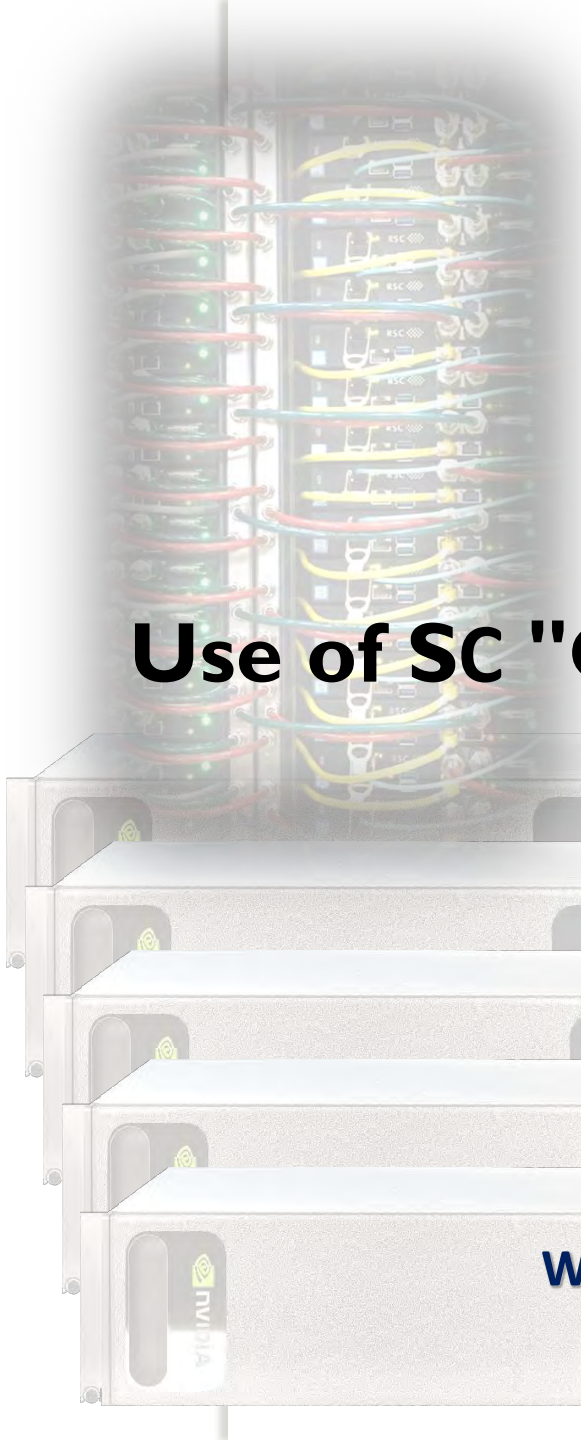


Use of SC "Govorun" for tasks of the NICA mega project

Dmitry Podgainy

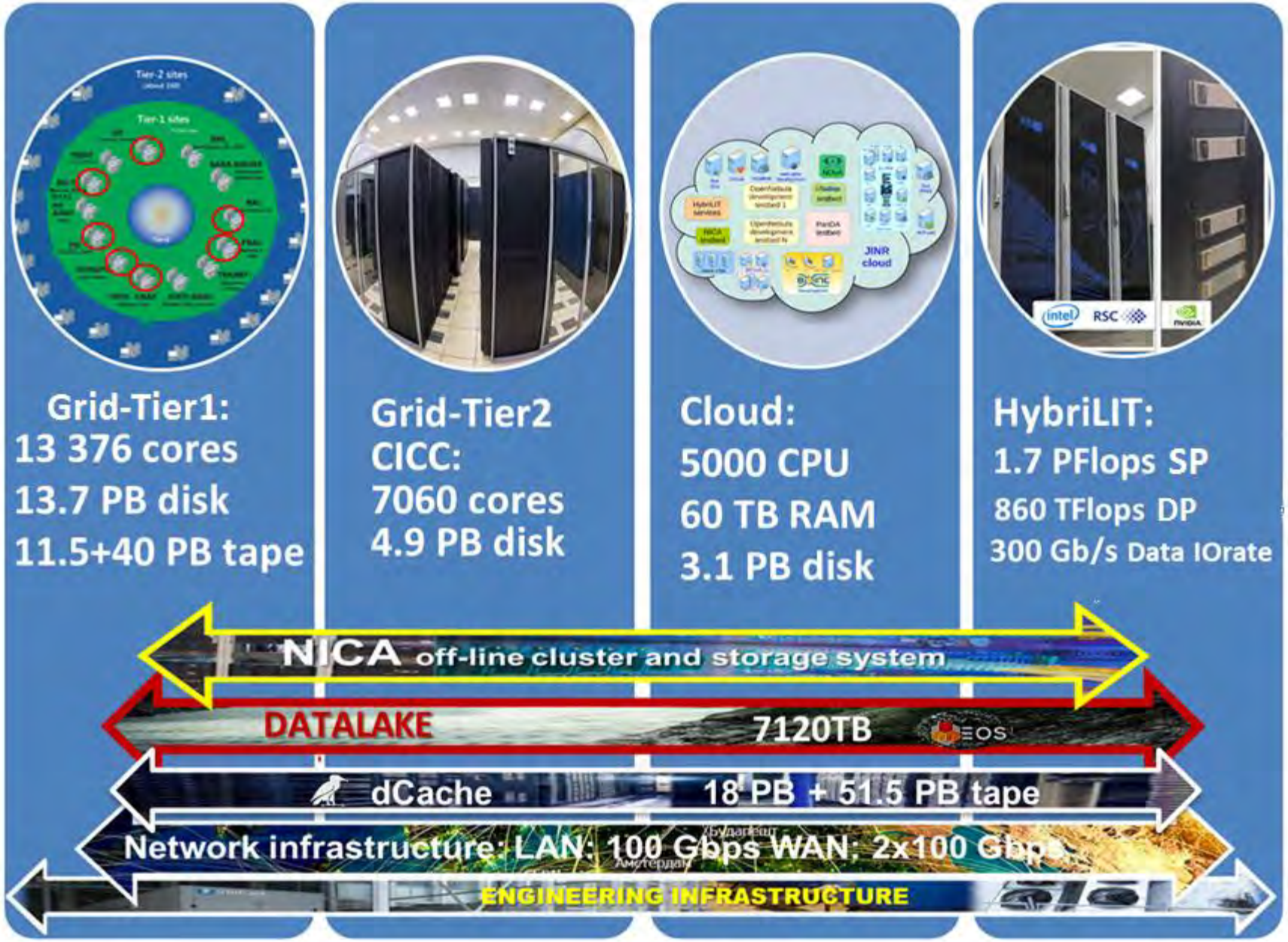
Meshcheryakov Laboratory of Information Technologies

Joint institute for nuclear research

Workshop on physics performance studies at NICA (NICA-2022)

13-15 December 2022

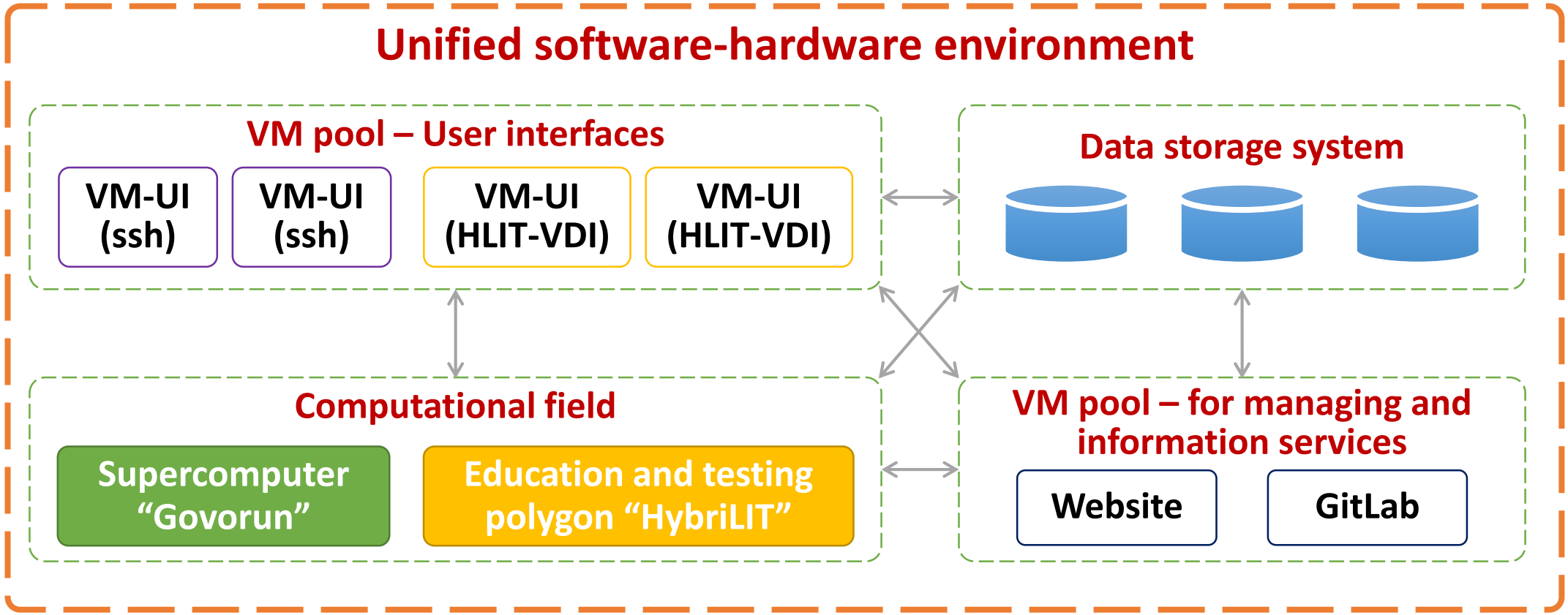
Multifunctional Information and Computing Complex



The **MICC** meets the requirements for a modern highly performant scientific computing complex: multi-functionality, high performance, task adapted data storage system, high reliability and availability, information security, scalability, customized software environment for different user groups, high-performance telecommunications and modern local network.

