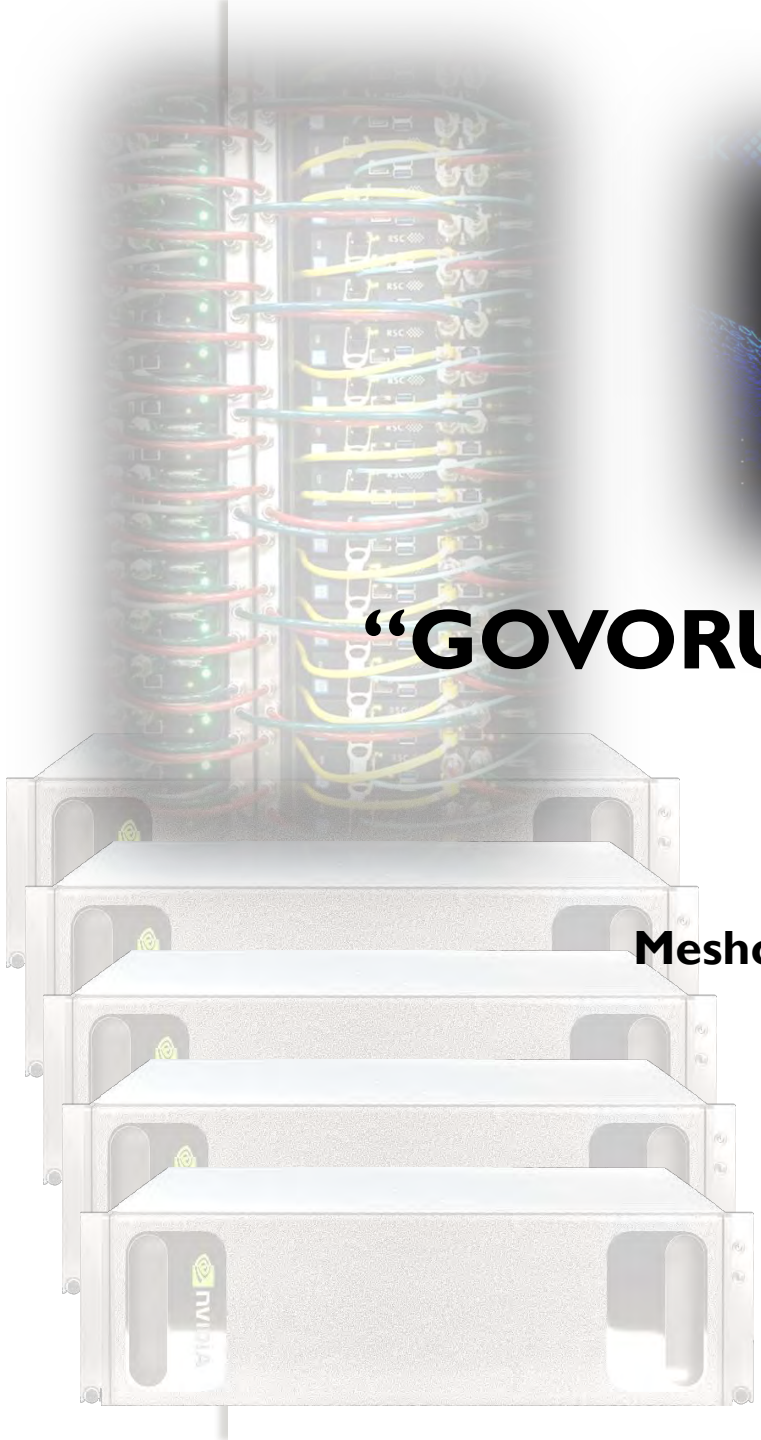
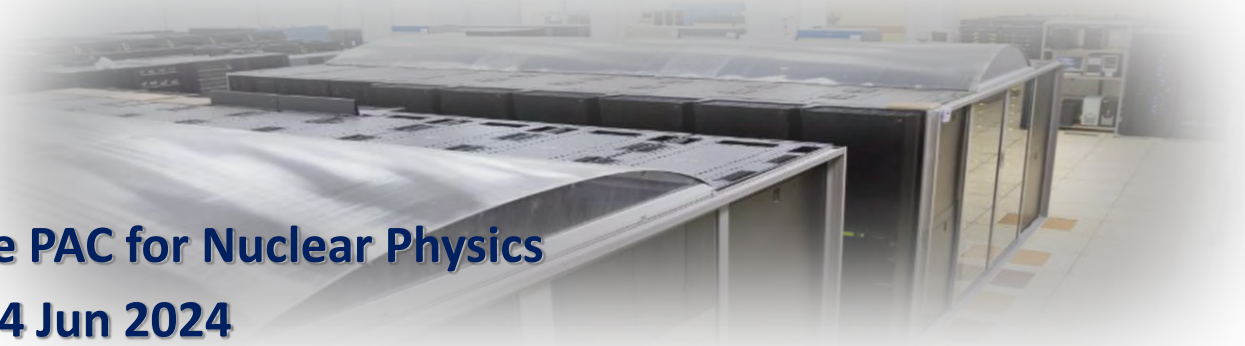


“GOVORUN” supercomputer for JINR tasks

D.V. Podgainy

Meshcheryakov Laboratory of Information Technologies



59th meeting of the PAC for Nuclear Physics

13–14 Jun 2024

History

The Laboratory of Computing Techniques and Automation of the Joint Institute for Nuclear Research in Dubna was founded in August 1966.

The main directions of the activities at the Laboratory are connected with the provision of networks, computer and information resources, as well as mathematical support of a wide range of research at JINR in high energy physics, nuclear physics, condensed matter physics, etc.

Computing is an integral part of theory, experiment, technology development

(17.09.1910 – 24.05.1994)

(18.03.1930 – 21.07.1989)

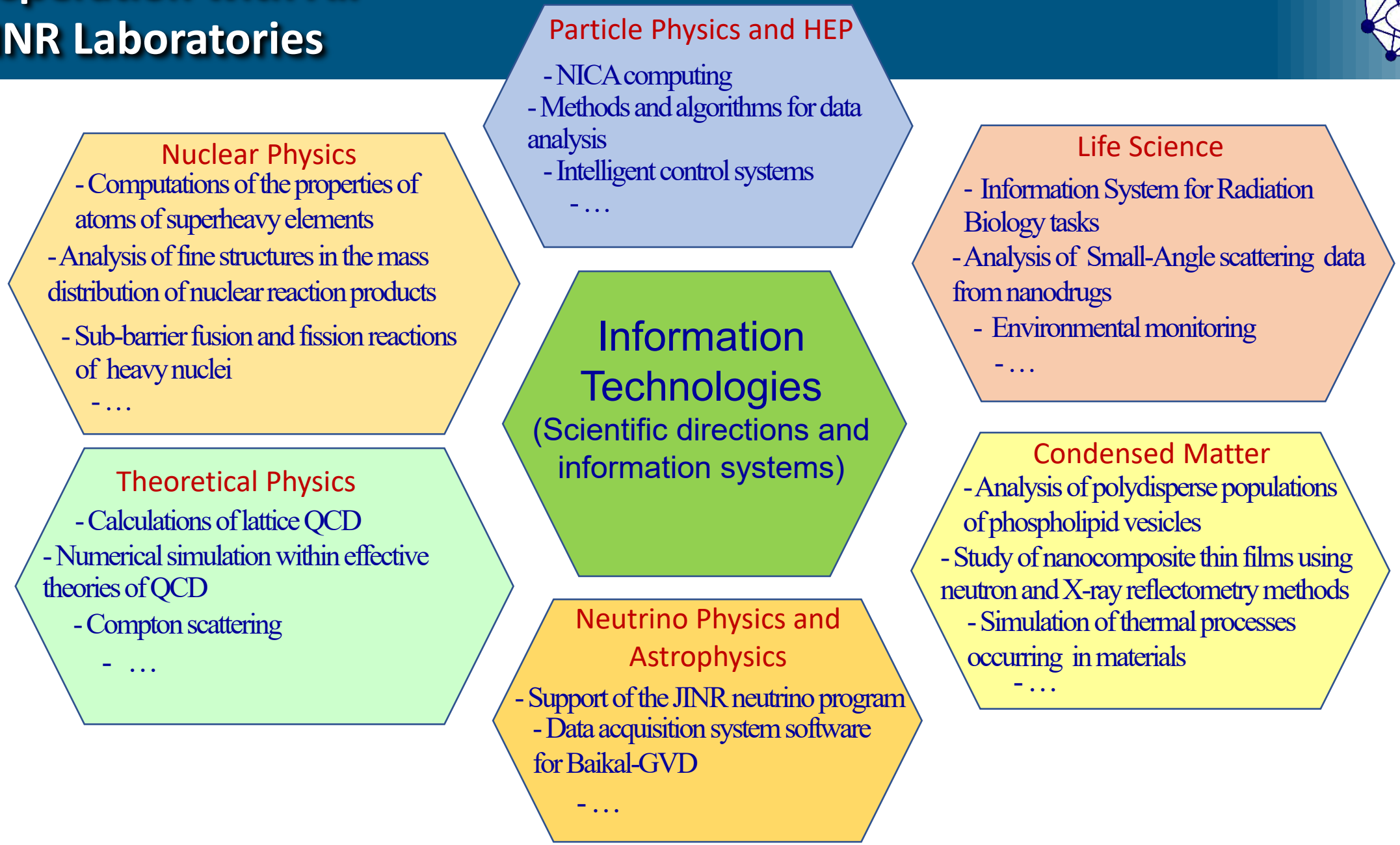
On 25 March 2021 the Committee of Plenipotentiary Representatives of the Governments of the JINR Member States **decided to name the Laboratory of Information Technologies after M. G. Meshcheryakov** for his outstanding contribution to the creation and development of the network infrastructure and the Information and Computing Complex of the Laboratory, the Institute, and the Member States.

MLIT today: Scientific IT-ecosystem

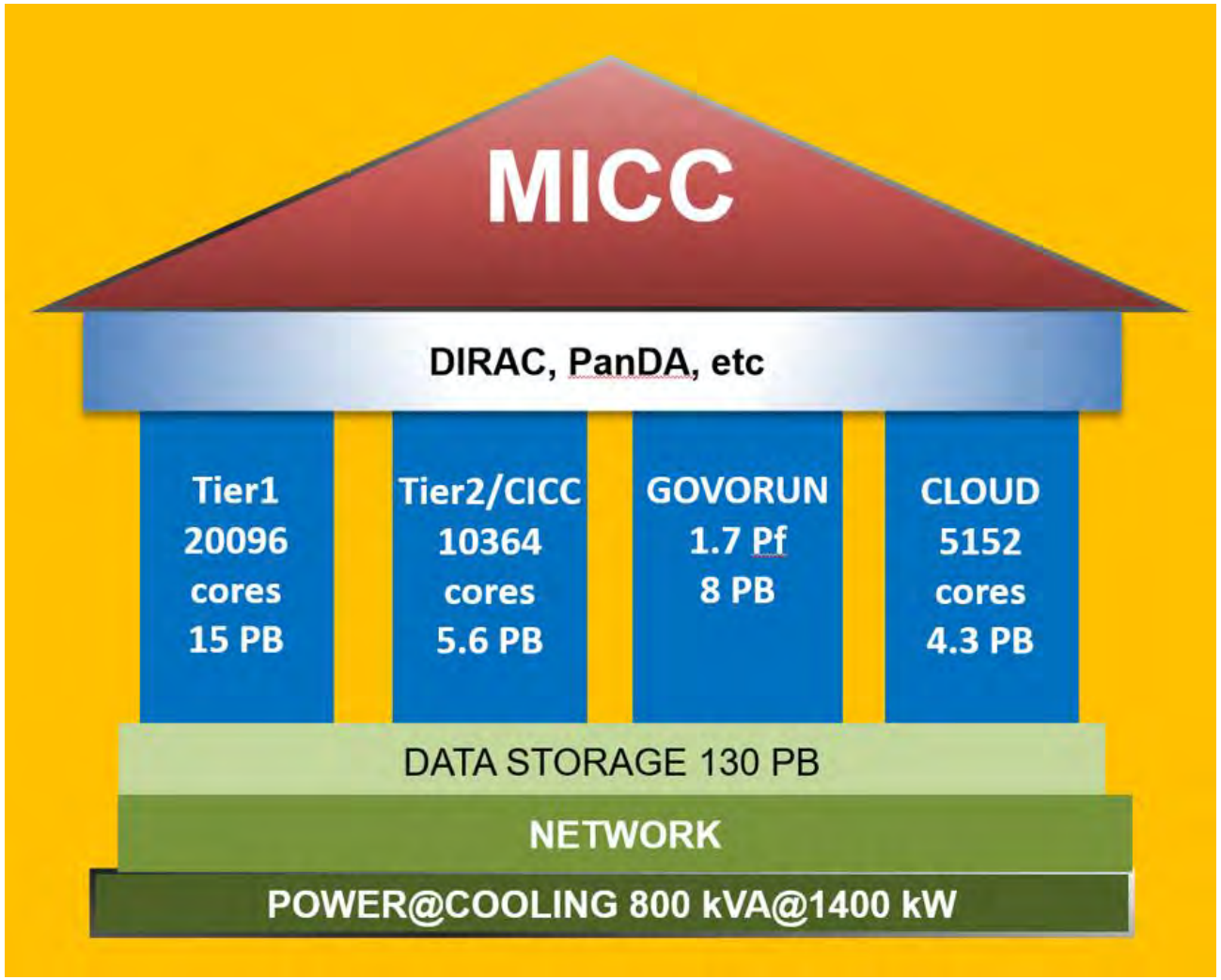
Staff: 311
Scientists: 108
Doctors of Science: 23
Candidates of Science: 61
Campus network 2x100 Gbps
Multisite network 4x100 Gbps
Telecommunication channel 3x100 Gbps
Grid Tier1 and Tier2 for global data processing
JINR Cloud computing
JINR Member States' Cloud environment
"Govorun" supercomputer

- The coordinated development of interconnected IT technologies and computational methods
- Providing the IT services necessary for the fulfillment of the JINR Topical Plan on Research and International Cooperation in an efficient manner.
- Building world-class competence in IT and computational physics.
- 24x7 support of the computing infrastructure and services.

