“GOVORUN” supercomputer for JINR tasks

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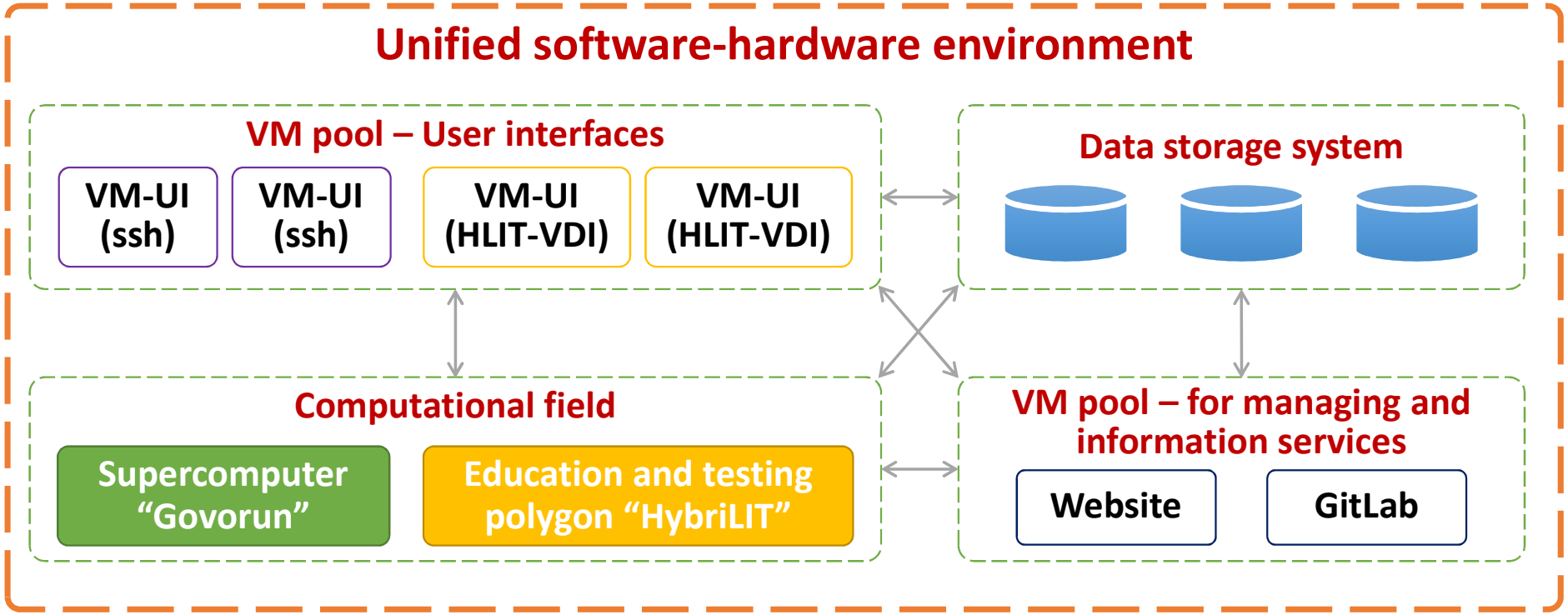
16-20 October 2023

MICC component: HybriLIT platform



The unified software and information environment of the HybriLIT platform allows users to use the education and testing polygon is aimed at exploring the possibilities of novel computing architectures, IT-solutions, to develop and debug their applications, furthermore, carry out calculations on the supercomputer, which allows them to effectively use the supercomputer resources.

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

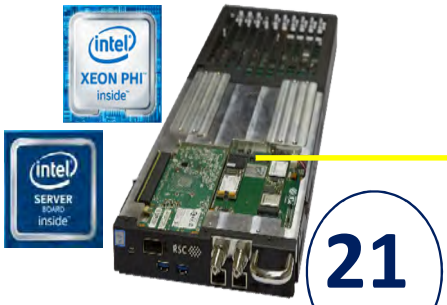
"Govorun" supercomputer
First stage 2018:
Full peak performance :
1 PFlops for single precision
500 TFlops for double precision
9th in the current edition of the IO500 list (July 2018)

#10 в Top50

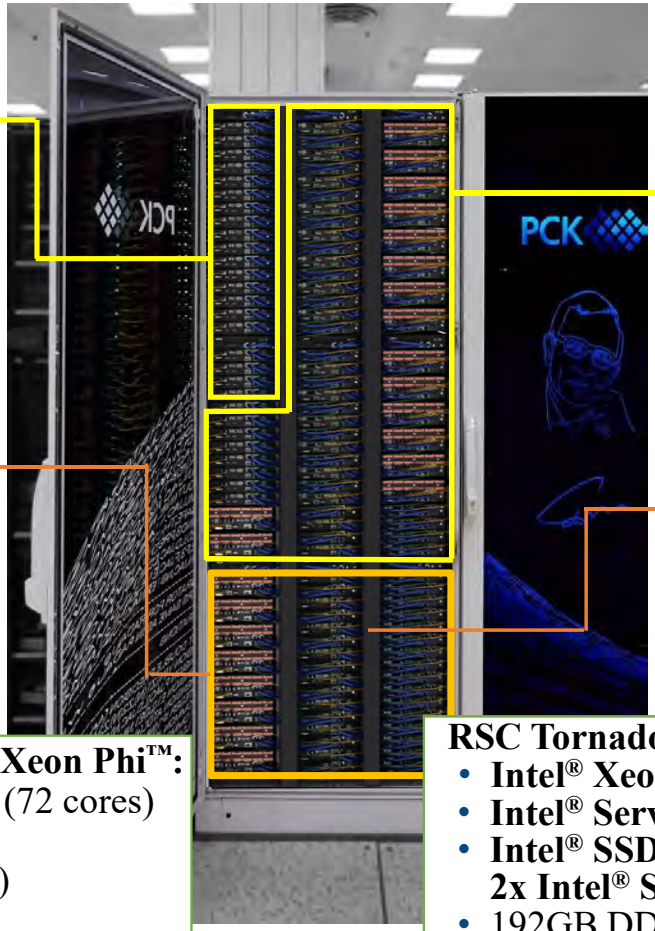
"Govorun" supercomputer
Second stage 2019:
Full peak performance :
1.7 PFlops for single precision
860 TFlops for double precision
288 ТВ ССХД with I/O speed >300 Gb/s
17th in the current edition of the IO500 list (July 2020)

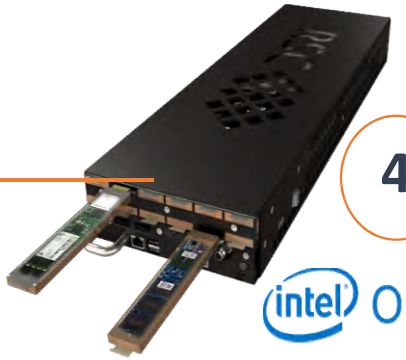
Russian DC Awards 2020 in "The Best IT Solution for Data Centers"

The CPU-component of the “Govorun” Supercomputer



Modules of fast scalable parallel file system (*Lustre, EOS* etc.)





RSC Tornado nodes based on Intel® Xeon Phi™:
- **Intel® Xeon Phi™ 7290** 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 2:
- **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**

"Govorun" supercomputer modernization 2022

Computation field:
+32 hyperconverged compute nodes

Hierarchical Storage:
+8 distributed storage nodes

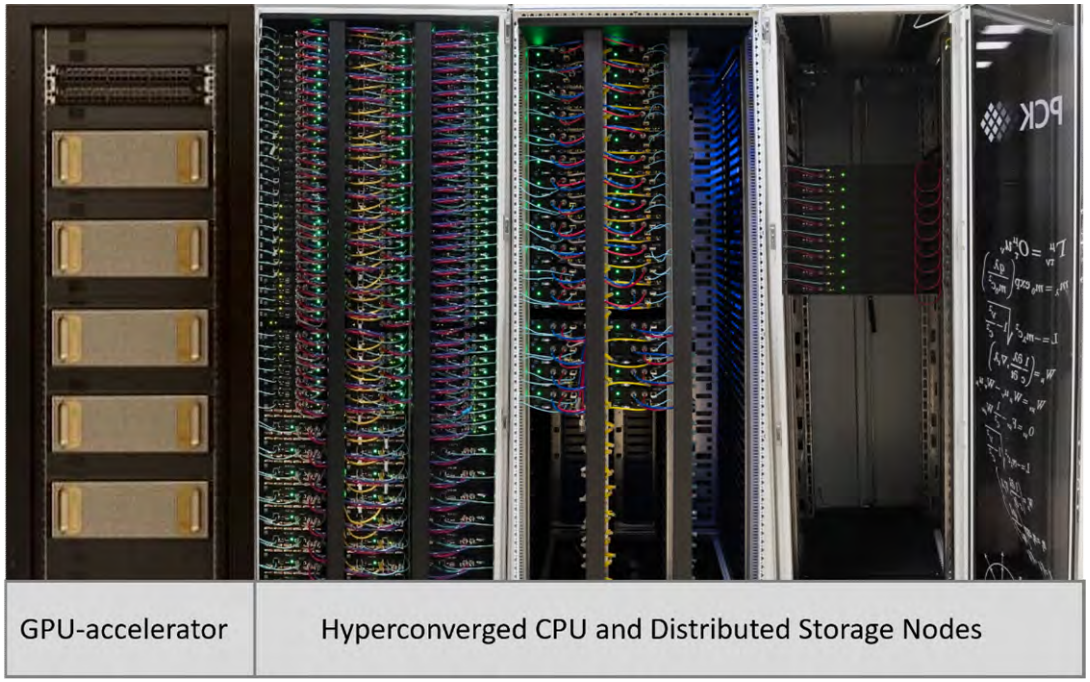
Performance: +239 Tflops
DAOS: +1.6 PB
Lustre, EOS: +8 PB

Current status:
- **138 hyperconverged compute nodes**
- **40 GPU** accelerators

Total peak performance:
- **1.1 PFlops DP**
- **2.2 PFlops SP**

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

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



+1,152 new computational cores for the MPD

Generated almost 31 million events less then month!!!

Performance "new cores"/"old cores" increase more than **1,5 times**

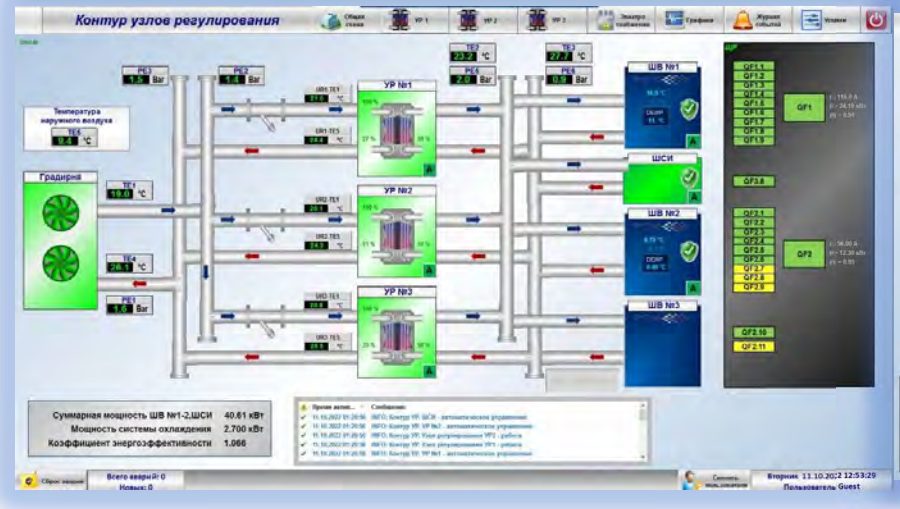
+0,4 PB for the MPD mass production storages integrated into the DIRAC File Catalog

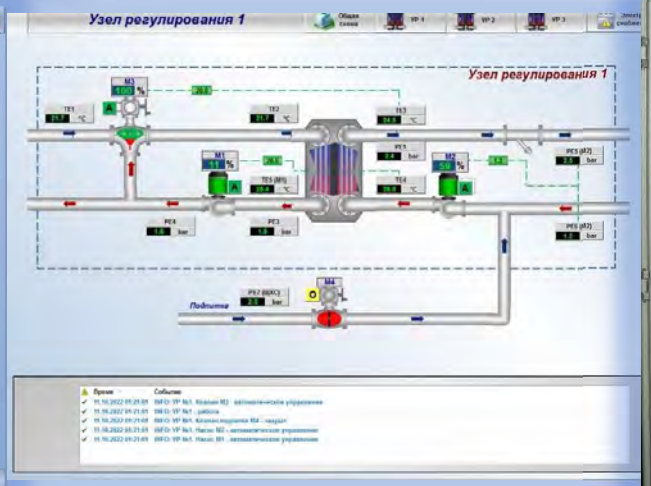
+1 PB for the MPD EOS storage

Engineering infrastructure

free cooling
24x7x365

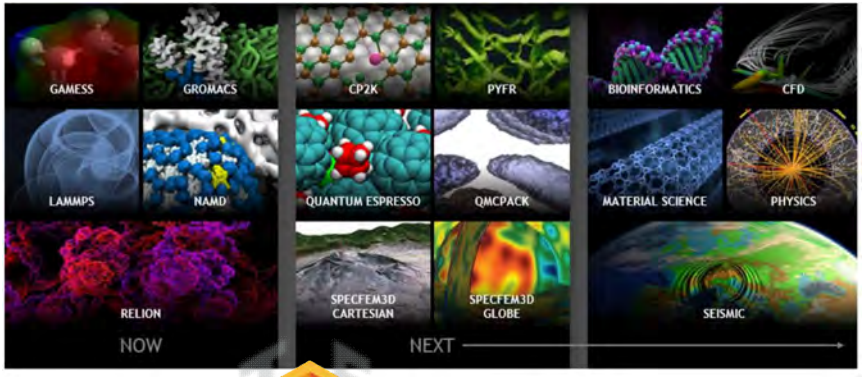
PUE ~ 1,06





The GPU-component of the “Govorun” Supercomputer

The GPU-component consists of **5 NVIDIA DGX-1 servers**. Each server has **8 GPU NVIDIA Tesla V100** based on the latest architecture NVIDIA Volta. Moreover, one server NVIDIA DGX-1 has **40960** cores CUDA, which are equivalent to 800 high-performance central processors. A whole number of novel technologies are used in DGX-1, including the NVLink 2.0 wire with the bandwidth up to 300 Gb/s.