LIT IT-infrastructure is the one of JINR basic facilities

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

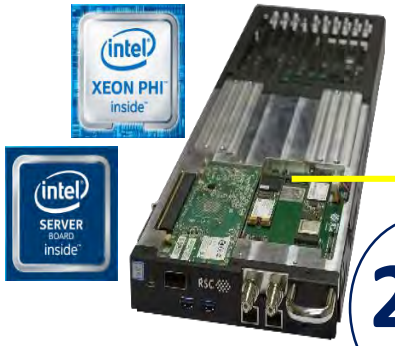
“Govorun” supercomputer
First stage 2018:
Full peak performance :
1 PFlops for single precision
500 TFlops for double precision
9th in the current edition of the IO500 list (July 2018)

#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



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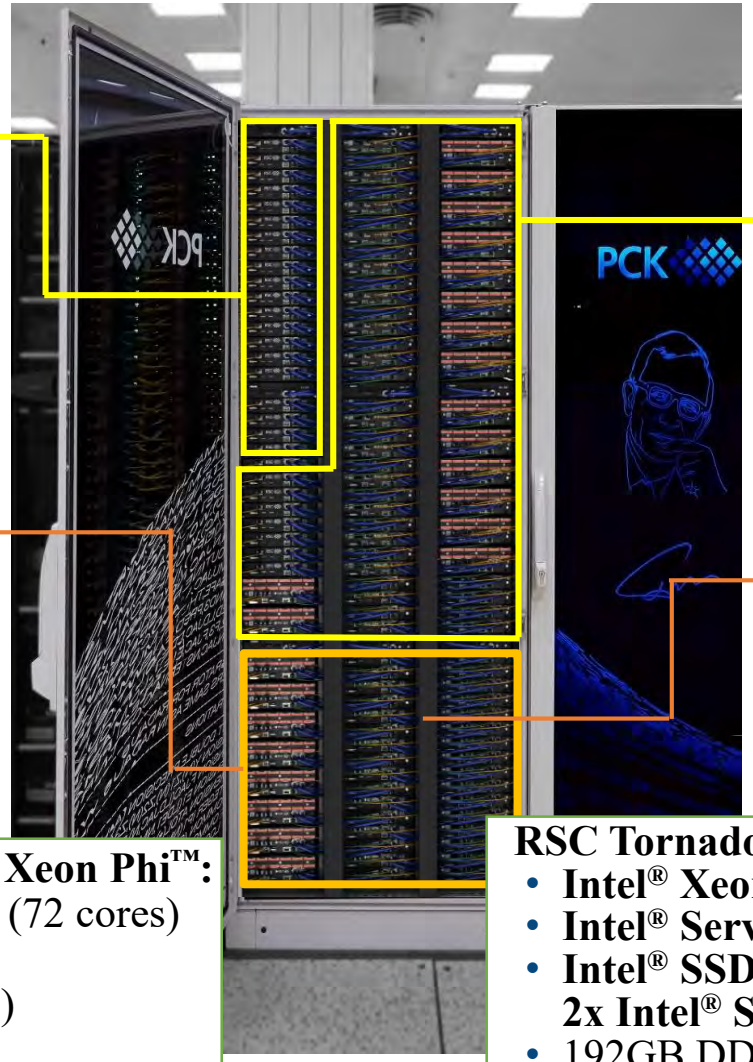

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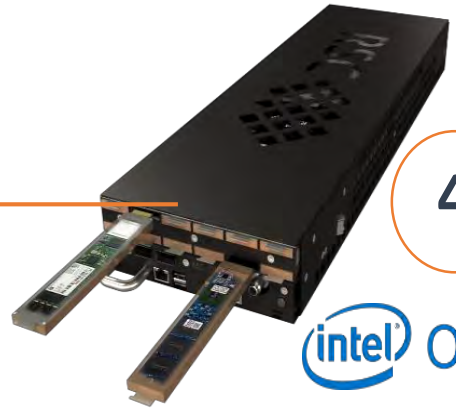
14

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



4

intel OPTANE™

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**

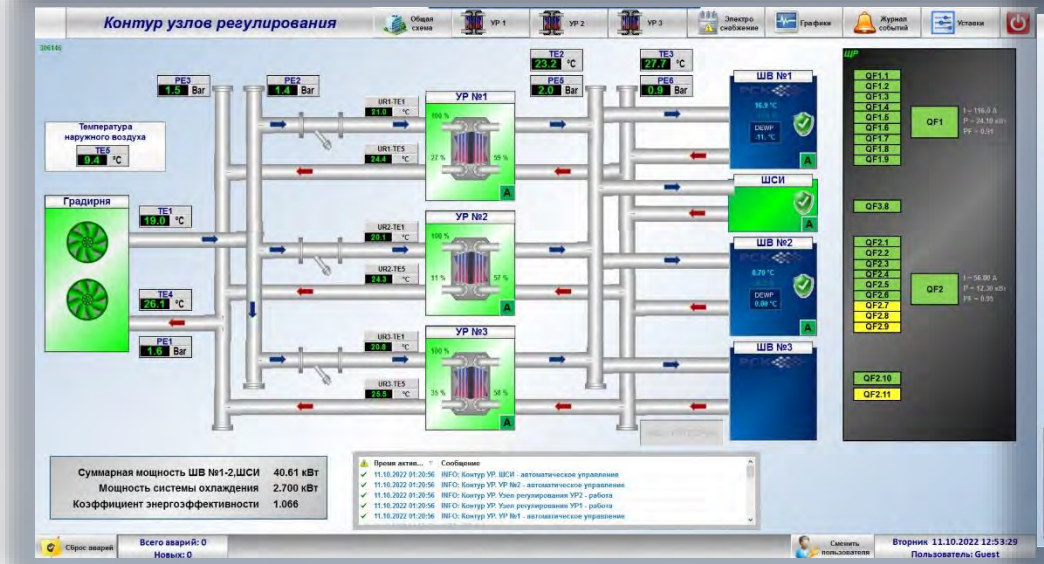
RSC Tornado nodes based on Intel® Xeon® Scalable gen 2:

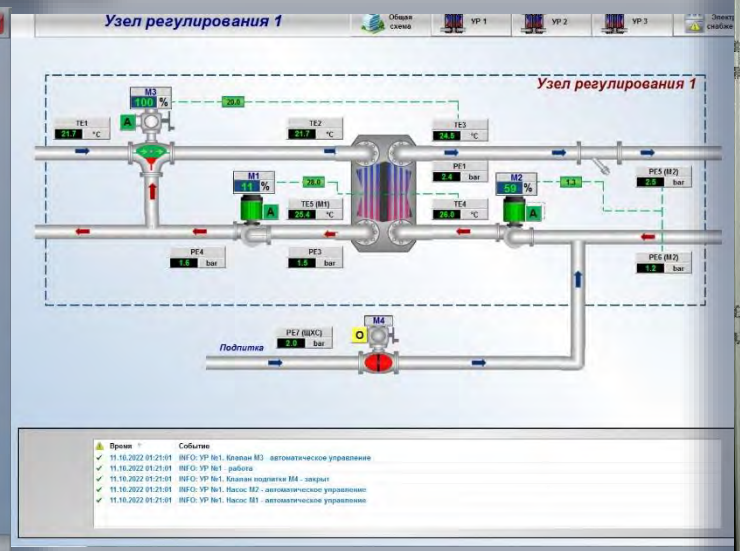
- **Intel® Xeon® Platinum 8268** processors (24 cores)
- **Intel® Server Board S2600BP**
- **Intel® SSD DC S4510** (SATA, M.2),
  2x Intel® SSD DC P4511 (NVMe, M.2) 2TB
- 192GB DDR4 2933 GHz RAM
- **Intel® Omni-Path 100 Gb/s adapter**

