

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





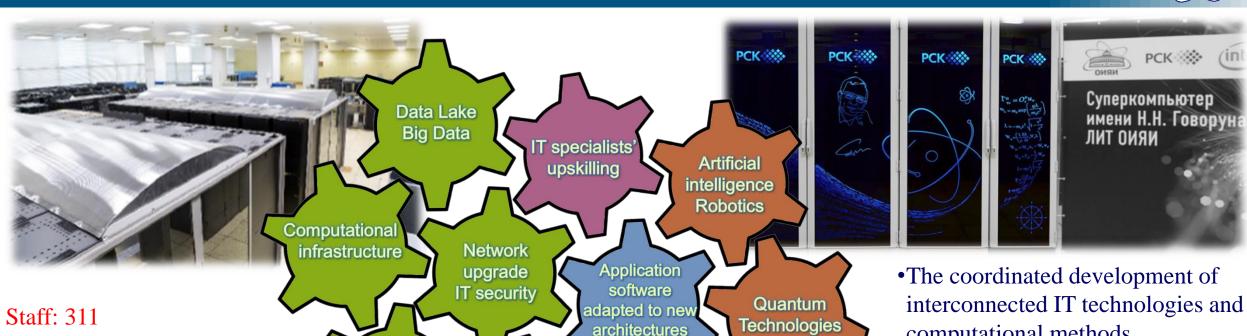
(17.09.1910 - 24.05.1994) (18.03.1930 - 21.07.1989)



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





Machine

& Deep

learning

Software

development

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

Data center nfrastructure

JINR Cloud computing

JINR Member States' Cloud environment

"Govorun" supercomputer

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

Nuclear Physics

- Computations of the properties of atoms of superheavy elements
- Analysis of fine structures in the mass distribution of nuclear reaction products
- Sub-barrier fusion and fission reactions of heavy nuclei

-...

Theoretical Physics

- Calculations of lattice QCD
- Numerical simulation within effective theories of QCD
 - Compton scattering

- ...

Particle Physics and HEP

- NICA computing
- Methods and algorithms for data analysis
 - Intelligent control systems

- . . .

Information Technologies

(Scientific directions and information systems)

Neutrino Physics and Astrophysics

- '- Support of the JINR neutrino program
 - Data acquisition system software for Baikal-GVD

- . . .



Life Science

- Information System for Radiation Biology tasks
- Analysis of Small-Angle scattering data from nanodrugs
 - Environmental monitoring

- . .

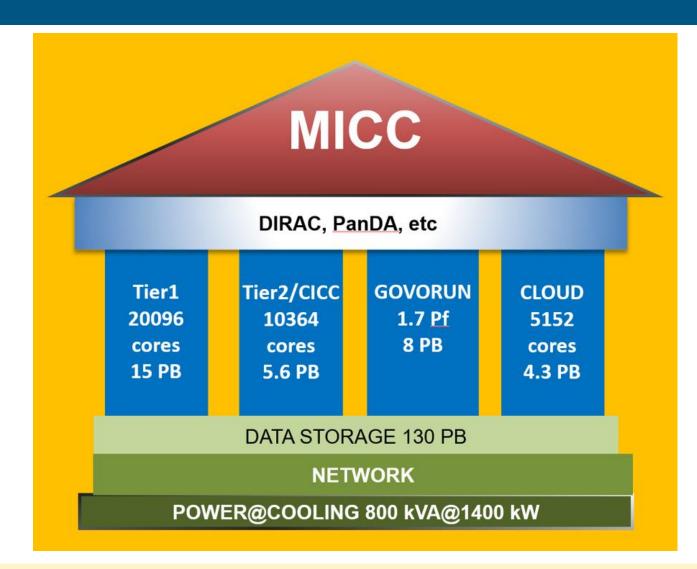
Condensed Matter

- Analysis of polydisperse populations of phospholipid vesicles
- Study of nanocomposite thin films using neutron and X-ray reflectometry methods
 - Simulation of thermal processes occurring in materials

- . .