Cooperation with All JINR Laboratories



Multifunctional Information and Computing Complex (MICC)



4 advanced software and hardware components

- Tier1 grid site
- Tier2 grid site
- hyperconverged "Govorun" supercomputer
- cloud infrastructure

Distributed multi-layer data storage system

- Disks
- Robotized tape library

Engineering infrastructure

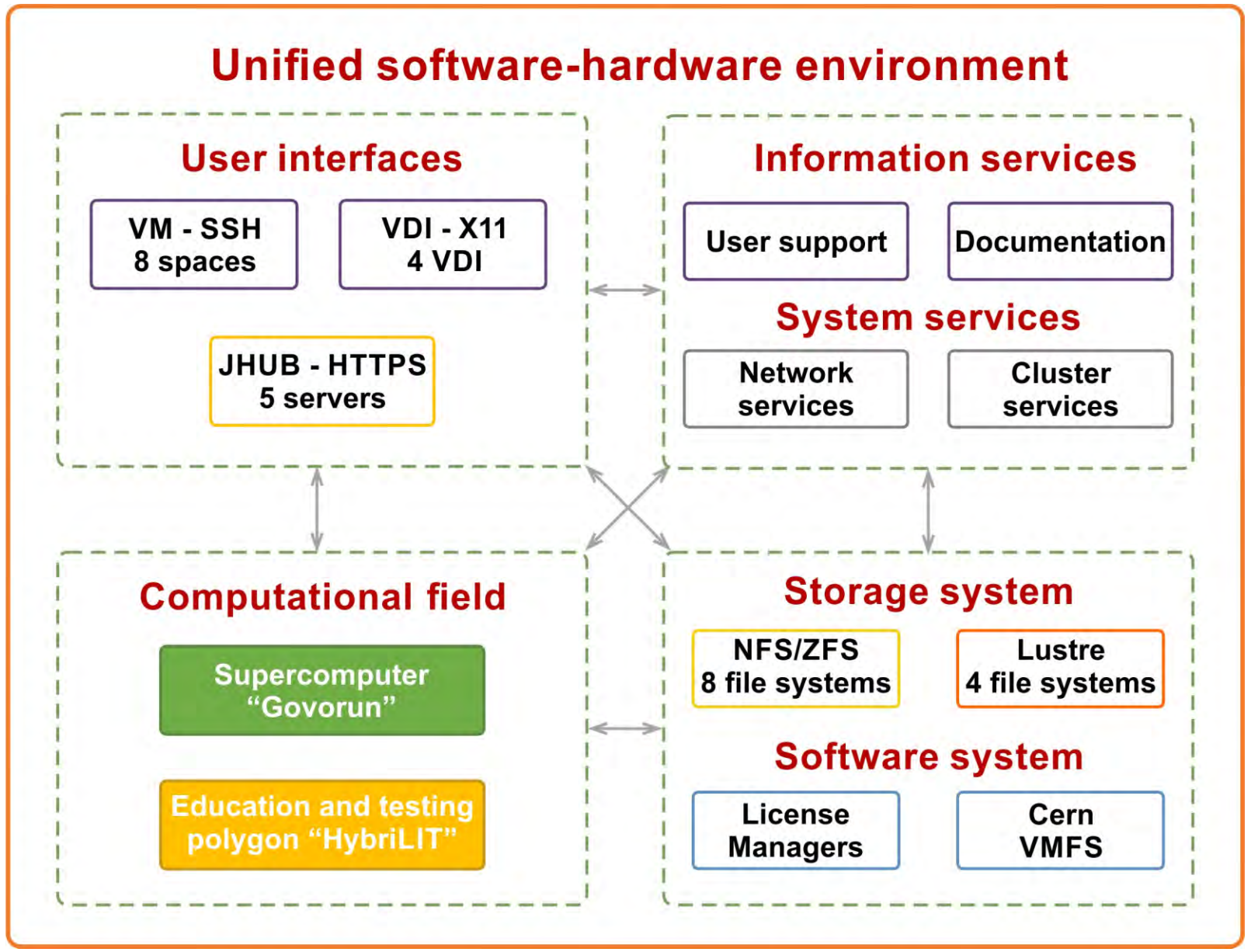
- Power
- Cooling

Network

- Wide Area Network
- Local Area Network

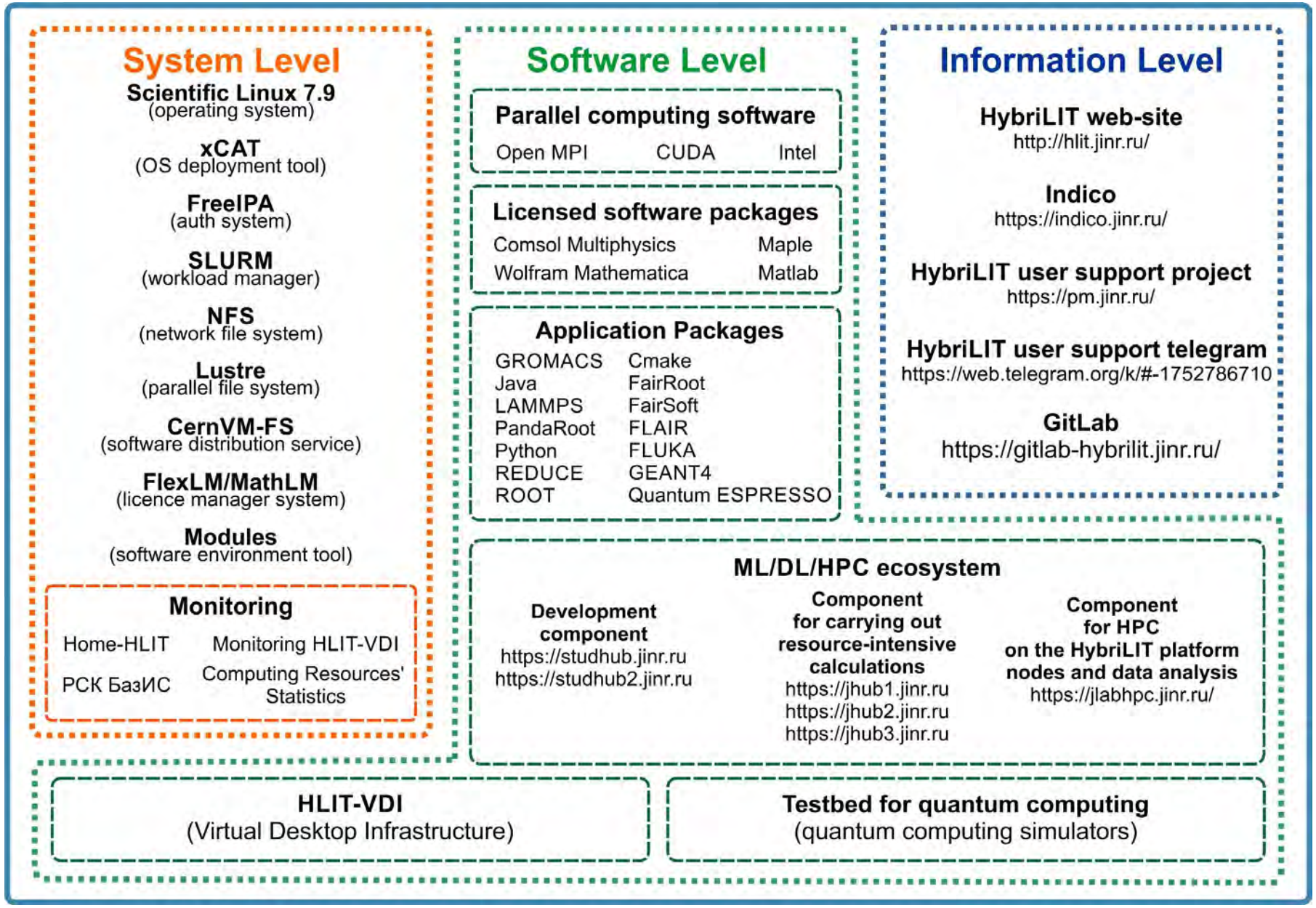
The main objective of the project is to ensure multifunctionality, scalability, high performance, reliability and availability in 24x7x365 mode for different user groups that carry out scientific studies within the JINR Topical Plan

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



Development of the heterogeneous HybriLIT platform

Cluster HybriLIT 2014:
Full peak performance:
140 TFlops for single precision;
50 TFlops for double precision

#18 в Top50

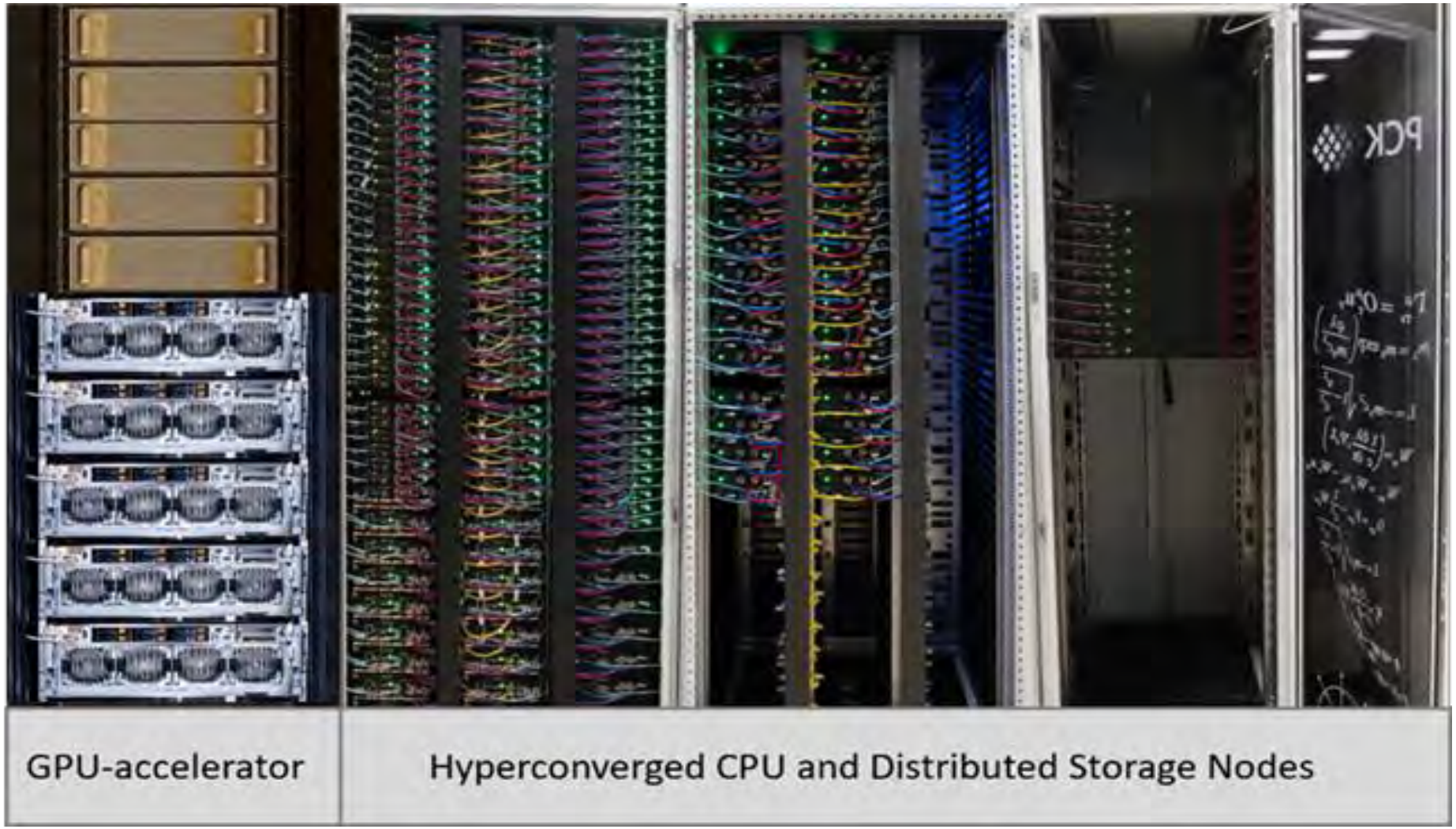
“Govorun” supercomputer
First stage 2018:
Full peak performance :
1 PFlops for single precision
500 TFlops for double precision
9th in the current edition of the IO500 list (July 2018)

#10 в Top50

“Govorun” supercomputer
Second stage 2019:
Full peak performance :
1.7 PFlops for single precision
860 TFlops for double precision
288 ТВ ССХД with I/O speed >300 Gb/s
17th in the current edition of the IO500 list (July 2020)

