"GOVORUN" supercomputer for JINR tasks

РСК 💥

PCK

D.V. Podgainy

Meshcheryakov Laboratory of Information Technologies

Рабочее совещание "ОИЯИ-ВШЭ" 14 June 2024

Development of the heterogeneous HybriLIT platform



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

#18 в Тор50

"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 Тор50

РСК

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

РСК

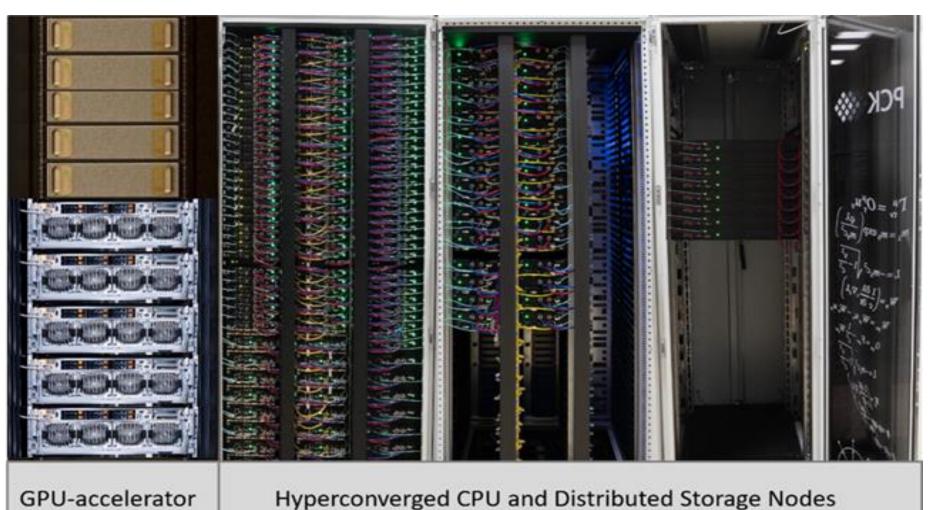


PCK 🐝

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

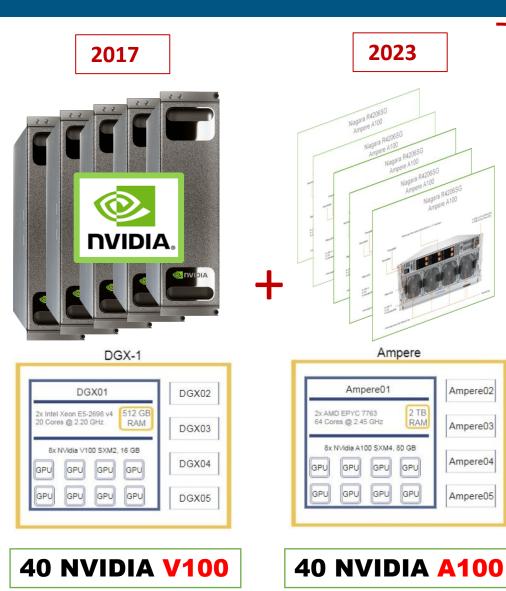
Total capacity of Hierarchical Storage: 8.6 PB

Data IO rate: 300 Gb/s

The GPU-component of the "Govorun" Supercomputer

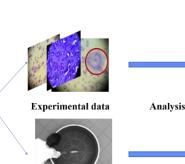
ŝ

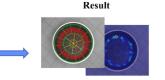




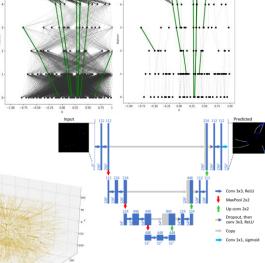
Total peak performance of the GPU-component: 900 Tflops for Double-Precision computations 26 Pflops for Half-Precision computations

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.