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

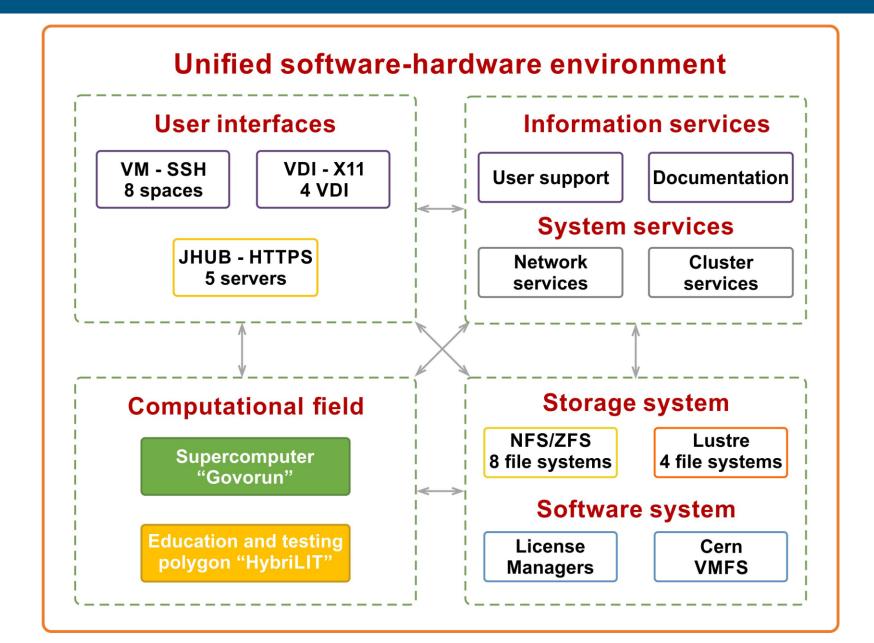
Network

- ➤ 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





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

MICC component: HybriLIT platform



System Level

Scientific Linux 7.9 (operating system)

xCAT (OS deployment tool)

FreeIPA (auth system)

SLURM (workload manager)

NFS (network file system)

Lustre (parallel file system)

CernVM-FS (software distribution service)

FlexLM/MathLM (licence manager system)

Modules (software environment tool)

Monitoring

Home-HLIT Monitoring HLIT-VDI

PCK БазИС Computing Resources'
Statistics

Software Level

Parallel computing software

Open MPI CUDA Intel

Licensed software packages

Comsol Multiphysics Maple
Wolfram Mathematica Matlab

Application Packages

GROMACS Cmake
Java FairRoot
LAMMPS FairSoft
PandaRoot FLAIR
Python FLUKA
REDUCE GEANT4
ROOT Quantum ESPRESSO

Information Level

HybriLIT web-site

http://hlit.jinr.ru/

Indico

https://indico.jinr.ru/

HybriLIT user support project https://pm.iinr.ru/

HybriLIT user support telegram https://web.telegram.org/k/#-1752786710

GitLab

https://gitlab-hybrilit.jinr.ru/

ML/DL/HPC ecosystem

Development component

https://studhub.jinr.ru https://studhub2.jinr.ru

Component for carrying out resource-intensive calculations

https://jhub1.jinr.ru https://jhub2.jinr.ru https://jhub3.jinr.ru Component for HPC on the HybriLIT platform nodes and data analysis https://jlabhpc.jinr.ru/

HLIT-VDI

(Virtual Desktop Infrastructure)

Testbed for quantum computing

(quantum computing simulators)

Development of the heterogeneous HybriLIT platform





Cluster HybriLIT 2014:

Full peak performance:

140 TFlops for single precision;

50 TFlops for double precision

"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 B Top50

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 10500

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 DP3.4 PFlops SP

<u>Total capacity of Hierarchical</u> <u>Storage</u>:

