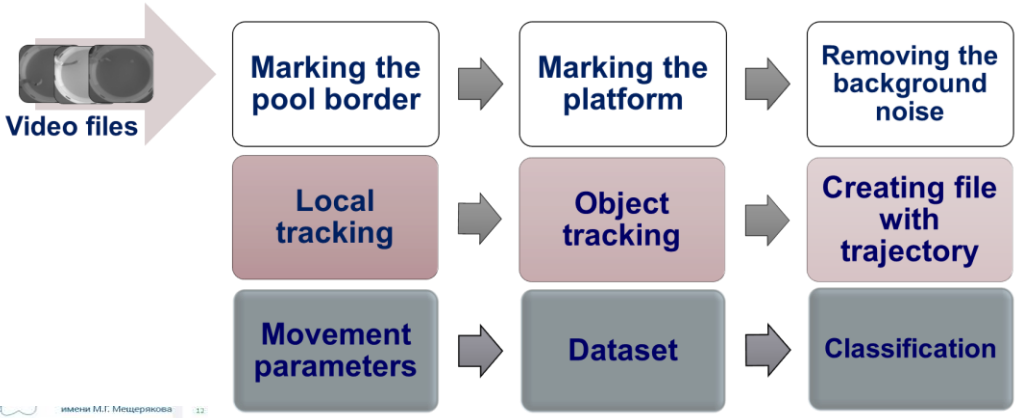
OpenCV
pandas
jupyter
Caffe
NumPy
scikit learn
Keras
PyTorch
JB
TensorFlow
theano
ultralytics
CVAT
FreeSurfer
kornia
Nipype: Neuroimaging in Python Pipelines and Interfaces
Joblib
Numba
matplotlib
Cirq
PENNYLANE

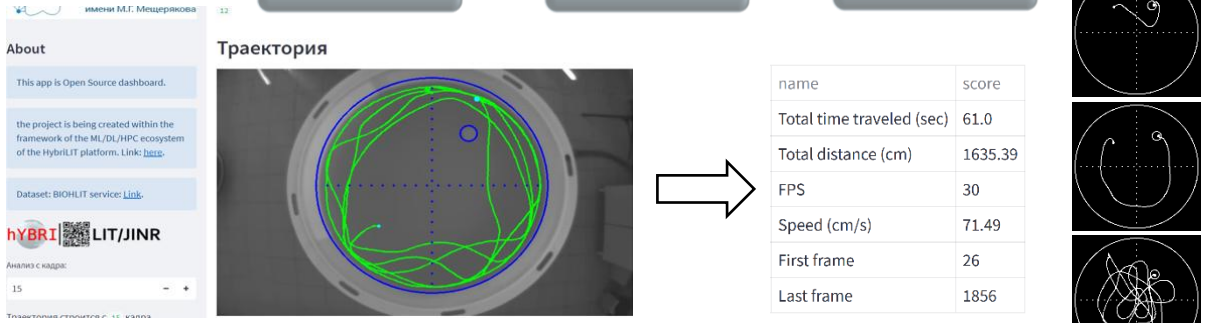
Services for BioProjects on ML/DL/HPC ecosystem of the HybriLIT platform

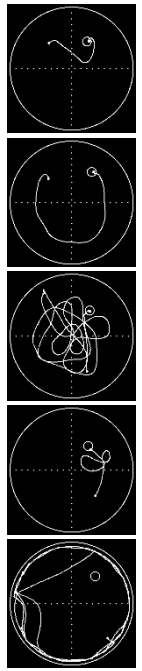
MLIT in collaboration with LRB JINR

Web service for «Morris Water Maze» behavioral test

http://bio-dashboards.jinr.ru/morris/Morris_tracking





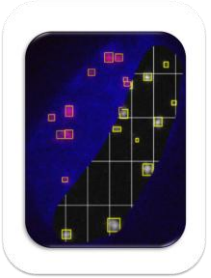


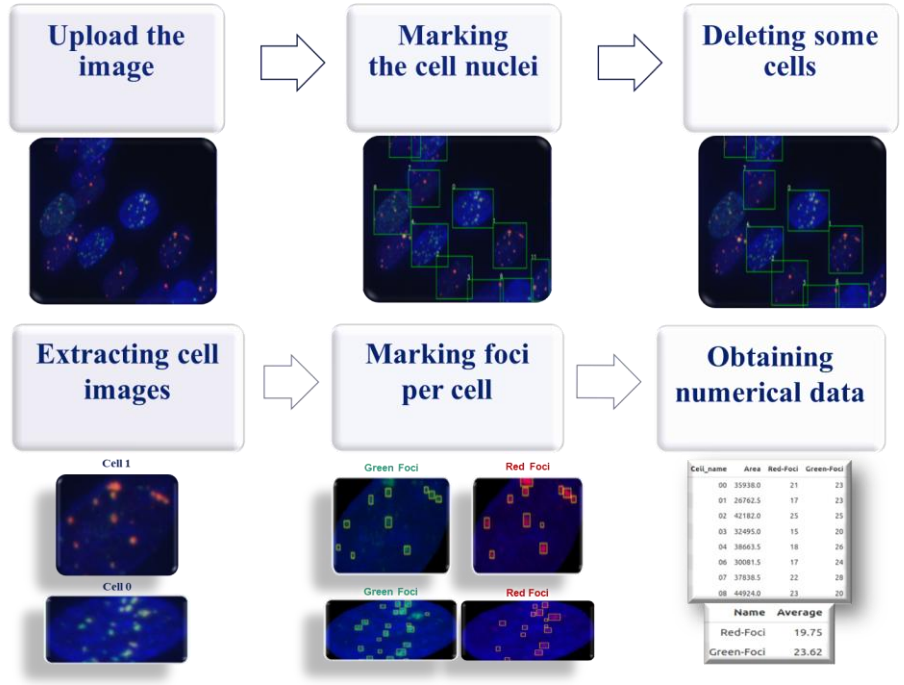
Developed web service for the trajectory analysis of laboratory animals in the «Morris Water Maze» behavioral test

