

"Govorun" supercomputer for JINR tasks

M. Zuev on behalf on HybriLIT heterogeneous group

The International Conference Mathematical Modeling and Computational Physics, 2024 (MMCP2024) 20-25 October 2024

Development of the heterogeneous platform HybriLIT

Cluster HybriLIT **2014**: Peak performance: **50 TFLOPS** double precision **140 TFLOPS** single precision #18 in Top50 Supercomputer "Govorun" First stage 2018 Peak performance: 500 TFLOPS double precision 1 PFLOPS single precision



#10 in Top50

РСК

Supercomputer "Govorun" Second stage 2019 Peak performance: 860 TFLOPS double precision 1.7 PFLOPF single precision 288 TB UDSS with I/O >300 Gb/s 17th in the IO500 list (July 2020)

РСК

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

РСК



"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: 800 TFLOPS 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

Peak performance:

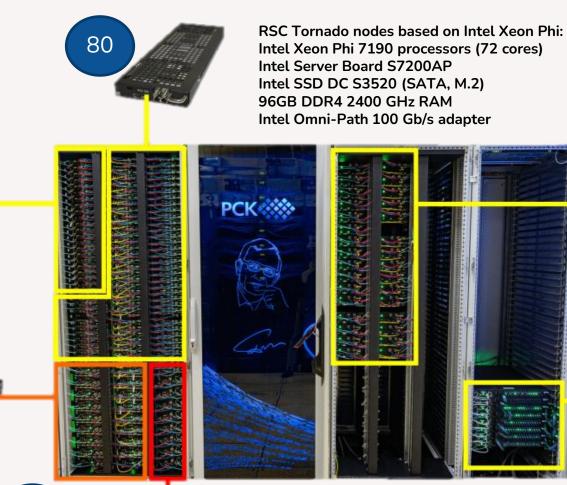
900 TFLOPS double precision 26 PFLOPS half precision

Storage system: 8.6 PB



Total peak performance 1.7 PFLOPS double precision 3.4 PFLOPS single precision

The CPU component of "Govorun" supercomputer



Current status:

163 hyperconverged compute nodes 8552 compute cores

Total peak performance: 800 TFLOPS double precission

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



32

<u>Total capacity of</u> <u>Hierarchical Storage</u>: **8.6 PB** <u>Data IO rate</u>: **300 Gb/s**

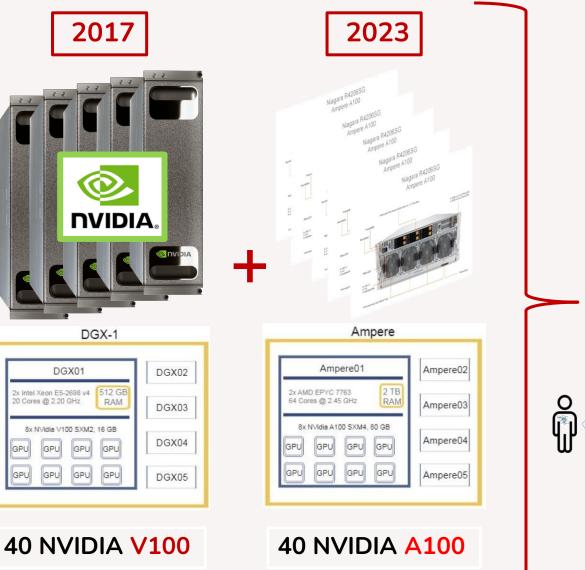


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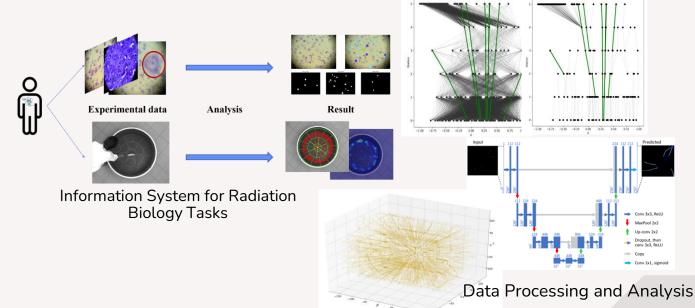
RSC Tornado nodes based on Intel Xeon Scalable gen 2 (TDN511S): Intel Xeon Platinum 8280 processors (28 cores) Intel Server Board S2600BP Intel SSD DC S4510(SATA, M.2), 2x Intel SSD DC P4511 (NVMe, M.2) 2TB / 4x Intel (PMem) 450 GB 192GB DDR4 2933 GHz RAM Intel Omni-Path 100 Gb/s adapter