Russian DC Awards 2020 in “The Best IT Solution for Data Centers”

"Govorun" supercomputer



Current status:

163 hyperconverged compute CPU nodes

80 GPU accelerators

Total peak performance:

1.7 PFlops DP

3.4 PFlops SP

Total capacity of Hierarchical Storage:

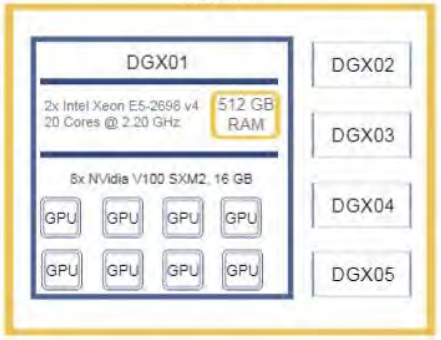
8.6 PB

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

The GPU-component of the “Govorun” Supercomputer

2017

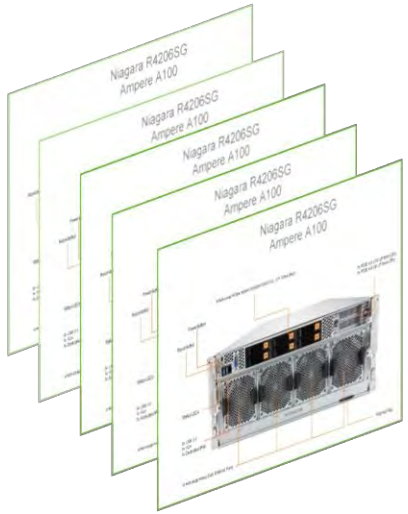
DGX-1



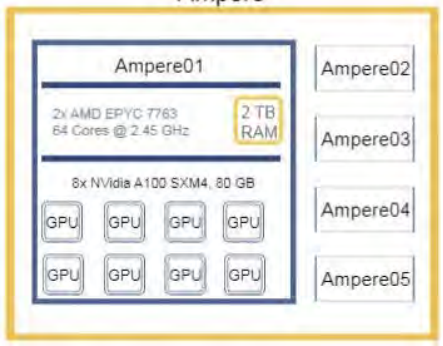
40 NVIDIA V100

+

2023



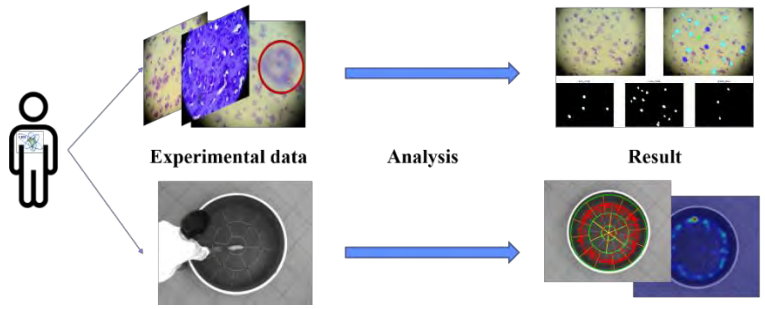
Ampere



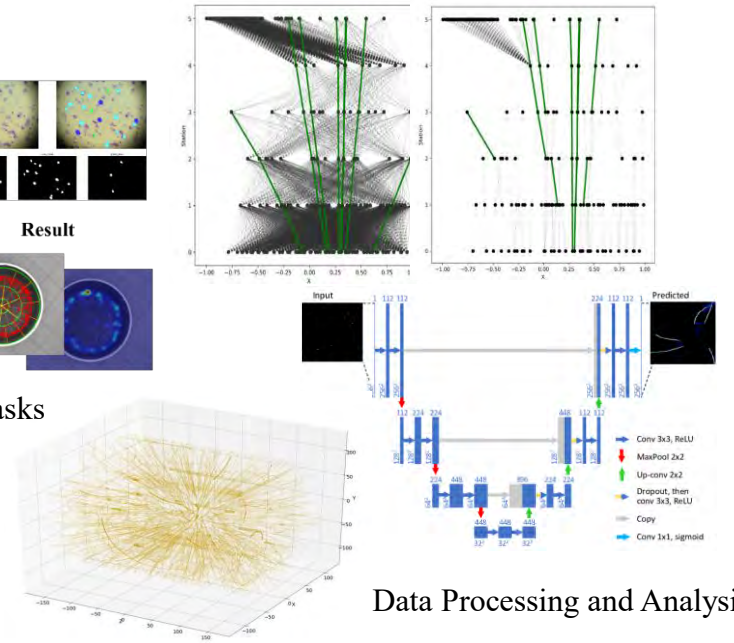
40 NVIDIA A100

Total peak performance of the GPU-component:
900 Tflops for Double-Precision computations
26 Pflops for Half-Precision computations

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.

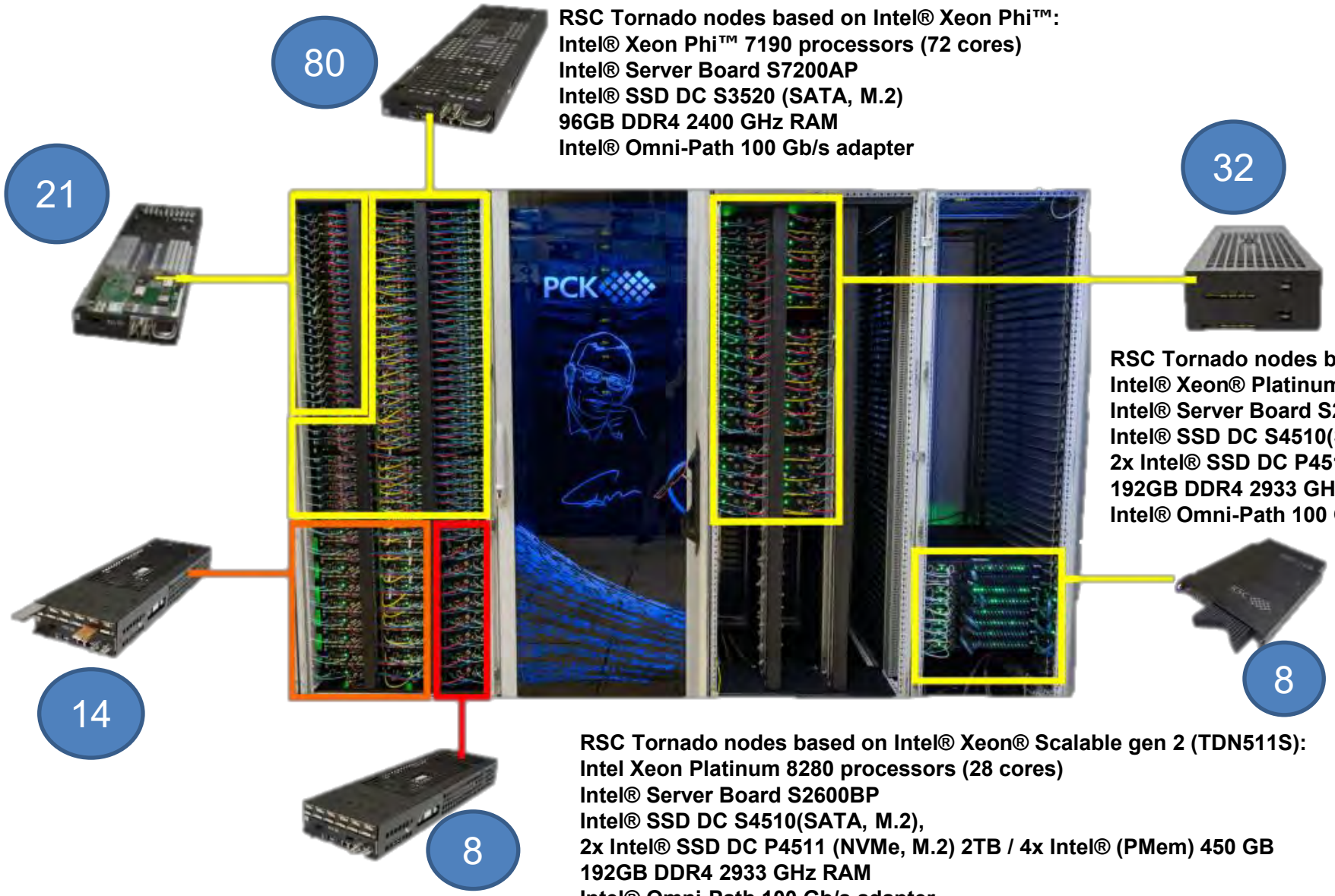


Information System for Radiation Biology Tasks



Data Processing and Analysis

The CPU-component of the “Govorun” Supercomputer



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

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

Current status:

163 hyperconverged compute CPU nodes

8552 compute cores

Total peak performance:

800 TFlops Double-Precision computations

Total capacity of Hierarchical Storage: **8.6 PB**

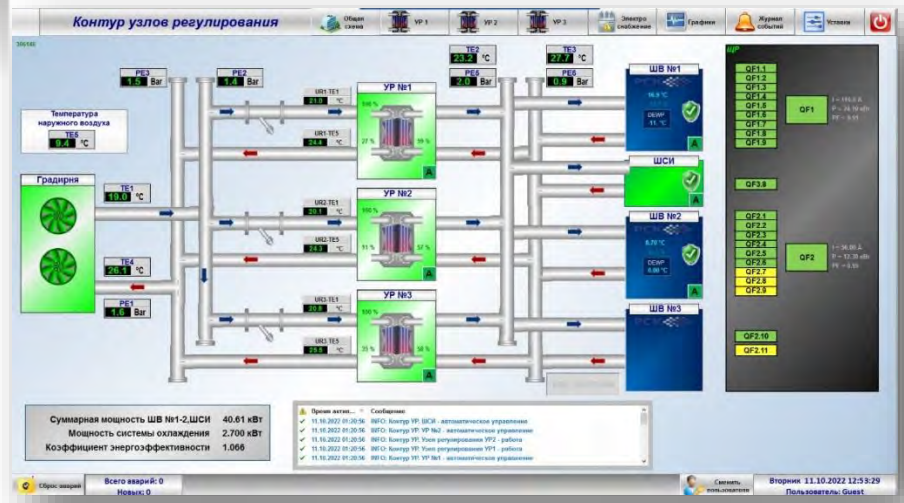
Data IO rate: **300 Gb/s**

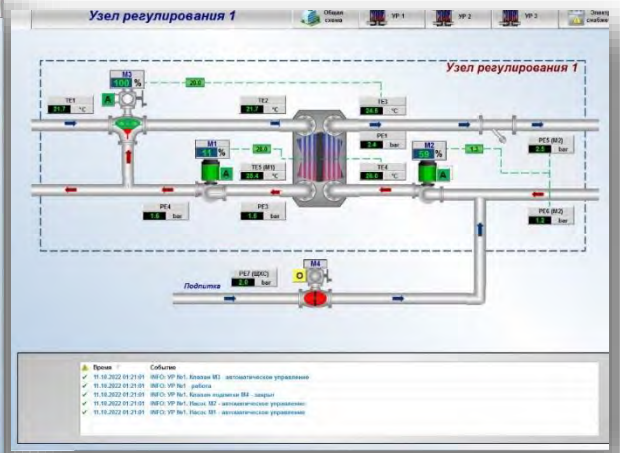
Supercomputer "Govorun". Hot water cooling.

PUE ~ 1,06

Power usage effectiveness

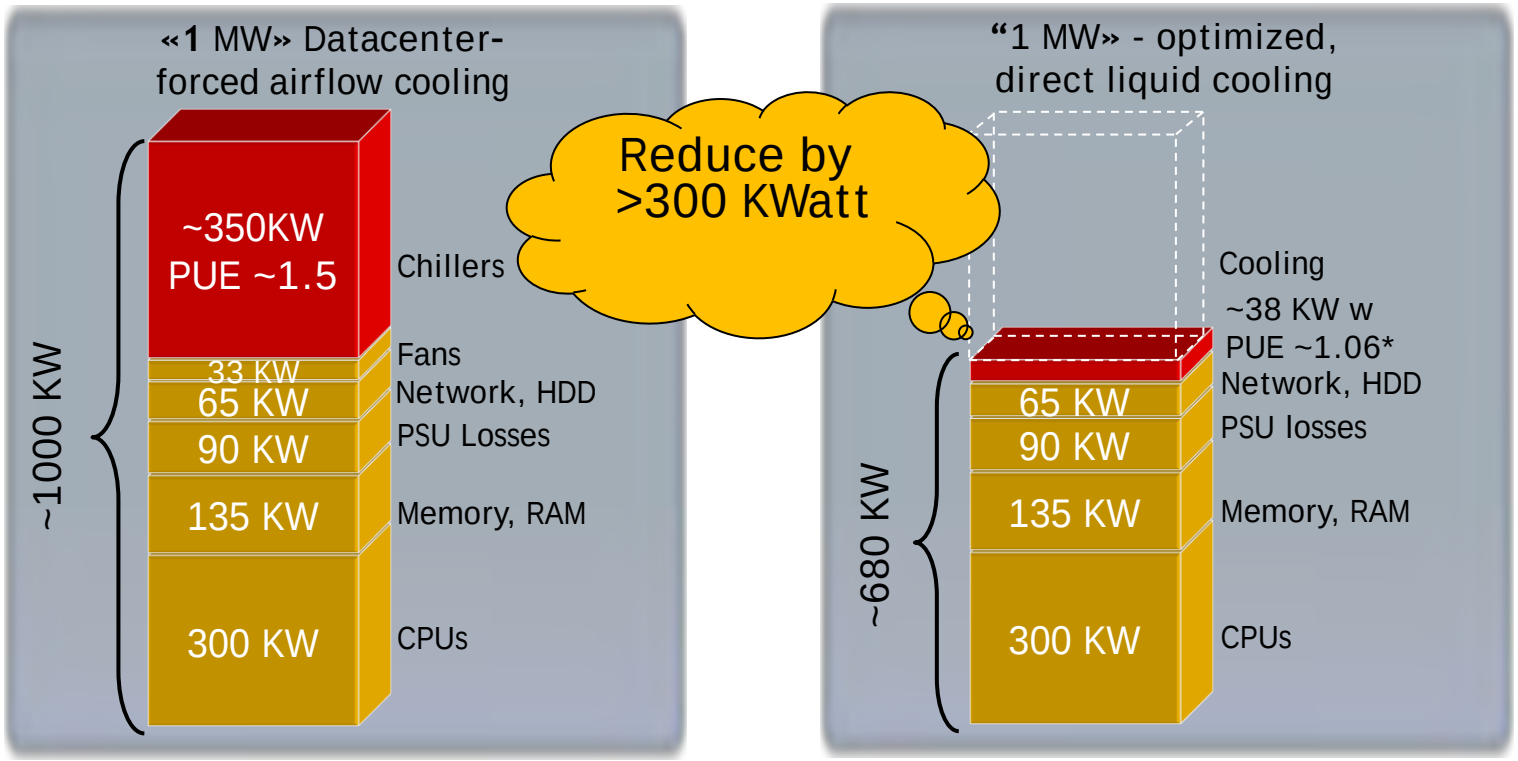
The supercomputer receives water cooled to a temperature of 45 degrees. Having passed through the entire circuit in the supercomputer, water heated to 50 degrees returns to the heat exchanger, where it is cooled, transferring thermal energy to the hydraulic circuit of the dry cooling tower.