8.6 PB

Data IO rate: 300 Gb/s

GPU-accelerator

Hyperconverged CPU and Distributed Storage Nodes

The GPU-component of the "Govorun" Supercomputer



2017



DGX01

2x Intel Xeon E5-2698 v4
20 Cores @ 2.20 GHz

8x NVidia V100 SXM2, 16 GB

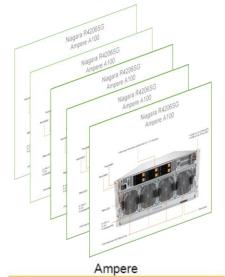
GPU GPU GPU GPU

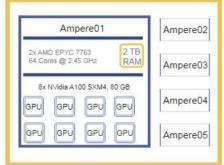
GPU GPU GPU

GPU GPU DGX05

40 NVIDIA V100

2023

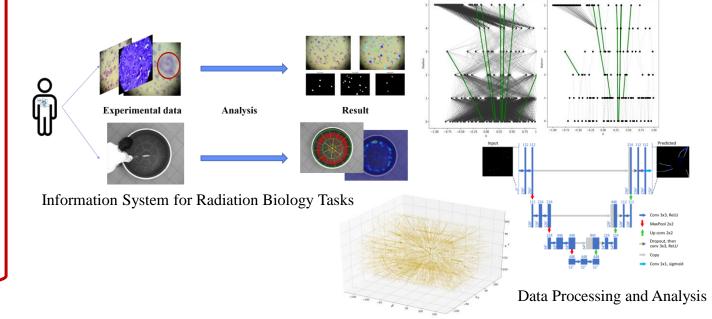




40 NVIDIA A100

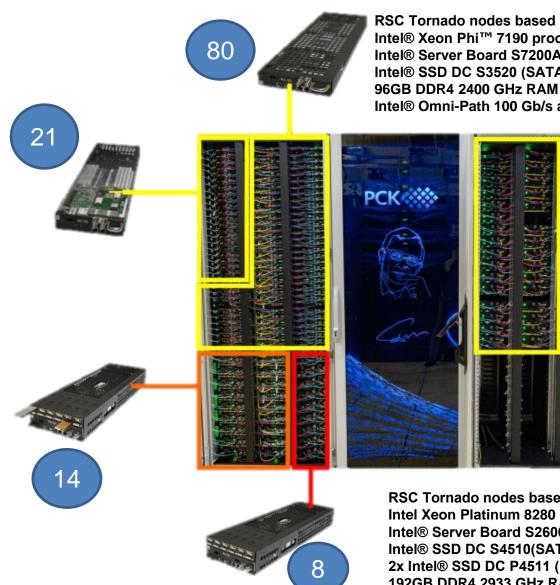
Total peak performance of the GPU-component: 900 Tflops for Double-Precision computations 26 Pflops for Half-Precision computations

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.



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)

Intel® Omni-Path 100 Gb/s adapter



Current status:

163 hyperconverged compute **CPU** nodes 8552 compute cores

<u>Total peak performance:</u> **800 TFlops Double-Precision** computations

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



Total capacity of

Hierarchical Storage: 8.6 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

Supercomputer "Govorun". Hot water cooling.

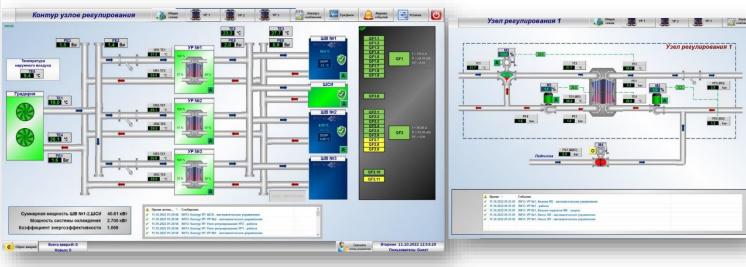






Power usage effectiveness

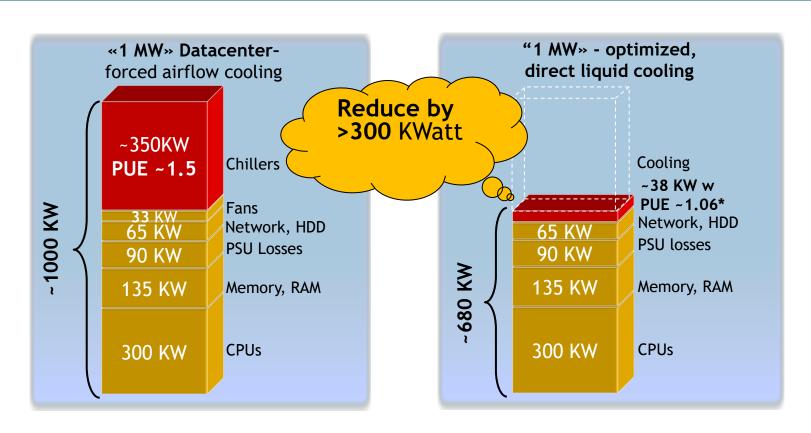
The supercomputer receives water cooled to a temperature of 45 degrees. Having passed through the entire circuit in the supercomputer, water heated to 50 degrees returns to the heat exchanger, where it is cooled, transferring thermal energy to the hydraulic circuit of the dry cooling tower.