Engineering infrastructure

free cooling
24x7x365

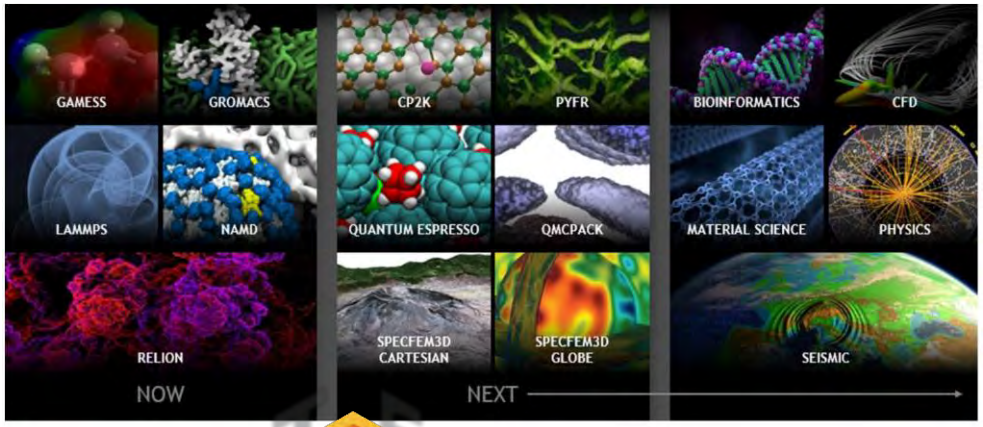
PUE ~ 1,06





The GPU-component of the “Govorun” Supercomputer

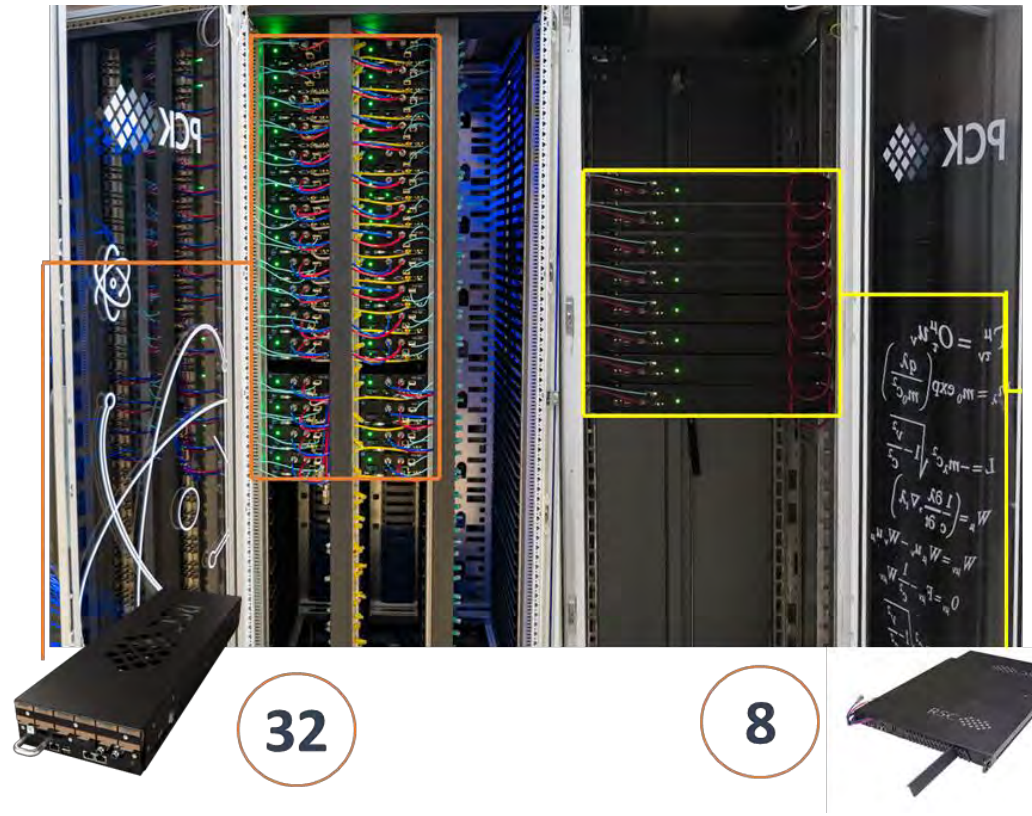
The GPU-component consists of **5 NVIDIA DGX-1 servers**. Each server has **8 GPU NVIDIA Tesla V100** based on the latest architecture NVIDIA Volta. Moreover, one server NVIDIA DGX-1 has **40960** cores CUDA, which are equivalent to 800 high-performance central processors. A whole number of novel technologies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

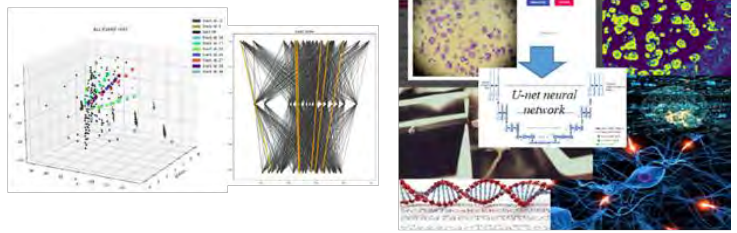


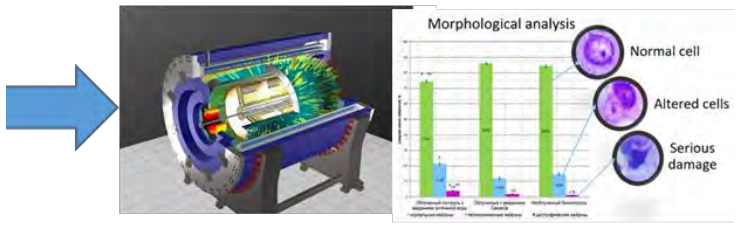
The GPU-component gives a users of the supercomputer a possibility to allow as massively parallel computation for general-purpose tasks using such technologies as CUDA and OpenCL, as well as use applications already adapted for this architecture. Also, GPU-component allow to use machine learning and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

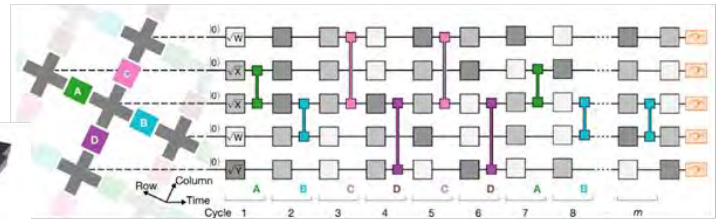
TensorFlow PYTORCH theano APACHE mxnet The Microsoft Cognitive Toolkit Caffe

"Govorun" supercomputer modernization 2022









The expansion of the “Govorun” supercomputer by 32 hyperconverged compute nodes and 8 distributed storage nodes made it possible to:

- enhance its performance by 239 Tflops (Total peak performance: 1.1 PFlops DP);
- increase the DAOS data processing and storage subsystem to 1.6 PB;
- enlarge the volume of the "warm data" storage subsystem by 8 PB with support for the creation of dynamic storage systems such as Luster, DAOS, EOS, dCache, NFS.

The continuous increase in the expansion of the range of tasks to be solved in order to ensure the solution of the theoretical and experimental tasks of JINR has required

- The constant re-equipment of the “Govorun” SC with computing resources;
- Permanent implementation of the novel IT solutions;
- Creating an environment for supercomputer modeling and the solution of compute-intensive and data-intensive tasks.

The CPU-component of the “Govorun” Supercomputer

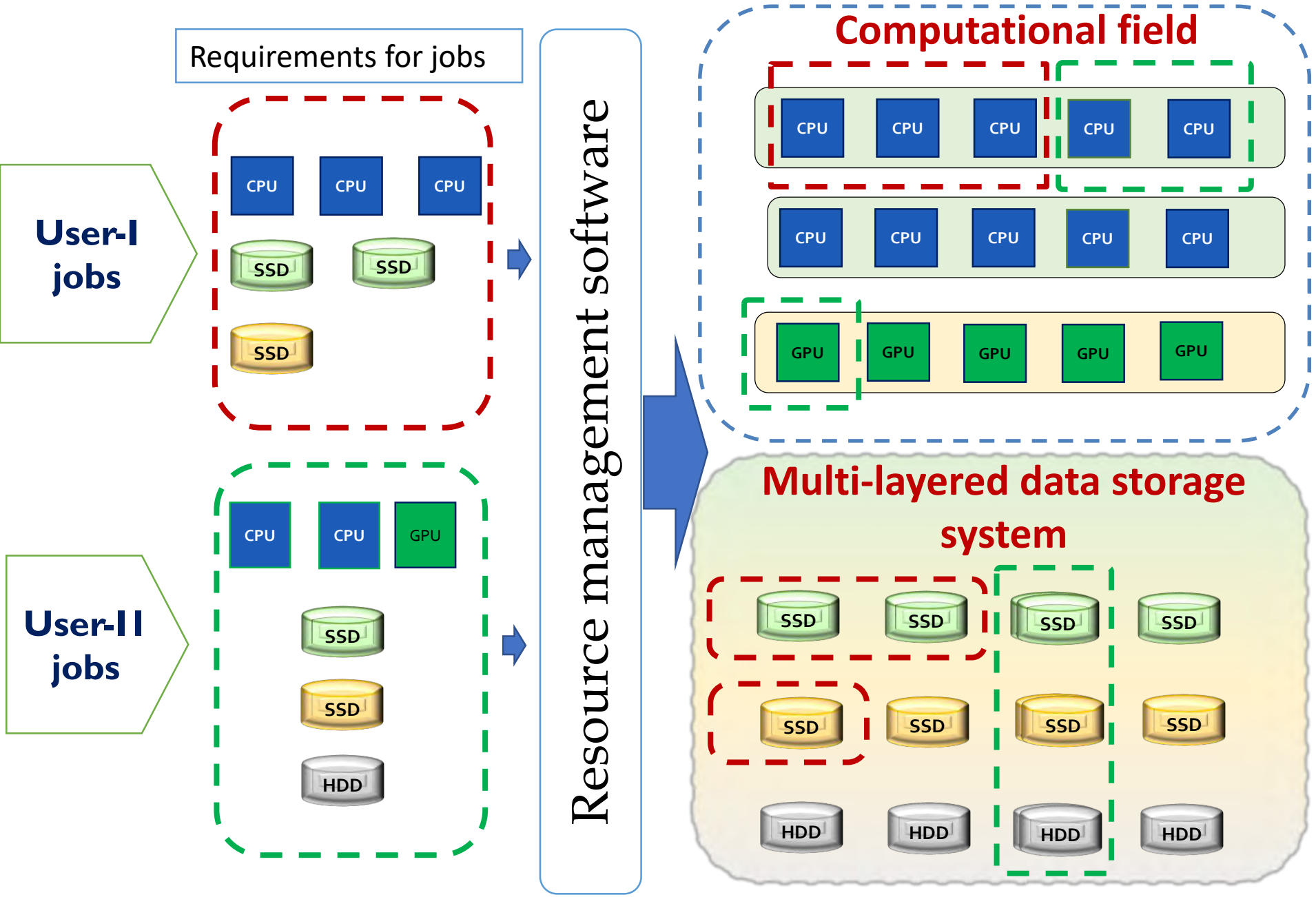
RSC Tornado nodes based on Intel® Xeon® Scalable gen 3:

- **Intel® Xeon® Platinum 8368Q** processors (38 cores)
- **DDR-T PMEM 200 Series, 256 GB - 8 pc. total 2 048 GB**
- **Intel® SSD EDSFF E1.S 4TB – 4 pc. total 16 TB**
- 256GB DDR4 2933 GHz RAM
- **Intel® Omni-Path 200 Gb/s adapter**

RSC Tornado nodes based on Intel® Xeon® Scalable gen 2:

- **Intel® Xeon® Gold 6248R** processors (24 cores)
- **Intel® Server Board S2600BP**
- **Intel® SSD NVMe EDSFF E1.L (RULER) 30,72 TB - 32 pc., total 983 TB**
- 384 GB DDR4 2933 GHz RAM
- **Intel® Omni-Path 200 Gb/s adapter**

Orchestration and hyperconvergence on the “Govorun” supercomputer



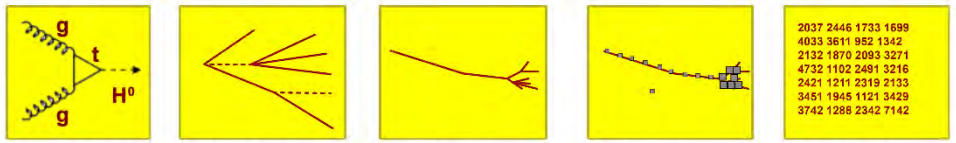
The “Govorun” supercomputer has unique properties for the flexibility of customizing the user’s job.

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.