The GPU-component gives a users of the supercomputer a possibility to allow as massively parallel computation for general-purpose tasks using such technologies as CUDA and OpenCL, as well as use applications already adapted for this architecture. Also, GPU-component allow to use machine learning and deep learning algorithms for solving applied problems by neural network approach.

TensorFlow PYTORCH theano APACHE mxnet The Microsoft Cognitive Toolkit Caffe

Expanding the Opportunities of the Govorun Supercomputer to Solve ML/DL Task

GPU component

5 NVIDIA DGX-1 servers
with
8 NVIDIA Tesla V100 GPUs
in each

+

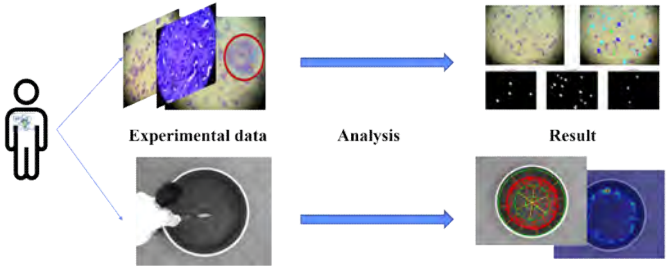
NEW!

5 Niagara R4206SG servers
with
8 NVidia A100 GPUs in each

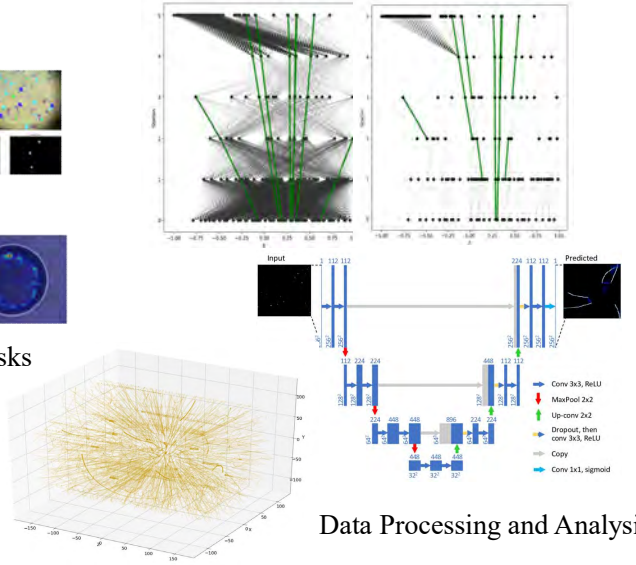
+ 40 GPU accelerators: 5 Niagara R4206SG servers with **8 NVIDIA A100 GPUs** in each.

Total performance of the GPU: 300+600 Tflops for DP
Total peak performance of the SC "Govorun": 1.7 Pflops for DP

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.

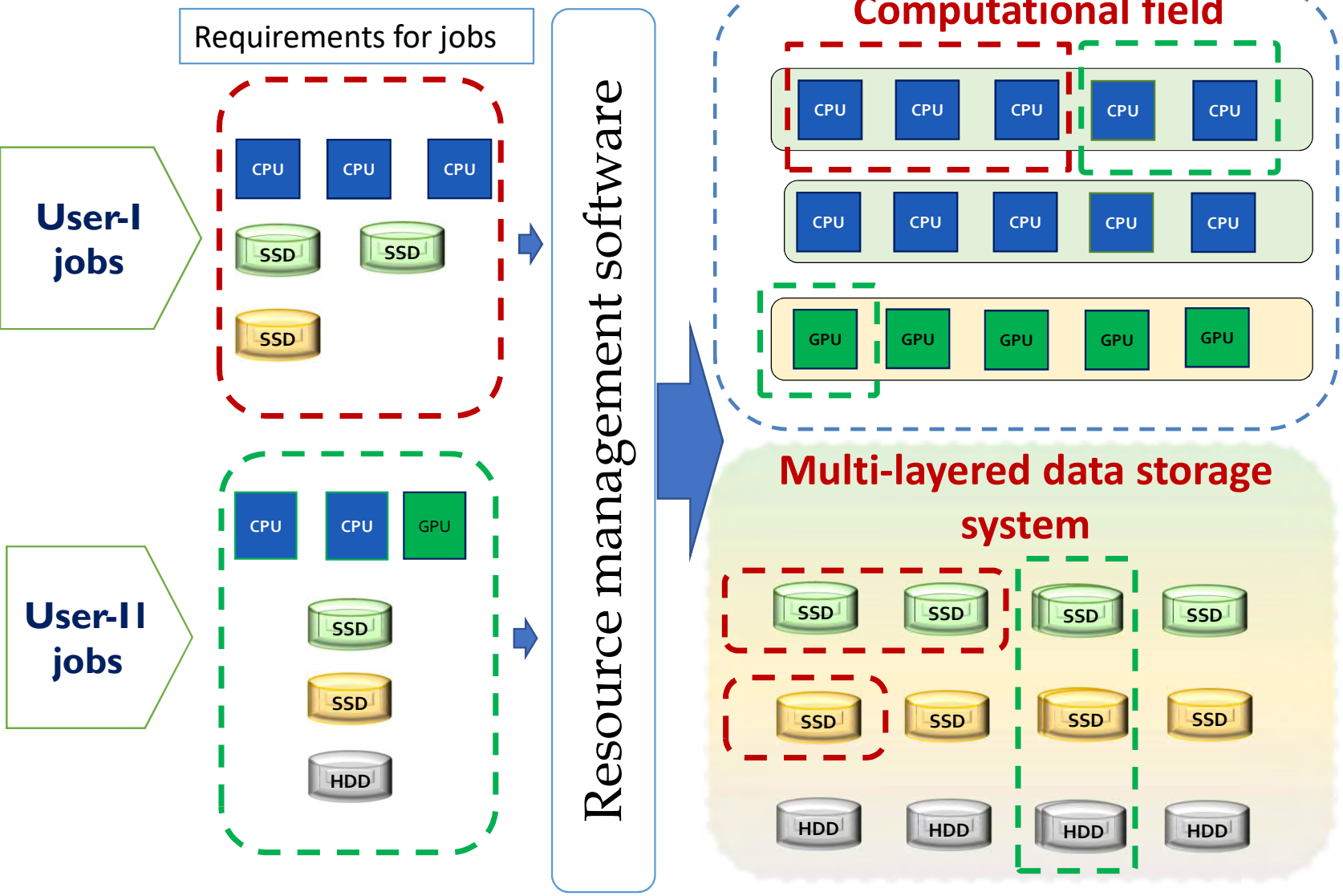


Information System for Radiation Biology Tasks



Data Processing and Analysis

Orchestration and hyperconvergence on the “Govorun” supercomputer

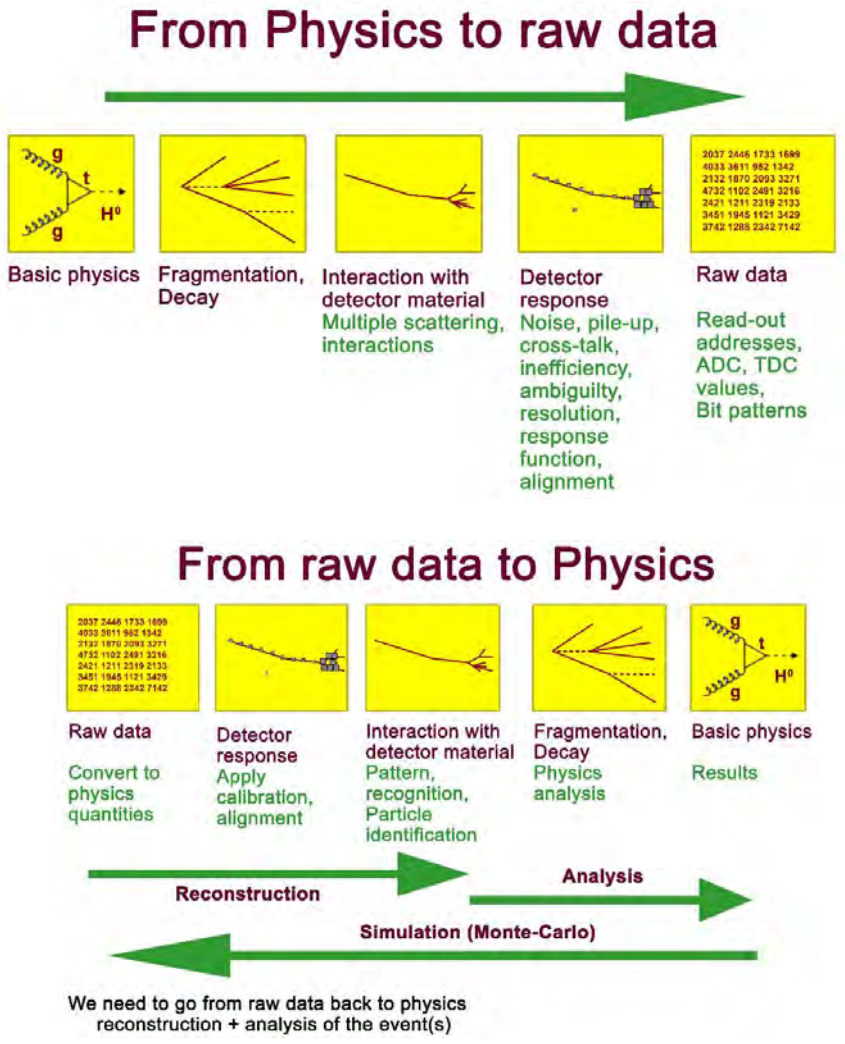


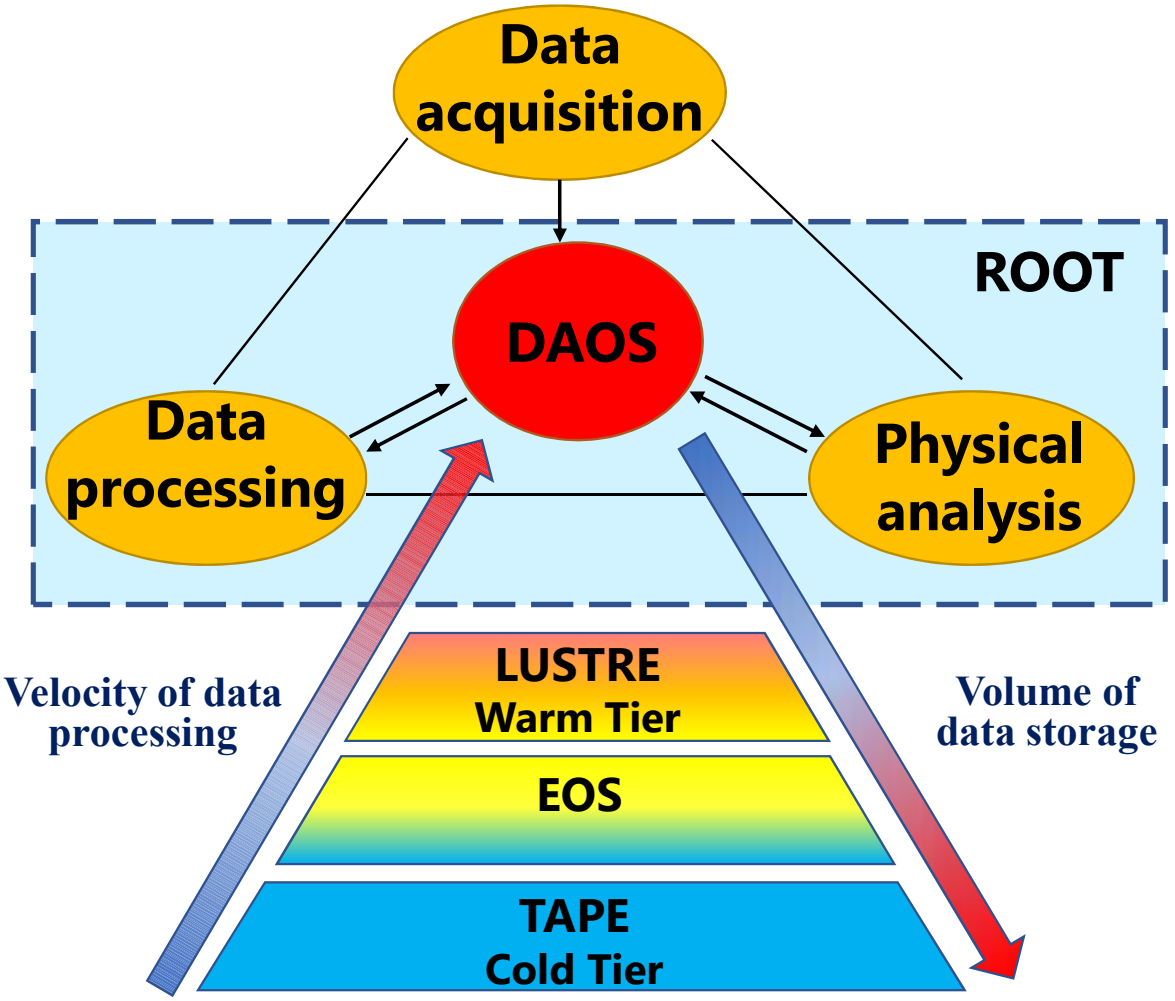
The “Govorun” supercomputer has unique properties for the flexibility of customizing the user’s job.

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.