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

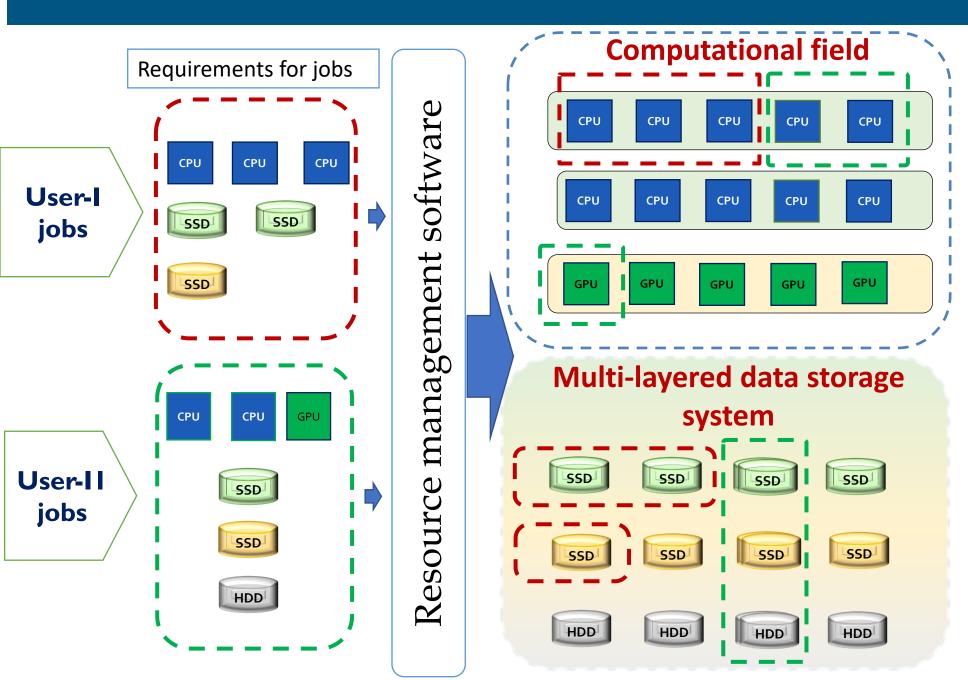


Top500 Rank	System	Cooling technology	Top500 Rank	System	Cooling technology
1	Frontier	Direct cold water cooling	11	Explorer-WUS3	
2	Fugaku	Direct cold water cooling	12	Adastra	Direct cold water cooling
3	LUMI	Direct cold water cooling	13	JUWELS Booster Module	Direct warm water cooling
4	Leonardo	Direct warm water cooling	14	Pre-Eos 128 Node DGX SuperPOD	Direct cold water cooling
5	Summit	Direct cold water cooling	15	HPC5	Airflow cooling
6	Sierra	Direct cold water cooling	16	Voyager-EUS2	Airflow cooling
7	Sunway TaihuLight	Airflow cooling	17	Setonix – GPU	Direct cold water cooling
8	Perlmutter	Direct cold water cooling	18	Discovery 5	Direct cold water cooling
9	Selene	Airflow cooling	19	Polaris	Airflow cooling
10	Tianhe-2A	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.

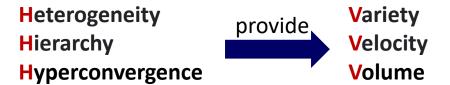
For his job the user can allocate the required number and type of computing nodes and the required volume and type of data storage systems.

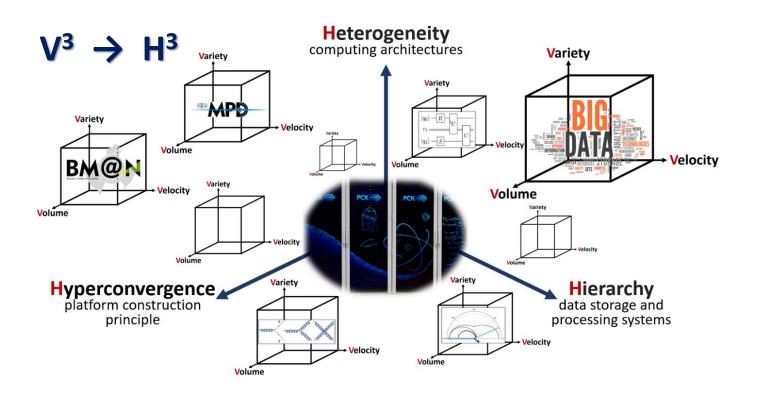
This property enables the effective solution of different tasks, which makes the "Govorun" supercomputer a unique tool for research underway at JINR.