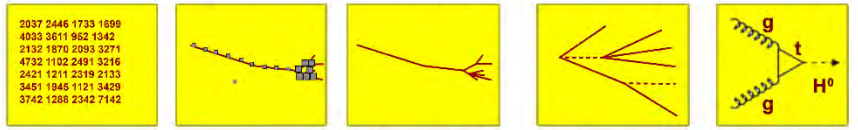
HEP experiments data flow

From Physics to raw data



Basic physics | Fragmentation, Decay | Interaction with detector material Multiple scattering, interactions | Detector response Noise, pile-up, cross-talk, inefficiency, ambiguity, resolution, response function, alignment | Raw data Read-out addresses, ADC, TDC values, Bit patterns

From raw data to Physics



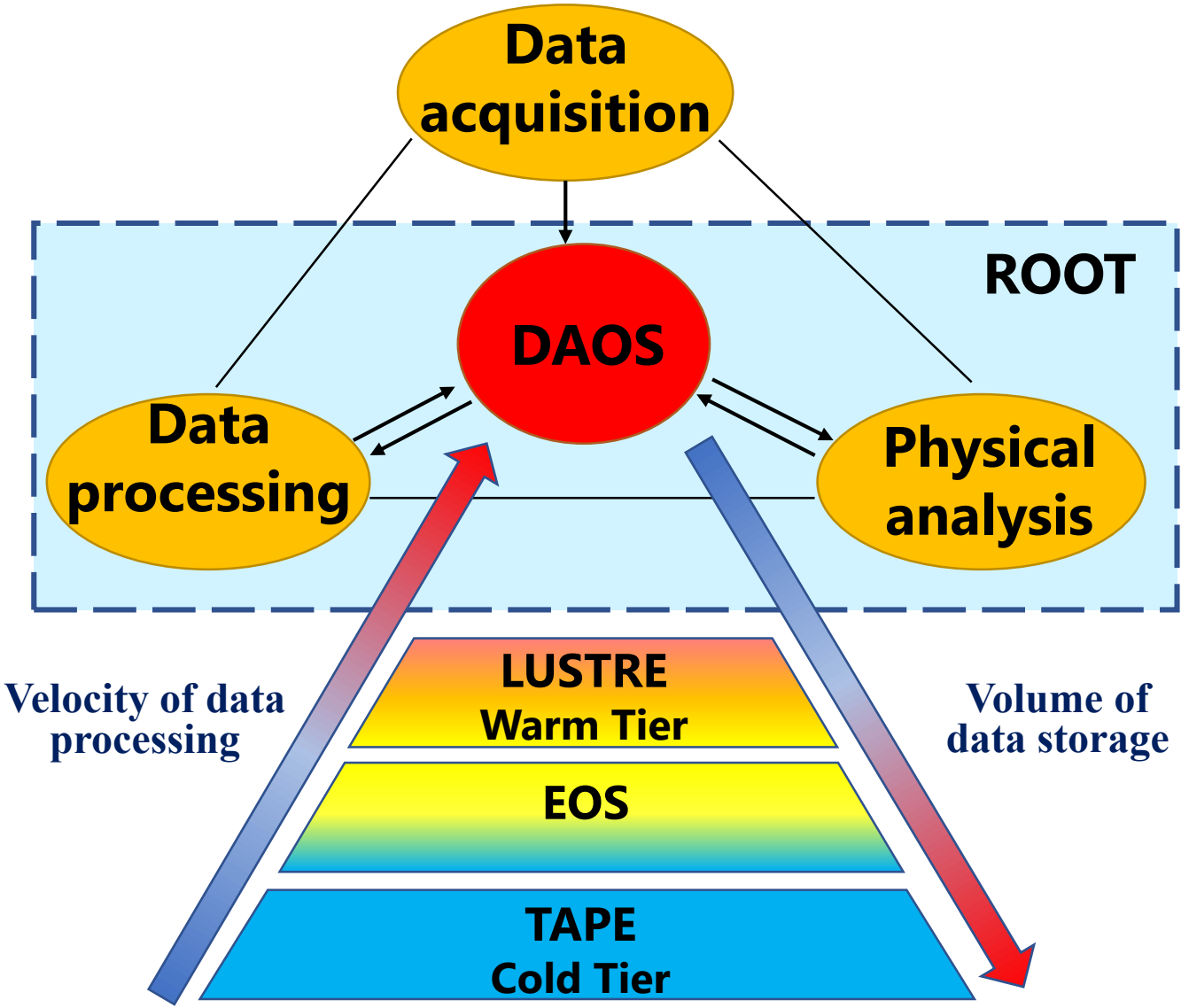
Raw data Convert to physics quantities | Detector response Apply calibration, alignment | Interaction with detector material Pattern, recognition, Particle identification | Fragmentation, Decay Physics analysis | Basic physics Results

Reconstruction

Analysis

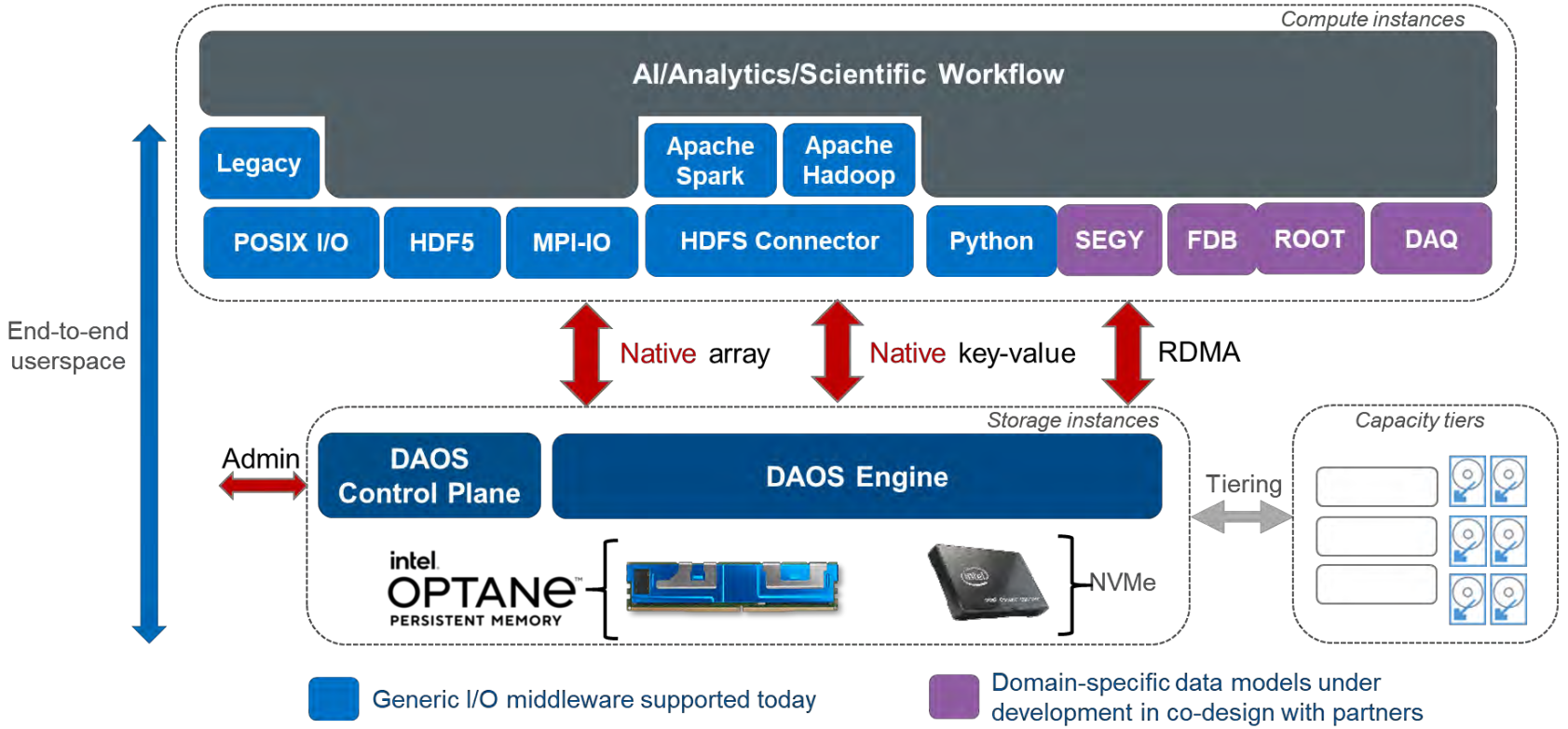
Simulation (Monte-Carlo)

We need to go from raw data back to physics reconstruction + analysis of the event(s)



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

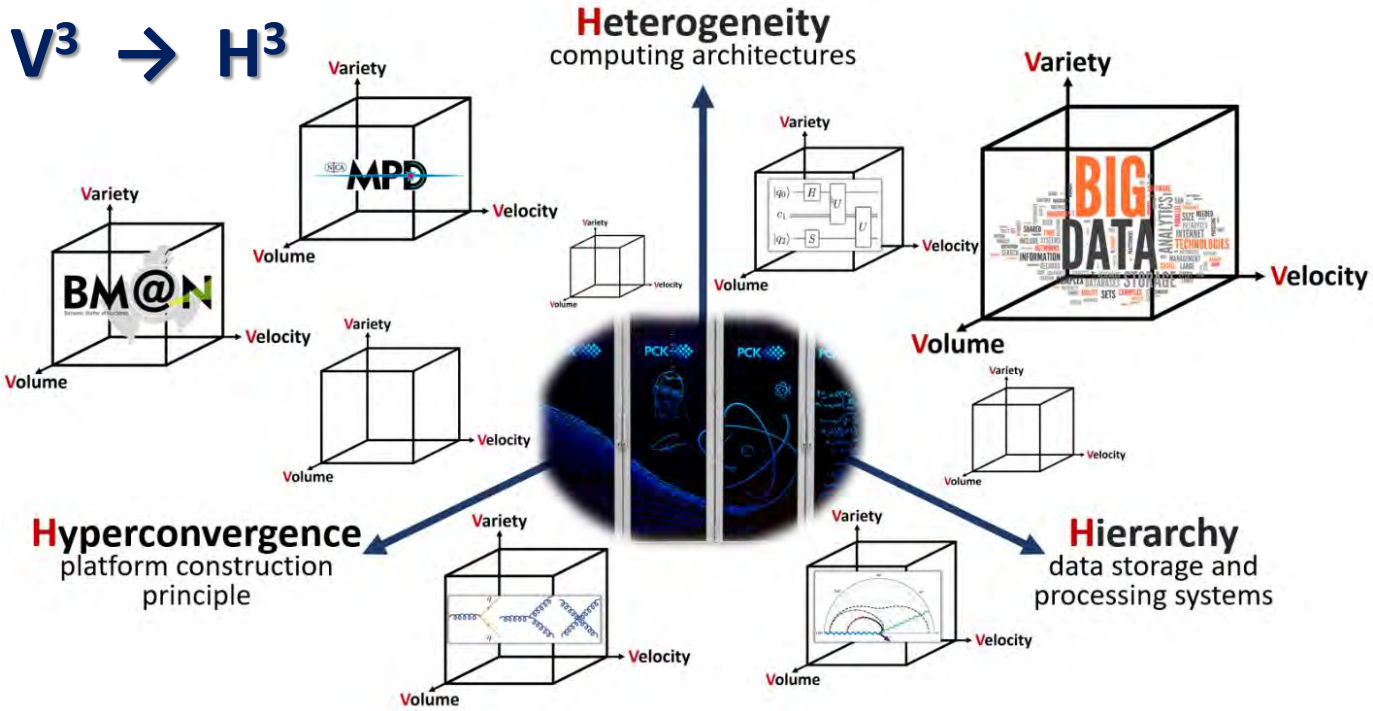
Big Data on the “Govorun” Supercomputer for NICA megaproject