The GPU component of "Govorun" supercomputer



Total peak performance of the GPU-component: 900 TFLOPS double precision 26 PFLOPS half precision

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.

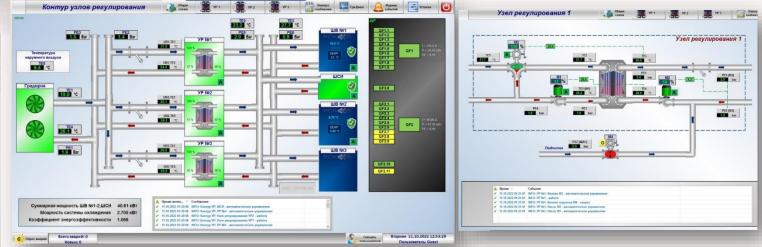


"Govorun" supercomputer. Hot water cooling



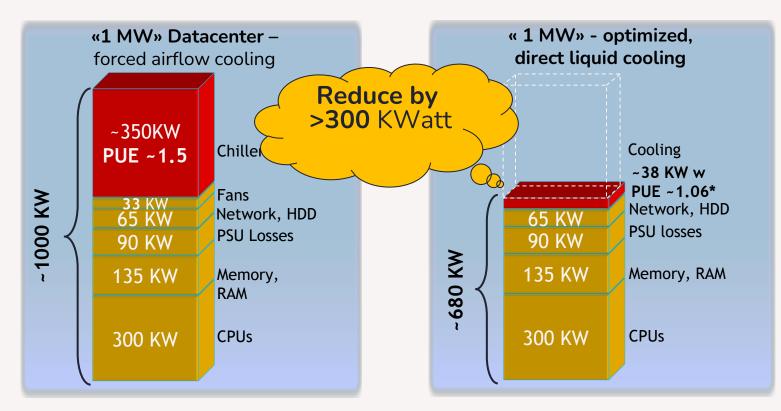


The supercomputer receives water cooled to a temperature of **45 degrees**. Having passed through the entire circuit in the supercomputer, water heated to **50 degrees** returns to the heat exchanger, where it is cooled, transferring thermal energy to the hydraulic circuit of the dry cooling tower.



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: 1 MW datacenter example



Cooling is a major optimization option in datacenter

Additional benefits:

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

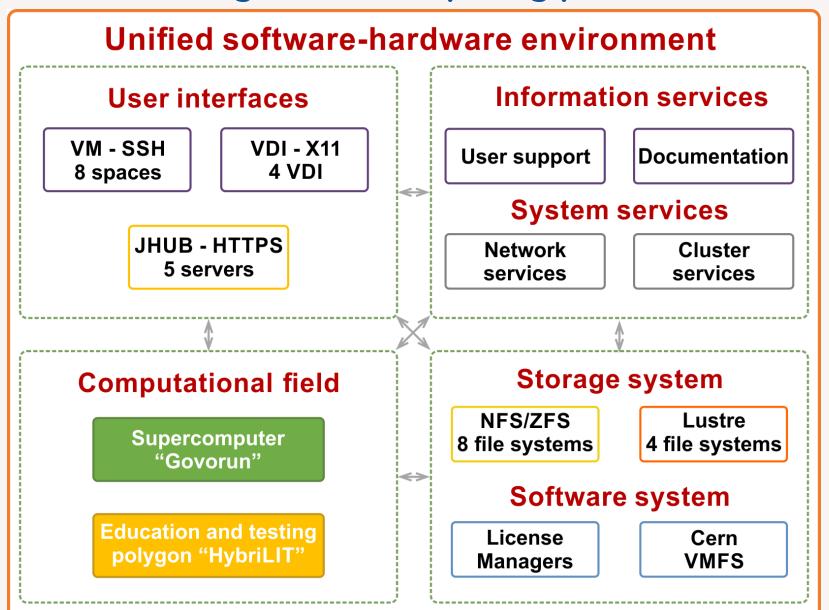
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Liquid cooling for supercomputers