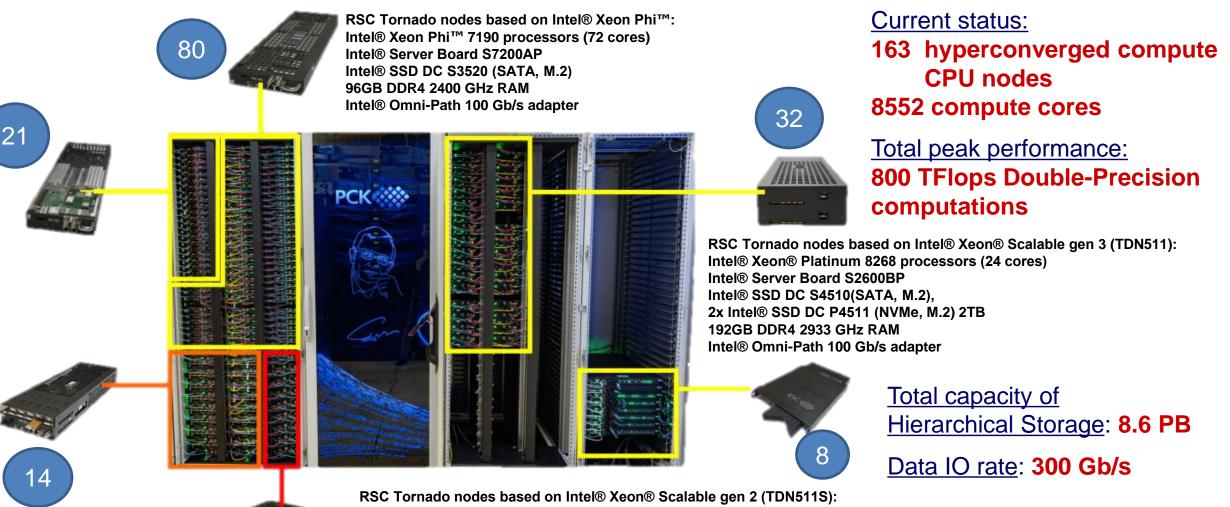
Information System for Radiation Biology Tasks



Data Processing and Analysis

The CPU-component of the "Govorun" Supercomputer





RSC Tornado nodes based on Intel® Xeon® Scalable gen 2 (TDN511 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.

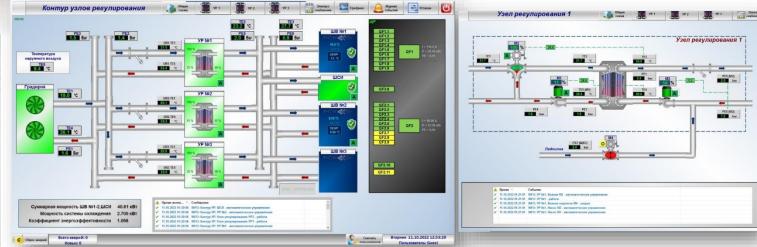








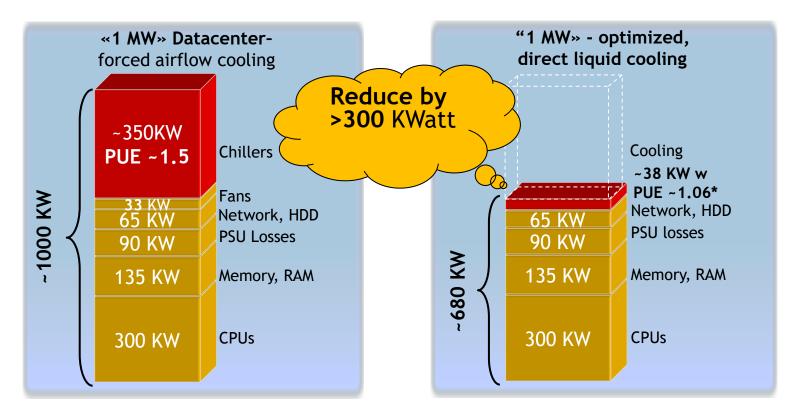
The supercomputer receives water cooled to a temperature of 45 degrees. Having passed through the entire circuit in the supercomputer, water heated to 50 degrees returns to the heat exchanger, where it is cooled, transferring thermal energy to the hydraulic circuit of the dry cooling tower.