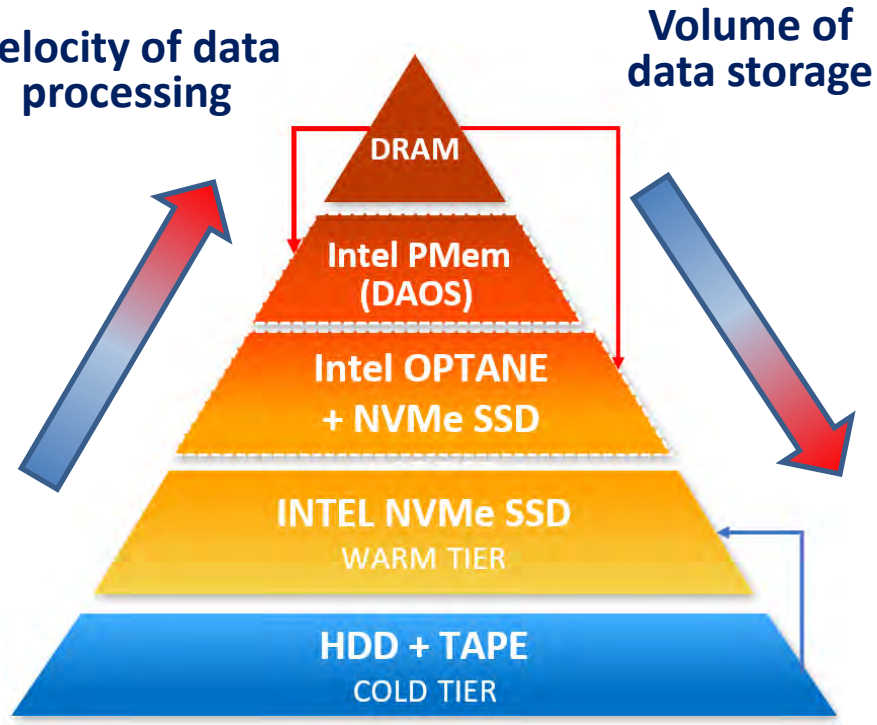
The DAOS polygon of the “Govorun” supercomputer takes the **1st** place among Russian supercomputers in terms of the data processing rate in the current **IO500 list**.

Heterogeneity
Hierarchy
Hyperconvergence

provide

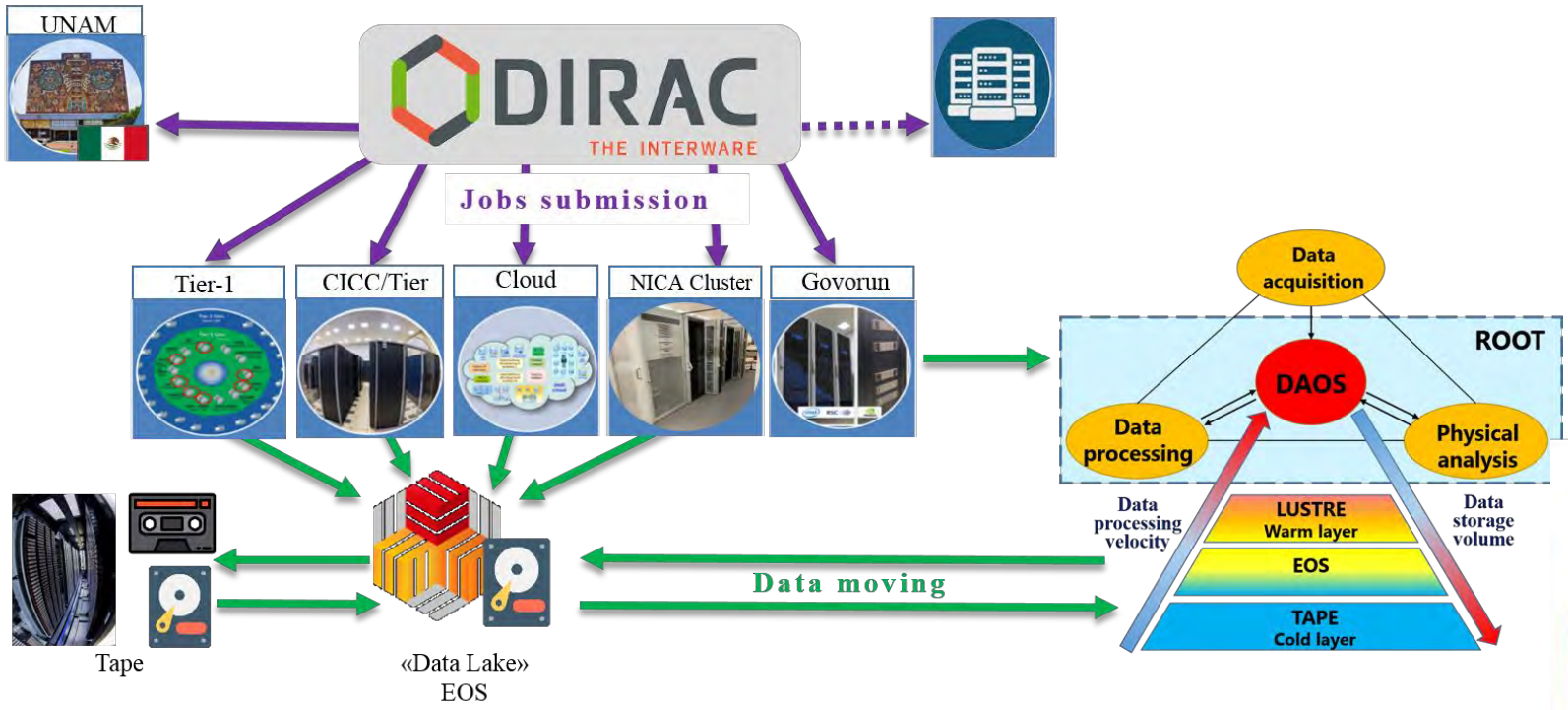
Variety
Velocity
Volume





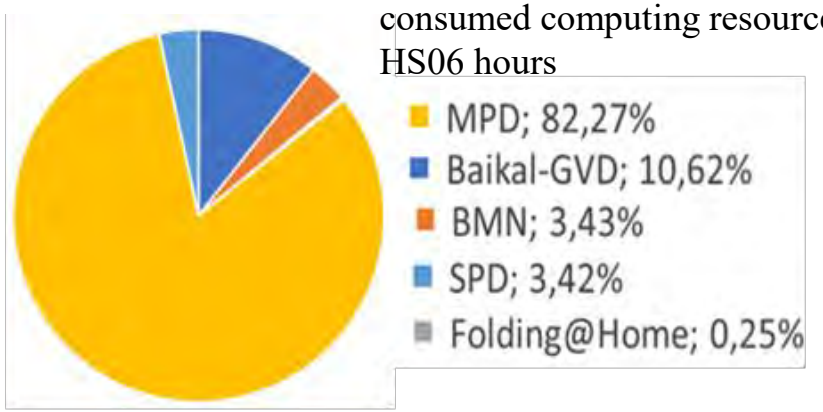
Heterogeneous distributed computing environment

A heterogeneous computing environment, based on the DIRAC platform, was created. for processing and storing data of the experiments conducted at JINR. By the end of 2021, all the MICC components, the clouds of the JINR Member States, the NICA cluster, as well as the cluster of the National Autonomous University of Mexico (NAUM, within the cooperation on the MPD project), were integrated into DIRAC. For the time being, the distributed infrastructure is used by the following experiments: MPD, Baikal-GVD, BM@N, SPD.