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

Software and hardware structure and services of the HybriLIT heterogeneous computing platform



Software and information environment of the Platform

Information Level

HybriLIT web-site http://hlit.jinr.ru/	HybriLIT user support project https://pm.jinr.ru/ HybriLIT user support telegram https://web.telegram.org/k/#-1752786710	Indico https://indico.jinr.ru/ GitLab https://gitlab-hybrilit.jinr.ru/	Jupyter Book http://studhub.jinr.ru:8080/jjbook http://studhub.jinr.ru:8080/books
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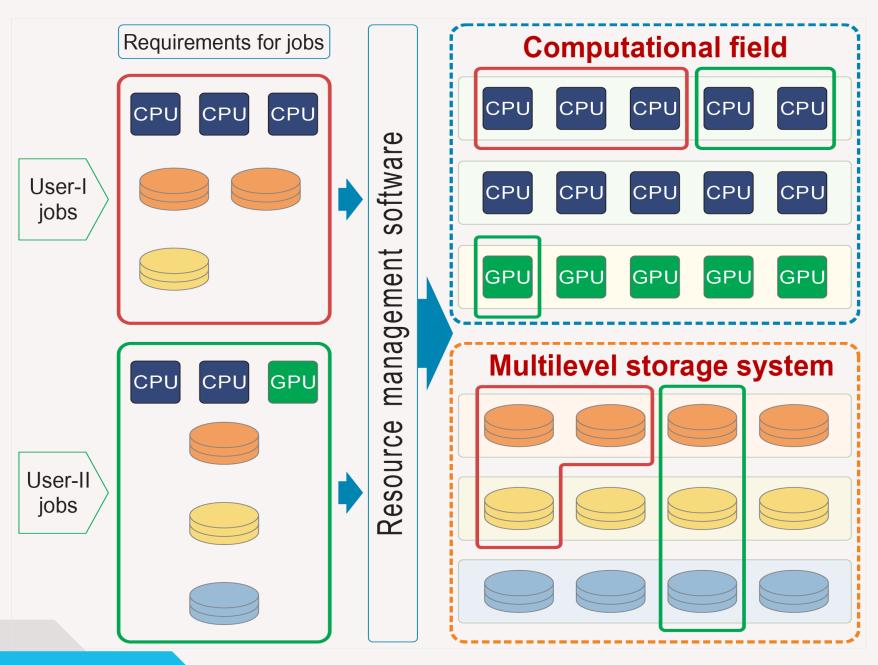
Software Level

Testbed			HLIT-VDI			
for quantu Cirq Qiskit	I m computing PennyLane QuTiP	ht ht	Development component tps://studhub.jinr.ru :ps://studhub2.jinr.ru	Component for carrying out resource-intensive calculations https://jhub1.jinr.ru https://jhub2.jinr.ru	Component for HPC on the HybriLIT platform nodes and data analysis https://jlabhpc.jinr.ru/	
Parallel computing software		Application Packages		BIOHLIT	NICA	
Open MPI	CUDA	Intel	GROMACS Java	Cmake FairRoot	BIO Dashboards	MPD Event Display
	software pack	I	LAMMPS PandaRoot Vthon	FairSoft FLAIR FLUKA	Datasets	Parametric Databas DIRAC interware
Comsol Multi Wolfram Mat		Maple Matlab	REDUCE ROOT	GEANT4 Quantum ESPRESSO	CVAT	integration

System Level

Scientific Linux 7.9 (operating system)	FreeIPA	NFS	CernVM-FS (software distribution service)	Мс	onitoring
xCAT (OS deployment tool)	(auth system)	(network file system)	FlexLM/MathLM (licence manager system)	Home-HLIT	Monitoring HLIT-VDI
Puppet (configuration management tool)	(workload manager)	(parallel file system)	Modules (software environment tool)	РСК БазИС	Computing Resources' Statistics