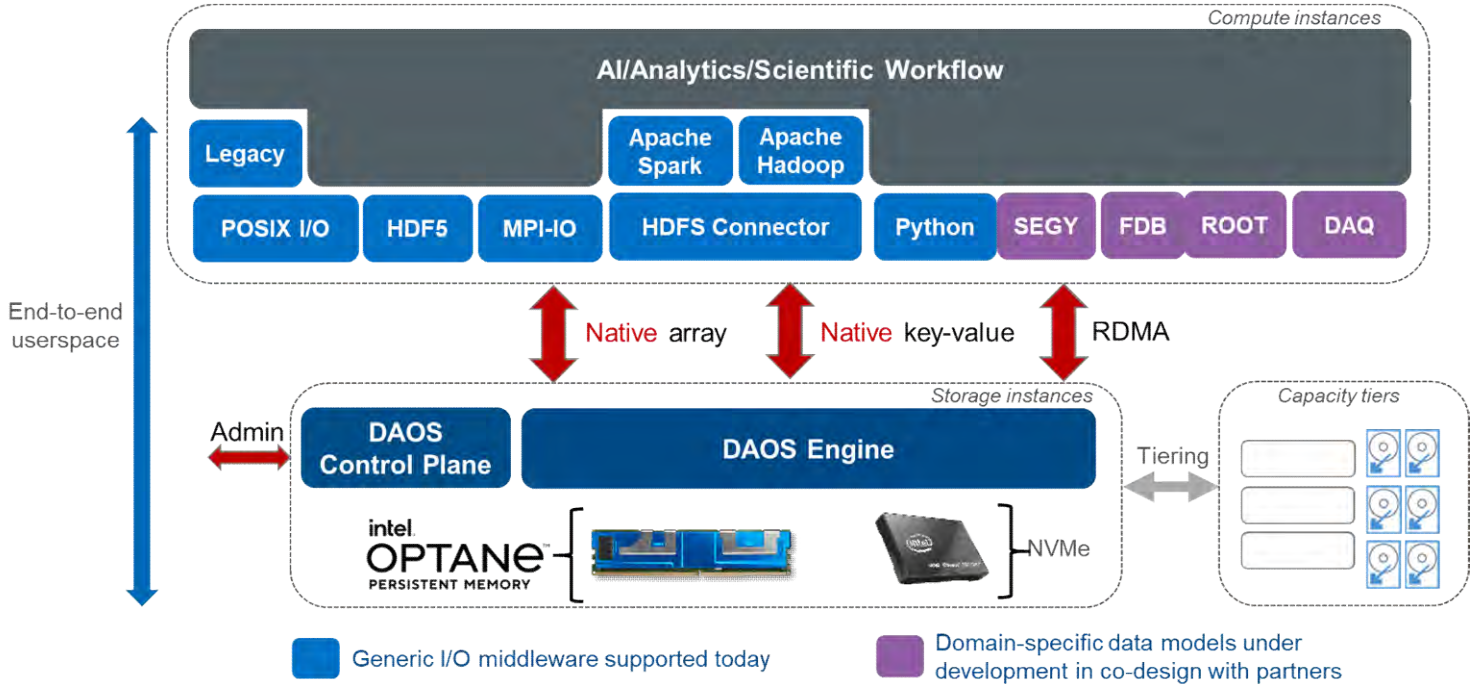
HEP experiments data flow





DAOS: Promising technology for HPC, Big Data, AI

DAOS (Distributed Asynchronous Object Storage) Software Ecosystem

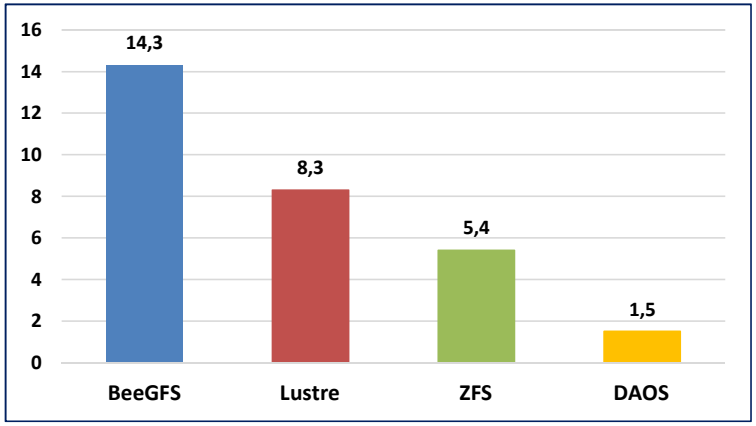


- Complex approach to build a hierarchical storage system
- DAOS is significant part of data acquisition and processing
- Different types of containers are used for different data processing stages
- No need of POSIX file system for most data operations
- Great system performance even for a few DAOS clients
- RSC Storage on-Demand software offers unique flexibility, speed, and convenience for DAOS users

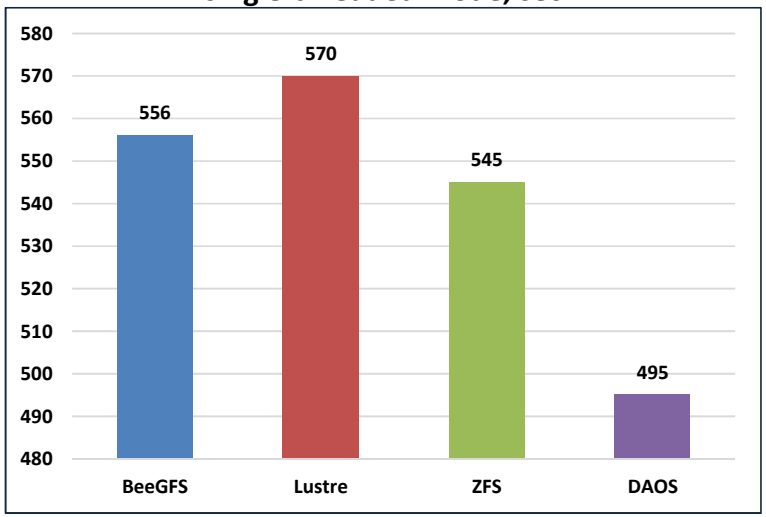
The DAOS polygon on the supercomputer “Govorun” take the 1st place among Russian supercomputers in the current IO500 list

DAOS Testing. Results

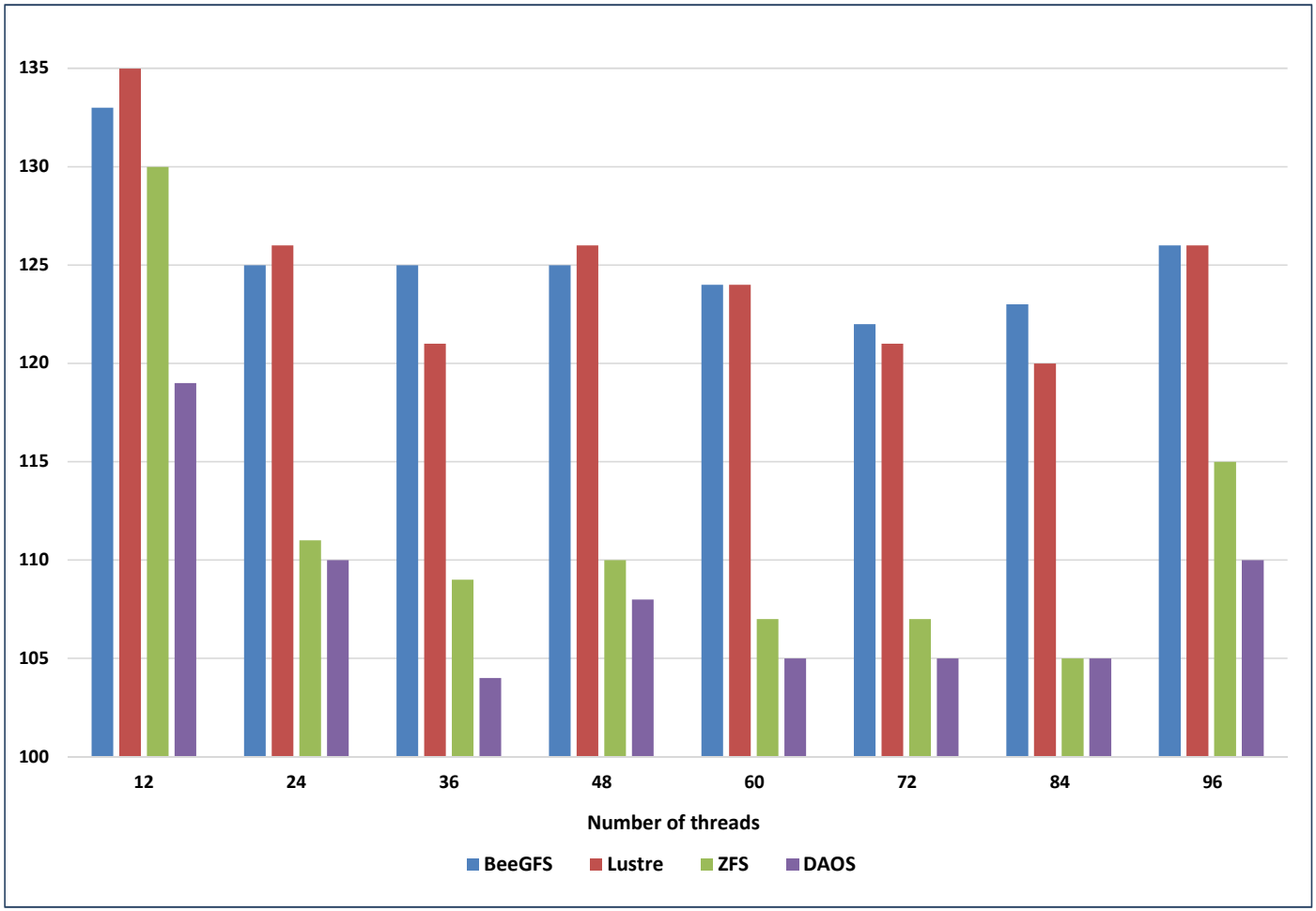
Time to load data into the model, sec



Average training time of one epoch in single-threaded mode, sec



Average training time of one training epoch, sec



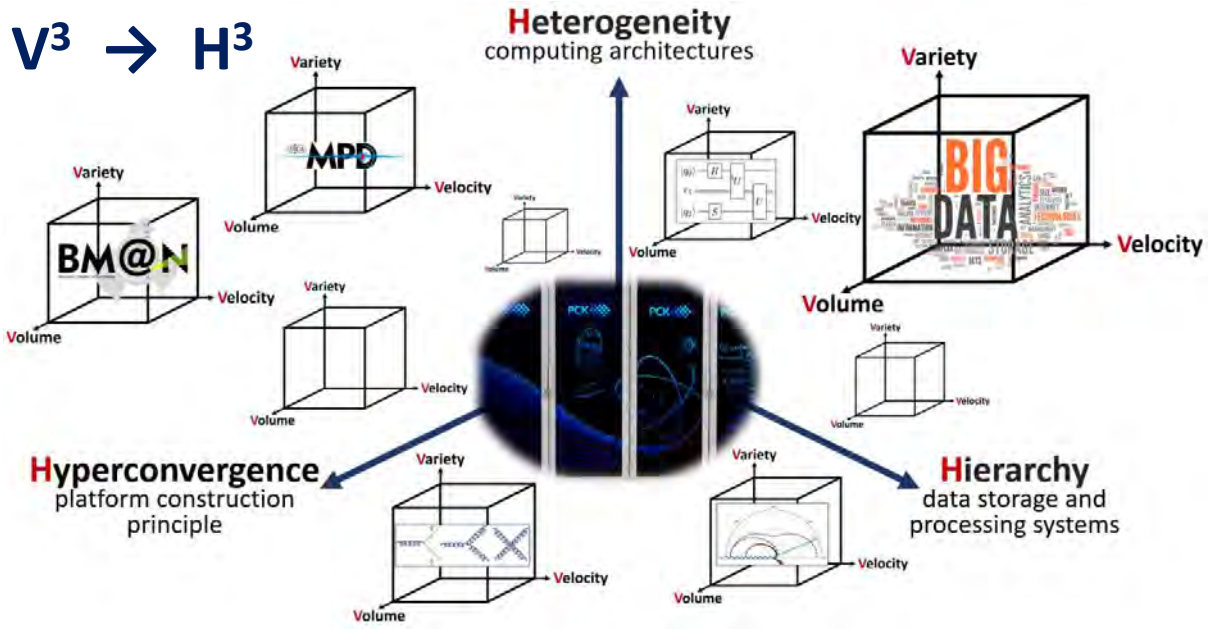
Big Data on the “Govorun” Supercomputer for NICA megaproject

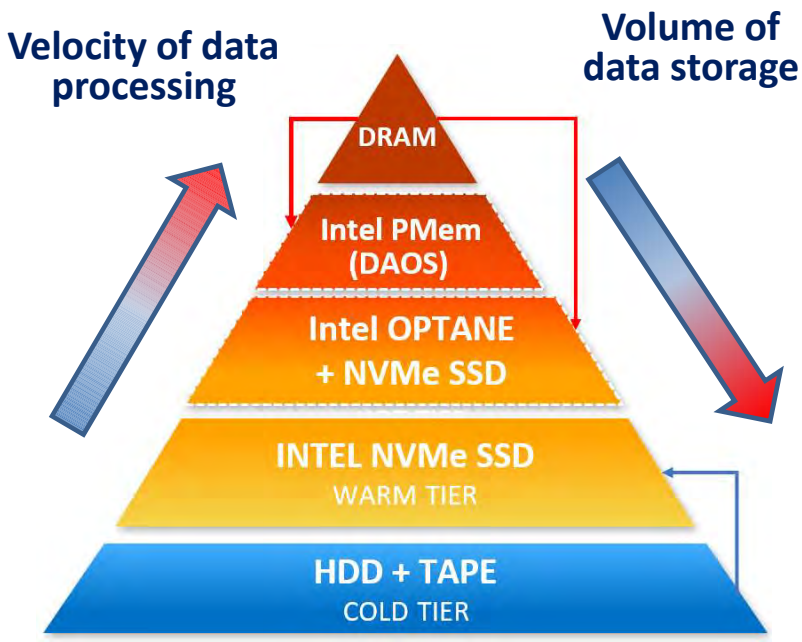
The DAOS polygon of the “Govorun” supercomputer takes the **1st** place among Russian supercomputers in terms of the data processing rate in the current **IO500 list**.