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.

Reason for liquid cooling: 1MW datacenter example



Cooling is a major optimization option in datacenter

Additional benetits:

1) Compact design enabled
2) Top bin CPU even in dense blade package
3) More reliability

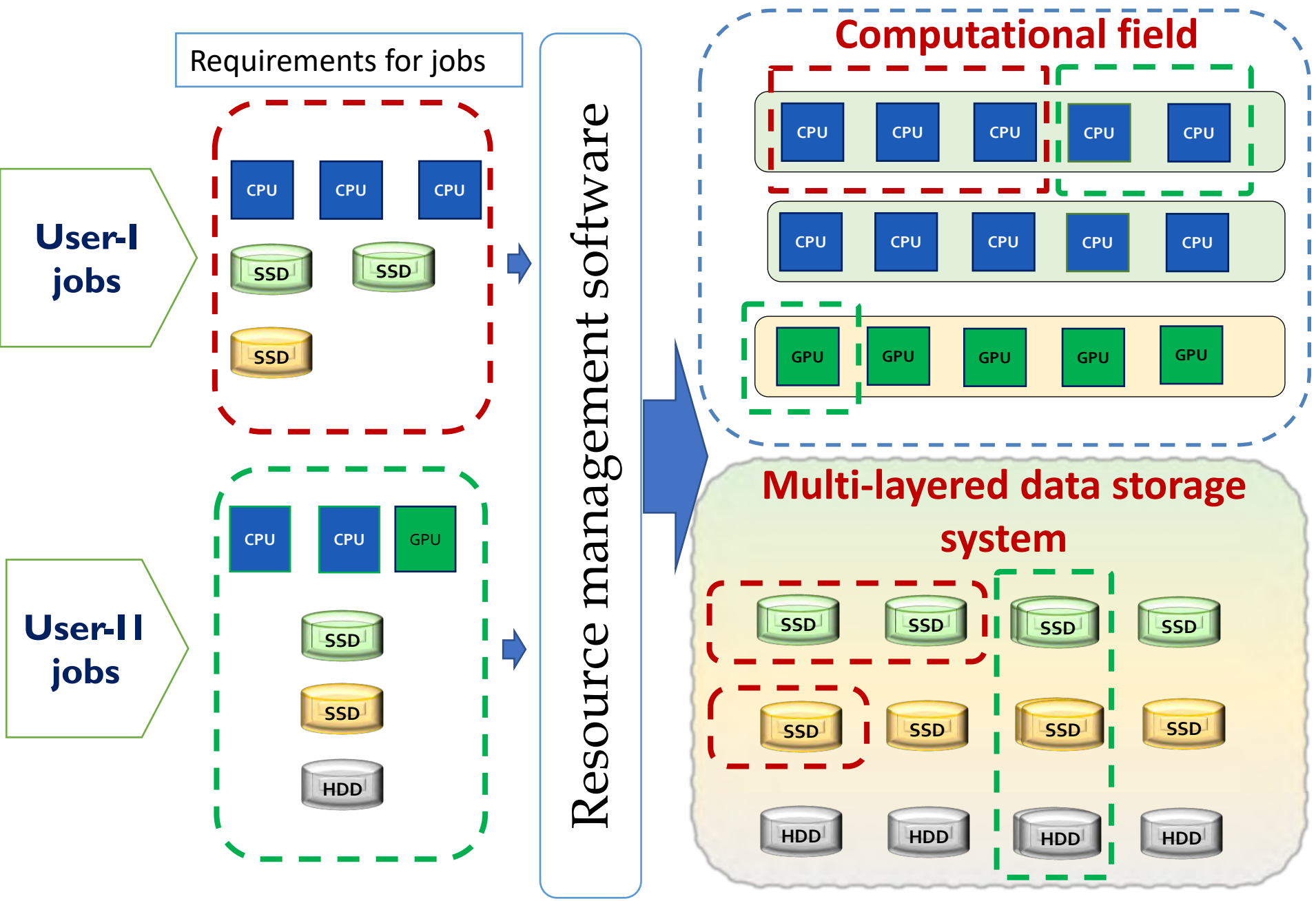
Liquid cooling for supercomputers

Top500 Rank	System	Cooling technology
1	Frontier	Direct cold water cooling
2	Fugaku	Direct cold water cooling
3	LUMI	Direct cold water cooling
4	Leonardo	Direct warm water cooling
5	Summit	Direct cold water cooling
6	Sierra	Direct cold water cooling
7	Sunway TaihuLight	Airflow cooling
8	Perlmutter	Direct cold water cooling
9	Selene	Airflow cooling
10	Tianhe-2A	Airflow cooling

Top500 Rank	System	Cooling technology
11	Explorer-WUS3	Airflow cooling
12	Adastra	Direct cold water cooling
13	JUWELS Booster Module	Direct warm water cooling
14	Pre-Eos 128 Node DGX SuperPOD	Direct cold water cooling
15	HPC5	Airflow cooling
16	Voyager-EUS2	Airflow cooling
17	Setonix – GPU	Direct cold water cooling
18	Discovery 5	Direct cold water cooling
19	Polaris	Airflow cooling
20	SSC-21	Airflow cooling

Liquid cooking systems take 12 positions among the first 20 places in the list of the Top500 most productive supercomputers in the world.

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.

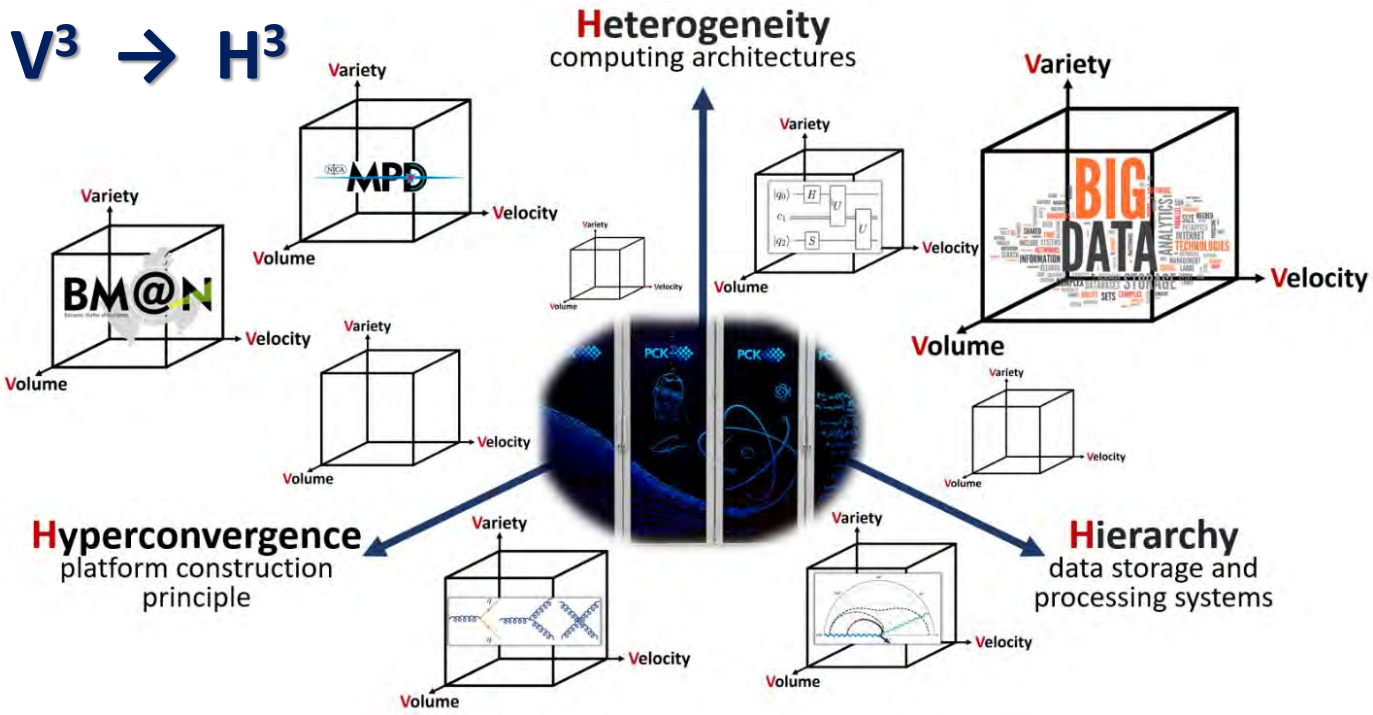
Big Data on the “Govorun” Supercomputer for NICA megaproject

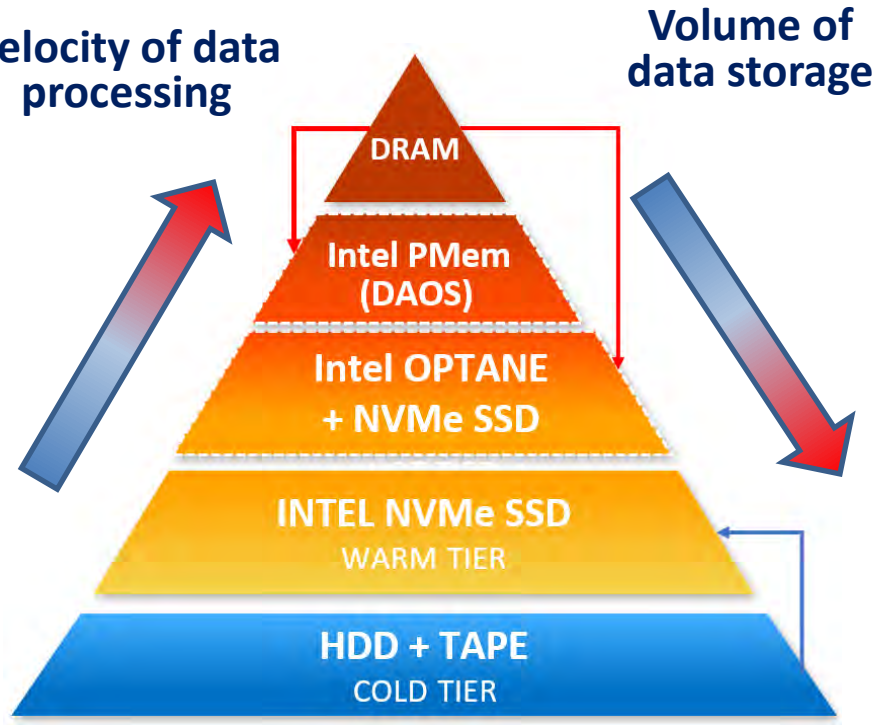
The DAOS polygon of the “Govorun” supercomputer takes the **1st** place among Russian supercomputers in terms of the data processing rate in the current **IO500 list**.