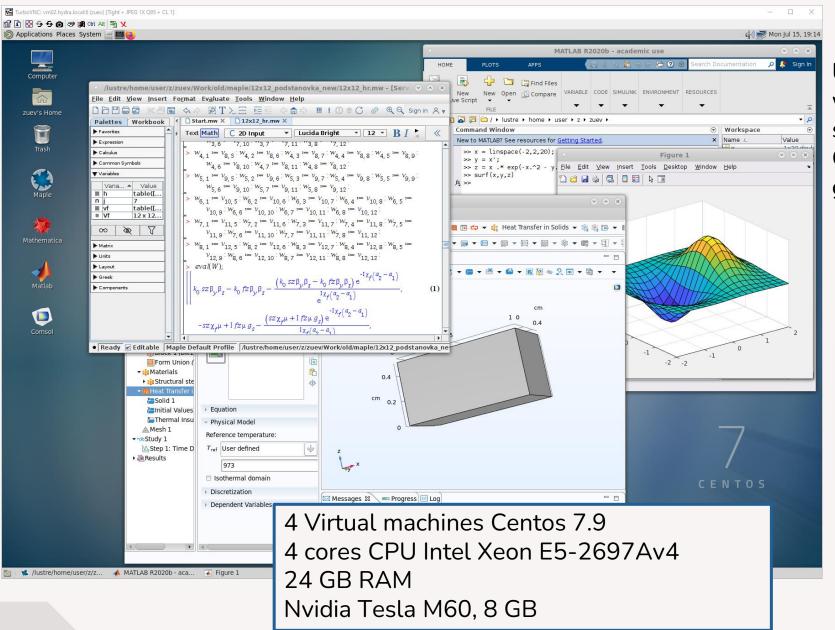
Orchestration and hyperconvergence



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

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

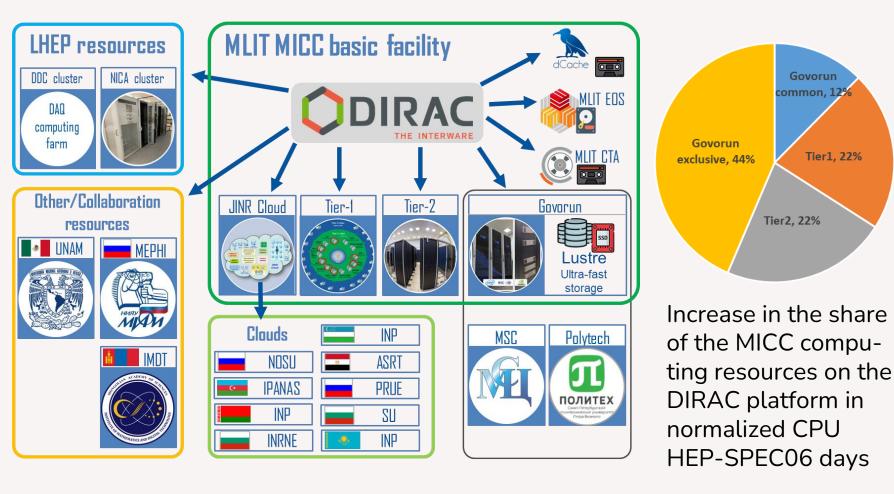
HLIT-VDI Remote Desktop

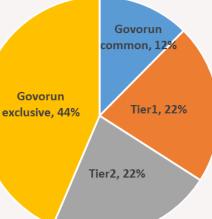


Users have the opportunity to work with mathematical and physical software (Matlab, Mathematica, Maple, COMSOL, Geant4, ROOT) through a graphical user interface (GUI).