Heterogeneity
Hierarchy
Hyperconvergence

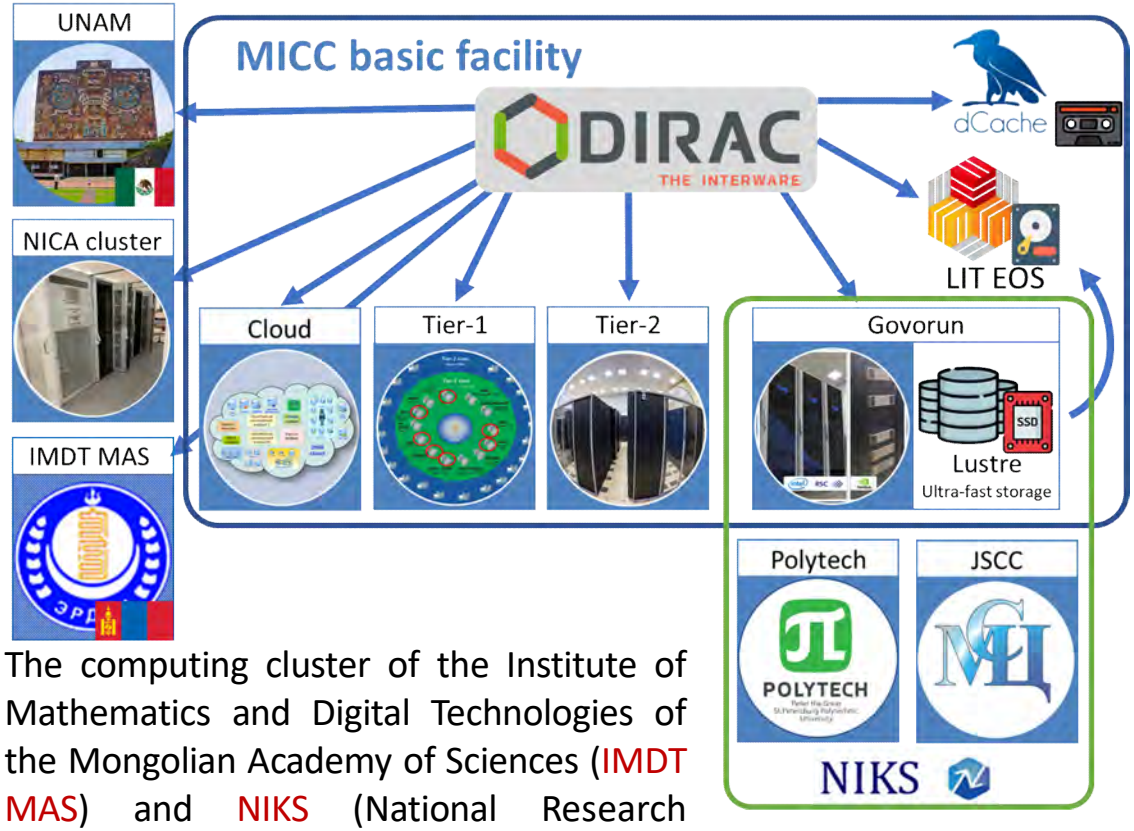
provide

Variety
Velocity
Volume

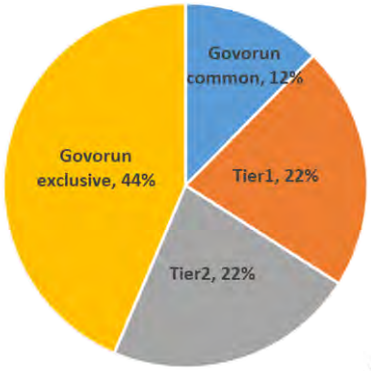




Heterogeneous distributed computing environment

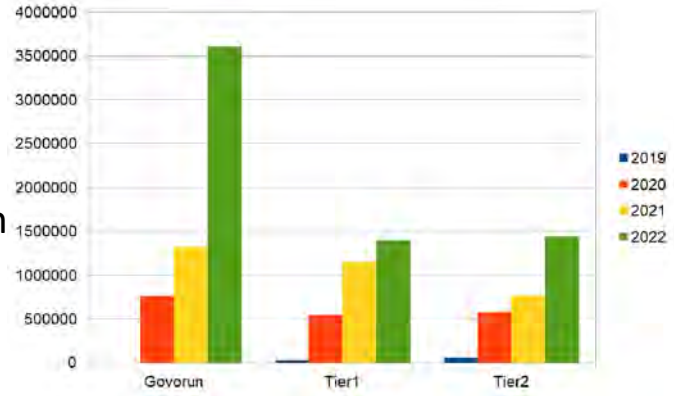


The computing cluster of the Institute of Mathematics and Digital Technologies of the Mongolian Academy of Sciences (IMDT MAS) and NIKS (National Research Computer Network, the Russia's largest research and education network) were integrated into the heterogeneous distributed environment based on the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

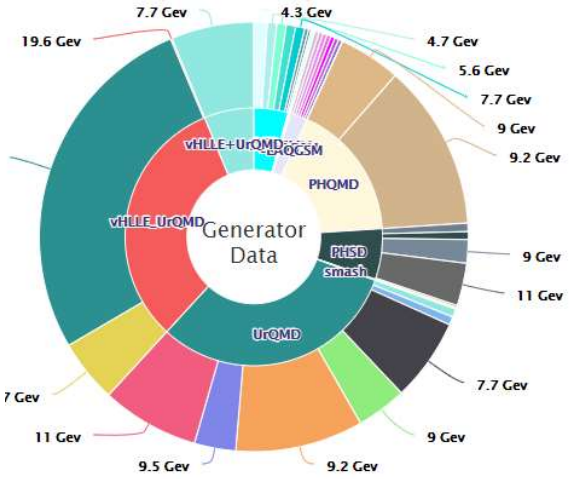


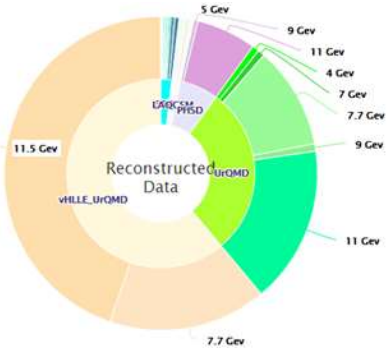
Summary statistics of using the DIRAC platform for MPD tasks in 2019-2022

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

Heterogeneous distributed computing environment for the MPD experiment

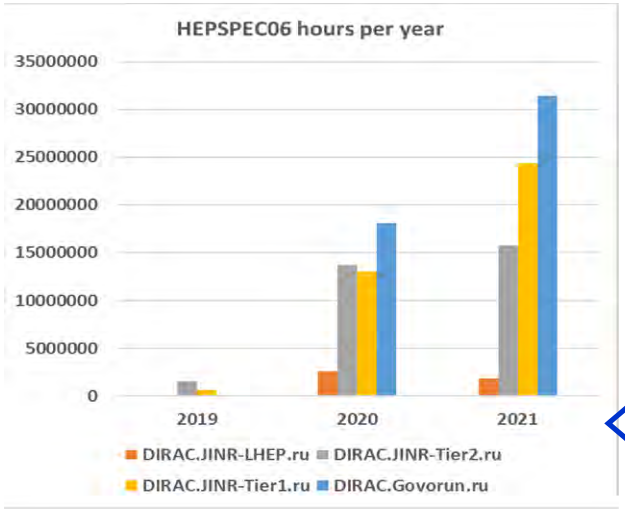
✓$1200 * 10^6$events were generated using *UrQMD, PHQMD, PHSD* and other models





✓$392 * 10^6$events were reconstructed

"Govorun" up to **40%**



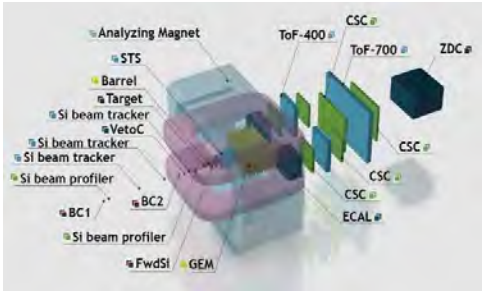
Available resources of the DIRAC platform for the MPD experiment:

- "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.

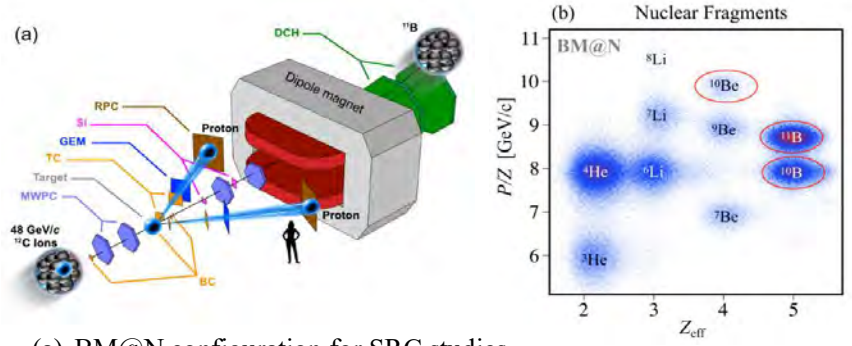
The mass production storages integrated into the Dirac File Catalog are 1.5 PB in size.

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

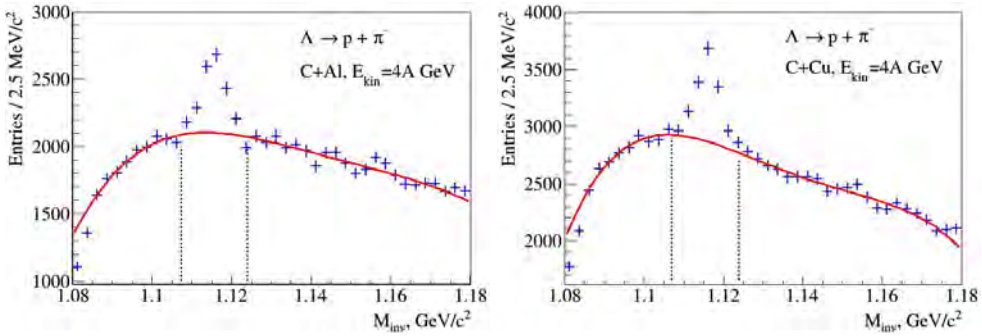
Computing for the NICA megaproject "Govorun" supercomputer for BM@N tasks



Full BM@N configuration for heavy ion studies in 2018.



(a) BM@N configuration for SRC studies.
(b) isolation of nuclear fragments in the experiment under the SRC program.

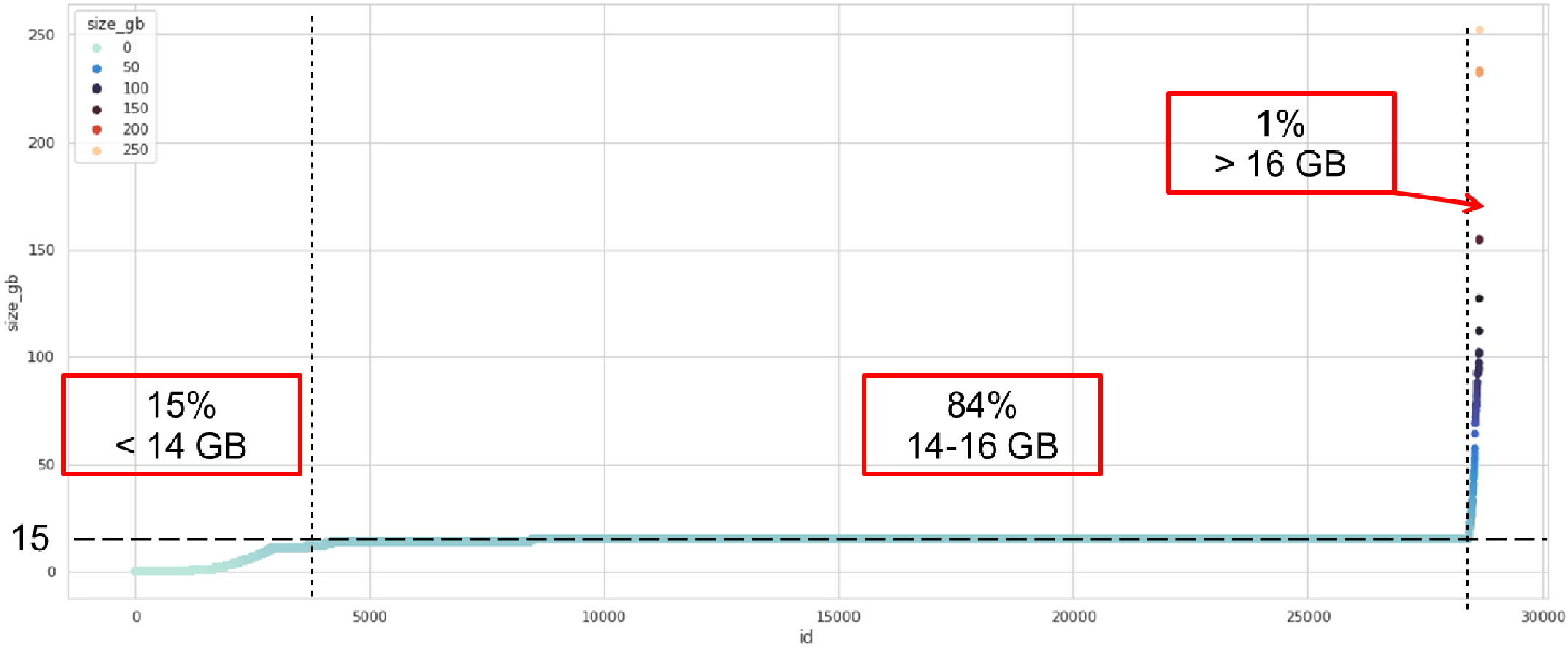


Signals of Λ-hyperons in the spectra of invariant masses (p,π-) measured in C+Al and C+Cu interactions.