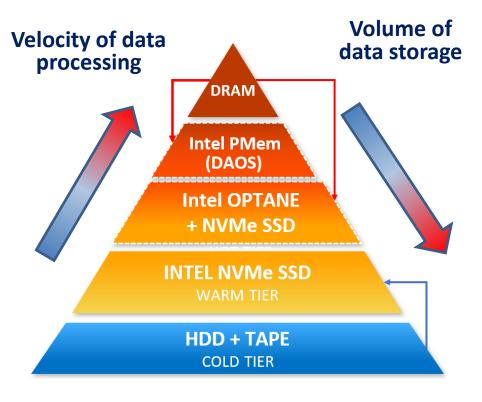
Big Data on the "Govorun" Supercomputer for NICA megaproject



The DAOS polygon of the "Govorun" supercomputer takes the 1st place among Russian supercomputers in terms of the data processing rate in the current 10500 list.

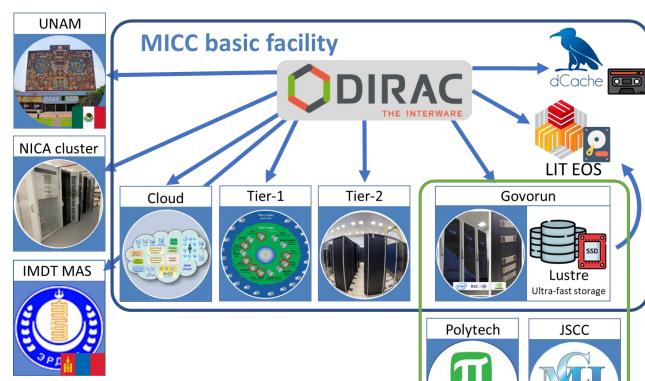




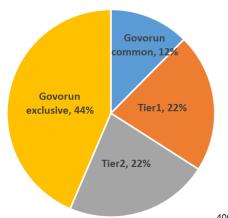


Heterogeneous distributed computing environment



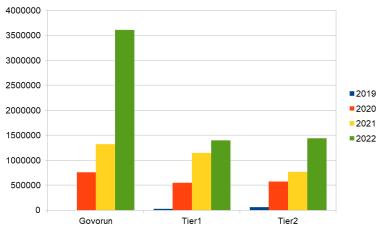


The computing cluster of the Institute of Mathematics and Digital Technologies of the Mongolian Academy of Sciences (IMDT MAS) and NIKS (National Research Computer Network, the Russia's largest research and education network) were integrated into the heterogeneous distributed environment based on the 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
1500000



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



NIKS 🐼











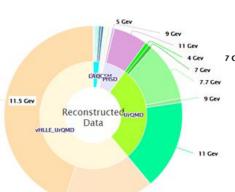


Heterogeneous distributed computing environment for the MPD experiment





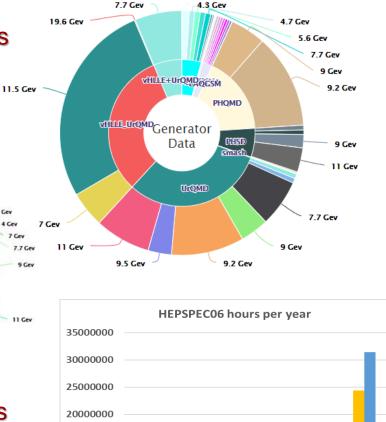
were generated using *UrQMD*, *PHQMD*, *PHSD* and other models



✓392*10⁶ events were

reconstructed

"Govorun" up to 40%



15000000

10000000

5000000

2019

2020

DIRAC.JINR-LHEP.ru ■ DIRAC.JINR-Tier2.ru

DIRAC.JINR-Tier1.ru DIRAC.Govorun.ru

2021

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.

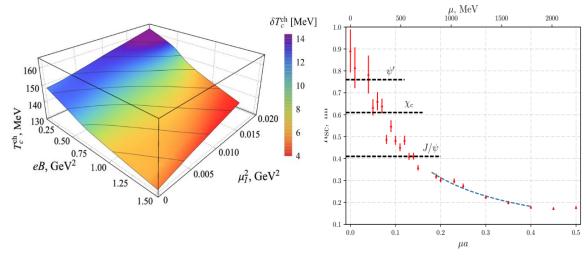
The mass production storages integrated into the Dirac File Catalog are 1.5 PB in size.