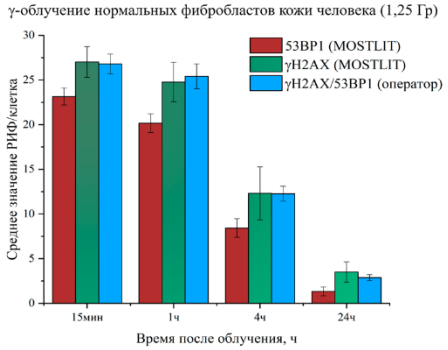
- ✓ Developed and tested algorithm for trajectory construction
- ✓ Received trajectories are annotated
- ✓ Created a dataset for classification
- ✓ Currently improving our Web service to classify the trajectories

MOSTLIT. Service for FOCI detection and analysis

https://mostlit.jinr.ru

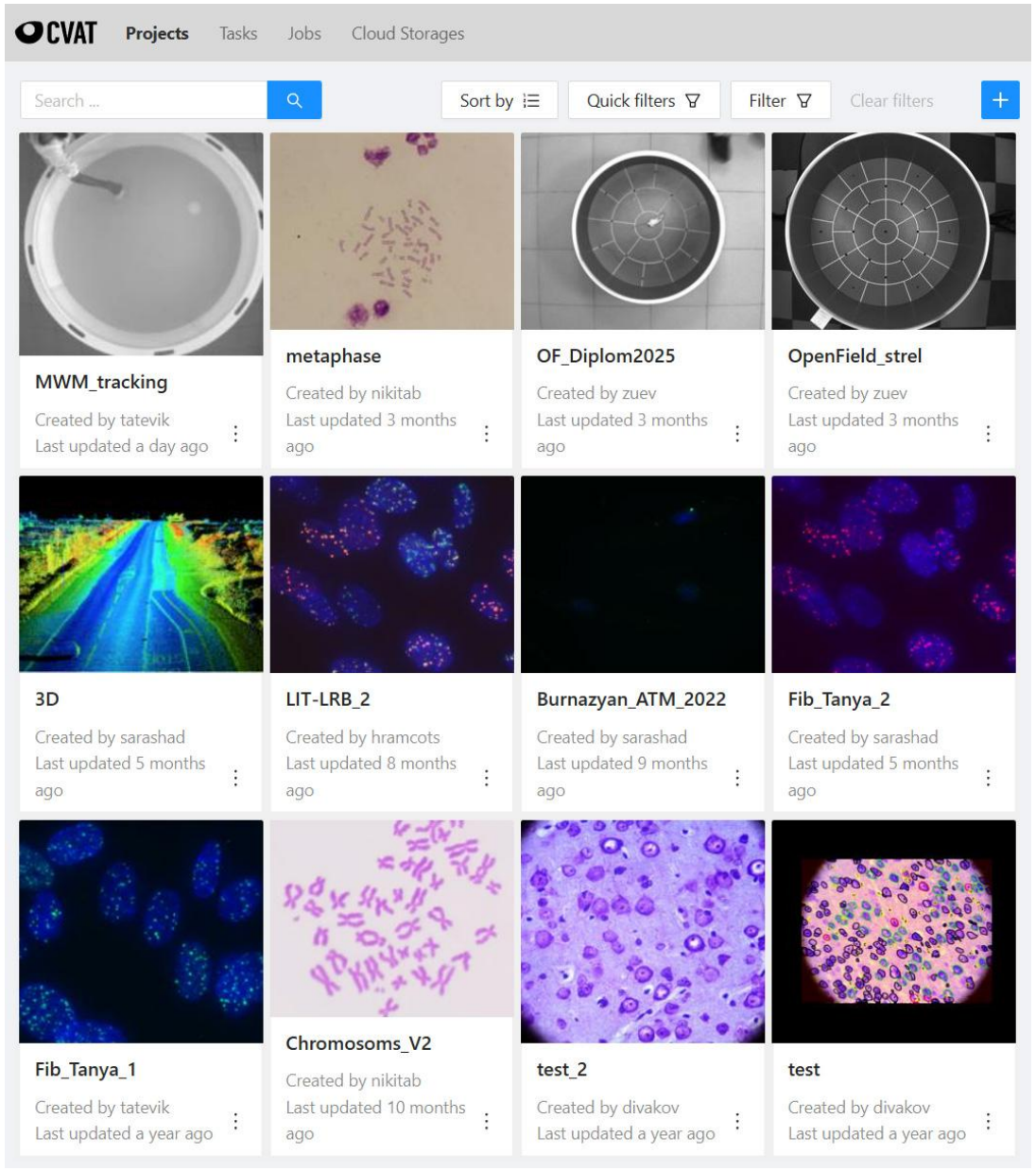


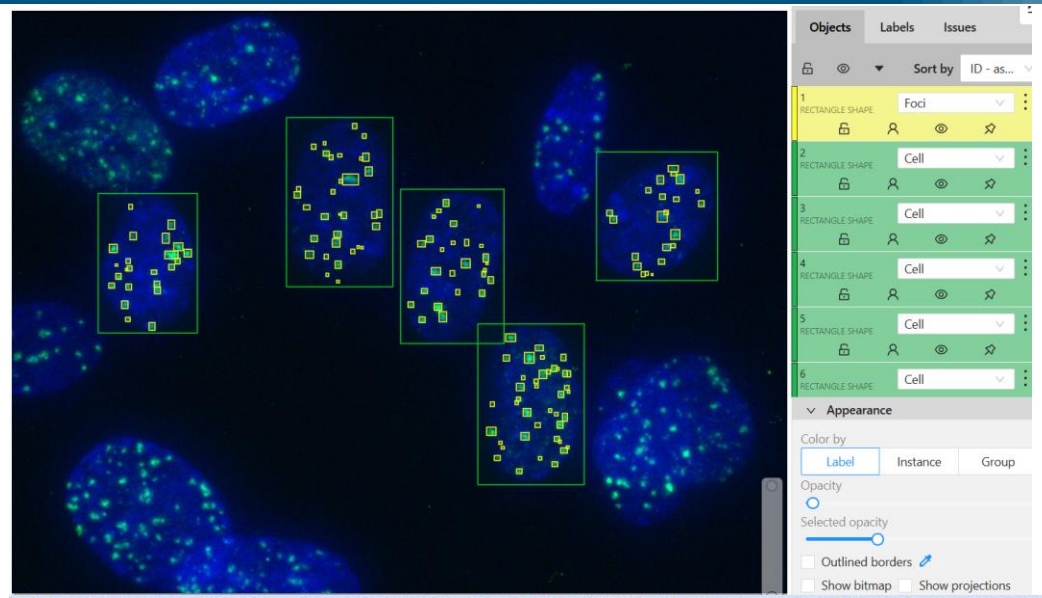


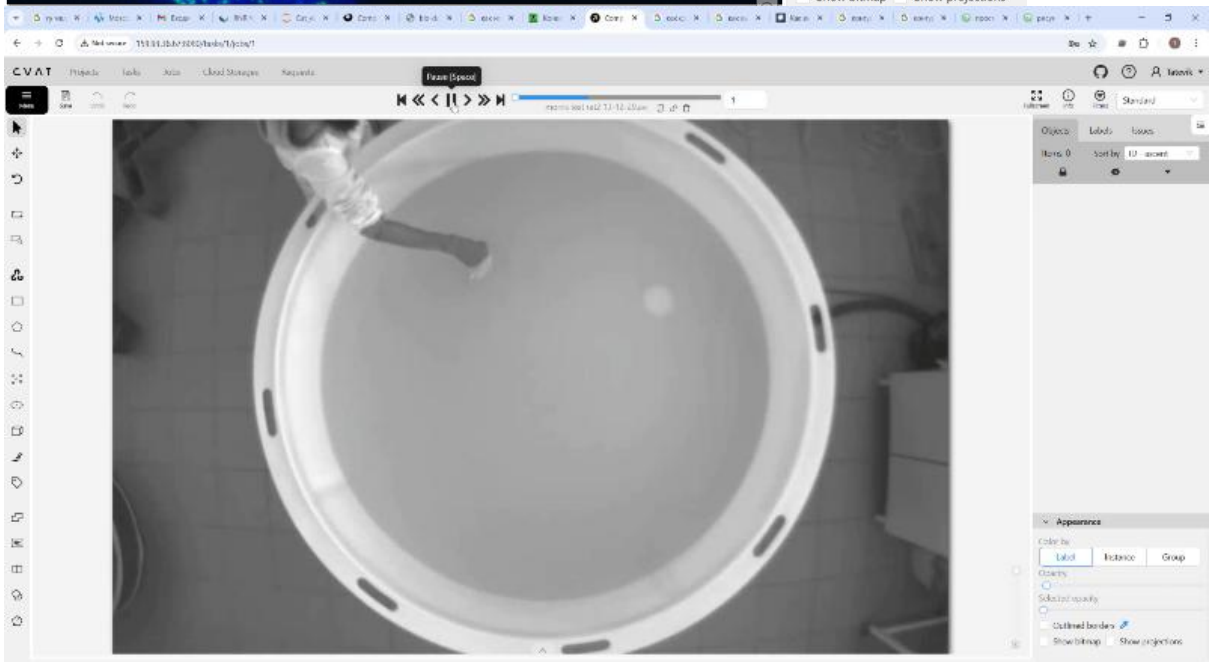


Developed web service to extract the cells from each data image and count the number of radiations induced foci. Functionality of the service allowed to analyze the group of images of an experiment, provide analytic information about average foci per cell, foci area and some other parameters.

CVAT. Image & Video Data Annotation Platform



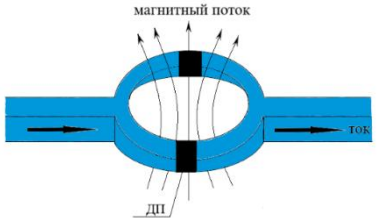




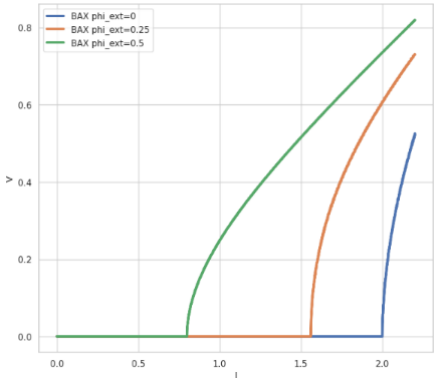
Josephson Junction Modeling on ML/DL/HPC Ecosystem on HybriLIT Platform