BM@N Collaboration. Production of Λ hyperons in 4 and 4.5 AGeV 2 carbon-nucleus interactions at the Nuclotron // The European Physical Journal A (awaiting publication)

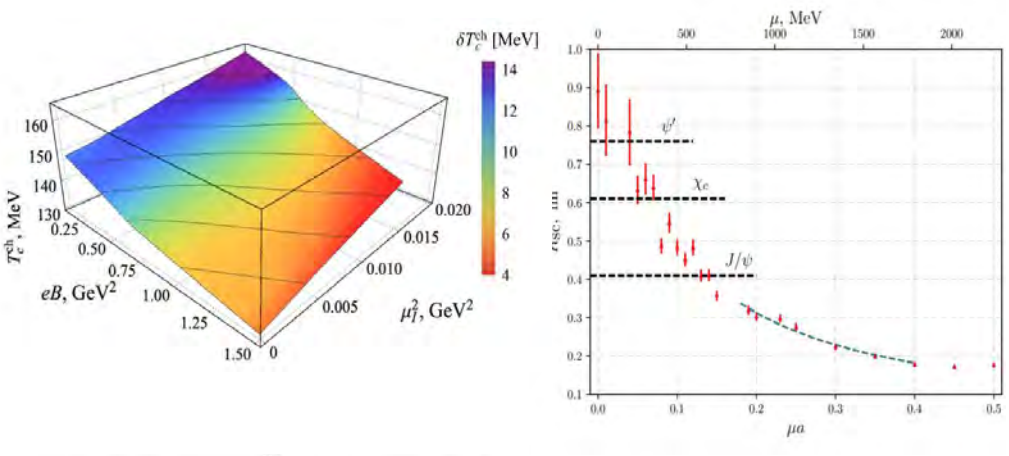
- The analysis of experimental data acquired during the Nuclotron runs in 2016-2018 was performed. Special attention is paid to the study of interactions between beams of carbon and argon ions with fixed targets of different types. The reconstruction of particle tracks was carried out using the method of "cellular automata".
- The modeling of the work of the experiment using generators of physical models, such as DCM-QGSM and URQMD, and the embedding procedure were performed.
- The staff of the BM@N collaboration from Russia, the USA, Israel, Germany, France and JINR, working on the program for the study of short-range correlations (SRC) of nucleons in nuclei, developed and applied a new experimental method for investigating the internal structure of the atomic nucleus in carbon-hydrogen interactions. A publication based on the results of the SRC program of the BM@N experiment was sent to the scientific journal Nature.
- The polarization of Λ-hyperons was studied using the model data of the DCM-QGSM generator of the BM@N experiment.

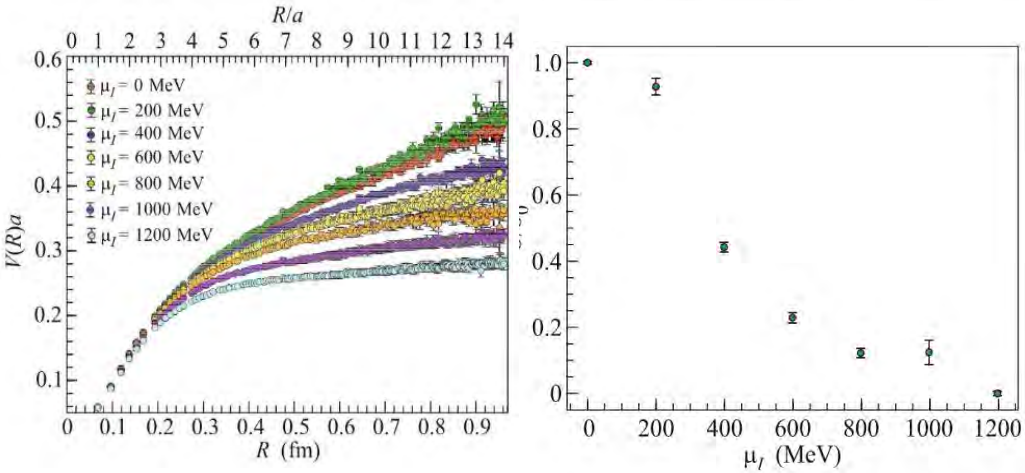
Computing for the NICA megaproject
“Govorun” supercomputer for BM@N tasks



Из презентации И.С. Пелеванюка

“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.

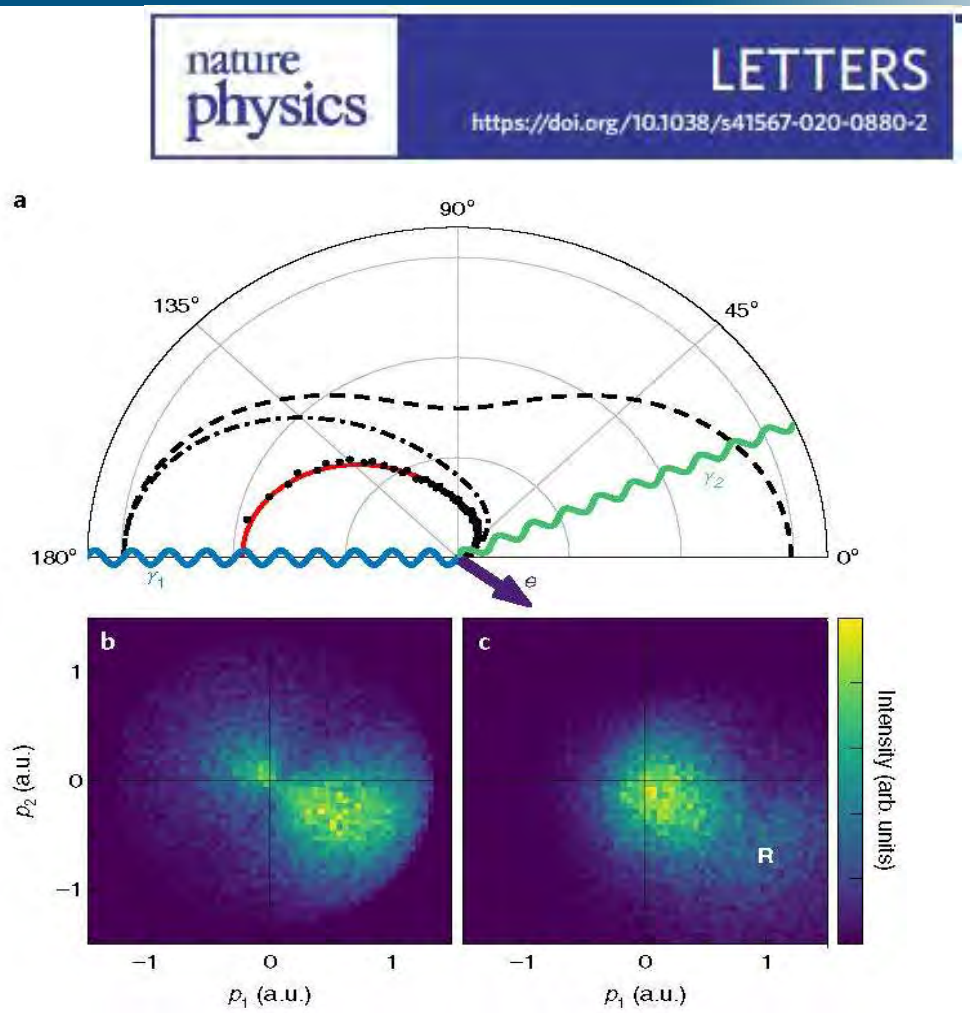
- The influence of the external magnetic field on the electromagnetic conductivity of quark-gluon plasma was investigated.

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

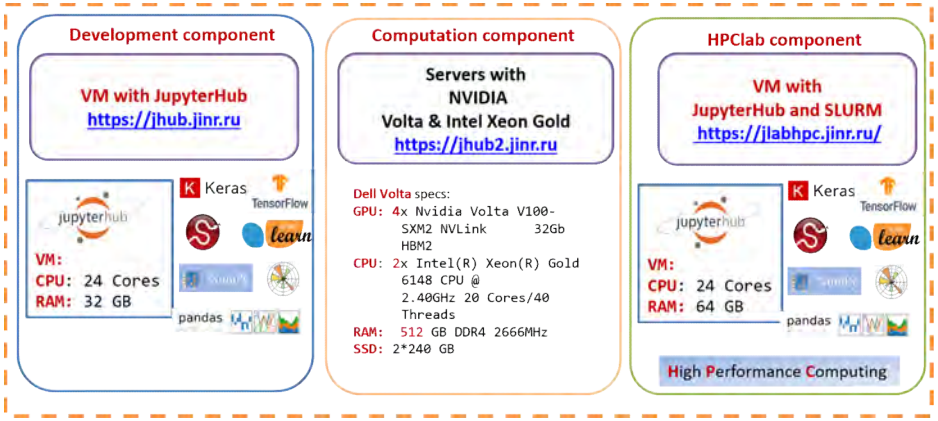
Kinematically complete experimental study of Compton scattering at helium atoms near the threshold

On 13 April, a scientific paper by an international scientific group was published in **Nature Physics**. A LIT staff member *O. Chuluunbaatar* and a BLTP employee *Yu. V. Popov* were members of the group in the frames of JINR international cooperation. The group conducted a kinematically complete experimental measurement of characteristics of Compton scattering at free atoms using the highly efficient method of COLD Target Recoil Ion Momentum Spectroscopy (COLTRIMS). The group also provided a relevant theoretical description of it which was carried out at the supercomputer "Govorun".

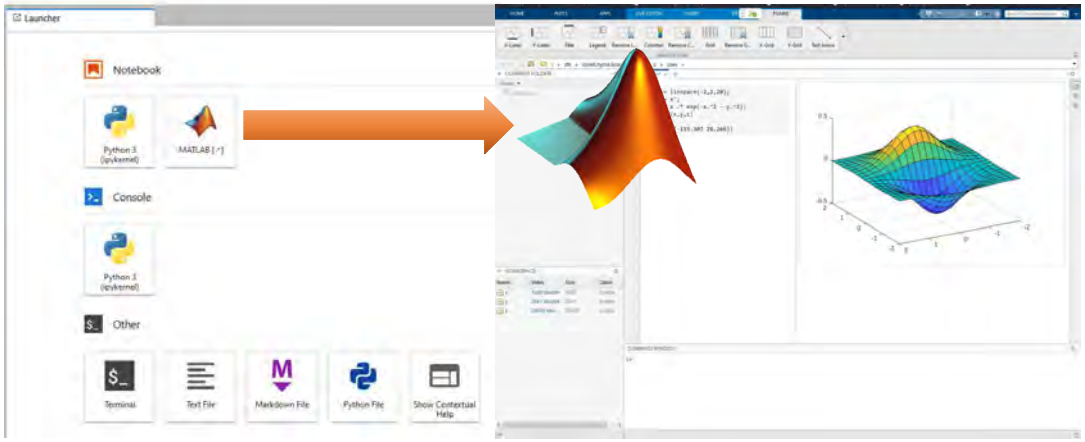


Scheme of ionization by Compton scattering at hν= 2.1 keV

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.

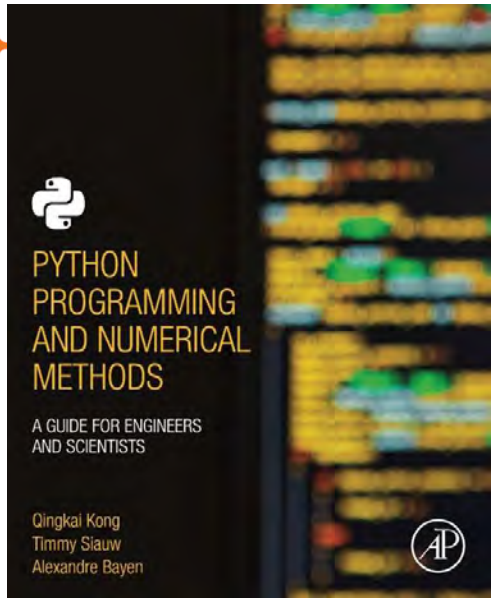


The ML/DL/HPC ecosystem is now actively used for machine and deep learning tasks. At the same time, the accumulated tools and libraries can be more widely used for scientific research, including:

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

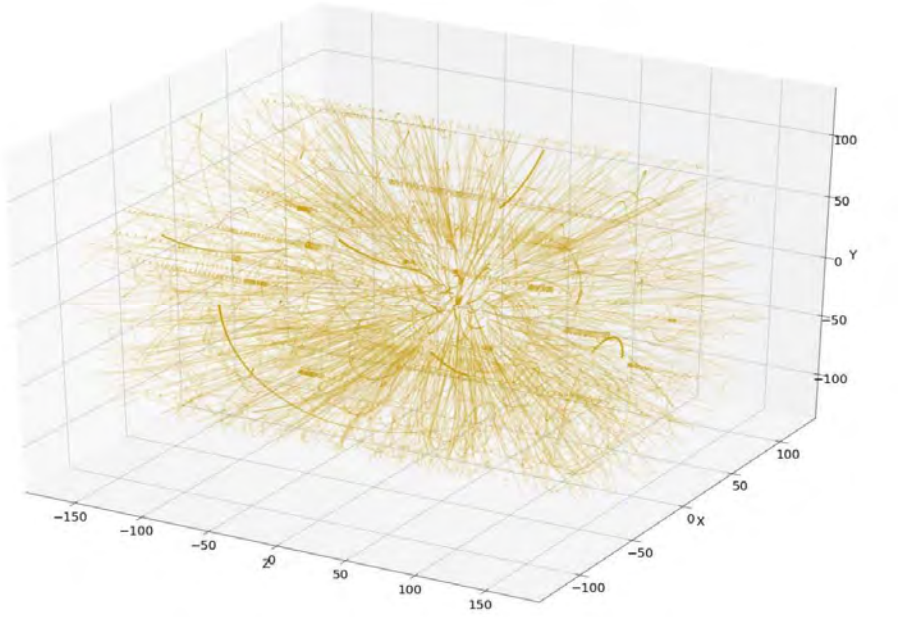
Parallel computations with Joblib

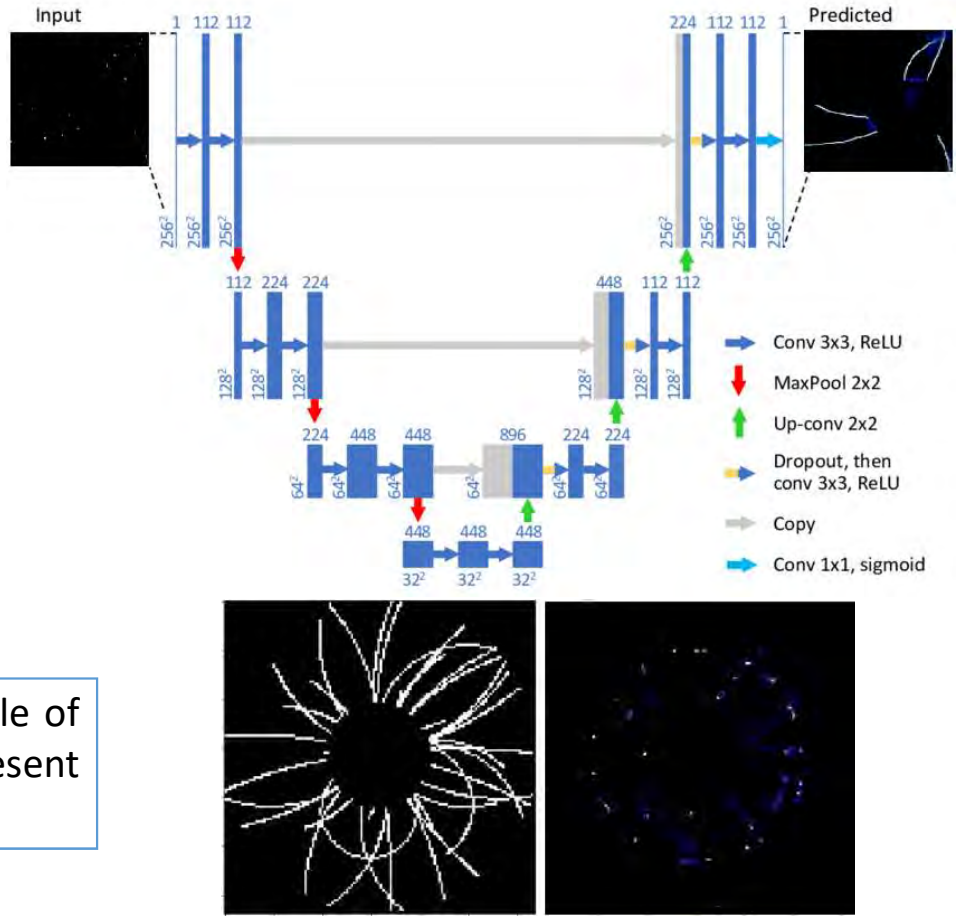
Python Numerical Methods



Computing for the NICA megaproject
Machine learning for MPD tracking tasks

A large number of tracks in events requires the development of approaches that have constant computational complexity regardless of the number of tracks in an event. The use of deep neural network architectures allows developing tracking one-pass algorithms that work in just single step.

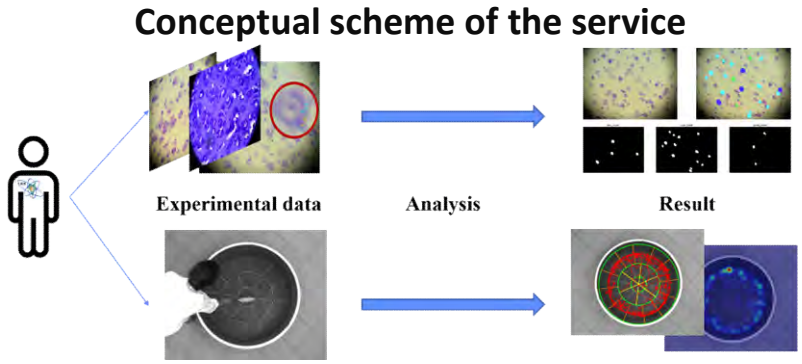




Model experiments show that neural network models are capable of both interpolating tracks and creating an internal model to represent the results in the phase space of the track parameters.

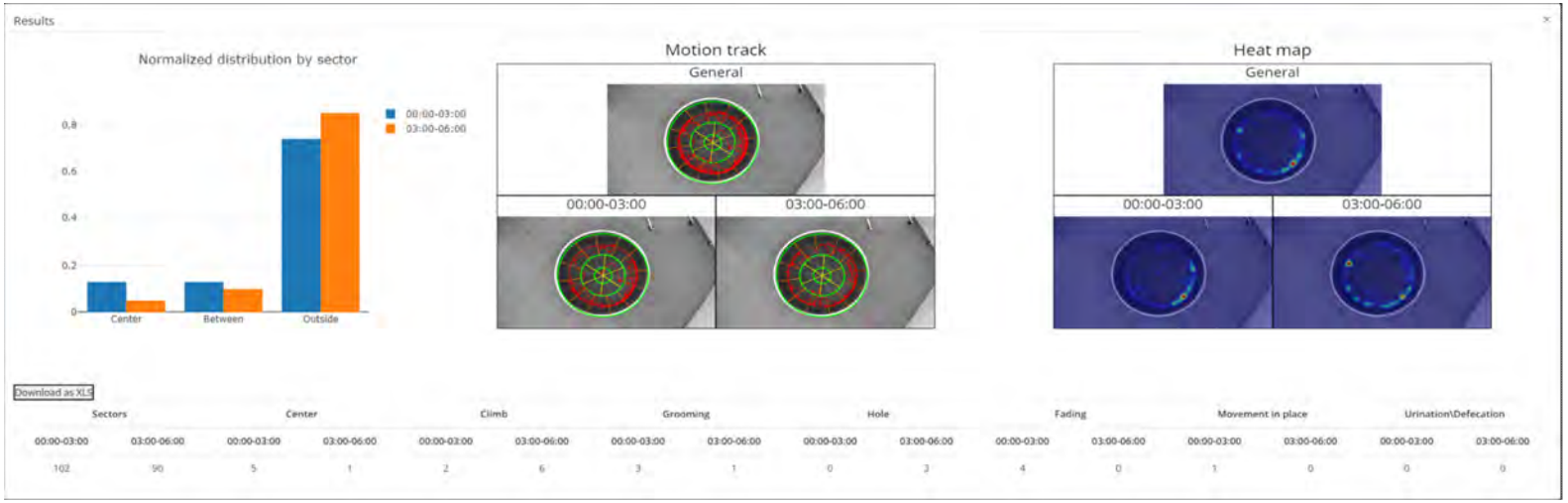
BIOHLIT information system for radiobiological studies

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.



Developed algorithms:

- algorithms for the automated marking of the field of experimental setups,
- algorithms for tracking the animal's position in experimental setups of different types,
- algorithms for evaluating the animal's behavioral patterns.



The obtained information is stored in different forms:

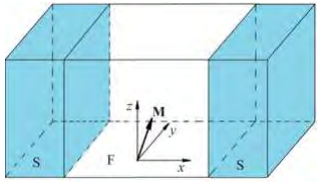
- visualized track of the animal's movement,
- video file with tracking the animal's position,
- heat map by sectors,
- file that stores all the information for subsequent statistical analysis.

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:

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

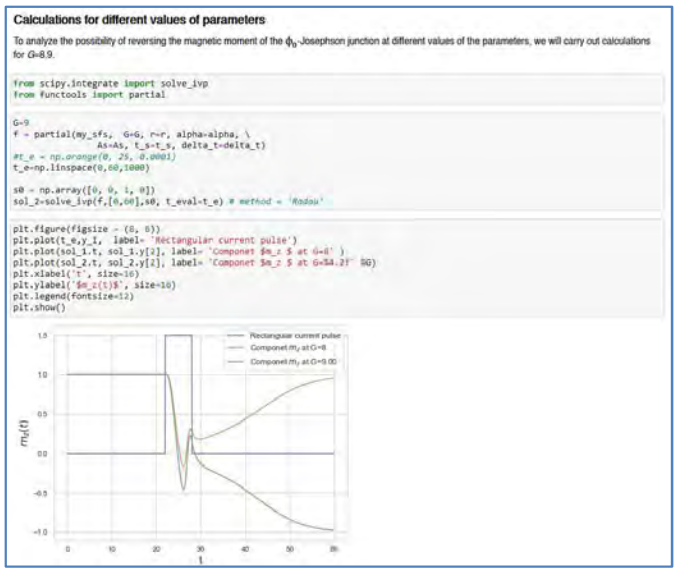
$M = [m_x, m_y, m_z]$ are the magnetic moment components; the effective field components $H = [H_x, H_y, H_z]$ depend on the Josephson phase difference ϕ and are defined as follows:

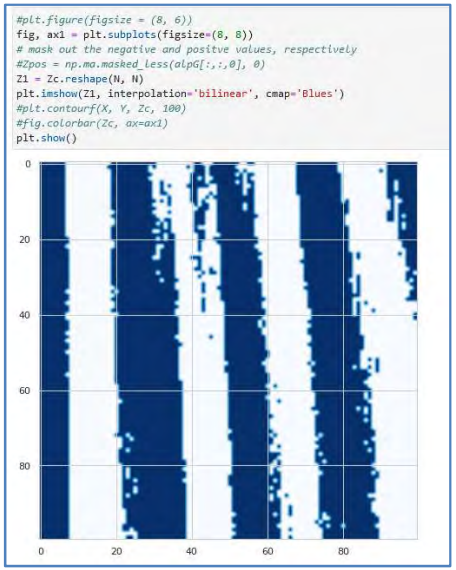


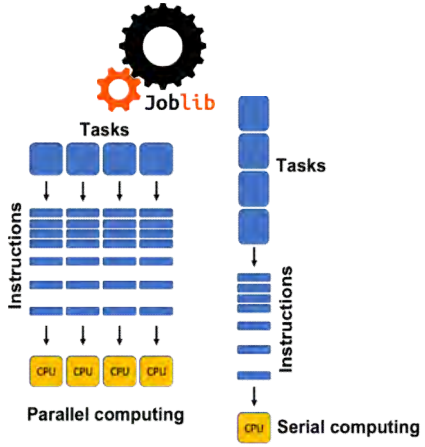
$$H_x(t) = 0,$$
$$H_y = Gr\sin(\phi(t) - tm_y(t)),$$
$$H_z(t) = m_z(t).$$

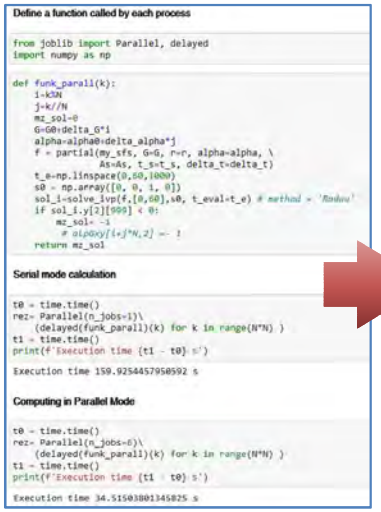
The equation for the Josephson phase difference $\phi(t)$ is determined from the equation for the electric current I flowing through the Josephson junction, measured in units of the critical current I_c :

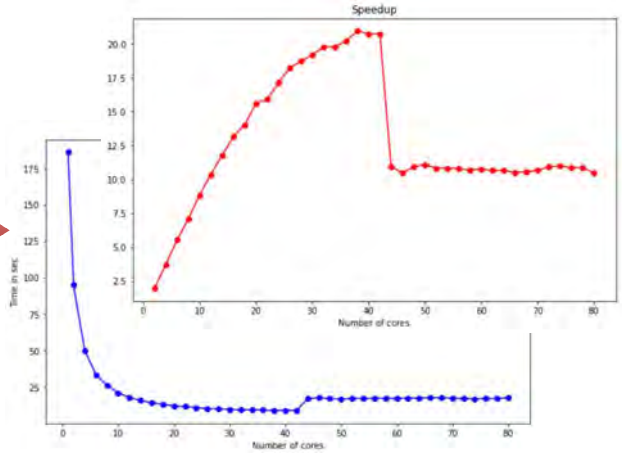
$$\frac{d\phi}{dt} = -\frac{1}{w}\left(\sin(\phi - rm_y) + r\frac{dm_y}{dt}\right) + \frac{1}{w}I,$$







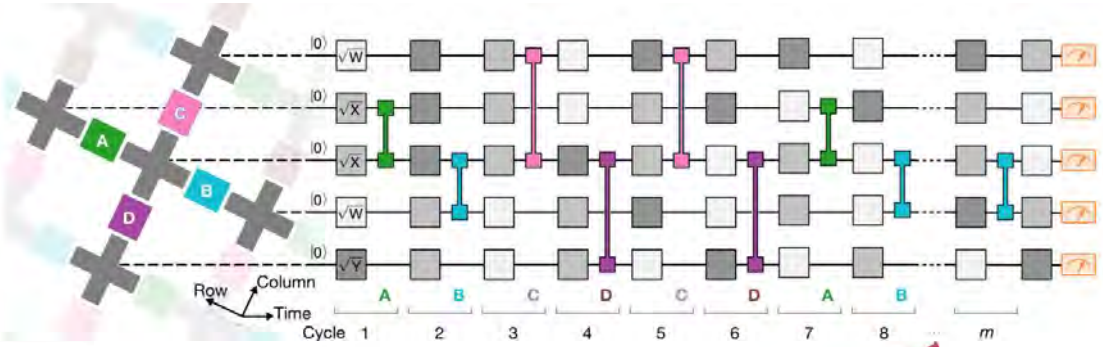


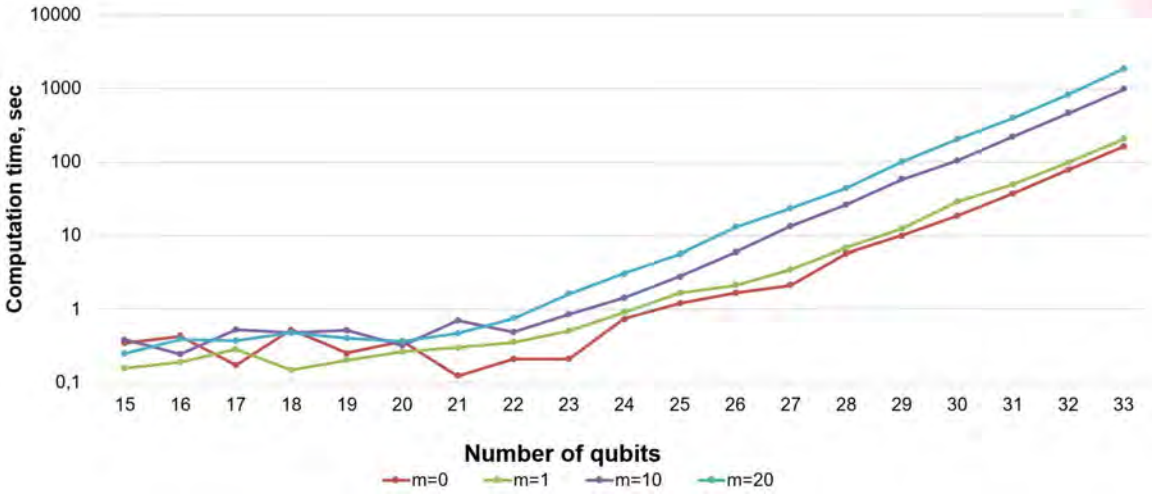


Quantum polygon

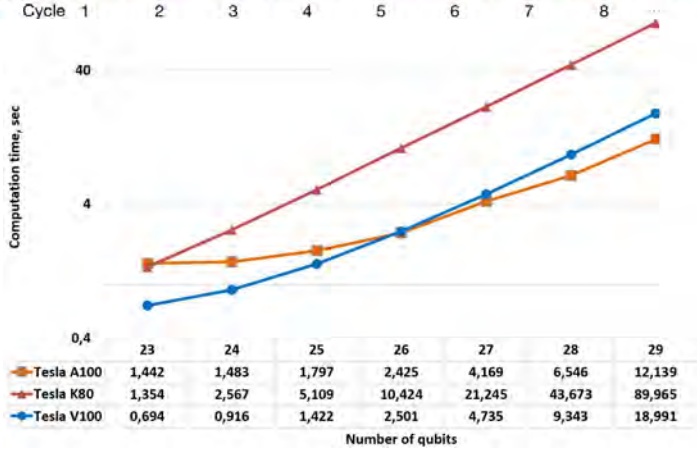
Quantum Exact Simulation Toolkit
https://quest.qtechtheory.org/