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

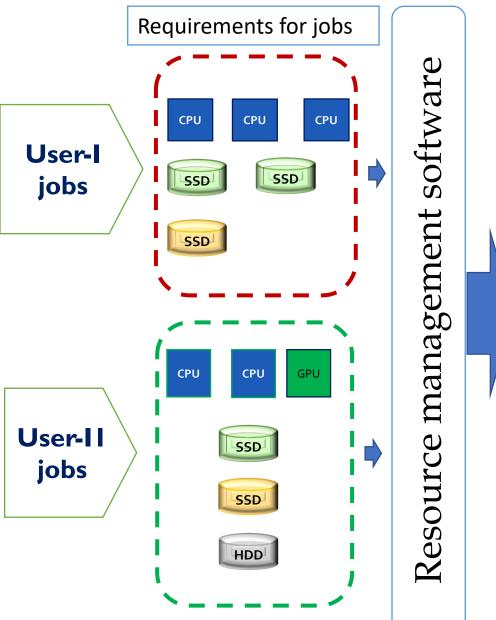


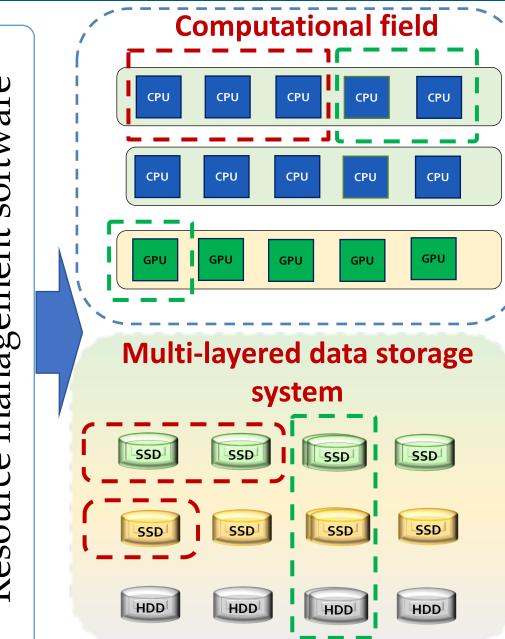
Top500 Rank	System	Cooling technology	Top500 Rank	System	Cooling technology
1	Frontier	Direct cold water cooling	11	Explorer-WUS3	
2	Fugaku	Direct cold water cooling	12	Adastra	Direct cold water cooling
3	LUMI	Direct cold water cooling	13	JUWELS Booster Module	Direct warm water cooling
4	Leonardo	Direct 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	
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

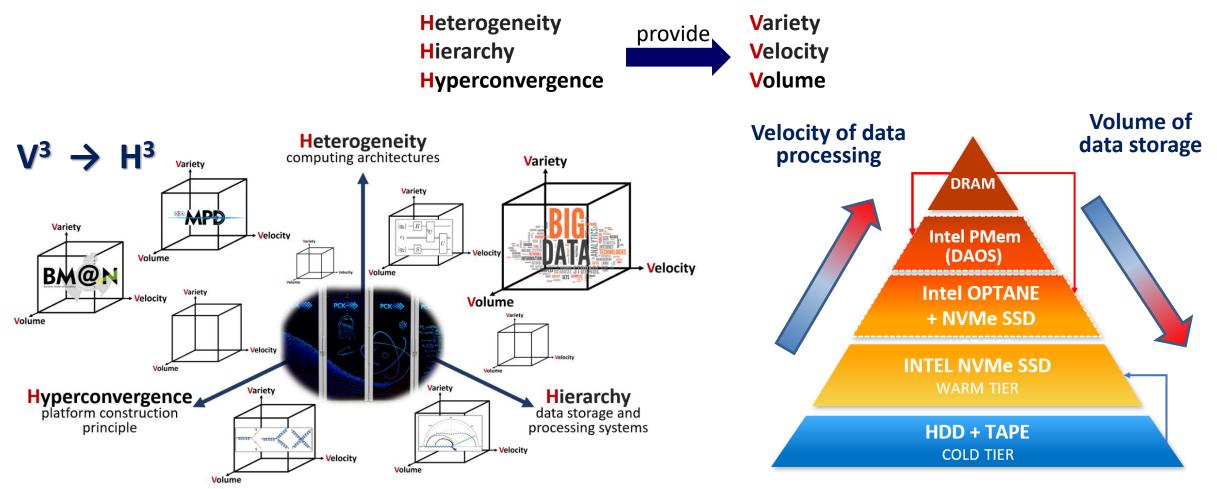
tasks, which makes the "Govorun" supercomputer a unique tool for research underway at JINR.

Big Data on the "Govorun" Supercomputer for NICA megaproject

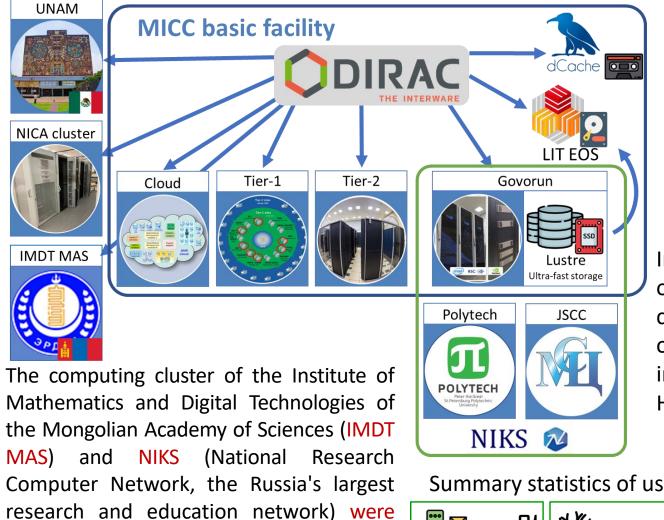


The DAOS polygon of the "Govorun" supercomputer takes the **1**st place among Russian supercomputers in terms

of the data processing rate in the current **IO500 list**.