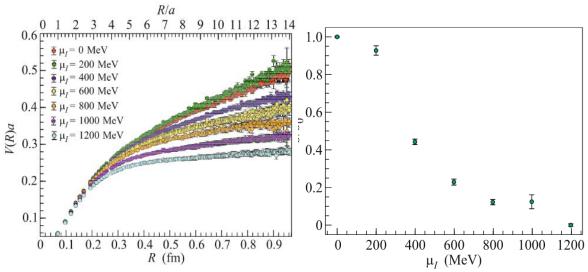
The histogram illustrates the accounting data from the centers. The metric shown is Sum CPU Work, grouped by center and year.



"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-, squarks 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

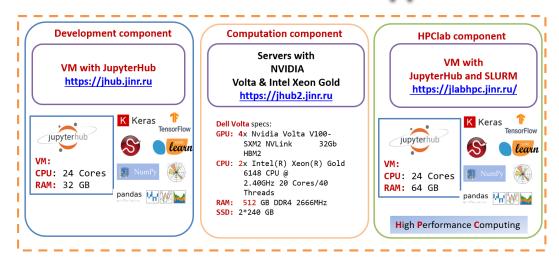
For calculations of electronic properties of superheavy elements. an on-demand computing system was created. It containing 380 physical cores (760 logical cores) and 80 TB file storage managed by the NFS file system. Intensive calculations were carried out on this system using AMS, DIRAC, KANTBP, etc. 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:

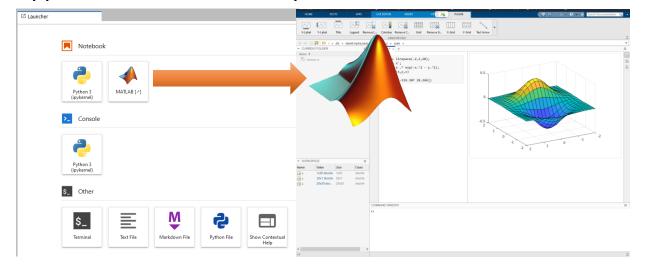
- 1) Kotov A. A., Kozhedub Y. S., Glazov D. A., Ilias M., Pershina V., Shabaev V. M. // ChemPhysChem. 2023. No 24. C. E202200680;
- 2) Ryzhkov A., Pershina V., Ilias M. and Shabaev V. // Phys. Chem. Chem. Phys. 2023. No 25. C. 15362;
- 3) Savelyev I. M., Kaygorodov M. Y., Kozhedub Y. S., Malyshev A. 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.

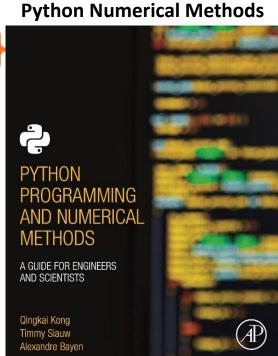


The ML/DL/HPC ecosystem is now actively used for machine and deep learning tasks. At the same time, the accumulated tools and libraries can be more widely used for scientific research, including:

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

| Jupyter | Jupyter | book | K | Keras | pandas | pandas | matpletlib | seaborn | Doblib | Parallel computations