Amsterdam Modeling Suite





Time dependency on the number of qubits for CPU calculations with OpenMP technology



	23	24	25	26	27	28	29
Tesla A100	1,442	1,483	1,797	2,425	4,169	6,546	12,139
Tesla K80	1,354	2,567	5,109	10,424	21,245	43,673	89,965
Tesla V100	0,694	0,916	1,422	2,501	4,735	9,343	18,991

Time dependency calculations on the number of qubits for various GPUs

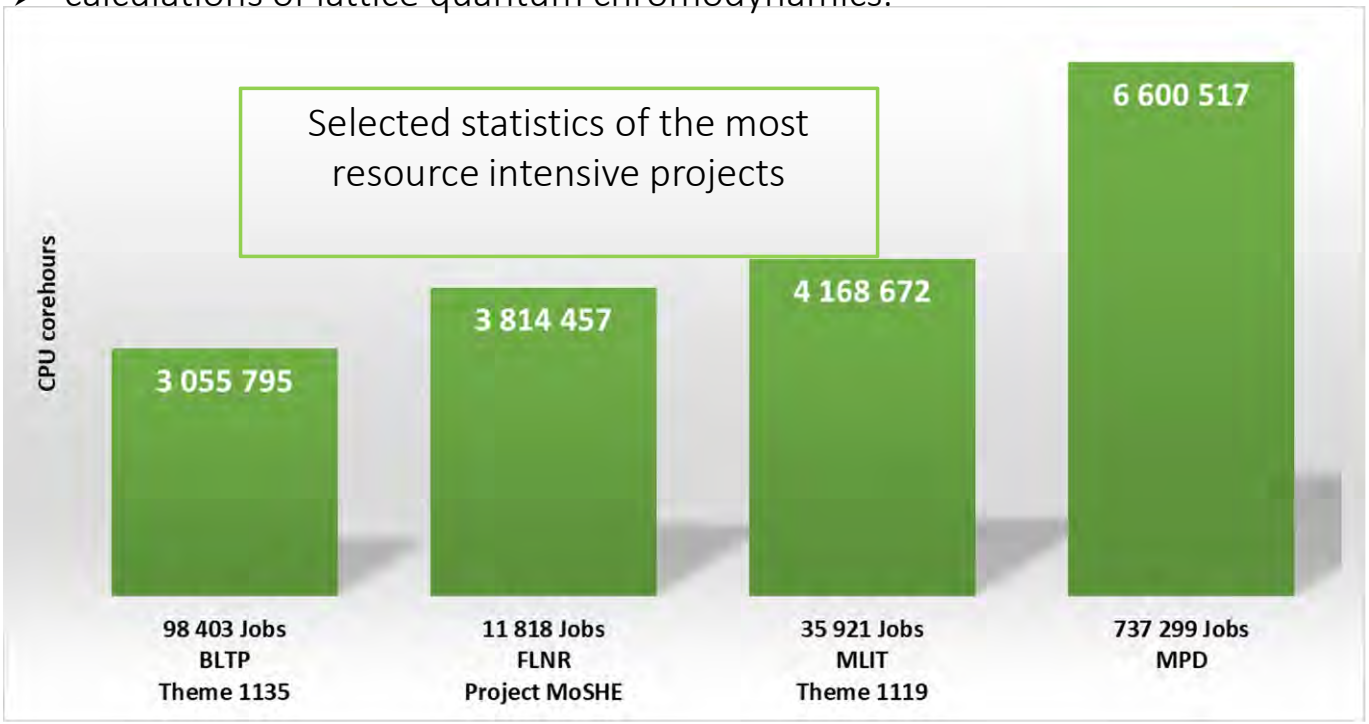
Для задач, решаемых в рамках Проекта была создана вычислительная система по требованию, содержащую 288 физических ядер (576 логических ядер) и файловое хранилище емкостью 7 ТБ под управлением файловой системы NFS. На этой системе проводились интенсивные расчеты с использованием ПО AMS, DIRAC, QuEST и др. для расчетов электронных свойств сверхтяжелых элементов. За время выполнения проекта было решено 4200 задач на которые было затрачено 740 000 ядро-часов

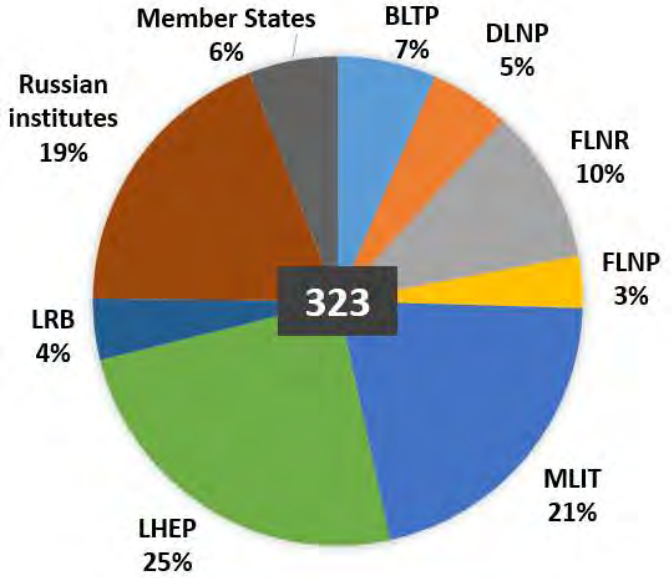
Using of the “Govorun” Supercomputer in 2022

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.





During 2022, 890,911 jobs were performed on the CPU component of the “Govorun” SC, which corresponds to 18,543,076 core hours.

“Govorun” Supercomputer for JINR Tasks

The resources of the “Govorun” supercomputer are used by scientific groups from all the Laboratories of the Institute within 25 themes of the JINR Topical Plan for solving a wide range of tasks in the field of theoretical physics, as well as for the modeling and processing of experimental data.

Research results obtained using the supercomputer resources are presented in 260 publications.

Using the results obtained at the Govorun SC, 2 publications were prepared in Nature Physics:

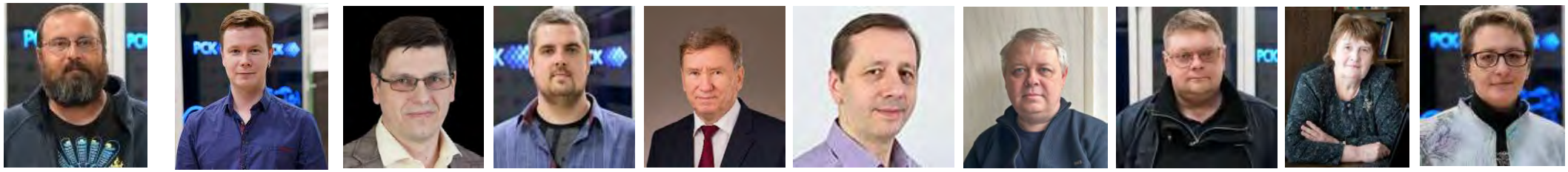
- M. Kircher … , **O. Chuluunbaatar** et al. Kinematically complete experimental study of Compton scattering at helium atoms near the threshold. Vol. 16. № 4. Pp. 756-760
- BM@N Collaboration. Unperturbed inverse kinematics nucleon knockout measurements with a 48 GeV/c carbon beam. Vol. 17. Pp. 693-699

Applied Physics Research

First Prize

"Hyperconverged "Govorun" supercomputer for the implementation of the JINR scientific program"

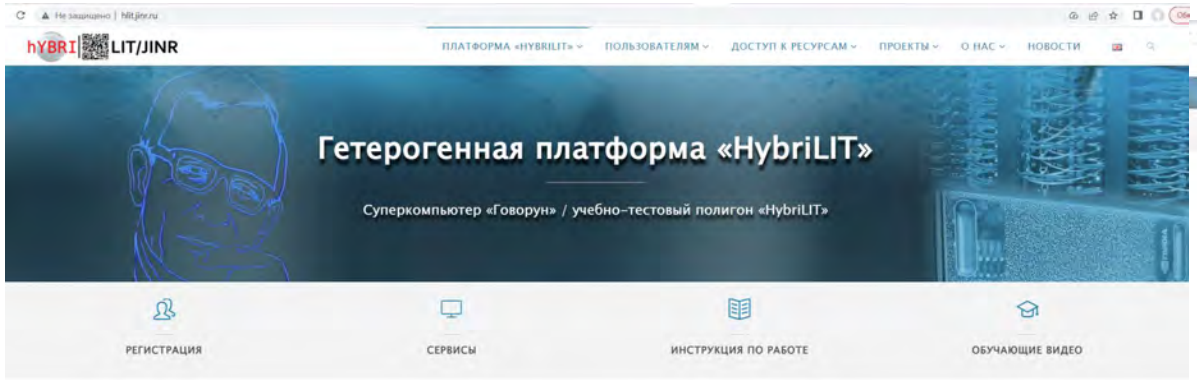
D.V. Belyakov, A.S. Vorontsov, E.A. Druzhinin, M.I. Zuev, V.V. Korenkov, Yu.M. Migal, A.A. Moshkin, D.V. Podgainy, T.A. Strizh, O.I. Streltsova

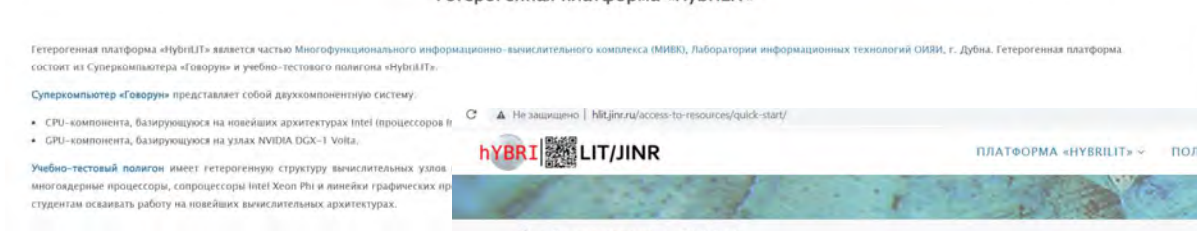


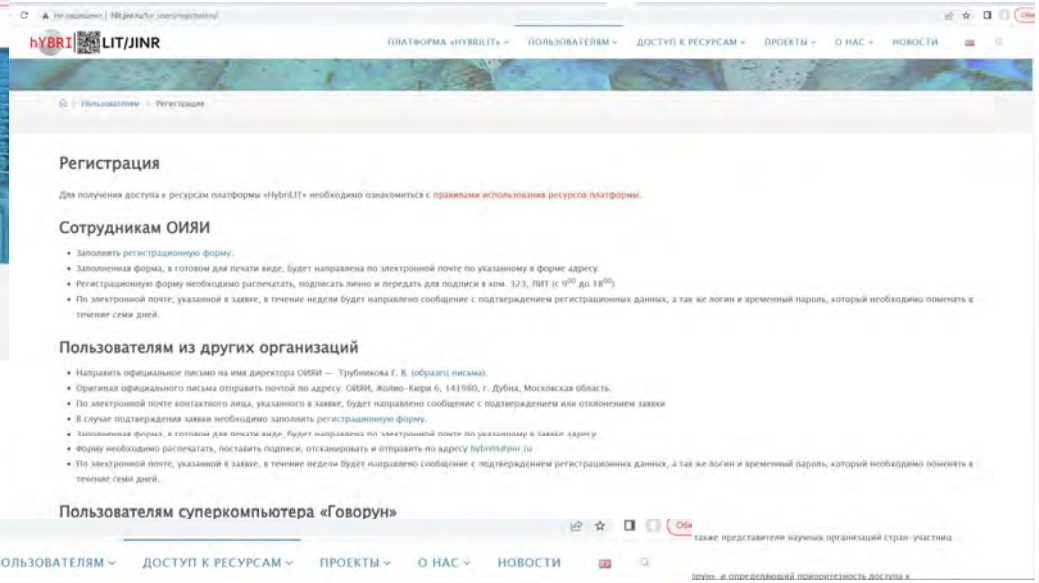
The creation of the "Govorun" supercomputer at JINR is an essential technological achievement being of great importance for the implementation of the JINR scientific program and international cooperation. The "Govorun" supercomputer is a unique scalable computing system with a hyperconverged and software-defined architecture. The technology of direct liquid cooling of CJSC "RSC Technologies" was chosen for the CPU component of the supercomputer. Due to liquid cooling, the average annual PUE indicator of the system, reflecting the level of energy efficiency, is less than 1.06. The operation experience of the SC "Govorun" has shown the relevance and effectiveness of using both novel hyperconverged computing architectures and the hierarchical data processing and storage system being part of it. The results obtained using the resources of the "Govorun" supercomputer are reflected in 204 user publications, two of them in the Nature Physics journal. At present, the resources of the "Govorun" spercomputer are used by scientific groups from all the Laboratories of the Institute within 25 themes of the JINR Topical Plan.