Heterogeneous distributed computing environment



heterogeneous

based on the

integrated

DIRAC platform.

into

distributed environment

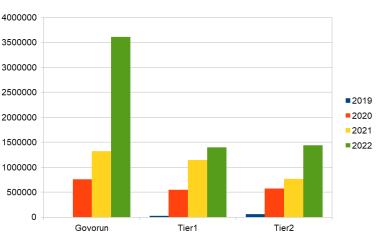
the

Govorun
exclusive, 44%Tier1, 22%Tier2, 22%4000000Increase in the share
of the MICC
computing resources
on the DIRAC platform
in normalized CPU3500000
200000
1500000Increase in the share
of the MICC
computing resources
on the DIRAC platform
15000003000000
200000
200000
500000

Govorun

ommon. 12%

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



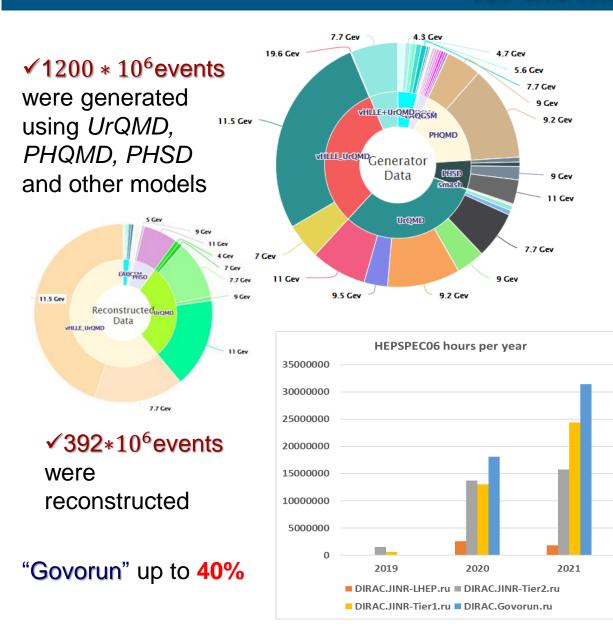
Summary statistics of using the DIRAC platform for MPD tasks in 2019-2022





Heterogeneous distributed computing environment for the MPD experiment





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.

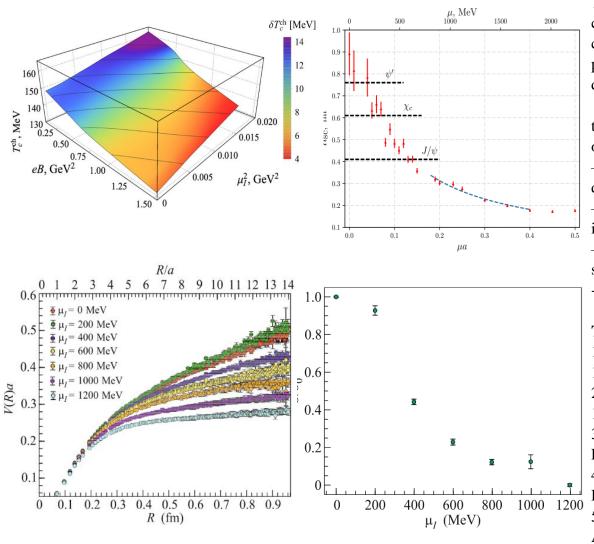
The mass production **storages** integrated into the Dirac File Catalog are **1.5 PB** in size.

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



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

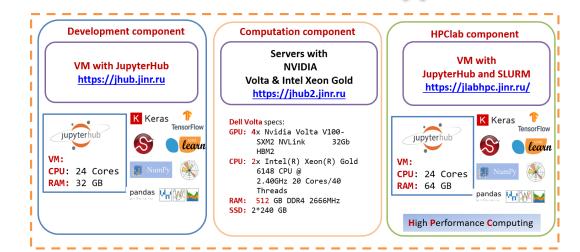
For calculations of electronic properties of superheavy elements. an on-demand computing system was created. It containing 380 physical cores (760 logical cores) and 80 TB file storage managed by the NFS file system. Intensive calculations were carried out on this system using AMS, DIRAC, KANTBP, etc.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