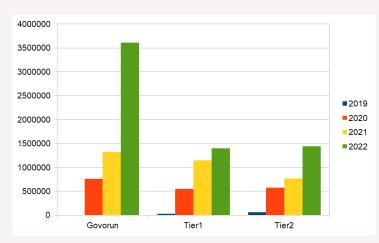


Heterogeneous distributed computing environment





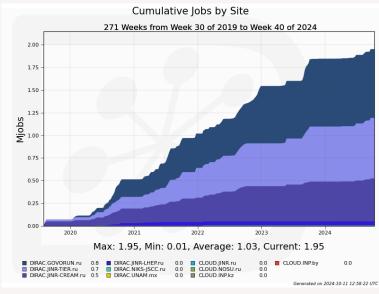
Share of the use of different MICC components for MPD tasks in 2022: "Govorun" resources are the most efficient for MPD tasks.



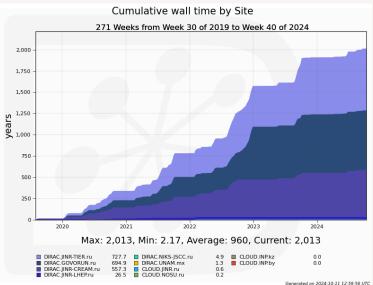
Summary statistics of using the DIRAC platform for MPD tasks in 2019-2024



Heterogeneous distributed computing environment for the MPD experiment



(NICA)



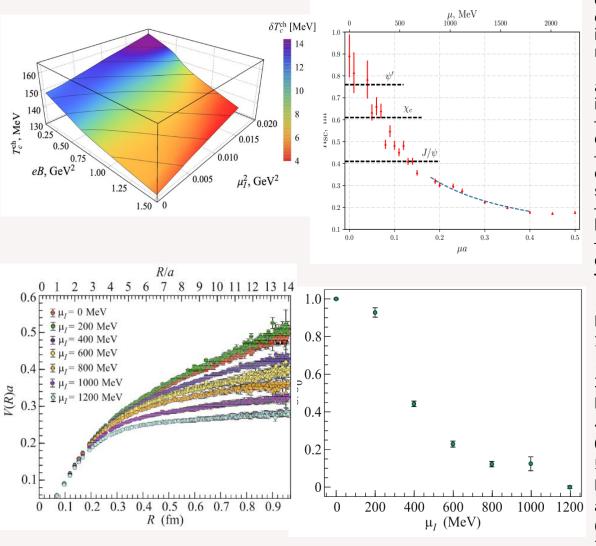
Available resources of the DIRAC platform for the MPD experiment:

- "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.



"Govorun" supercomputer for QCD tasks



The resources of "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 twocolor 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

– 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

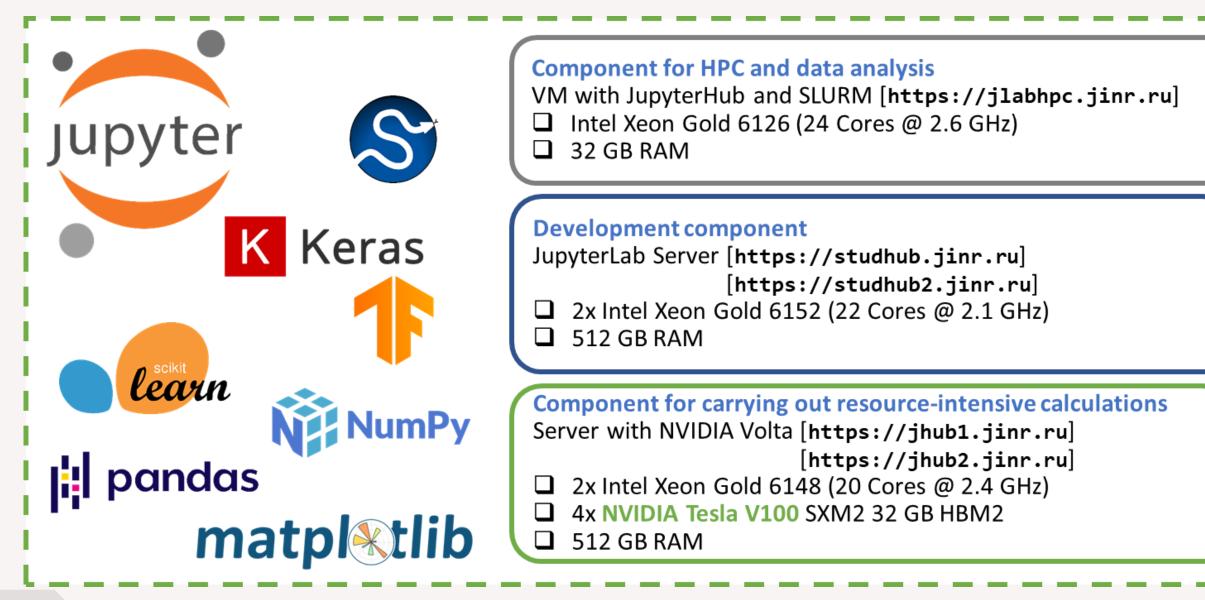
"Govorun" supercomputer for nuclear physics tasks