Heterogeneity
Hierarchy
Hyperconvergence

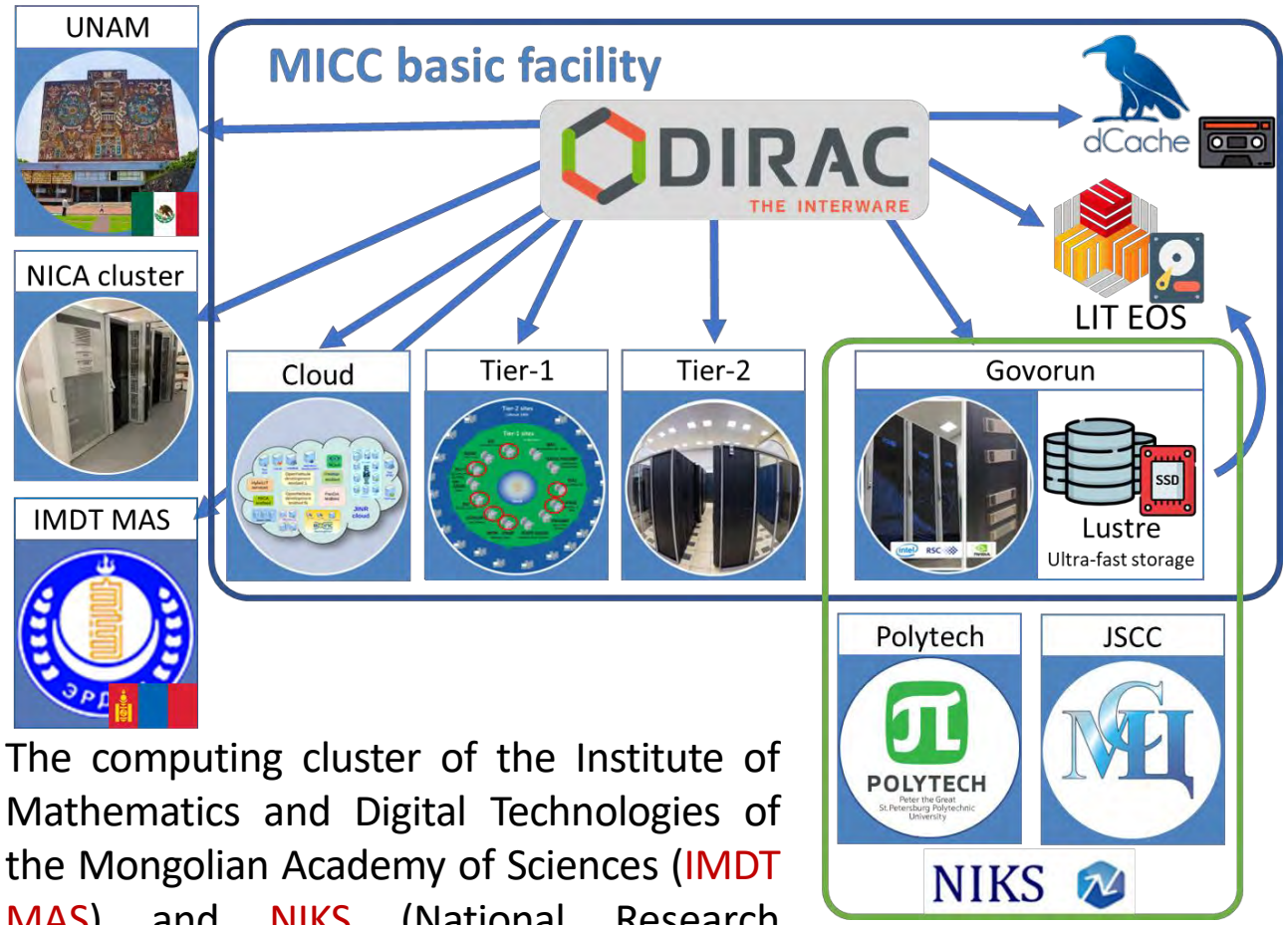
provide

Variety
Velocity
Volume

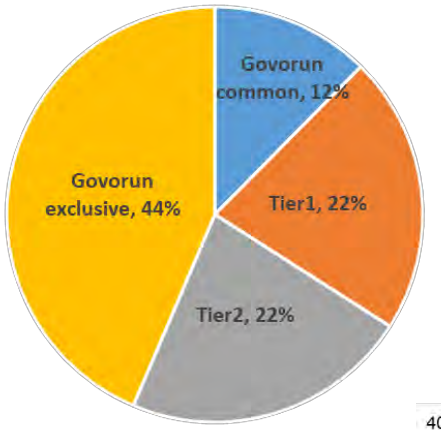




Heterogeneous distributed computing environment

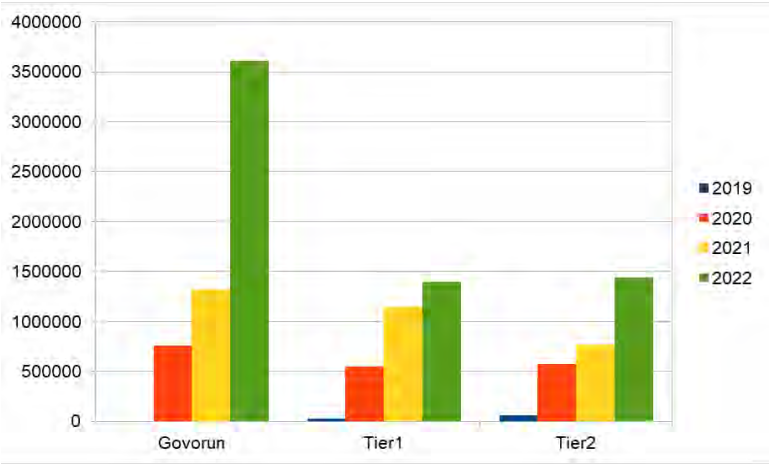


The computing cluster of the Institute of Mathematics and Digital Technologies of the Mongolian Academy of Sciences (IMDT MAS) and NIKS (National Research Computer Network, the Russia's largest research and education network) were integrated into the heterogeneous distributed environment based on the DIRAC platform.



Share of the use of different MICC components for MPD tasks in 2022: the SC "Govorun" resources are the most efficient for MPD tasks.

Increase in the share of the MICC computing resources on the DIRAC platform in normalized CPU HEP-SPEC06 days

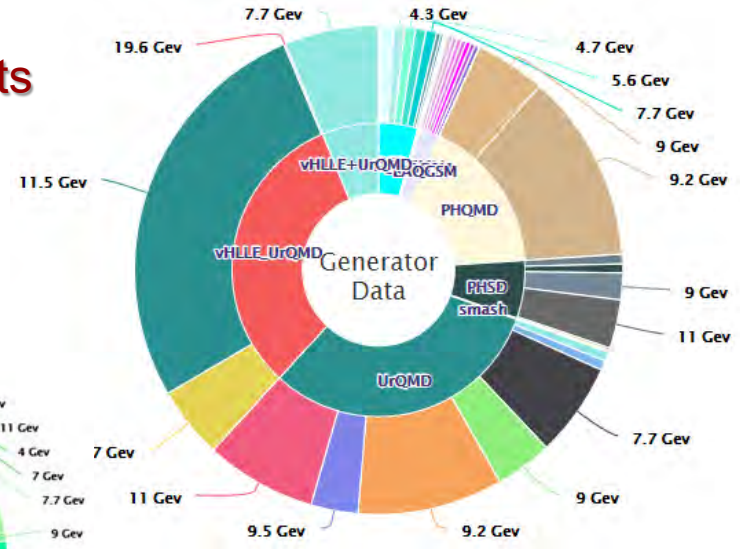


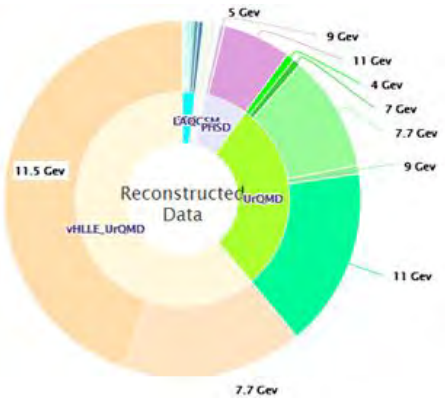
Summary statistics of using the DIRAC platform for MPD tasks in 2019-2022

31 data generation campaigns	1.283 B events generated	440M events reconstructed	1.5M jobs completed	1557 years total computation time	1.3 PB MPD data produced

Heterogeneous distributed computing environment for the MPD experiment

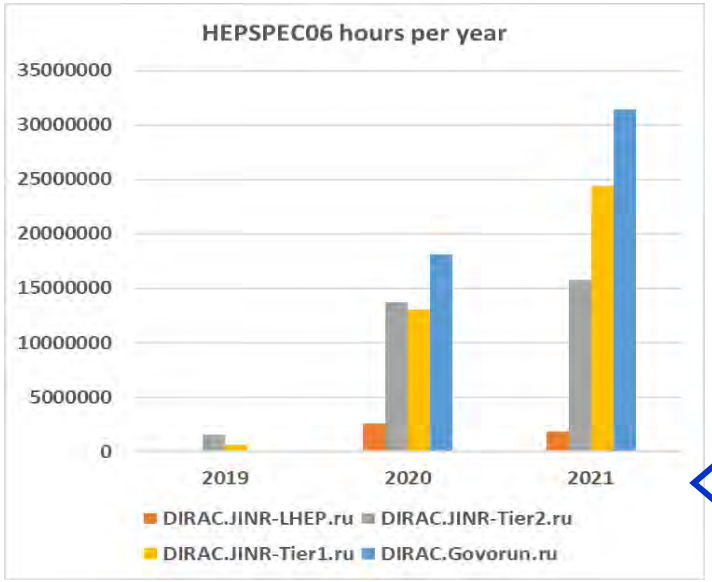
✓$1200 * 10^6$events were generated using *UrQMD*, *PHQMD*, *PHSD* and other models





✓$392 * 10^6$events were reconstructed

"Govorun" up to **40%**



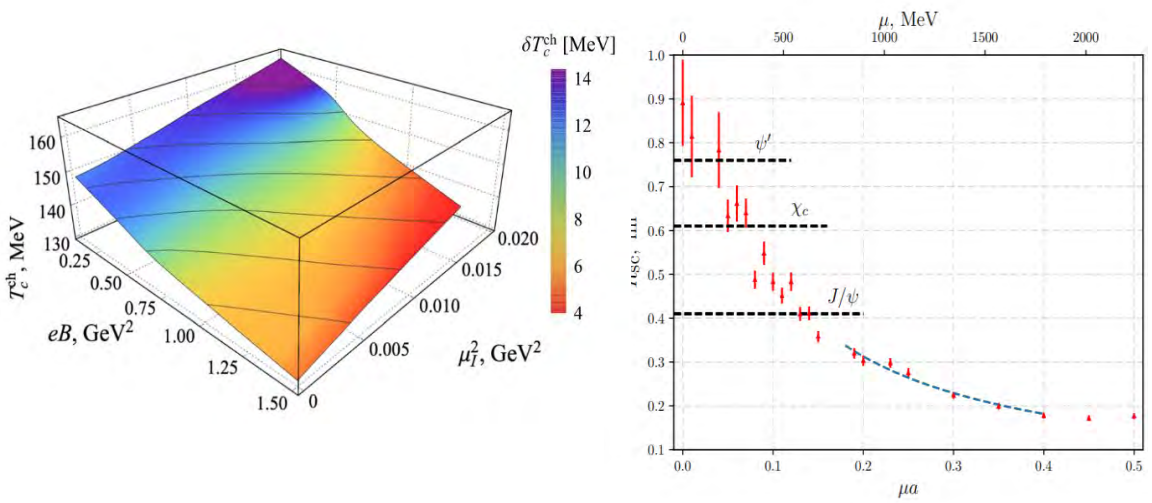
Available resources of the DIRAC platform for the MPD experiment:

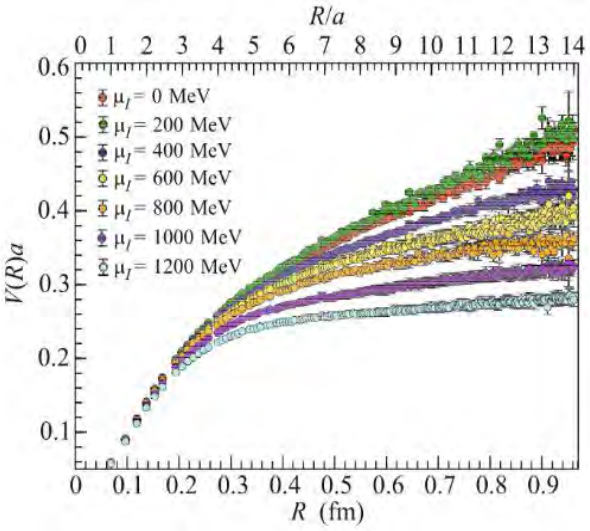
- "Govorun" supercomputer: up to 1,586 cores in the latest production
- Tier1: 920 cores
- Tier2: 1,000 cores
- Clouds (JINR and JINR Member States): 70 cores
- NICA offline cluster: 300 cores (limit for users)
- UNAM (Mexico University): 100 cores
- National Research Computer Network of Russia (NIKS, now resources from SPBTU and JSCC): 672 cores – New resource, added in 12.2021.

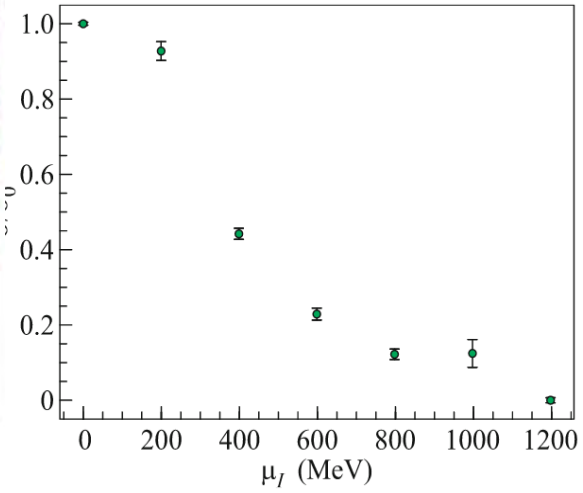
The mass production storages integrated into the Dirac File Catalog are 1.5 PB in size.