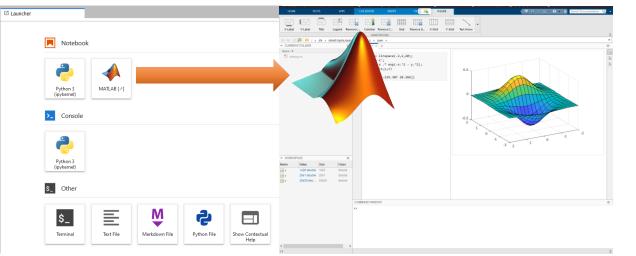
- Kotov A. A., Kozhedub Y. S., Glazov D. A., Ilias M., Pershina V., Shabaev V. M. // ChemPhysChem. 2023. No 24. C. E202200680;
- 2) Ryzhkov A., Pershina V., Ilias M. and Shabaev V. // Phys. Chem. Chem. Phys.2023. No 25. C. 15362;
- Savelyev I. M., Kaygorodov M. Y., Kozhedub Y. S., Malyshev A. V., Tupitsyn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



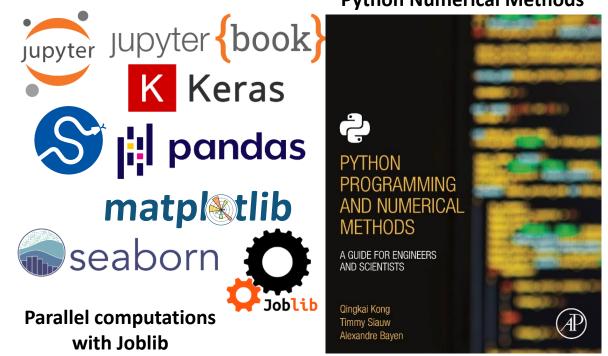


In 2022, on the ML/DL/HPC ecosystem, it became possible to run the MATLAB code in Jupyter Notebook, which allows one to effectively perform applied and scientific computations.



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:

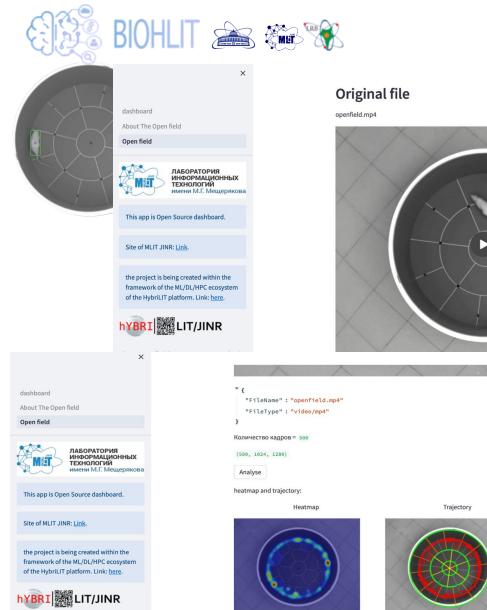
- numerical computations;
- parallel computing on CPUs and GPUs;
- visualization of results;
- accompanying them with the necessary formulas and explanations. Python Numerical Methods





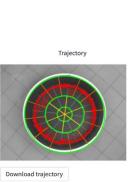
BIOHLIT information system for radiobiological studies





Download heatmap

The Open field test-system analysis



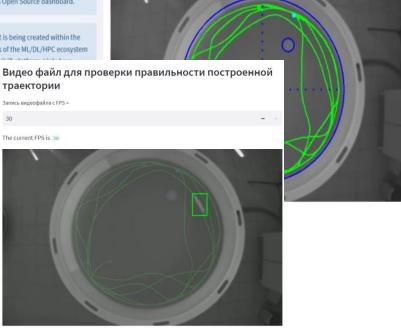
of the HybriLIT platform. Link: here.

Dataset: BIOHLIT service: Link.

HYBRI

MOUSE TRACK ANALYSIS DASHBOARD About Morris water trecking Morris water maze Upload file ЛАБОРАТОРИЯ ИНФОРМАЦИОННЫХ ТЕХНОЛОГИЙ Drag and drop file here MET Browse files mit 200MB per file • MP4, MOV. rat4 12-32-20.avi 1.9MB About 752 480 30 This app is Open Source dashboard he project is being created within the amework of the ML/DL/HPC ecosyster of the HybriLIT platform, Link; here, Dataset: BIOHLIT service: Link. YBRI LIT/JINR имени М.Г. Мешерякова ектория строится с 15 кадра bout This app is Open Source dashboard. the project is being created within the framework of the ML/DL/HPC ecosystem траектории Запись видеофайла с FPS = Morris water trecking 30 The current FPS is 30 ЛАБОРАТОРИЯ ИНФОРМАЦИОННЫХ ТЕХНОЛОГИЙ About This app is Open Source dashboard. the project is being created within the framework of the ML/DL/HPC ecosystem

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



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

Jobli

Tasks

CPU Serial computing

Tasks

Parallel computing



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

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

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

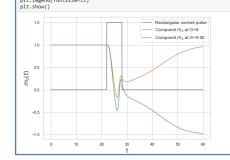
Calculations for different values of parameters

To analyze the possibility of reversing the magnetic moment of the ϕ_0 -Josephson junction at different values of the parameters, we will carry out calculations for G=8.9.