- 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**. 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;
- 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.

ML/DL/HPC ecosystem



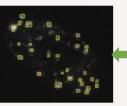
BIOHLIT information system for radiobiological studies

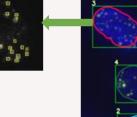


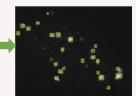


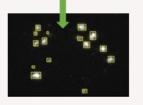
Within the framework of the joint project between Meshcheryakov Laboratory of Information Technologies (MLIT) and the Laboratory of Radiation Biology (LRB), the web services are developed and deployed based on the ML/DL/HPC ecosystem of the HybriLIT Heterogeneous Computing Platform.

Detecting DNA repair foci in cell nuclei



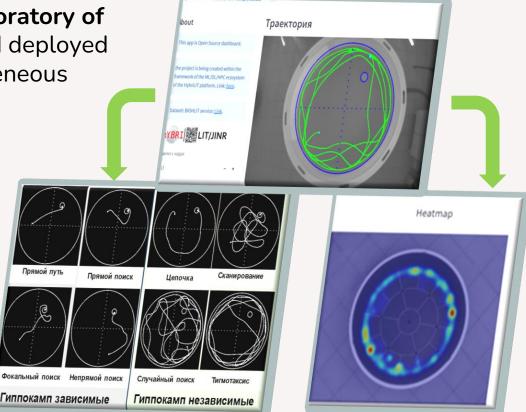












Our web service allows to process the group of fluorescent images with minimal operator's involvement and automate the analysis of radiation induced DNA double-strand breaks.

The developed web service allows one to study spatial learning, behavioral reactions and memory of small laboratory animals exposed to irradiations.

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

Μ

Tasks

Calculations for different values of parameters

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

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

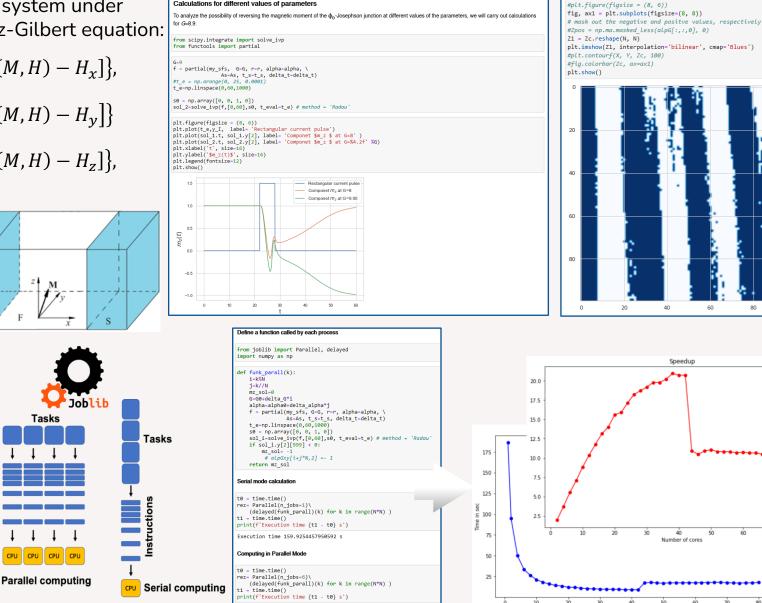
 $M = [m_x, m_y, m_z]$ are the magnetic moment components; the effective field components $H = [H_x, H_y, H_z]$ depend on the Josephson phase difference ϕ and are defined as follows:

$$H_x(t) = 0,$$

$$H_y = Gr \sin(\phi(t) - tm_y(t)),$$

$$H_z(t) = m_z(t).$$

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



Execution time 34,51503801345825

Number of cores

Software modules for modelling superconductor/magnetic hybrid nanostructures

http://studhub.jinr.ru:8080/jjbook, http://studhub.jinr.ru:8080/books

As part of a joint project between **MLIT** and **the Laboratory of Theoretical Physics (BLTP)** on modelling hybrid superconductor/magnetic nanostructures, a package of tools in the form of Jupyter Notebook, which are posted in the format of electronic publications **Jupyter Book** on the Platform resources has been developed.

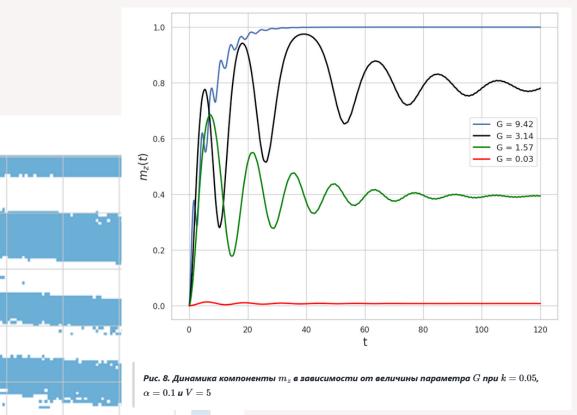
Математическая постановка задачи

Динамика магнитного момента *m* рассматриваемой системы описывается уравнением Ландау-Лифшица-Гильберта [1], которое в нормированных единицах покомпонентно имеет вид :

$$\begin{aligned} \frac{dm_x}{dt} &= \frac{\Omega_F}{1+m^2\alpha^2} \left[h_y(m_z - \alpha m_x m_y) - h_z(\alpha m_x m_z + m_y) + \alpha h_x(m_y^2 + m_x^2) \right],\\ \frac{dm_y}{dt} &= \frac{\Omega_F}{1+m^2\alpha^2} \left[-h_x(\alpha m_x m_z + m_z) + h_z(m_x - \alpha m_y m_z) + \alpha h_y(m_x^2 + m_z^2) \right]\\ \frac{dm_z}{dt} &= \frac{\Omega_F}{1+m^2\alpha^2 + \Omega_F \alpha \epsilon k(m_x^2 + m_y^2)} \left[\alpha \epsilon [\sin(Vt - km_z) + V](m_x^2 + m_y^2) - \frac{2\pi k^2 k(m_x^2 + m_y^2)}{2\pi k^2 k(m_x^2 + m_y^2)} \right] \end{aligned}$$

Зафиксированные физические параметры alpha = 0.1
k = 0.05
OmegaF = 0.5
V = 5
Параметры численного счеты
t0 = 0
tf = 120
nt = 600000





-0.925

Testbed 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.

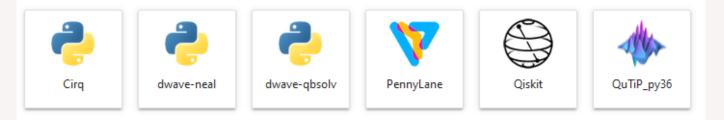
The work is organized in two modes:

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.