The histogram illustrates the accounting data from the centers. The metric shown is Sum CPU Work, grouped by center and year.

“Govorun” supercomputer for QCD tasks







The resources of the “Govorun” supercomputer were used to study the properties of quantum chromodynamics (QCD) and Dirac semimetals in a tight-binding mode under extreme external conditions using lattice modeling. The given study entails the inversion of large matrices, which is performed on video cards (GPU), as well as massive parallel CPU calculations, to implement the quantum Monte-Carlo method:

– The influence of the magnetic field on the confinement/deconfinement transition and the chiral transition at finite temperature and zero baryon density were investigated using the numerical modeling of lattice QCD with a physical quark mass.

– Quantum chromodynamics with non-zero isospin density taking into account dynamical u- d-, s-quarks in the Kogut-Susskind formulation was studied.

– The potential of the interaction between a static quark-antiquark pair in dense two-color QCD was investigated, and the confinement/deconfinement phenomenon was studied.

– The effect of the non-zero chiral chemical potential on dynamical chiral symmetry breaking for Dirac semimetals was studied.

- The influence of the external magnetic field on the electromagnetic conductivity of quark-gluon plasma was investigated.

The results are published in the articles:

1. V. V. Braguta, M. N. Chernodub, A. Yu. Kotov, A. V. Molochkov, and A. A. Nikolaev, Phys. Rev. D 100 (2019), 114503, DOI: 10.1103/PhysRevD.100.114503, arXiv:1909.09547
2. V.V. Braguta , A.Yu. Kotov, A.A. Nikolaev, JETP Lett. 110 (2019) no.1, 1-4, DOI: 10.1134/S0021364019130083 (JETP Letters, 110 (2019) no.1, 3-6)
3. N. Astrakhantsev, V. Bornyakov, V. Braguta, E.M. Ilgenfritz, A.Y. Kotov, A. Nikolaev, A. Rothkopf, PoS Confinement2018 (2019), 154, DOI: 10.22323/1.336.0154
4. V. V. Braguta, M. I. Katsnelson, A. Yu. Kotov, and A. M. Trunin, Phys.Rev. B100 (2019), 085117, DOI: 10.1103/PhysRevB.100.085117 , e-Print: arXiv:1904.07003
5. N. Yu. Astrakhantsev, V. G. Bornyakov, V. V. Braguta, E.-M. Ilgenfritz, A. Yu. Kotov, A. A. Nikolaev, A. Rothkopf, JHEP 1905 (2019) 171, DOI: 10.1007/JHEP05(2019)171,e-Print: arXiv:1808.06466
6. https://arxiv.org/abs/1902.09325
7. http://arxiv.org/abs/1910.08516

“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

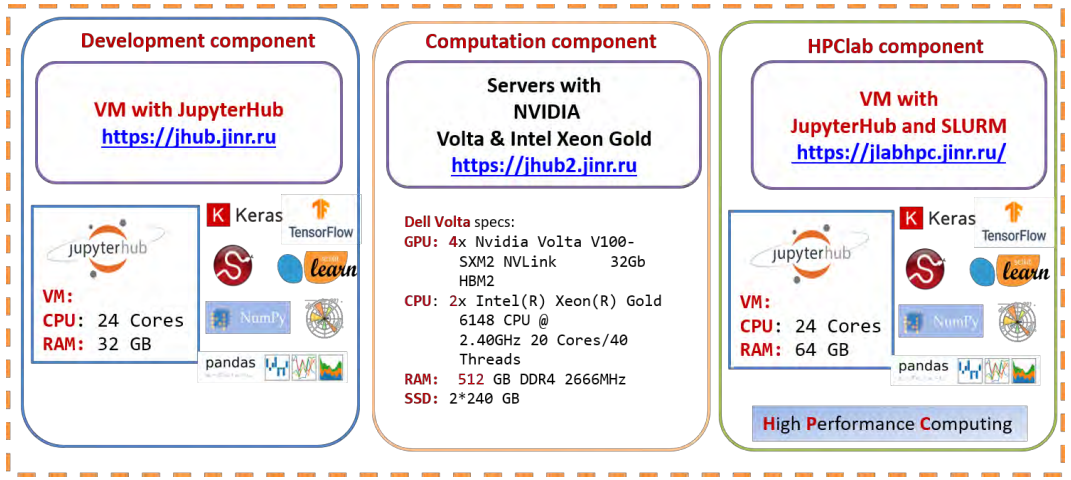
Modeling the kinetics of excitation and relaxation of dielectrics irradiated by fast heavy ions

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.

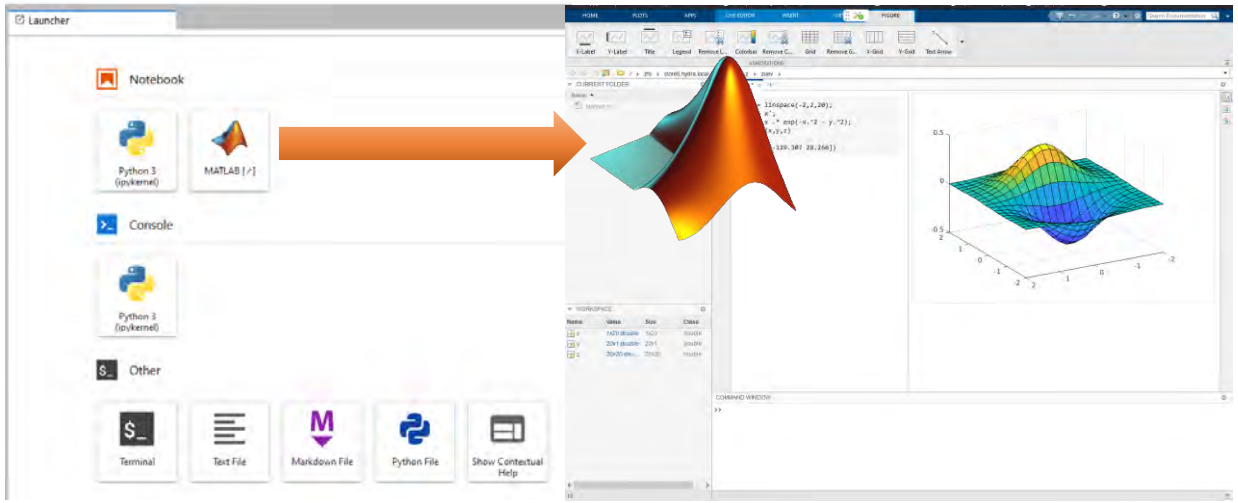
The results are presented in the next publications:

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: New Opportunities for Applied Research



In 2022, on the ML/DL/HPC ecosystem, it became possible to run the MATLAB code in Jupyter Notebook, which allows one to effectively perform applied and scientific computations.



The ML/DL/HPC ecosystem is now actively used for machine and deep learning tasks. At the same time, the accumulated tools and libraries can be more widely used for scientific research, including:

- numerical computations;
- parallel computing on CPUs and GPUs;
- visualization of results;
- accompanying them with the necessary formulas and explanations.

jupyter jupyter{book}

Keras

pandas

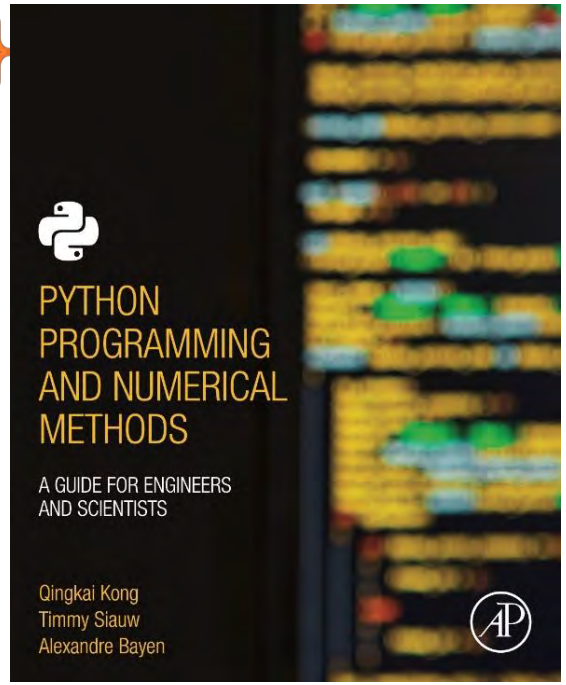
matplotlib

seaborn

Joblib

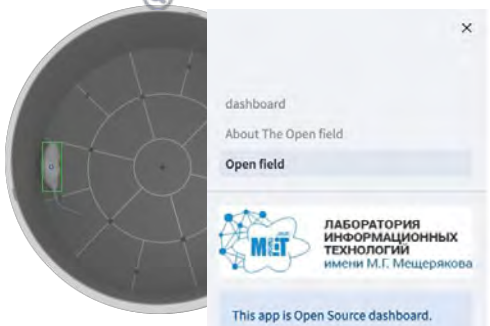
Parallel computations with Joblib

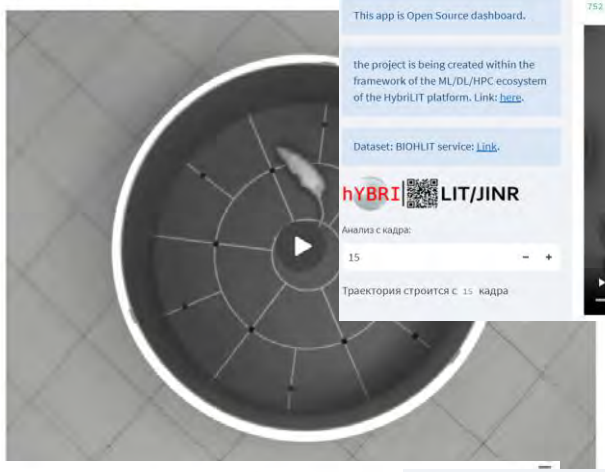
Python Numerical Methods

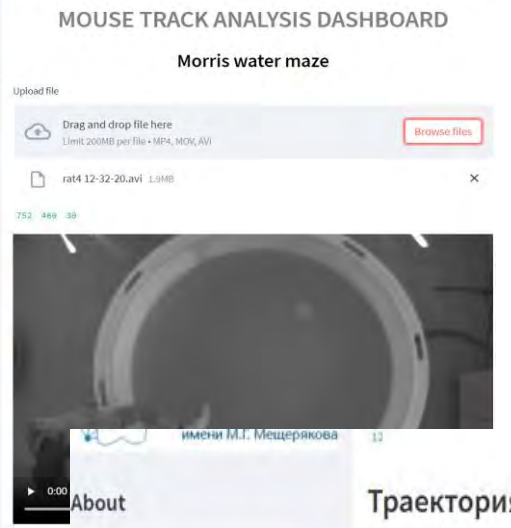


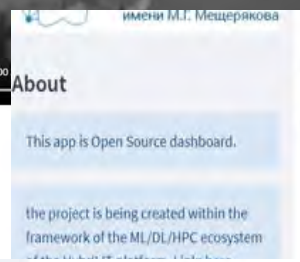
BIOHLIT information system for radiobiological studies