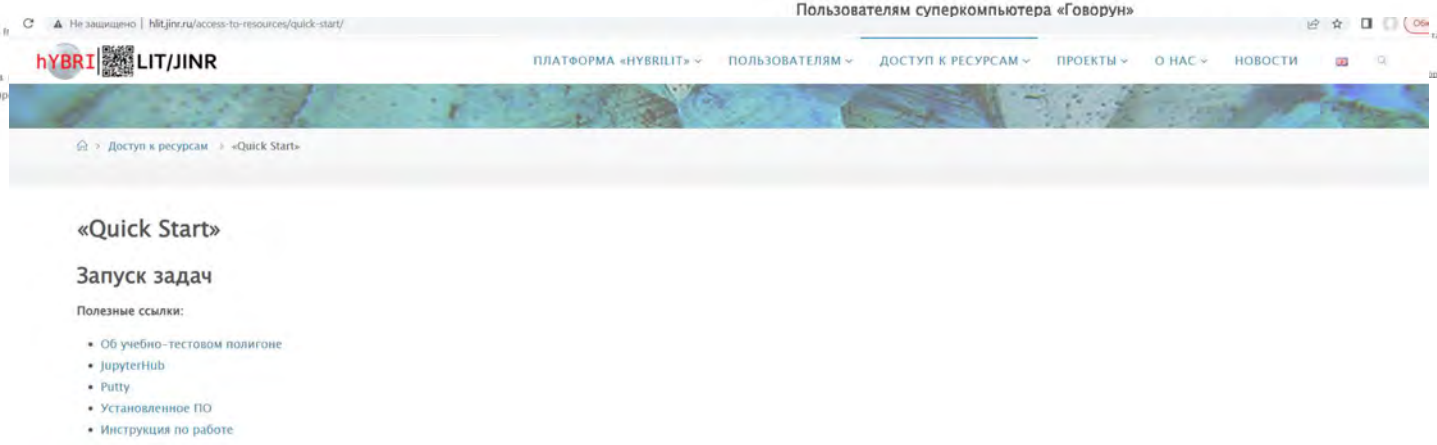
“Govorun” supercomputer

http://hlit.jinr.ru/









Thank you for your attention

HYBRILIT HETEROGENEOUS PLATFORM at MLIT JINR:

http://hlit.jinr.ru

SC Govorun included into unified supercomputer network of Russia

On 24 September, an agreement was signed in St. Petersburg on uniting three supercomputers, including the object of the scientific infrastructure of the JINR Member States – the "Govorun" supercomputer – into a single network. Its aim is to develop the National Research Computer Network of Russia.

Deputy Prime Minister of the Russian Federation Dmitry Chernyshenko

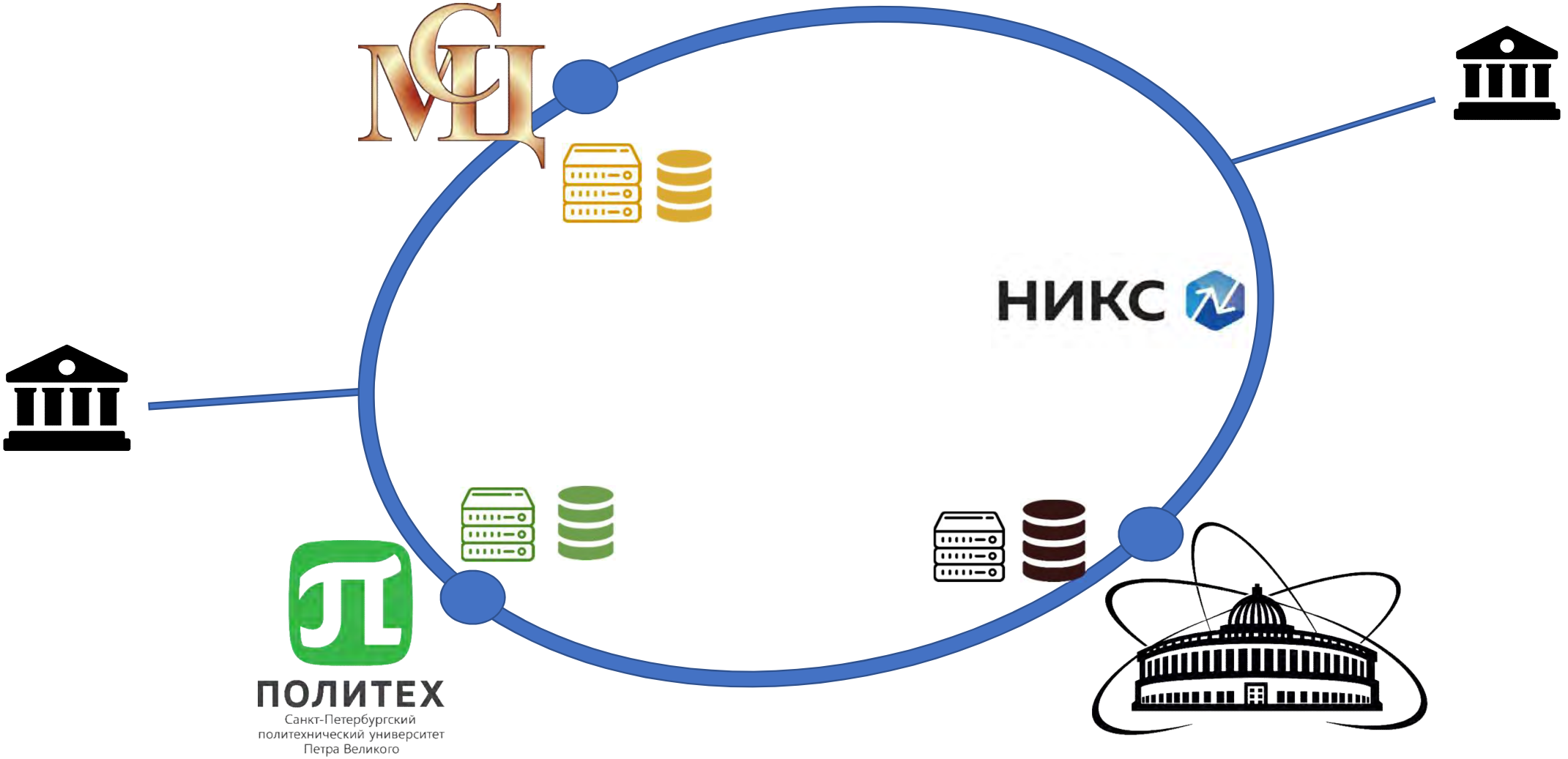
Director of the Meshcheryakov Laboratory of Information Technologies JINR Vladimir Korenkov

Rector of Peter the Great St. Petersburg Polytechnic University Andrey Rudskoi

Director of the Joint Supercomputer Centre of the Russian Academy of Sciences Boris Shabanov

There is a unified scientific and educational space of information technologies being formed in Russia. Scientific world-level centres, scientific-educational and engineering centres gain an opportunity for distributed work with big data at megascience scientific facilities in supercomputer centres. Researchers and developers will be provided with global access to services of machine learning, big data analysis, supercomputer resources.

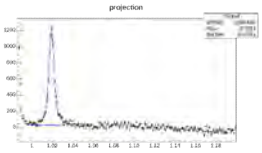
Объединенная географически распределенная суперкомпьютерная инфраструктура

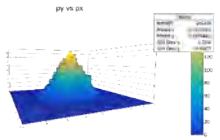


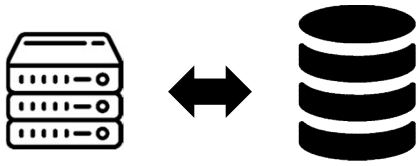
Объединенная географически распределенная суперкомпьютерная инфраструктура для мегапроекта NICA

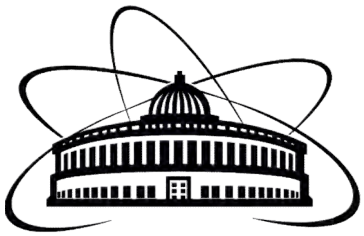
На основе интеграции суперкомпьютеров ОИЯИ, Межведомственного суперкомпьютерного центра РАН и Санкт-Петербургского политехнического университета Петра Великого создана масштабируемая исследовательская инфраструктура нового уровня. Такая инфраструктура востребована для задач меганауки NICA.

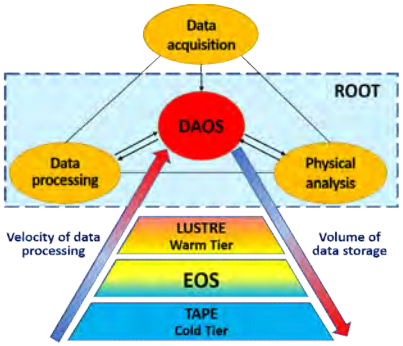
Реконструкция траекторий, Физический анализ







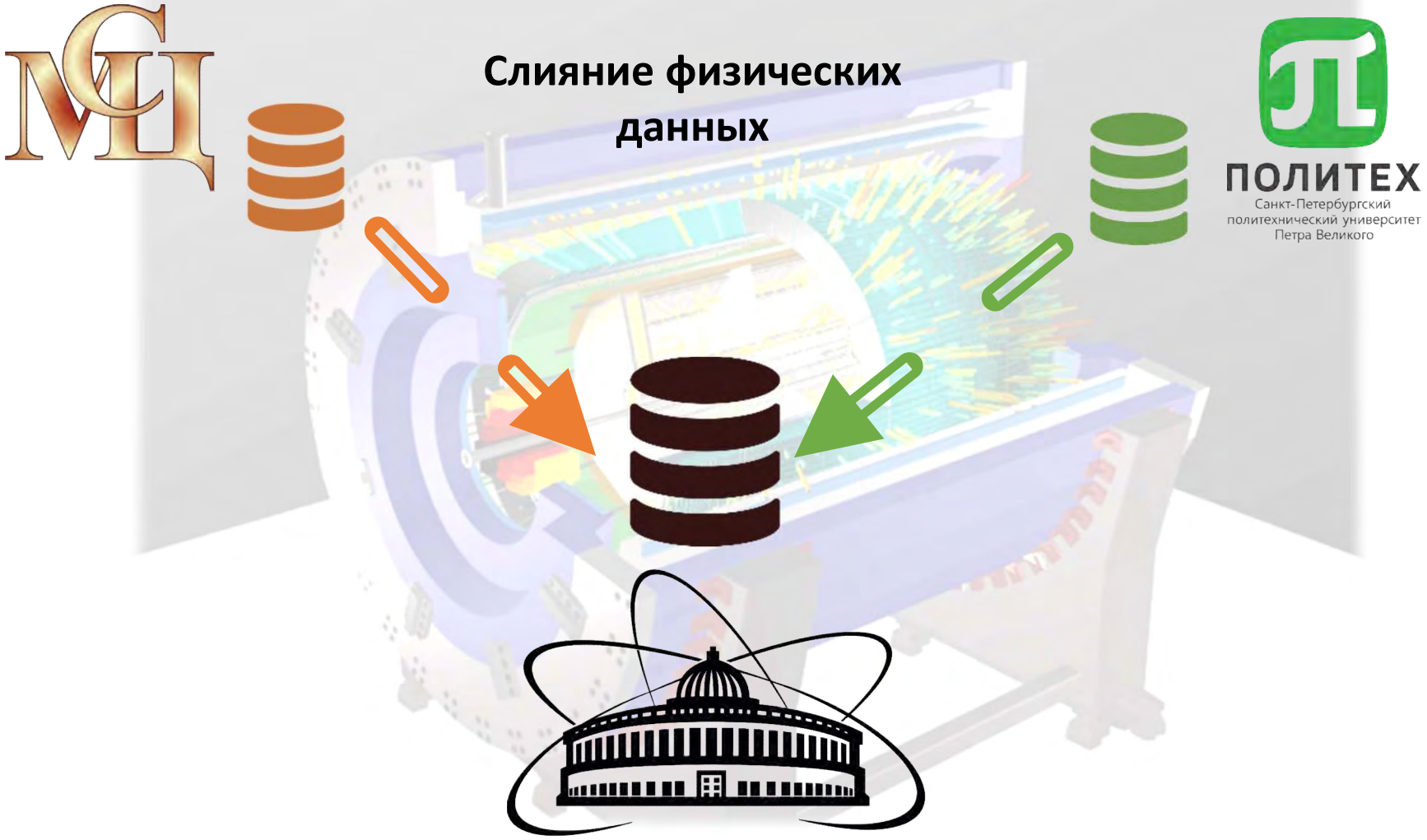




Основным направлениями развития создаваемой инфраструктуры являются:

- объединение суперкомпьютерных ресурсов в интегрированную территориально распределённую сеть;
- создание экосистемы профессионального сообщества пользователей суперкомпьютерными ресурсами;
- совместное развитие средств хранения и обработки больших объемов данных;
- создание облачных цифровых сервисов для доступа к суперкомпьютерным ресурсам;
- создание сервисов машинного обучения и аналитики больших данных, распределенных витрин данных для пользователей научных и образовательных организаций.

Объединенная географически распределенная суперкомпьютерная инфраструктура для мегапроекта NICA



Объединенная географически распределенная суперкомпьютерная инфраструктура для мегапроекта NICA

В январе 2022 года успешно завершен первый совместный эксперимент по использованию единой суперкомпьютерной инфраструктуры для задач мегасайенс-проекта NICA:

- ✓ для эксперимента MPD было запущено 3000 задач генерации данных;
- ✓ было сгенерировано порядка 3 миллиона событий;
- ✓ полученные данные были переданы на СК «Говорун» для дальнейшей обработки и физического анализа.