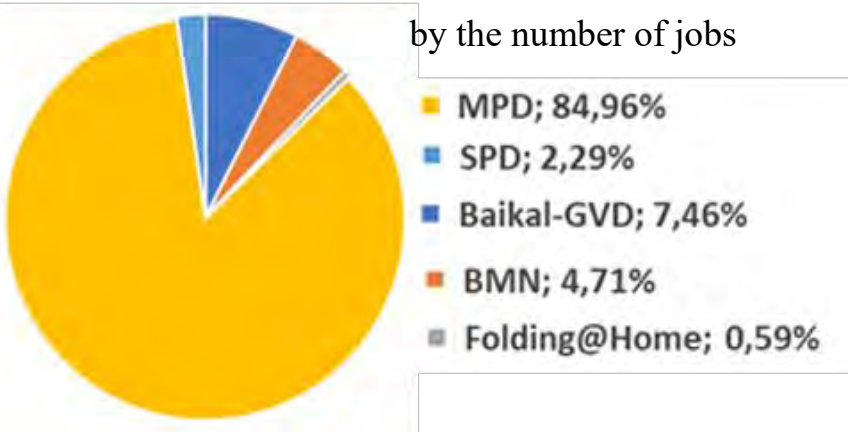


Usage of resources integrated into DIRAC by main users:

consumed computing resources in HS06 hours

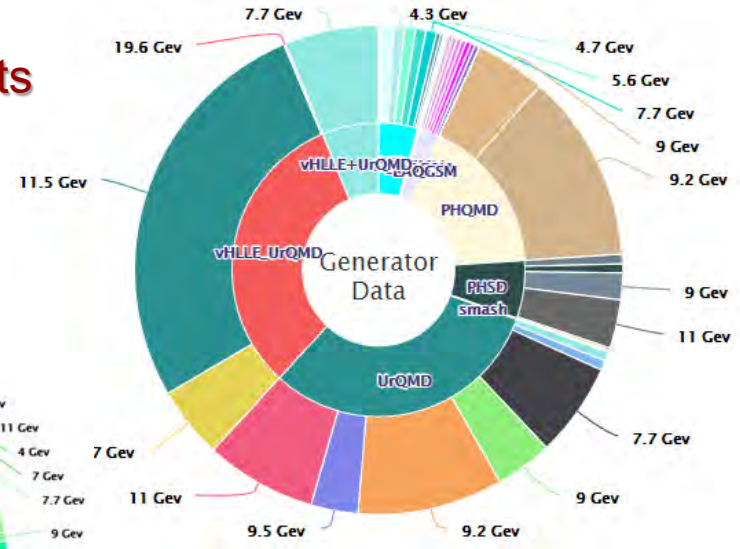


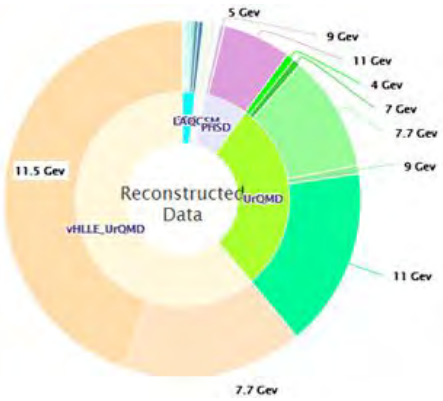
by the number of jobs



Heterogeneous distributed computing environment for the MPD experiment

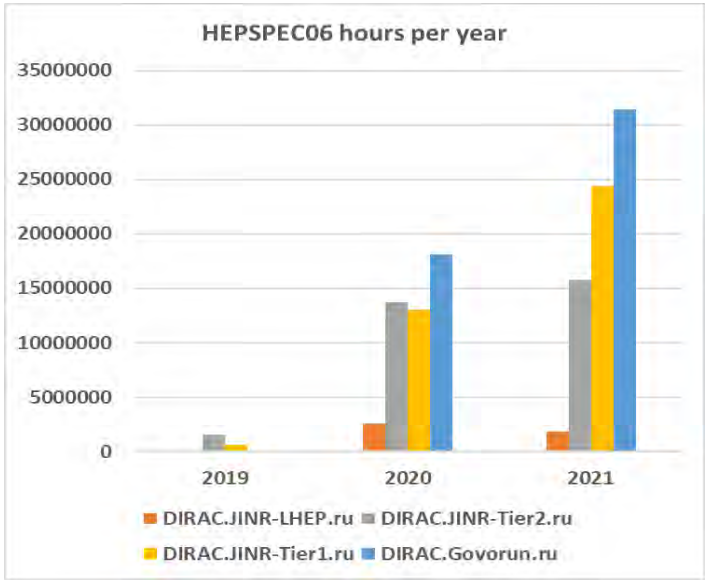
✓$1233 * 10^6$events were generated using *UrQMD*, *PHQMD*, *PHSD* and other models





✓$423 * 10^6$events were reconstructed

"Govorun" up to **40%**



Available resources of the DIRAC platform for the MPD experiment:

- "Govorun" supercomputer:

"Old" nodes up to 1,334 cores

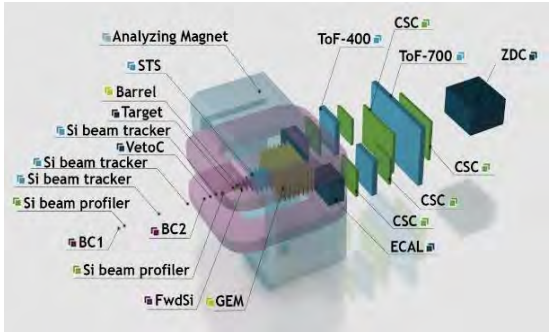
"New" nodes up to 1,152 cores (almost 31 million events less then mounth!)

- Tier1: 920 cores
- Tier2: 1,000 cores
- Clouds (JINR and JINR Member States): 70 cores
- NICA offline cluster: 500 cores
- 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.

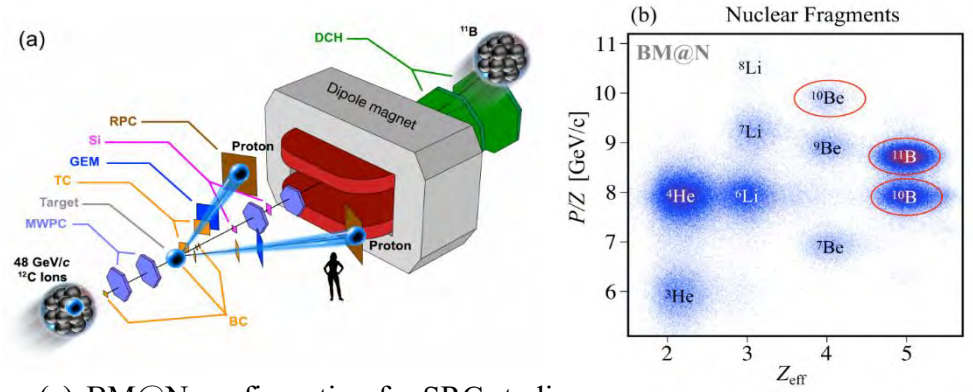
The mass production storages integrated into the Dirac File Catalog are 2,1 PB in size. 0,4 PB on the new Ruler Storage

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

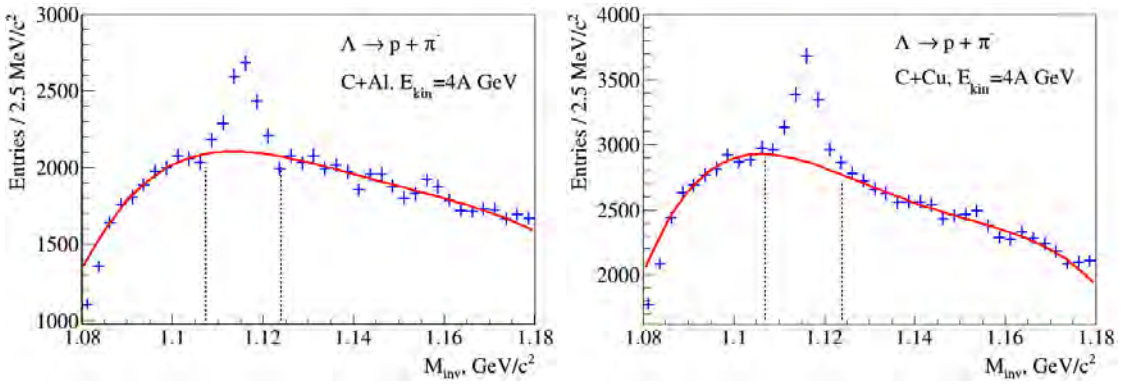
Computing for the NICA megaproject “Govorun” supercomputer for BM@N tasks



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.

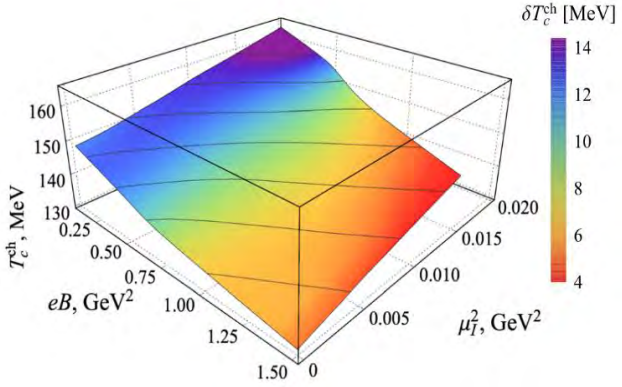


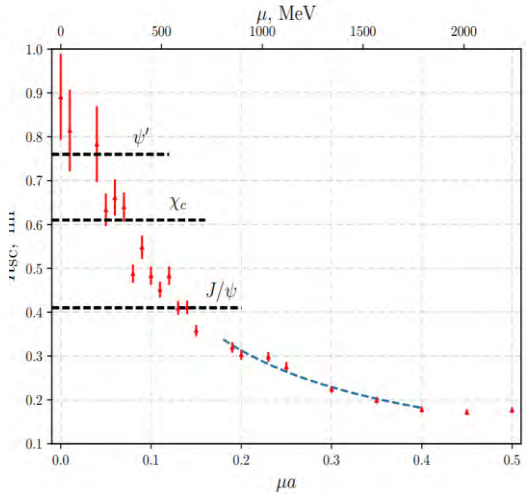
Signals of Λ-hyperons in the spectra of invariant masses (p,π-) measured in C+Al and C+Cu interactions.

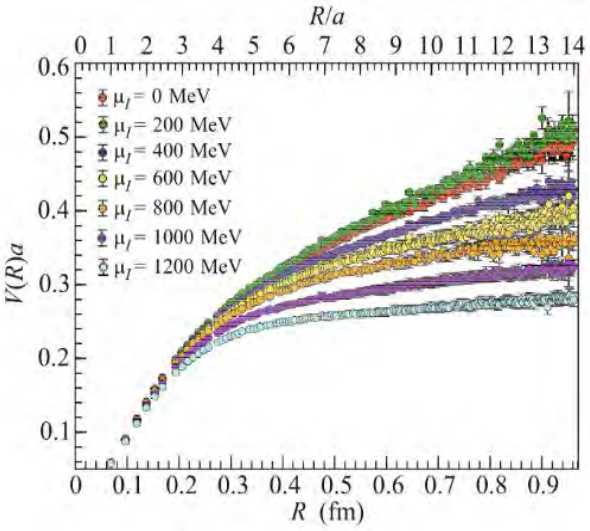
BM@N Collaboration. Production of Λ hyperons in 4 and 4.5 AGeV 2 carbon-nucleus interactions at the Nuclotron // The European Physical Journal A (awaiting publication)

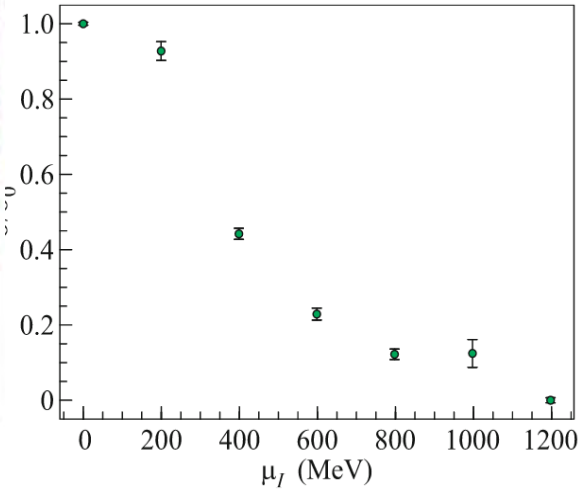
- The analysis of experimental data acquired during the Nuclotron runs in 2016-2018 was performed. Special attention is paid to the study of interactions between beams of carbon and argon ions with fixed targets of different types. The reconstruction of particle tracks was carried out using the method 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.