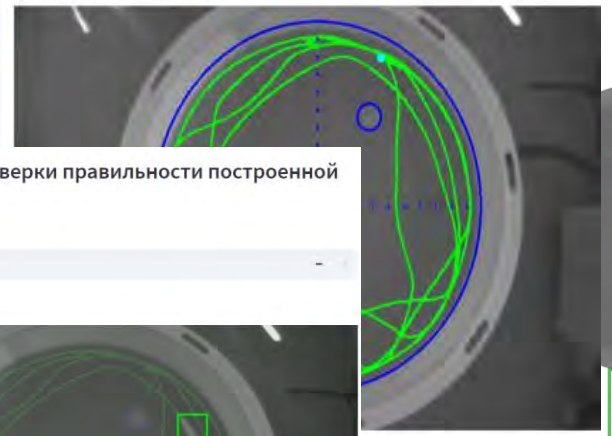
BIOHLIT

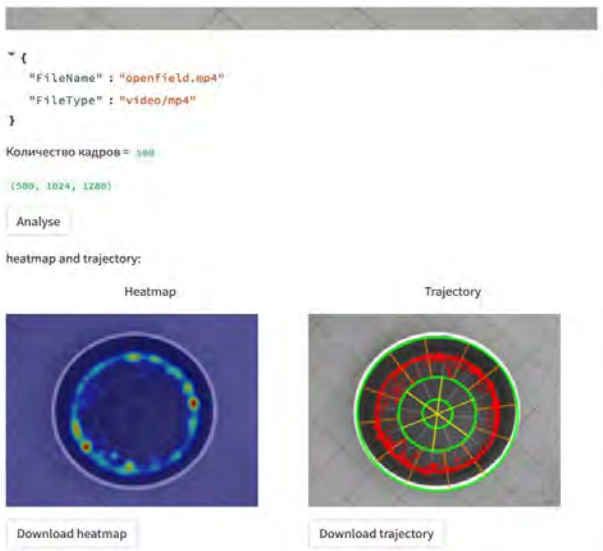


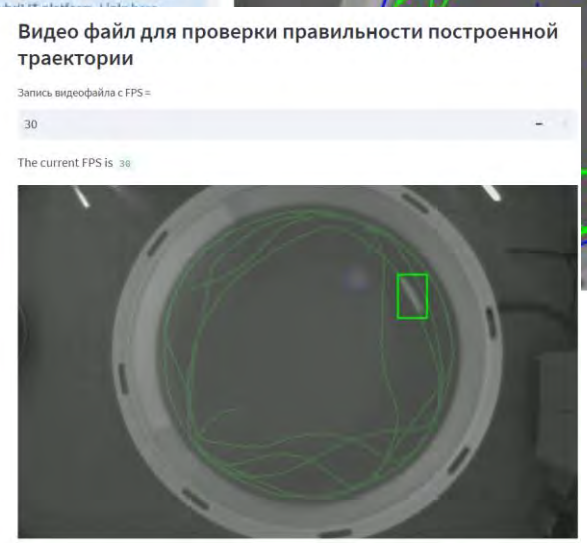


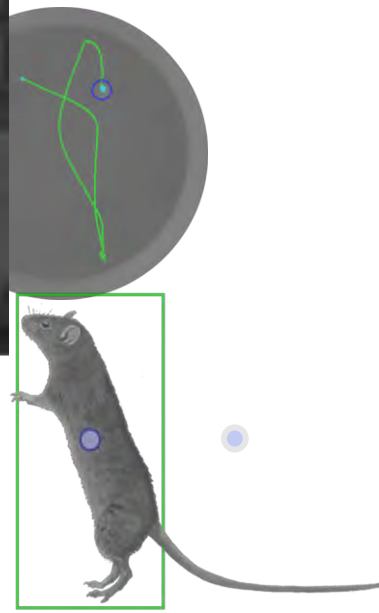












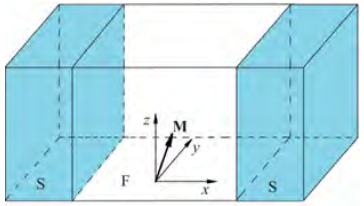
The information system allows one to store, quickly access and process data using a stack of neural network and classical algorithms of computer vision, providing a wide range of possibilities for automating routine tasks. It gives an increase in productivity, quality and speed of obtaining results.

Study the dynamics of magnetization in a Phi-0 Josephson Junction

The dynamics of the magnetic moment M of the system under consideration is described by the Landau-Lifshitz-Gilbert equation:

$$\frac{dm_x}{dt} = -\frac{1}{1+M^2\alpha^2}\{m_y H_z - m_z H_y + \alpha[m_x(M,H) - H_x]\},$$
$$\frac{dm_y}{dt} = -\frac{1}{1+M^2\alpha^2}\{m_z H_x - m_x H_z + \alpha[m_y(M,H) - H_y]\}$$
$$\frac{dm_z}{dt} = -\frac{1}{1+M^2\alpha^2}\{m_x H_y - m_y H_x + \alpha[m_z(M,H) - H_z]\},$$

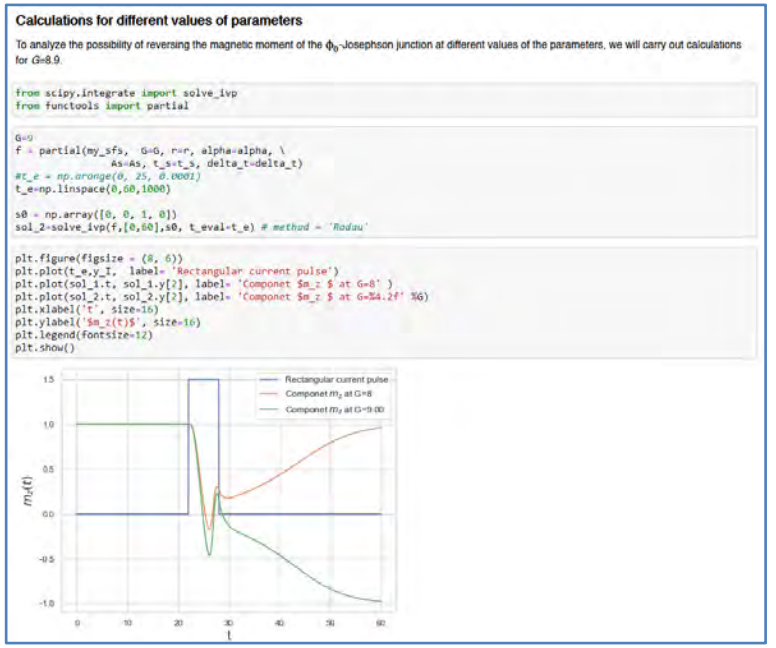
$M = [m_x, m_y, m_z]$ are the magnetic moment components; the effective field components $H = [H_x, H_y, H_z]$ depend on the Josephson phase difference ϕ and are defined as follows:

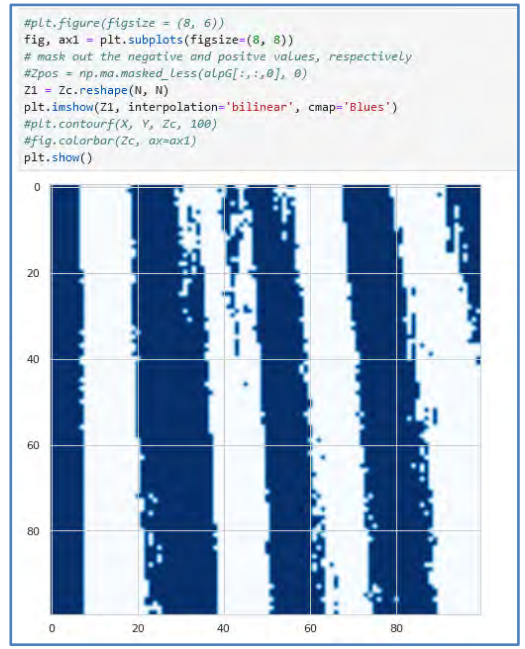


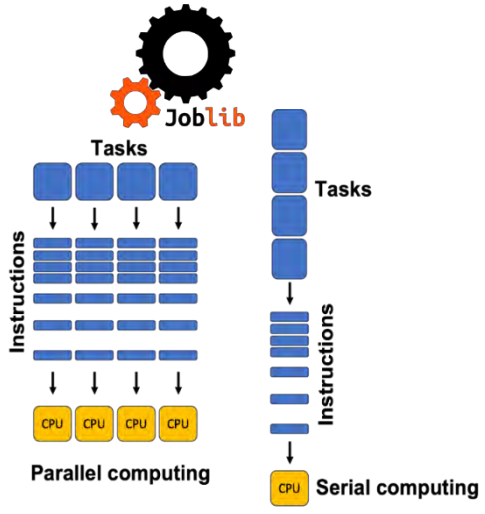
$$H_x(t) = 0,$$
$$H_y = Gr\sin(\phi(t) - tm_y(t)),$$
$$H_z(t) = m_z(t).$$

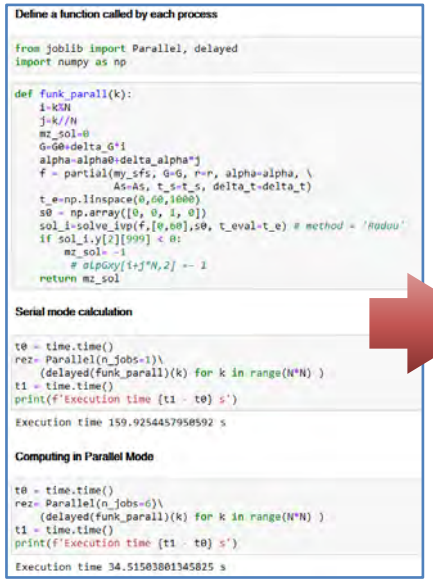
The equation for the Josephson phase difference $\phi(t)$ is determined from the equation for the electric current I flowing through the Josephson junction, measured in units of the critical current I_c :

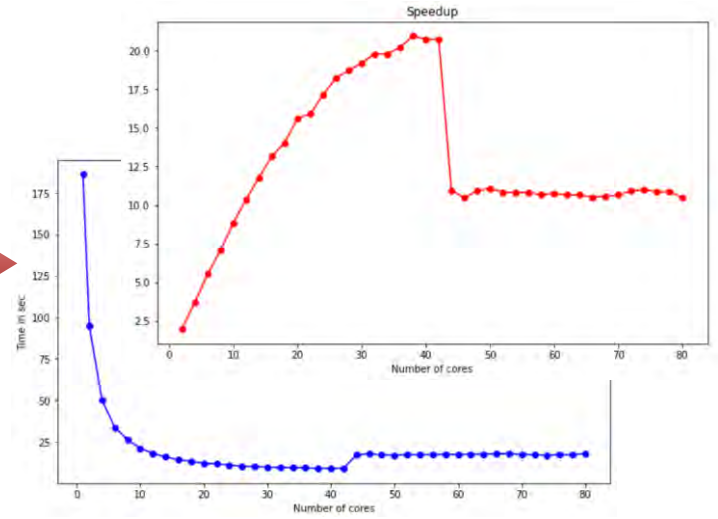
$$\frac{d\phi}{dt} = -\frac{1}{w}\left(\sin(\phi - rm_y) + r\frac{dm_y}{dt}\right) + \frac{1}{w}I,$$











Quantum polygon

Notebook

Python 3 (ipykernel) | Cirq | PennyLane | Qiskit

Console

Python 3 (ipykernel) | Cirq | PennyLane | Qiskit

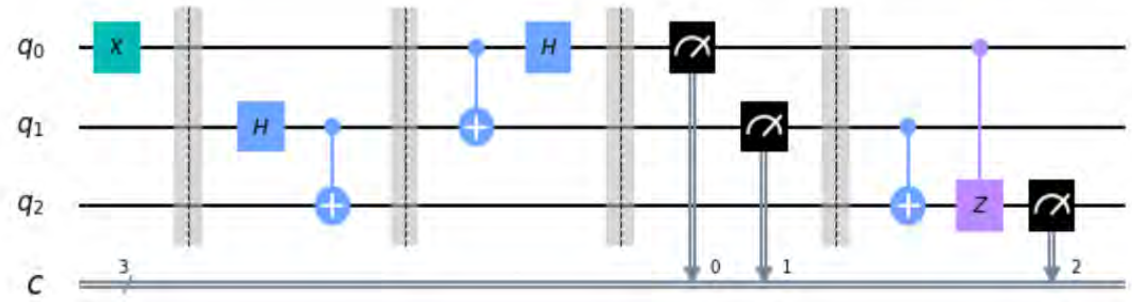
Other

Terminal | Text File | Markdown File | Python File | Show Contextual Help

https://jhub3.jinr.ru

Equipment:
- 2x Intel Xeon E5 2698v4 (20 Cores @ 2.2 GHz),
- 512 GB RAM,
- 8x NVIDIA Tesla V100 SXM2 16 GB HBM2

```
%matplotlib inline
circuit.draw(output='mpl')
```