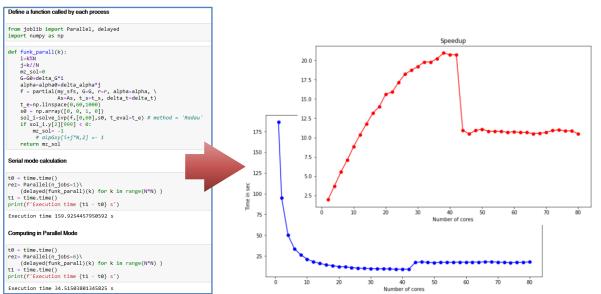
s0 = np.array([0, 0, 1, 0]) sol_2=solve_ivp(f,[0,60],s0, t_eval=t_e) # method = 'Radau'

plt.figure(figsize = (8, 6))
plt.plot(t_e,y_I, label= "Rectangular current pulse')
plt.plot(sol_1.t, sol_1.y(2), label= "Componet Sm_z S at G=8")
plt.plot(sol_2.t, sol_2.y(2), label= "Componet Sm_z S at G=%4.2f" %G)
plt.ylabel('t_, size=16)
plt.legen(frontSize=12)
plt.legen(frontSize=12)



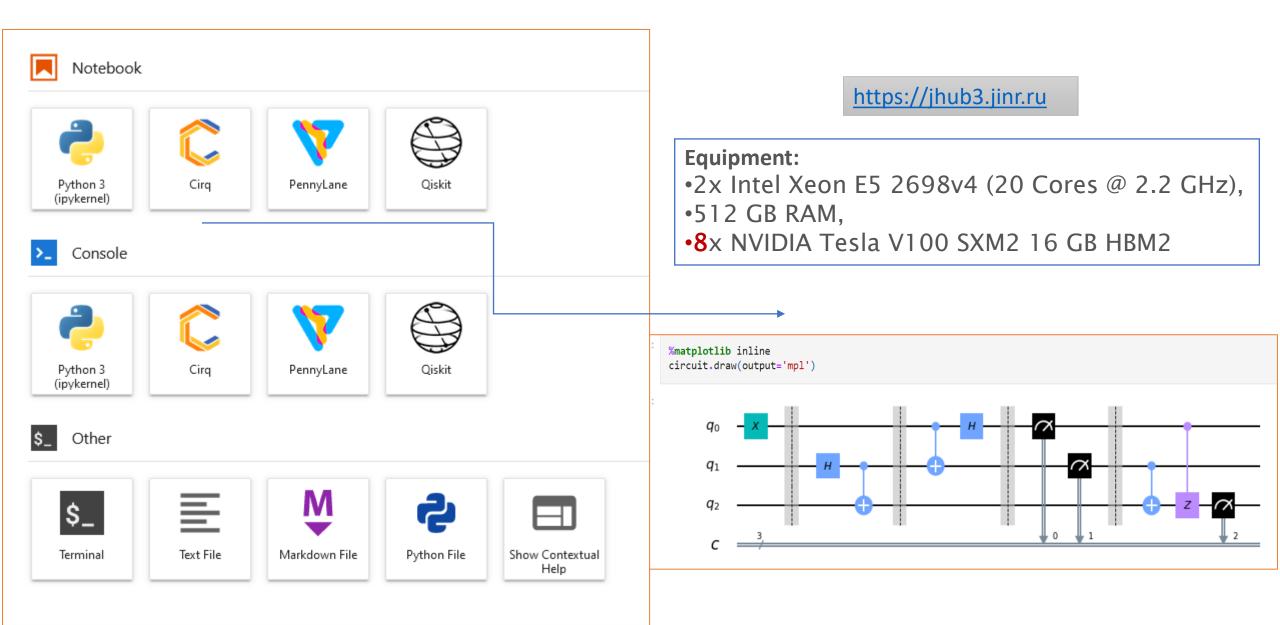


#plt.figure(figsize = (8, 6))