Collaboration of MLIT and BLTP

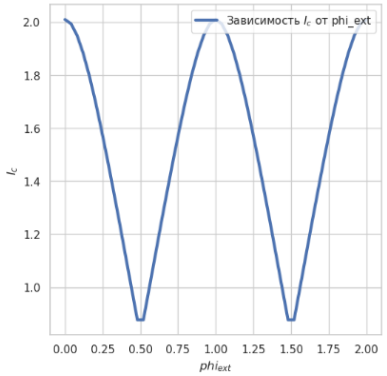
Python implementation of algorithms and tools for modeling the dynamics of a superconducting quantum interference device with two Josephson junctions (DC SQUID) http://studhub.jinr.ru:8080/jjbook/DC-SQUID.html



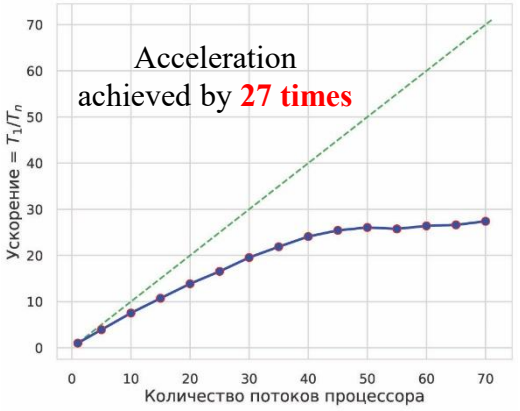
Schematic view of a SQUID



Calculated current-voltage characteristics for different values of external magnetic field flux



Dependence of the critical current on the magnitude of the external magnetic field flux



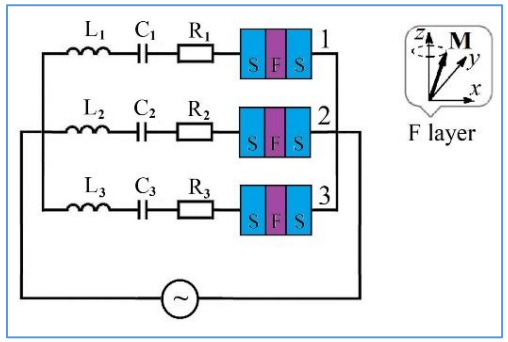
Numba

Acceleration of computing

A toolkit for modeling the physical properties of a superconducting quantum interference device with two Josephson junctions has been developed. Algorithms for calculation of the currant voltage characteristics (CVC) of a SQUID under the influence of an external magnetic field and the external magnetic field dependence of critical current of a SQUID have been implemented. The software implementation is performed using the Numba library.

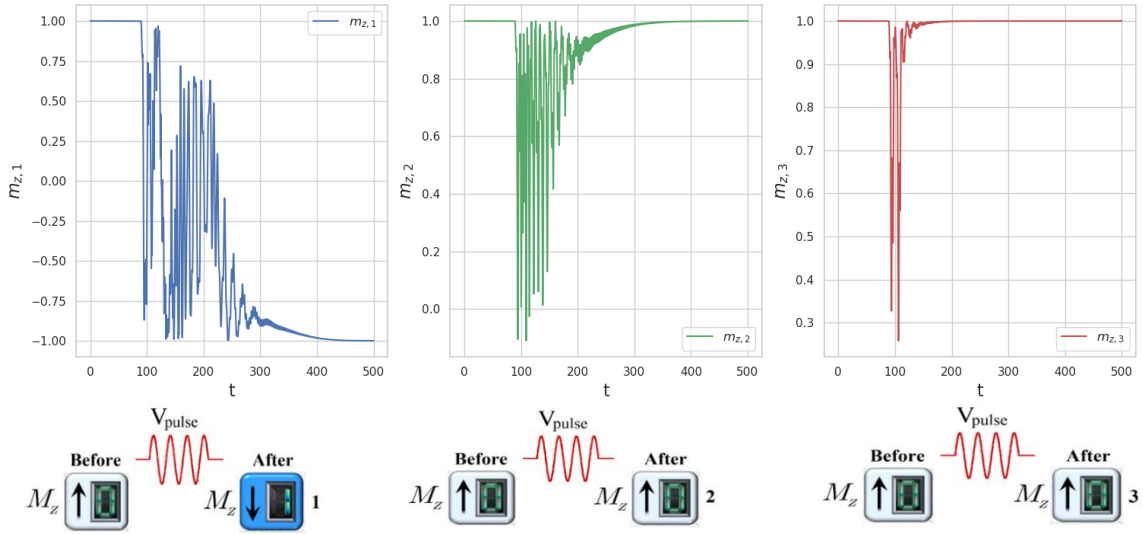
A. R. Rahmonova, O. I. Streltsova, M. I. Zuev, I. R. Rahmonov, A. V. Nechaevskiy, Proceedings of the All-Russian Conference with International Participation, pp. 347-353 (2024).

Python implementation of algorithms and toolkit for investigation of the controllable magnetization reversal in a system of three φ_0 junctions with LCR circuits



Equivalent circuit of a system consisting of three φ0 junctions connected to LCR circuits.