with Joblib





hYBRI LIT/JINR

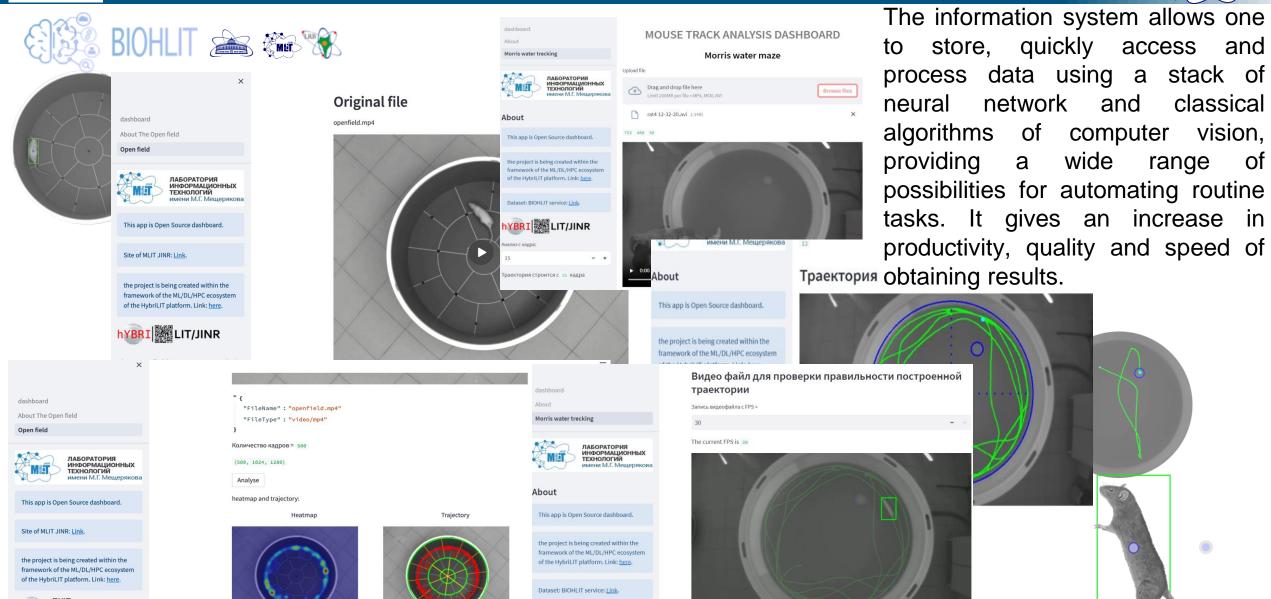
The Open field test-system analysis

Download heatmap

Download trajectory

BIOHLIT information system for radiobiological studies





YBRI LIT/JINR

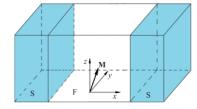
Study the dynamics of magnetization in a Phi-0 Josephson Junction

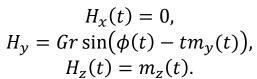


The dynamics of the magnetic moment M of the system under consideration is described by the Landau-Lifshitz-Gilbert equation:

$$\begin{split} \frac{dm_{x}}{dt} &= -\frac{1}{1 + M^{2}\alpha^{2}} \{ m_{y}H_{z} - m_{z}H_{y} + \alpha [m_{x}(M, H) - H_{x}] \}, \\ \frac{dm_{y}}{dt} &= -\frac{1}{1 + M^{2}\alpha^{2}} \{ m_{z}H_{x} - m_{x}H_{z} + \alpha [m_{y}(M, H) - H_{y}] \}, \\ \frac{dm_{z}}{dt} &= -\frac{1}{1 + M^{2}\alpha^{2}} \{ m_{x}H_{y} - m_{y}H_{x} + \alpha [m_{z}(M, H) - H_{z}] \}, \end{split}$$

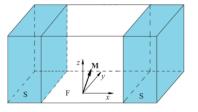
 $M = [m_x, m_y, m_z]$ are the magnetic moment components; the effective components $H = |H_x, H_y, H_z|$ on the Josephson phase depend and are defined as difference ϕ follows:

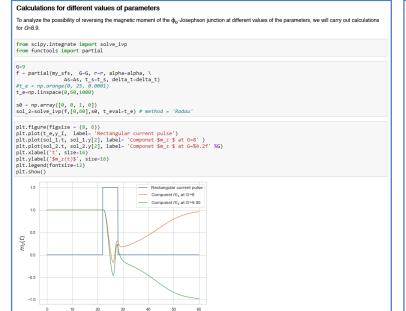


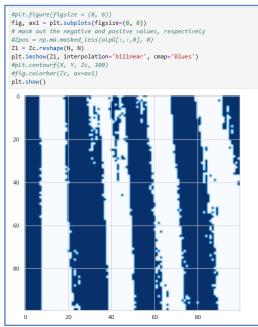


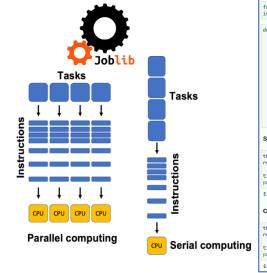
The equation for the Josephson phase difference $\phi(t)$ is determined from the equation for the electric current I flowing through the Josephson junction, measured in units of the critical current I_c :

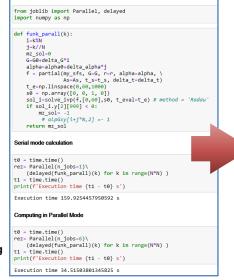
in units of the critical current
$$I_c$$
: $\frac{d\phi}{dt} = -\frac{1}{w} \left(\sin(\phi - r m_y) + r \frac{d m_y}{dt} \right) + \frac{1}{w} I$,