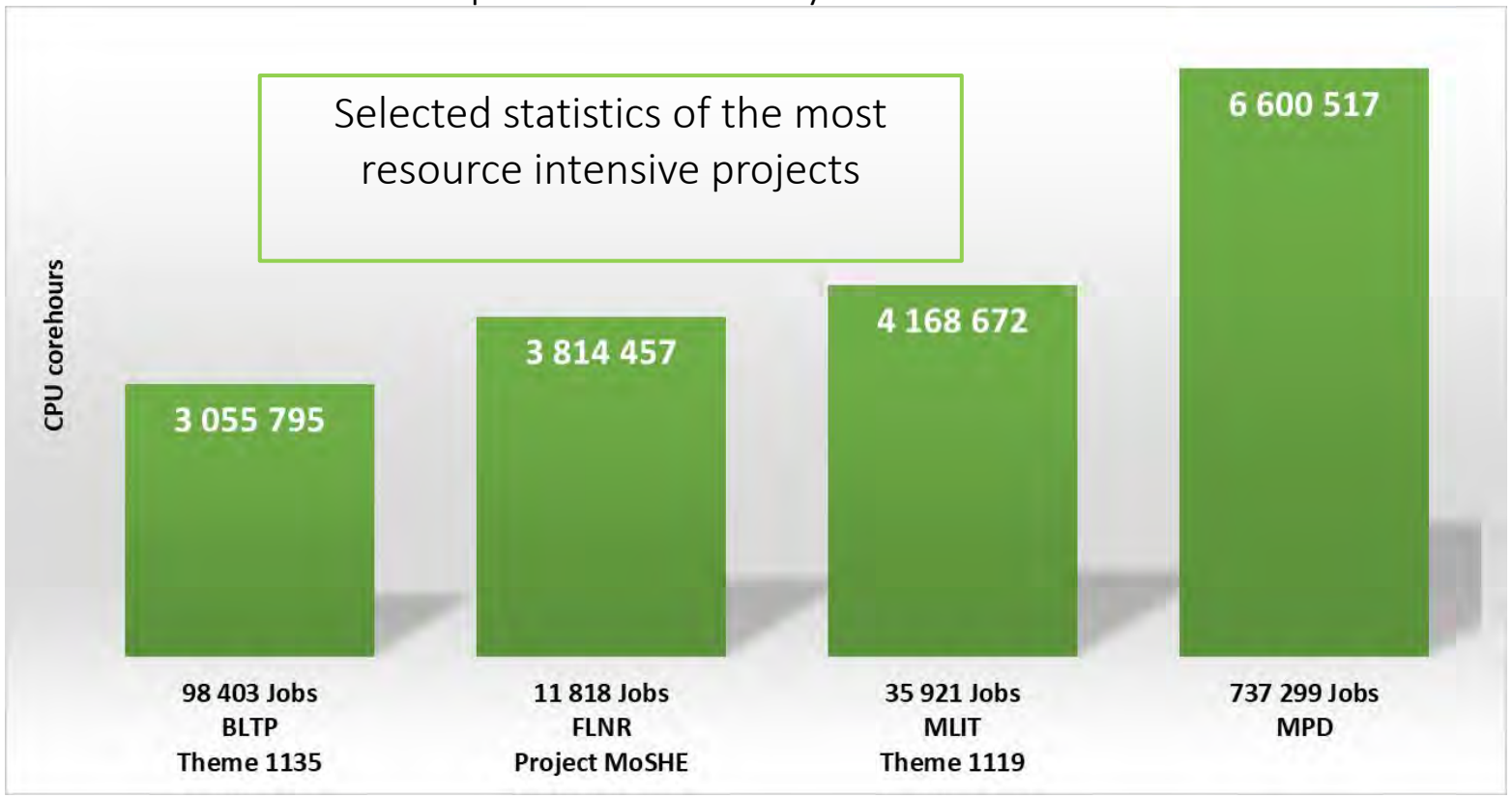


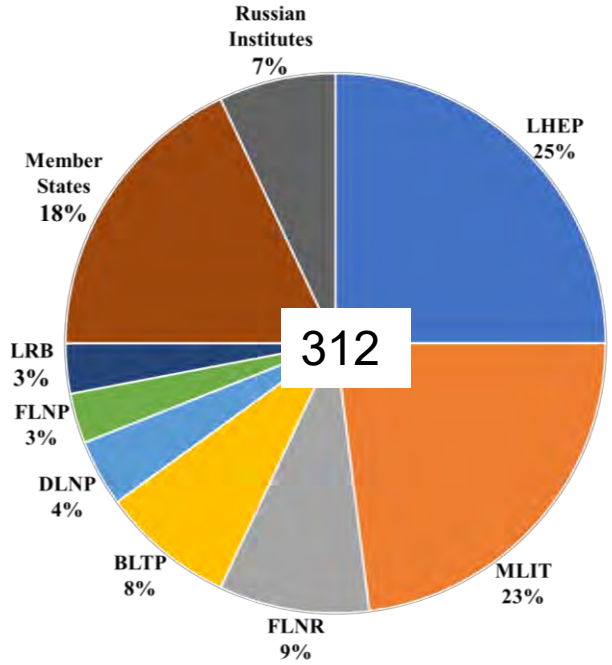
Using of the “Govorun” Supercomputer in 2023

The resources of the “Govorun” SC are used by scientific groups from all the Laboratories of the Institute within 25 themes of the JINR Topical Plan.

The projects that mostly intensive use the CPU resources of the “Govorun” SC:

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



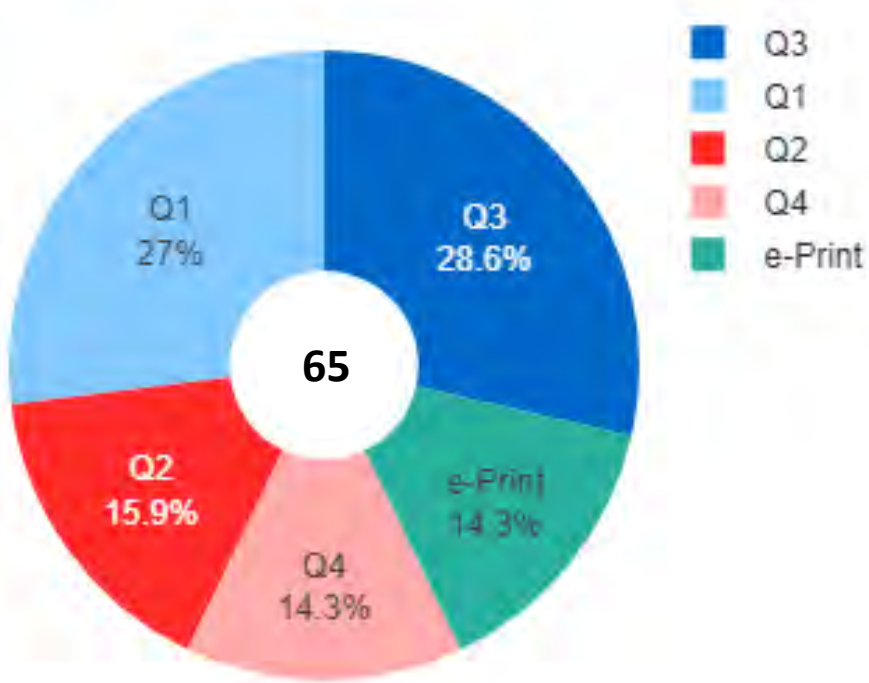


Within 2023, all groups of “Govorun” SC users completed 640,861 jobs on the CPU component, which corresponds to 16 million core hours, and 7,808 jobs on the GPU component, which corresponds to 45,400 GPU hours. The average load of the CPU component was 96.4%, while the GPU component load was 91.2%.

Publications

Over the past year, users of the heterogeneous HybriLIT platform published 65 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.



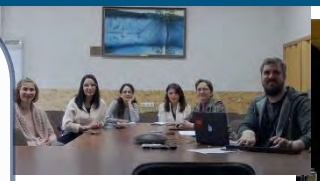
Research results obtained using the supercomputer resources since 2018 are presented in 325 publications. Two of them were prepared in Nature Physics:

- 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

Educational activities: training courses

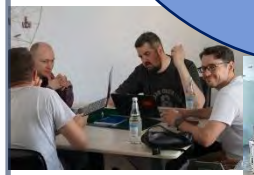
Modern information technologies in biology and medicine

The international workshop “Modern information technologies in biology and medicine”
22-24 November 2023.
«Tutorial on the use of Python for tasks in Bio-Medical research»
60 участников

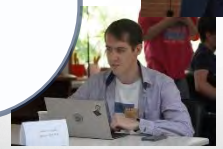




210
Participants in 2023 г.





СОГУ
ЦЕНТР ОТКРЫТОГО ОБРАЗОВАНИЯ НА РУССКОМ ЯЗЫКЕ

V Международная летняя школа молодых ученых «Современные информационные технологии для решения научных и прикладных задач» 14-17 Июня 2023.
"Инструментарий на основе Python-библиотек и экосистемы Jupyter для решения научных и прикладных задач"
70 участников

it SCHOOL JINR

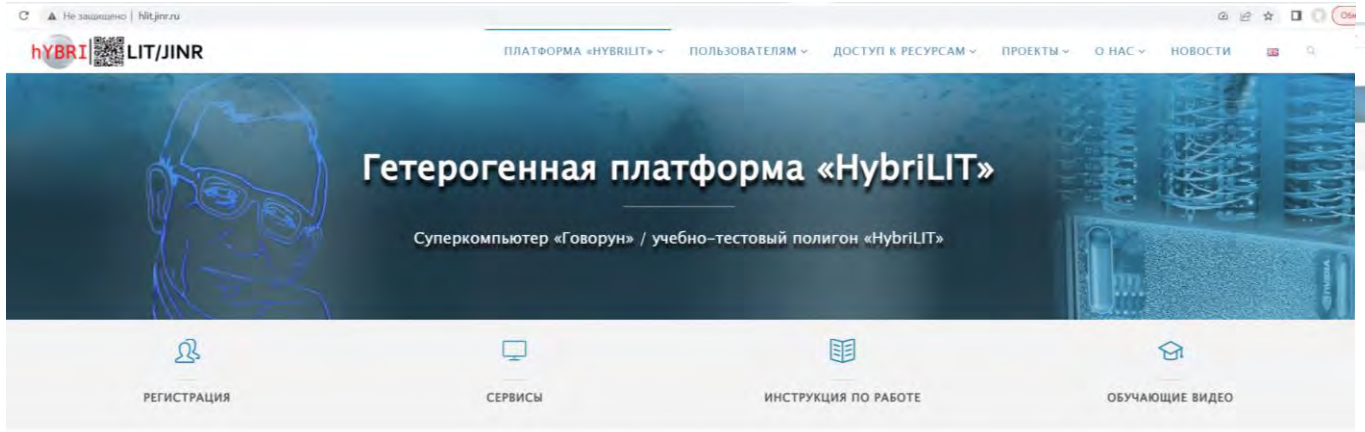
Осенняя Школа по информационным технологиям ОИЯИ 16-20 Октября 2023
«Инструментарий на основе Python-библиотек и экосистемы Jupyter для решения научных и прикладных задач»
Хакатон по параллельным вычислениям
60 участников

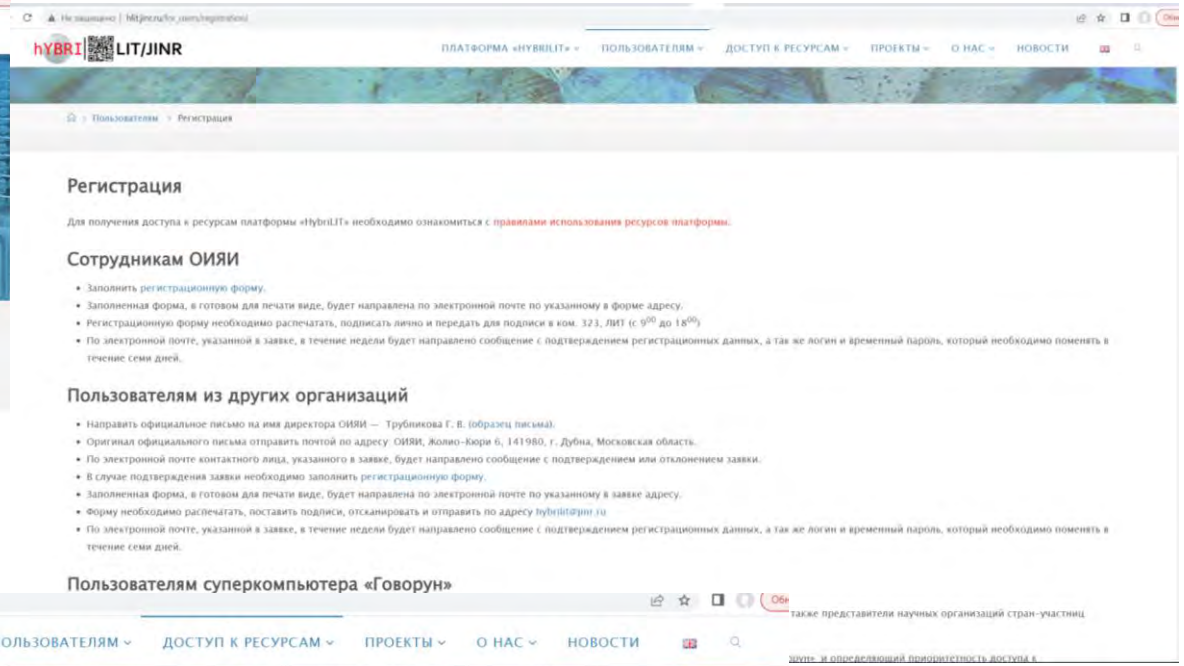
МИЦНТ СНГ

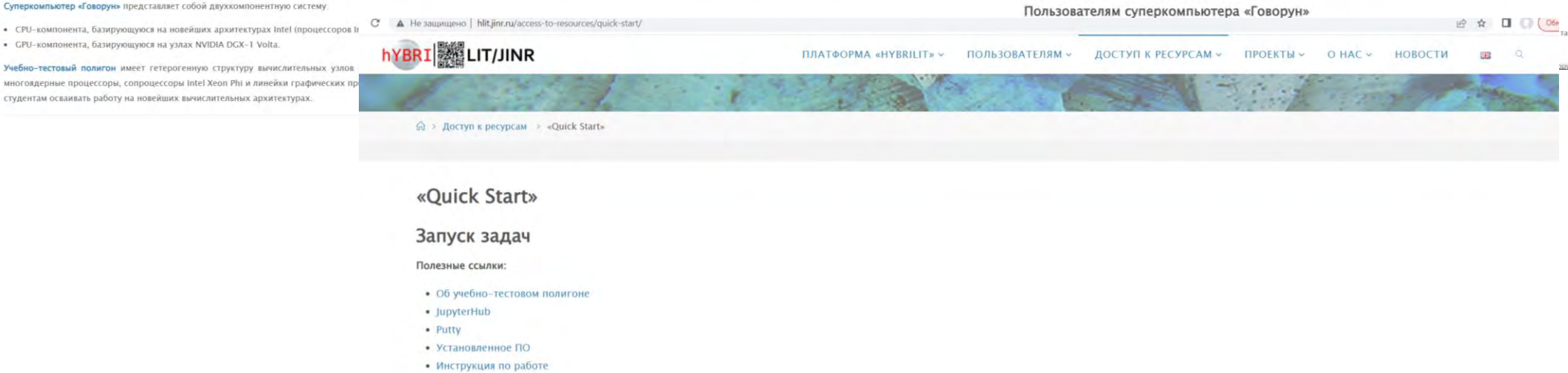
XVI Международная стажировка молодых ученых стран СНГ Май-Июнь 2023
«Как научить компьютер "видеть"»
20 участников

“Govorun” supercomputer

http://hlit.jinr.ru/







Thank you for your attention

HYBRILIT HETEROGENEOUS PLATFORM at MLIT JINR:

http://hlit.jinr.ru