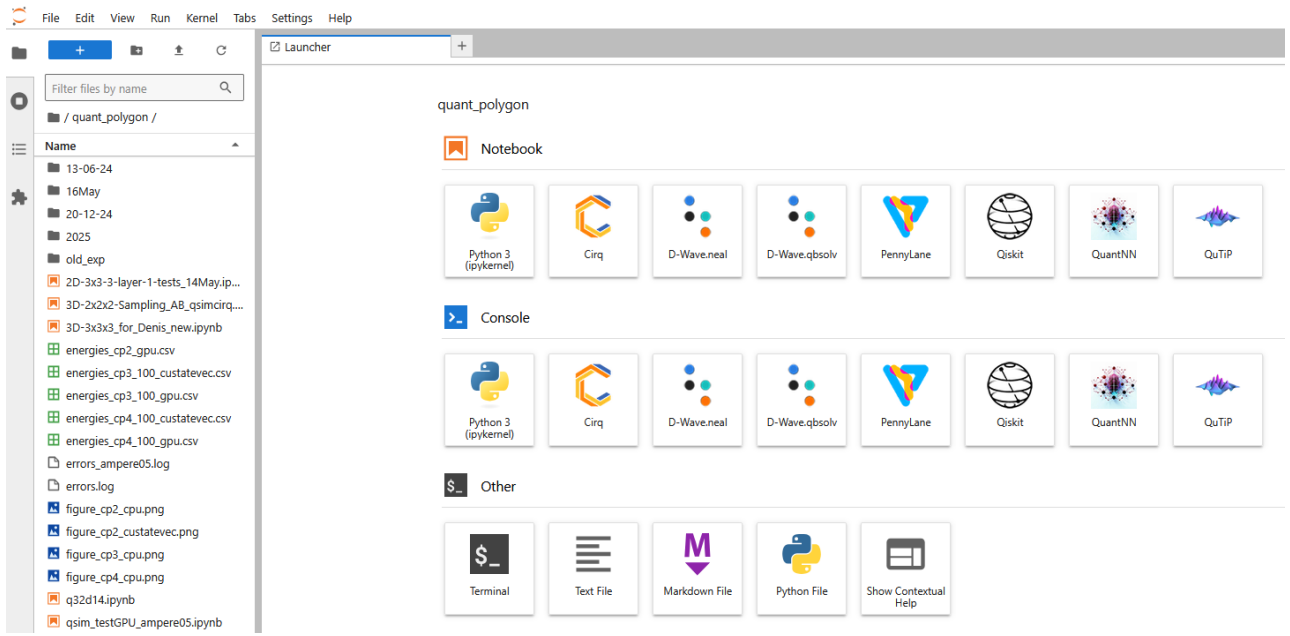
A system consisting of three φ_0-junctions, each of which is connected in series by LCR-circuits, is investigated. In this case, each LCR-circuit has a eigen frequency. Based on numerical simulation, it is shown that by applying an alternating voltage pulse with a frequency corresponding to the natural frequency of the selected LCR-circuit, it is possible to realize a magnetization reversal in the φ_0-junction connected to the LCR-circuit. The obtained results can be used in the development of superconducting electronics and spintronics devices, in particular in the development of cryogenic memory based on the φ_0-junction.

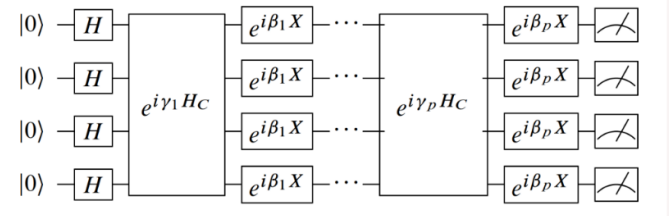


Polygon for quantum computing

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

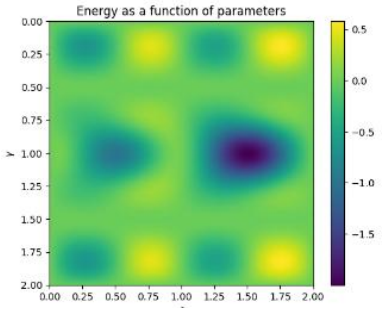
Technical implementation.
To work with quantum simulators, a separate server has been allocated, on which the Anaconda package is locally installed. Quantum simulators are installed in virtual environments. Due to this, it is possible to avoid conflicts between versions of libraries that are installed with simulators. Virtual environments are output to the JupyterLab interface by creating a computing core in an interactive ipython shell, which is installed in each environment separately.





A quantum circuit to the variation ansatz of QAOA

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



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 GBБ RAM GPU**.

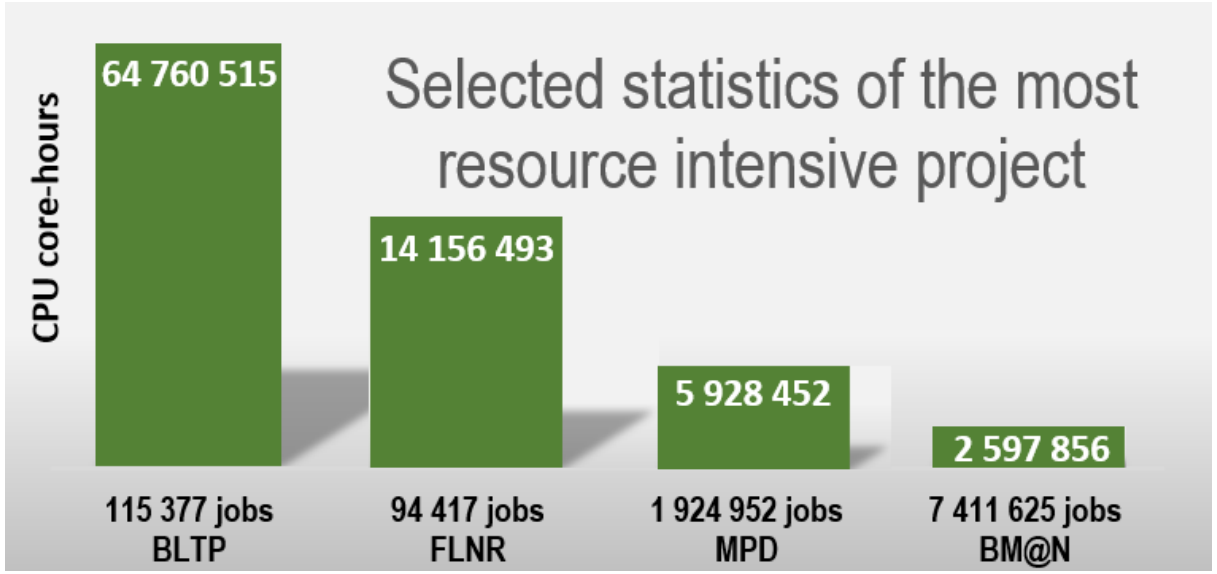
Ising Model 3x3x3 lattice 27 qubits	AMD EPYC 7763, 128 threads	Intel Xeon Platinum 8368Q, 128 threads	NVIDIA A100, cuStateVec
Computation time	3 h 20 min	3 h 10 min	**14 min 35 sec**