Quantum polygon



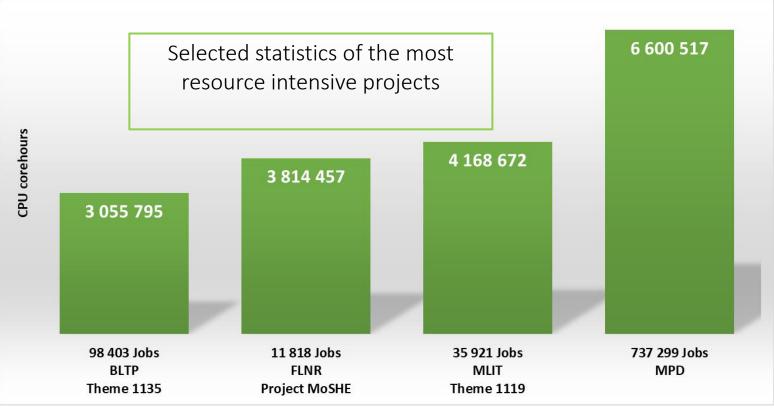


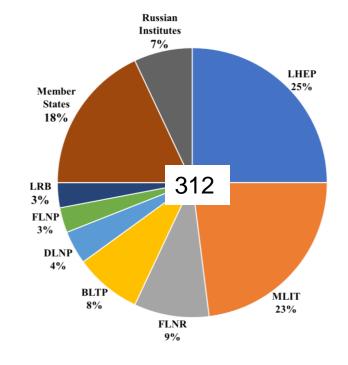
Using of the "Govorun" Supercomputer in 2023

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%.

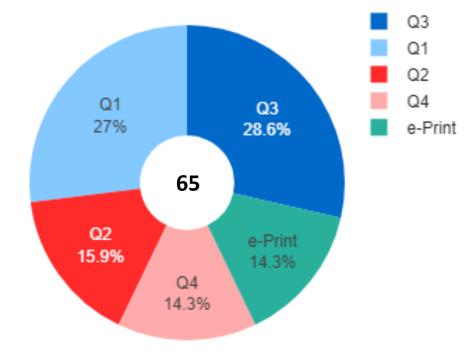
Publications



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





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



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

"Govorun" supercomputer



http://hlit.jinr.ru/

C 🔺 He защащено hiitjincru			@ @ ☆ □ 0				
hYBRI	ПЛАТФОРМА «HYBRILIT»	ОПОЛЬЗОВАТЕЛЯМ - ДОСТУП К РЕСУРСАМ - ПРОВ	ЕКТЫ 🗸 О НАС 🖌 НОВОСТИ 🖪 🔍				
				hybri Milling Infateorma «Hybrillin» Norboleaterram Qoctyri k Pecypicam Infotoerta Infateorma (Infateorma) (a) Norboleaterram Persectature Persectature Infateorma (Infateorma) Infateorma) Infateorma (Infateorma) Infateorma) Infateorma) <td< th=""></td<>			
		рогенная платформа «HybriLIT»		Регистрация Для получения доступа к ресурсам платформы «НуbriLT» необходимо ознакомиться с правилами использования ресурсов платформы. Сотрудникам ОИЯИ • Заполнить регистрационную форму.			
ß	D	匪	ଜ	 Регистрационную форму необходимо распечатать, подлисать лично и передать для подлиси в ком. 323, ЛИТ (с 9⁰⁰ до 18⁰⁰) По электронной почте, указанной в заявке, в течение недели будет направлено сообщение с подтверждением регистрационных данных, а так же логии и временный пароль, который необходимо поменять в 			
РЕГИСТРАЦИЯ	СЕРВИСЫ	ИНСТРУКЦИЯ ПО РАБОТЕ	обучающие видео	течение семи дней. Пользователям из других организаций			
Гетерогенная платформа «HybriLIT» является частью і состоит из Суперкомпьютера «Говорун» и учебно-тес	Многофункционального информационно-вычислителы	латформа «HybriLIT» ного комплекса (МИВК), Лаборатории информационных технологи	 Направить официальное письмо на имя директора ОИЯИ — Трубникова Г. В. (образец письма). Оригивал официального письма оптравить потой по адресу: ОИЯИ, Жолно-Кюри 6, 14198, Московская область. По электронной потех контактого лиць, эказиного в заявке, бодет направлено сообщение с подтверждением или отклонением заявки. В случае подтверждения заявки необходимо залолиить регистрациенирую форму. Заполненная форма, в тотовом для печати виде, будет направлено сообщение с подтверждением или отклонением заявки. В случае подтверждения заявки необходимо залолиить регистрациенирую форму. Заполненная форма, в тотовом для печати виде, будет направлена по электронной потте по указанному в заявке адресу. Форму необходимо распечатать, постявить подписов, отсканировать и отправлить по адресу hybrint@jinr.tu По электронной поте, указанной в заявке, в течение недели будет направлено сообщение с подтверждением регистрационных данных, а так же логии и временный пароль, который необходимо поменять в течение ски динай. 				
Суперкомпьютер «Говорун» представляет собой двух							
CPU-kownoneerra, базирурошурося на новейших архитектурах Intel (процессоров II							
• GPU-компонента, базирующуюся на узлах NVIDIA DCX-1 Volta. Учебно-тестовый полигон имеет гетерогенную структуру вычислительных узлов				ПОЛЬЗОВАТЕЛЯМ У ДОСТУП К РЕСУРСАМ У ПРОЕКТЫ У О НАС У НОВОСТИ 📪 Q			
многоядерные процессоры, сопроцессоры Intel Xeon студентам осваивать работу на новейших вычислител			in the second				
	က် > Дос	туп к ресурсам 🔿 «Quick Start»					
	«Qui	ck Start»					
	Запус	ск задач					
	Полезны	е ссылки:					
	• Об у • Jupyt	ебно-тестовом полигоне erHub					
	• Putty						
		новленное ПО рукция по работе					