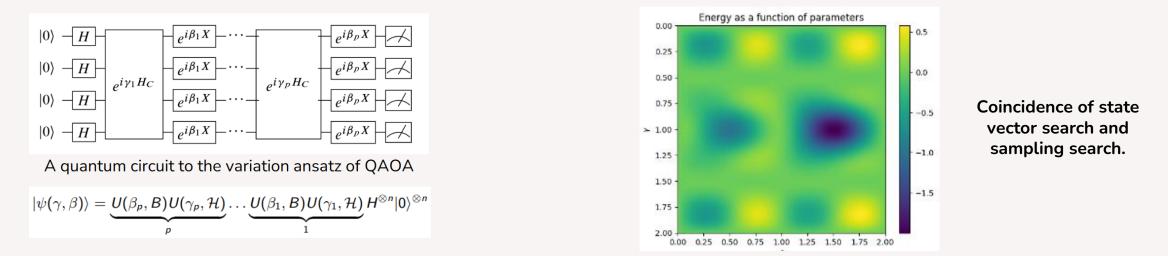


Testbed for quantum computing. Working in interactive mode. Cirq library

https://quantumai.google/cirq

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

The solution to the problem is to find a pair of parameters y, β , at which the energy value $\mathcal{E}(y, \beta)$ will be minimal. The problem statement is presented in detail in the work 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.



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 TE RAM CPU and ~1.5 FE RAM GPU.

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

Information level

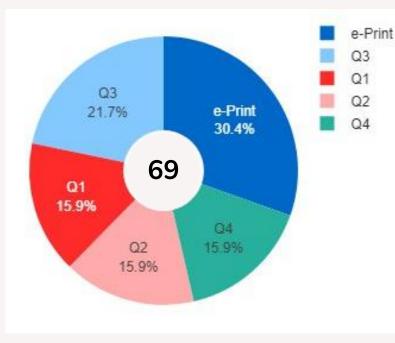
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- The website provides a detailed description of the platform: hardware and software structure, characteristics of computing resources, and examples for working with installed application software
- GitLab collaborative development service provides 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.
- To consult and resolve user questions regarding work on the Platform, the HybriLIT user support service is used, available in the JINR Project Management Service environment.
- A streaming channel HybriLIT user support on the Telegram social network is being used to promptly inform users

84 processed user requests (in 2023) via PM HybriLIT user support

41 events conducted (in 2023) via the **Indico** system

Using of the "Govorun" supercomputer in 2023

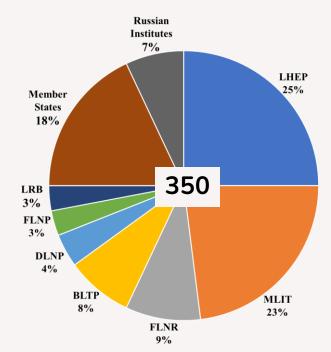


Over the past year, users of the heterogeneous HybriLIT platform published 69 articles in various fields:

- 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 **336** 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. Nº 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



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%.

Educational activities on the Platform

Platform resources are used as a base platform for studying new IT technologies and for training IT specialists. The International School on Information Technologies of JINR is held annually at LIT; it is aimed at attracting young specialists to solving JINR tasks using modern information technologies.

The **Dubna State University** regularly conducts training courses in such disciplines as:

- "Architecture and technologies of high-performance systems",
- "Parallel distributed computing",
- "Languages and technologies of data analysis",
- "High-performance computing technologies".
 Over the past academic year (2022-2023), 380 students participated in these courses.

"Software tools for mathematical calculations" course attended by **40 students** was held at **Tver State University**.



https://itschool.jinr.ru

Training courses, lectures, tutorials

MPQIT 27-28 May 2024 International Workshop Mathematical Problems in Quantum Information Technologies



JINR School of Information

Technologies

7-11 October 2024



The main focus was on the mathematical aspects of diverse problems in fundamental and applied quantum technologies, such as

- quantum information theory,
- quantum communications,
- quantum computing, simulation, and quantum algorithms. More than **60** participants from

Armenia,Great Britain,India,Romania,Belarus,Georgia,Kazakhstan,Serbia,Bulgaria,Egypt,Moldova,the Czech Republic

Russia was represented by specialists from Voronezh, Kazan, Moscow, St. Petersburg, Tver, Chelyabinsk and Dubna.



 Distributed and high-performance computing for experimental and theoretical research at JINR;

Mathematical modeling and numerical methods;

 Modern methods and technologies for information processing and analysis;

- JINR Digital EcoSystem;
- Support and development of the JINR Multifunctional Information and Computing Complex (MICC);



• Engineering infrastructure: automation and monitoring.



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Thank you for your attention!

Heterogeneous platform "HybriLIT" http://hlit.jinr.ru/



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