Yu. Palii, A. Bogolubskaya, and D. Yanovich: Quantum Approximation Optimization Algorithm for the Ising Model in an External Magnetic Field // PEPAN, V. 55, N. 3. Pp. 600-602, 2024.

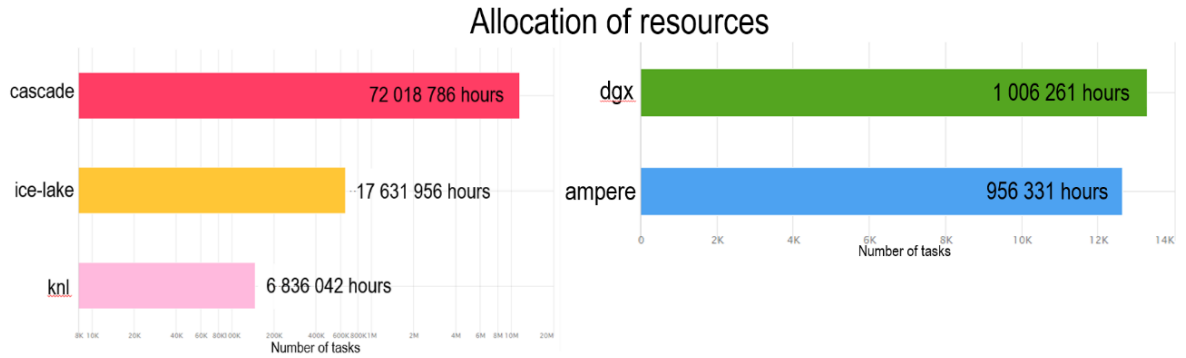
Using of the “Govorun” Supercomputer

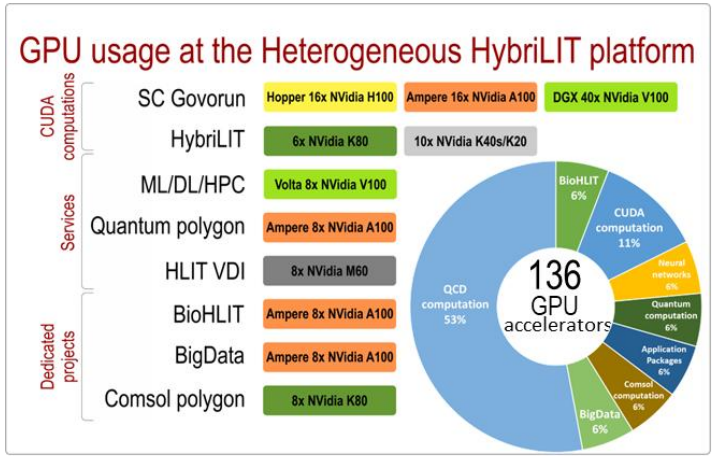
The resources of the “Govorun” SC are used by scientific groups from all the Laboratories of the Institute. The projects that mostly intensive use the CPU resources of the “Govorun” SC:

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

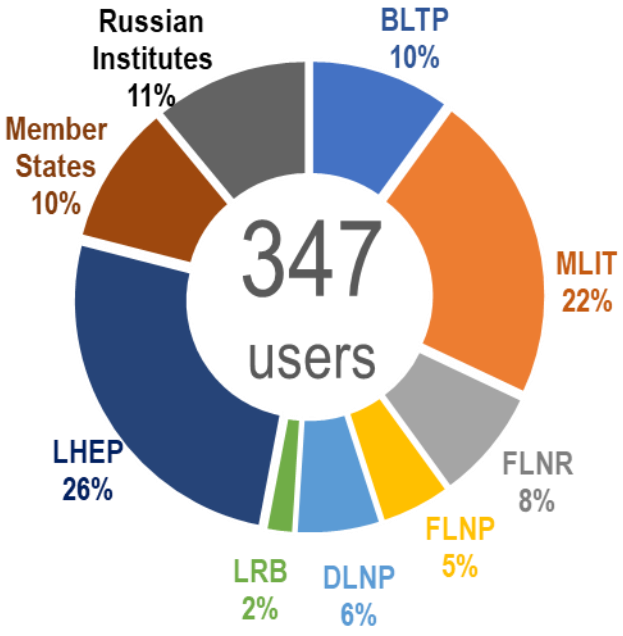


“Govorun” SC users completed 12,3 M jobs what corresponds to the 98 M core-hours.
The average load of the CPU component was 97.2%
The average load of the GPU component:
DGX load was 99.2%, Ampere load was 87,7%.