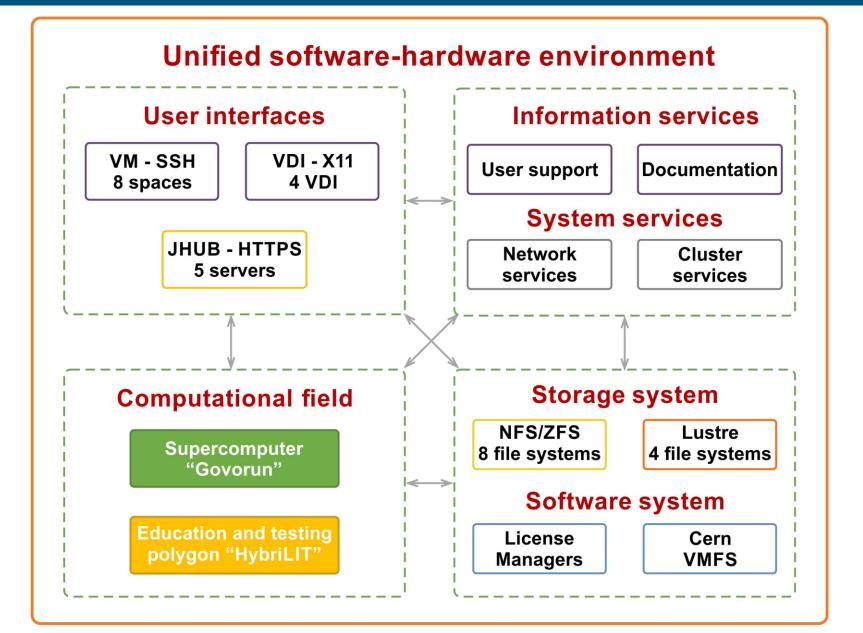
Thank you for your attention

HYBRILIT HETEROGENEOUS PLATFORM at MLIT JINR:

http://hlit.jinr.ru

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	Software Level	Information Level	
Scientific Linux 7.9 (operating system)	Parallel computing software	HybriLIT web-site	
xCAT (OS deployment tool)	Open MPI CUDA Intel	http://hlit.jinr.ru/	
FreeIPA (auth system)	Licensed software packages	Indico https://indico.jinr.ru/	
SLURM (workload manager)	Comsol Multiphysics Maple Wolfram Mathematica Matlab	HybriLIT user support project https://pm.jinr.ru/	
NFS (network file system) Lustre	Application Packages GROMACS Cmake Java FairRoot	HybriLIT user support telegram https://web.telegram.org/k/#-1752786710	
(parallel file system) CernVM-FS (software distribution service) FlexLM/MathLM (licence manager system)	LAMMPS FairSoft PandaRoot FLAIR Python FLUKA REDUCE GEANT4 ROOT Quantum ESPRESSO	GitLab https://gitlab-hybrilit.jinr.ru/	
Modules (software environment tool)	ML/DL/HP	C ecosystem	
Monitoring Home-HLIT Monitoring HLIT-VDI РСК БазИС ^{Computing Resources'} Statistics	Developmentfor carcomponentresourcehttps://studhub.jinr.rucalcuhttps://studhub2.jinr.ruhttps://jhhttps://studhub2.jinr.ruhttps://jh	ponent rying out e-intensive ulations hub1.jinr.ru hub2.jinr.ru hub3.jinr.ru	
HLIT-VDI (Virtual Desktop Infrastru	ed for quantum computing tum computing simulators)		