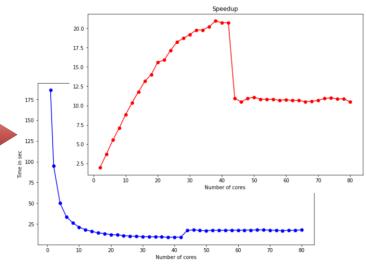






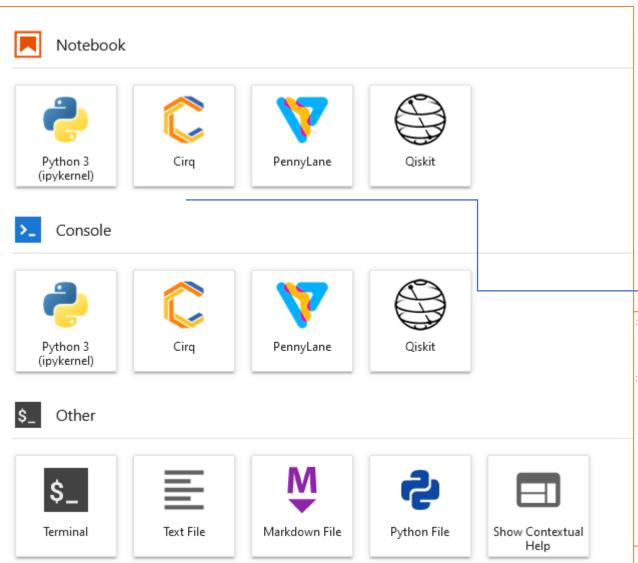






Quantum polygon

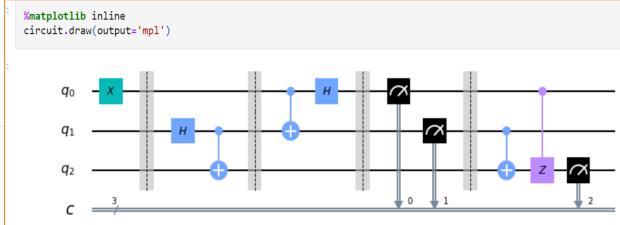




https://jhub3.jinr.ru

Equipment:

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

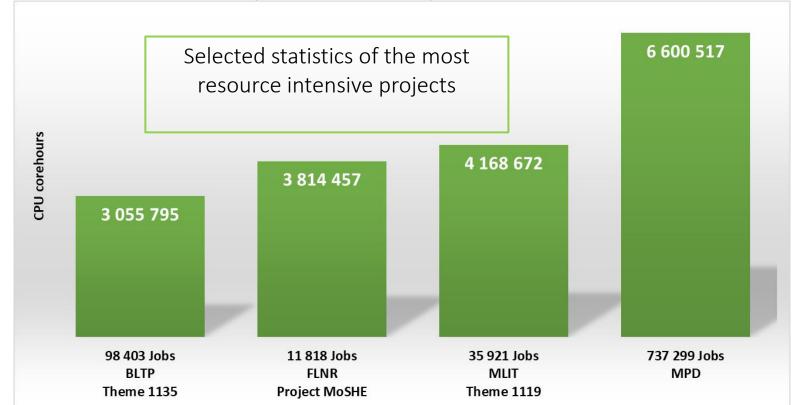


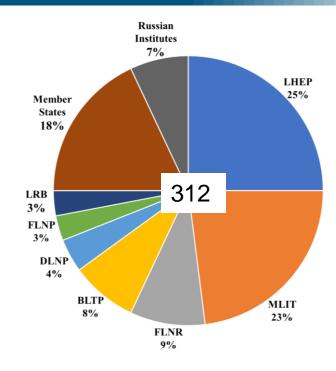
Using of the "Govorun" Supercomputer in 2023

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%.

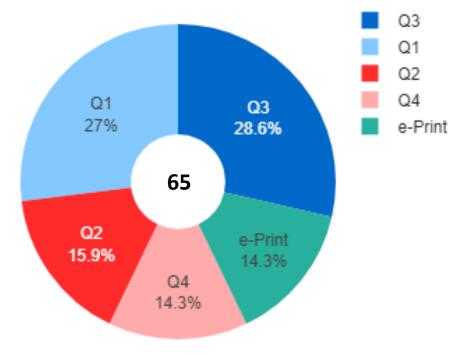
Publications



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







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



210

Participants in 2023 г.



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





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

"Govorun" supercomputer



http://hlit.jinr.ru/