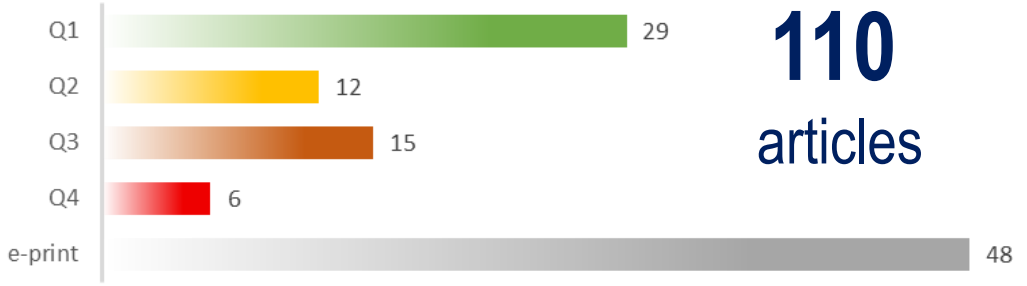


Publications



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.

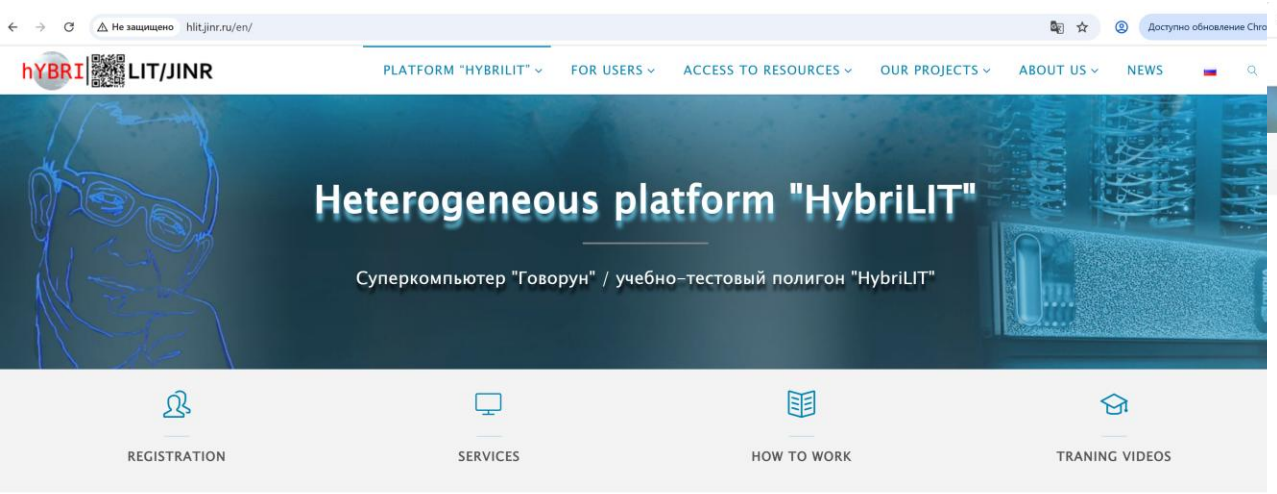


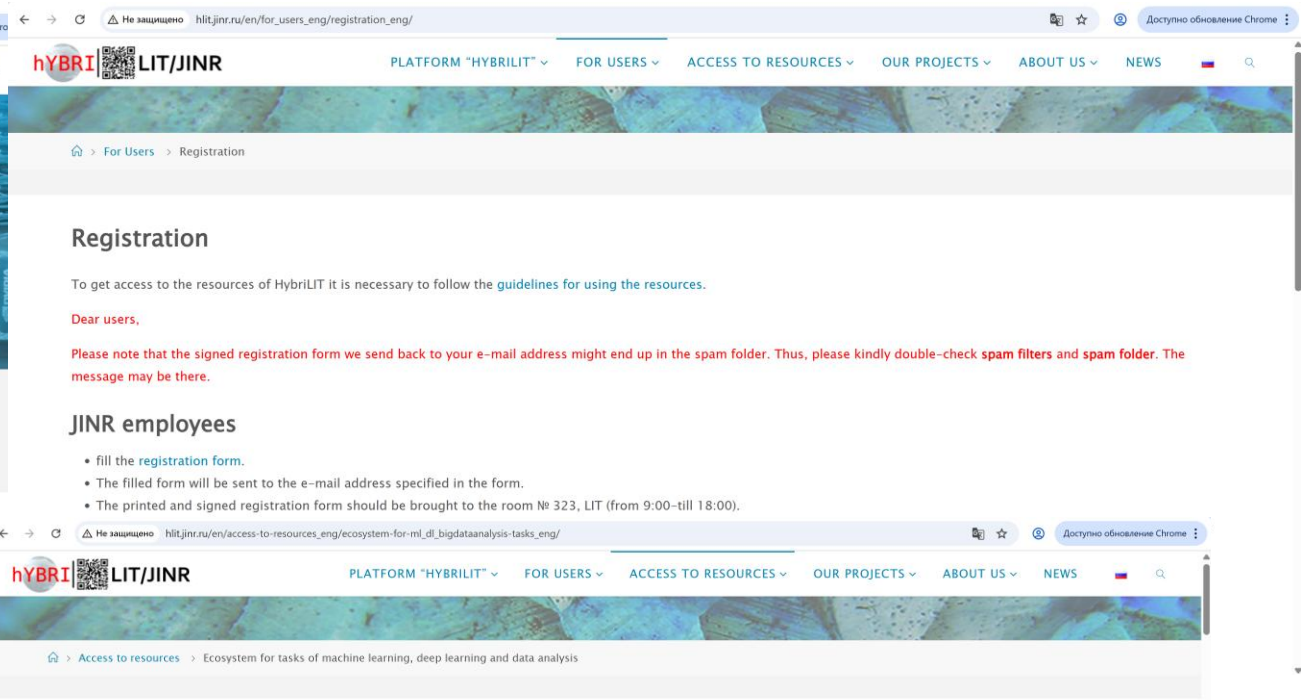
Research results obtained using the supercomputer resources since 2018 are presented in 501 publications. Two of them were prepared in Nature Physics:

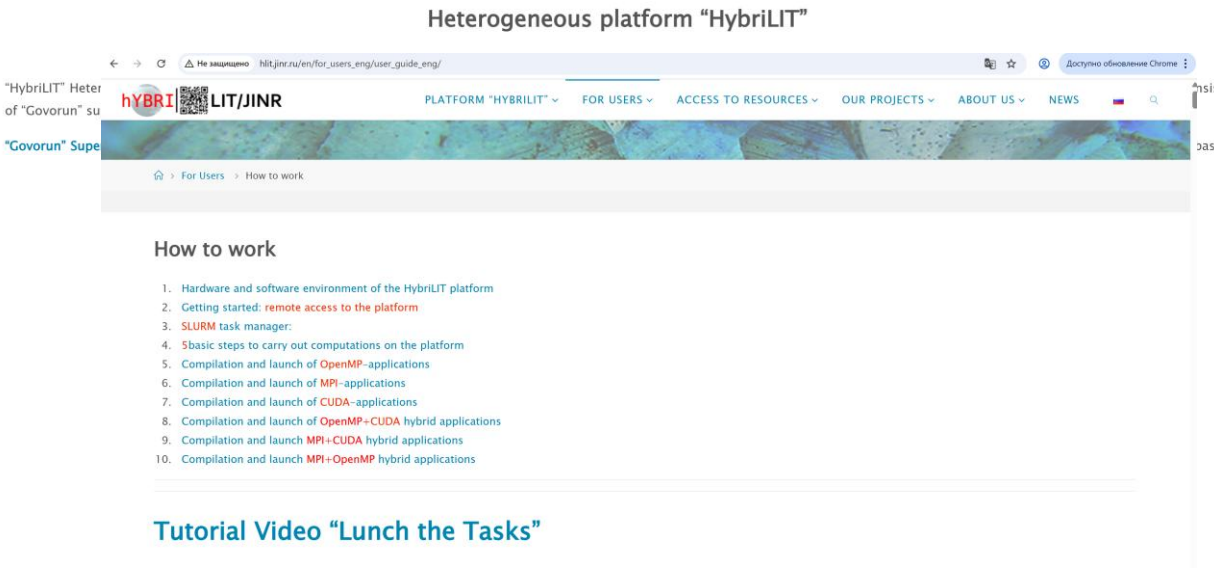
- M. Kircher … , O. Chuluunbaatar et al. Kinematically complete experimental study of Compton scattering at helium atoms near the threshold. Vol. 16. № 4. Pp. 756-760
- BM@N Collaboration. Unperturbed inverse kinematics nucleon knockout measurements with a 48 GeV/c carbon beam. Vol. 17. Pp. 693-699

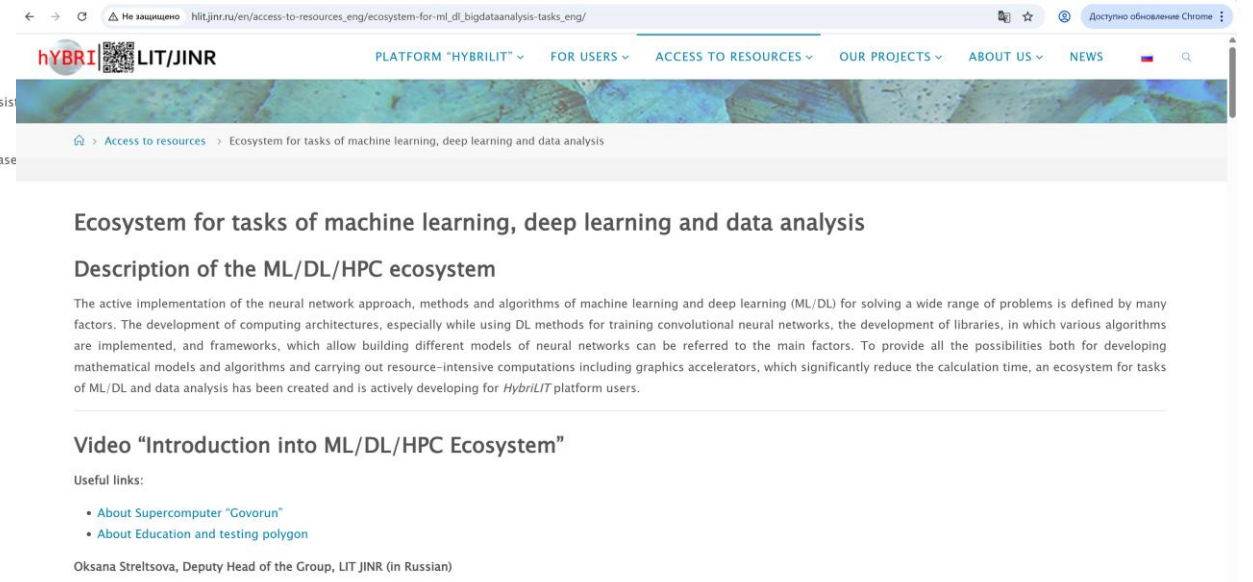
“Govorun” supercomputer

http://hlit.jinr.ru/









Thank you for your attention

HYBRILIT HETEROGENEOUS PLATFORM at MLIT JINR:

http://hlit.jinr.ru