“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.

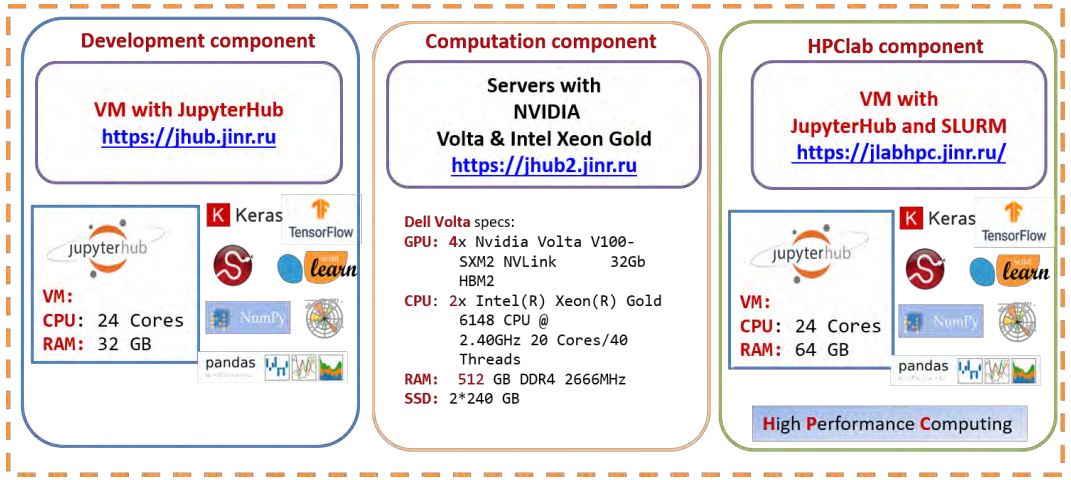
– The effect of the non-zero chiral chemical potential on dynamical chiral symmetry breaking for Dirac semimetals was studied.

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

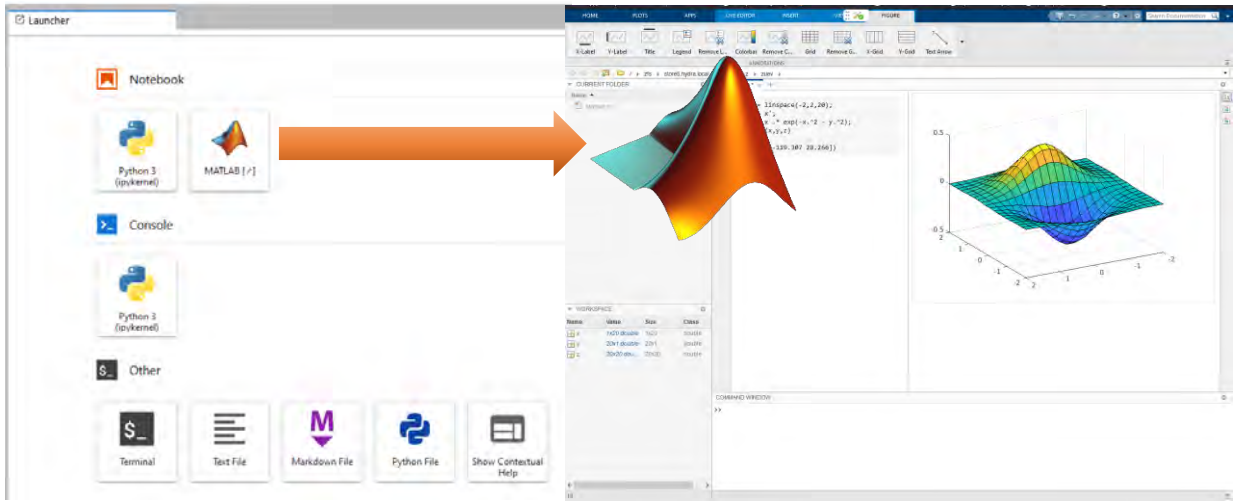
The results are published in the articles:

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

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.

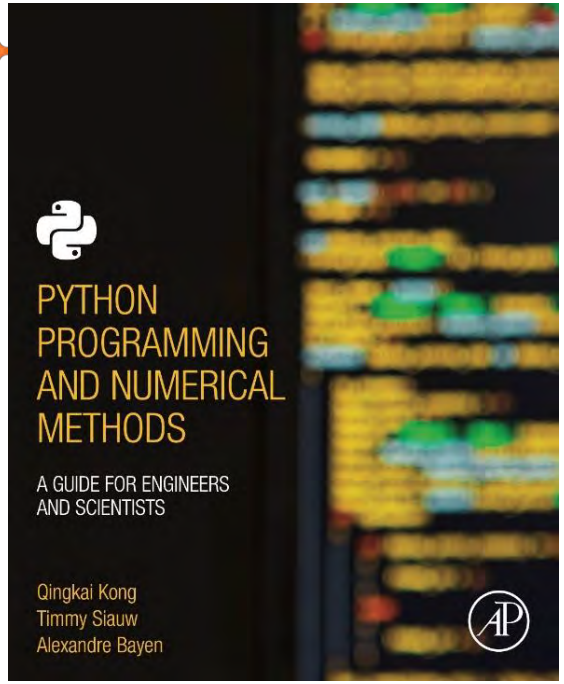


The ML/DL/HPC ecosystem is now actively used for machine and deep learning tasks. At the same time, the accumulated tools and libraries can be more widely used for scientific research, including:

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

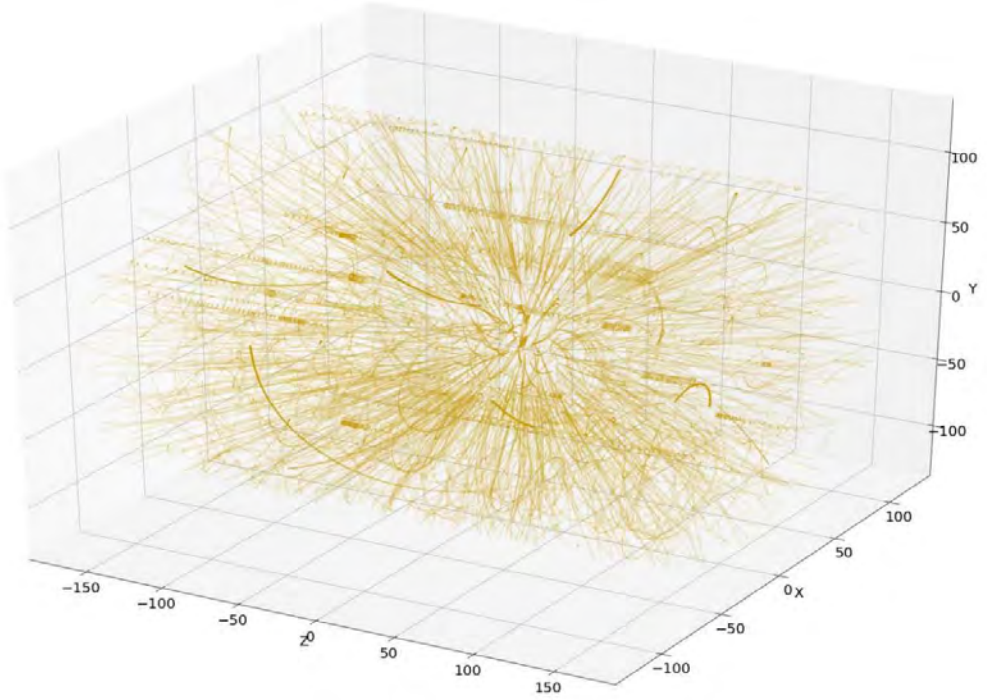
Parallel computations with Joblib

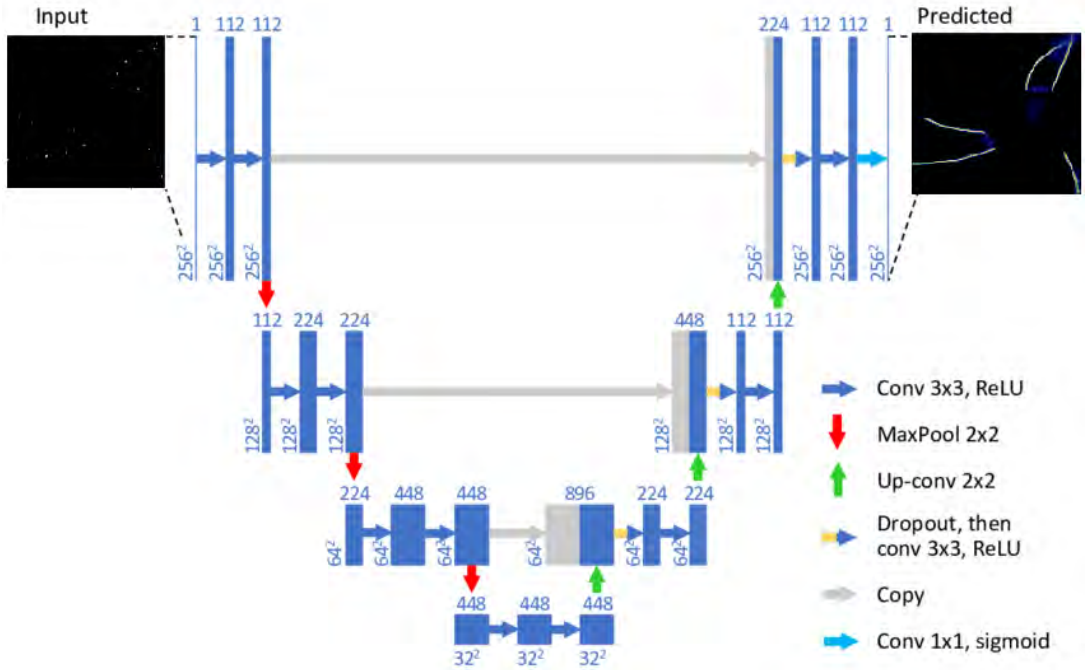
Python Numerical Methods

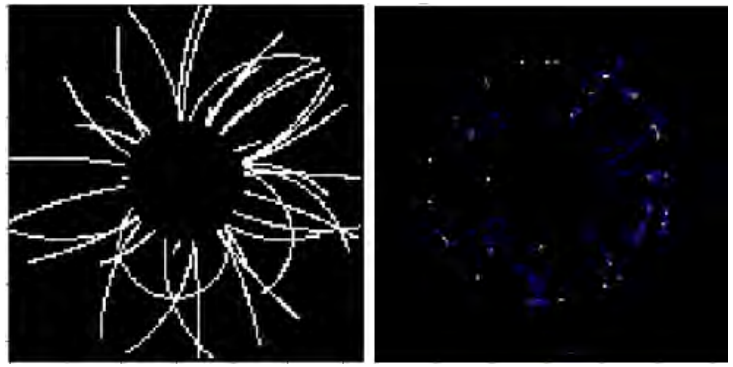


Computing for the NICA megaproject
Machine learning for MPD tracking tasks

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.



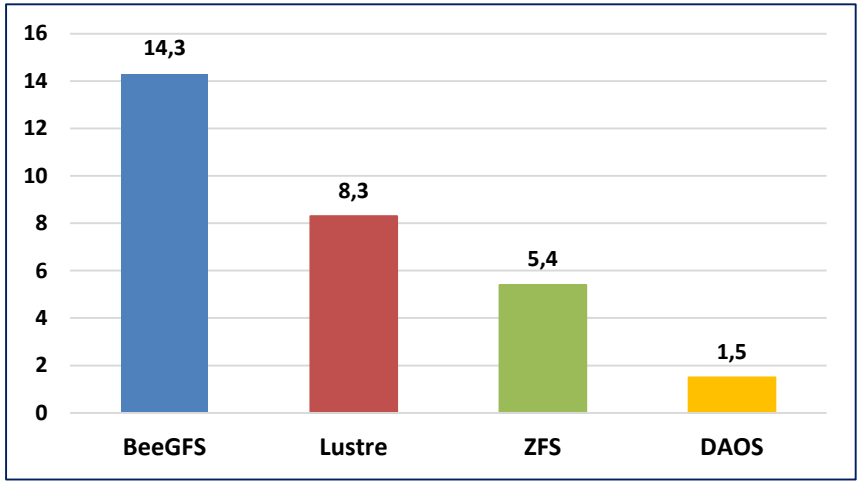




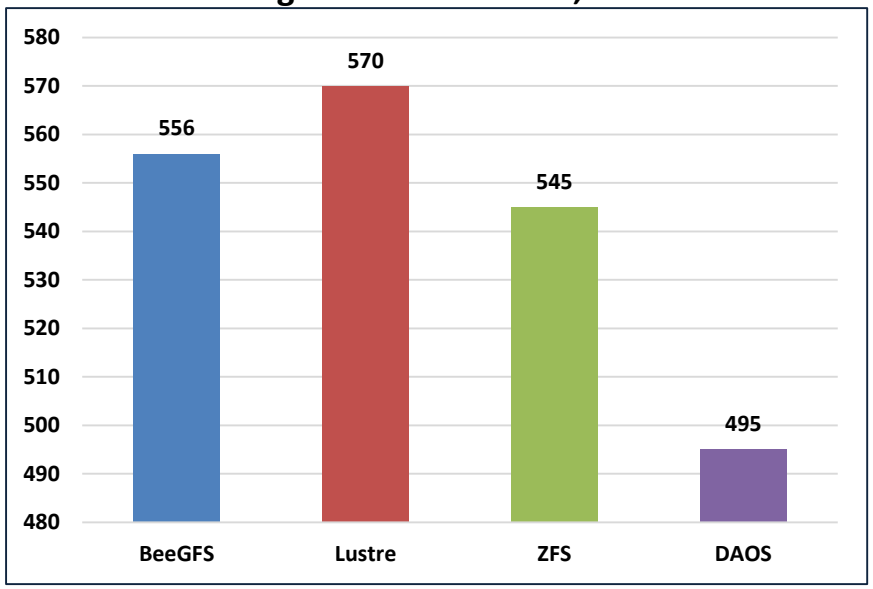
Model experiments show that neural network models are capable of both interpolating tracks and creating an internal model to represent the results in the phase space of the track parameters.

DAOS Testing. Results

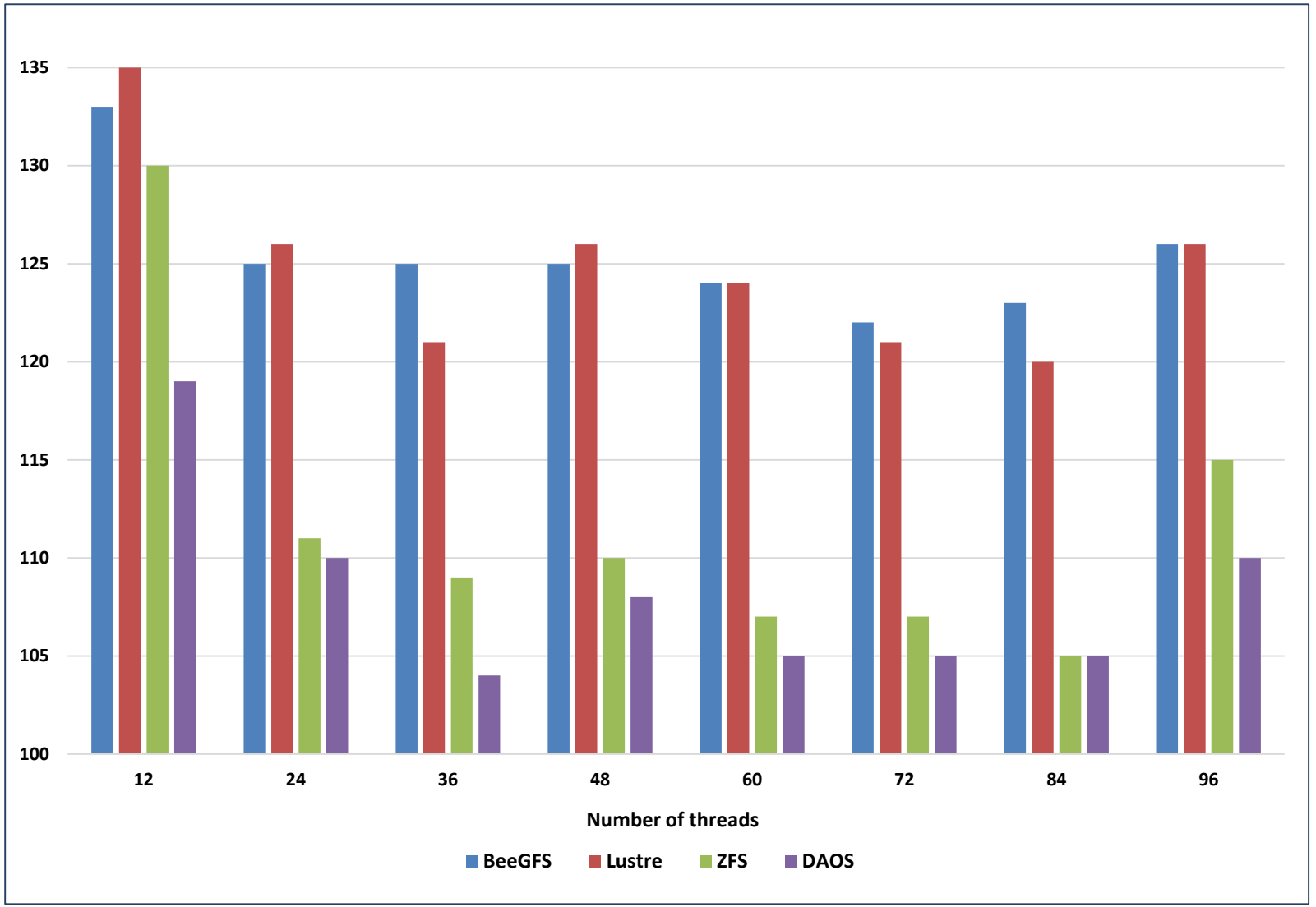
Time to load data into the model, sec



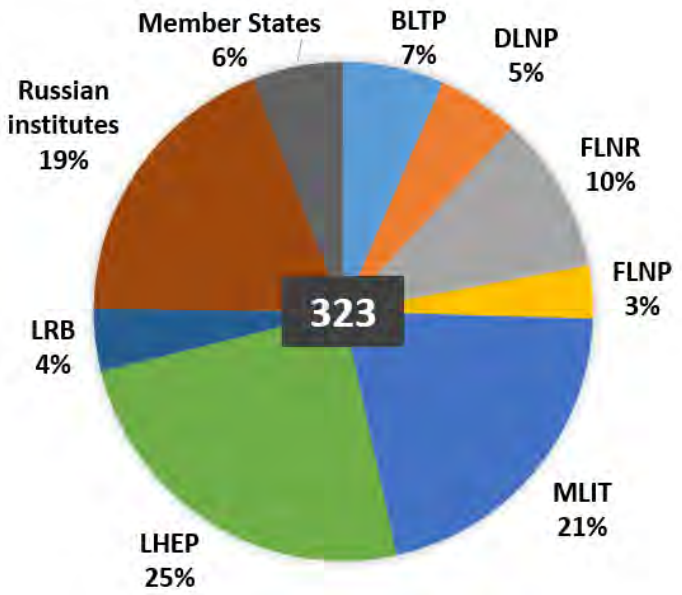
Average training time of one epoch in single-threaded mode, sec



Average training time of one training epoch, sec



“Govorun” supercomputer

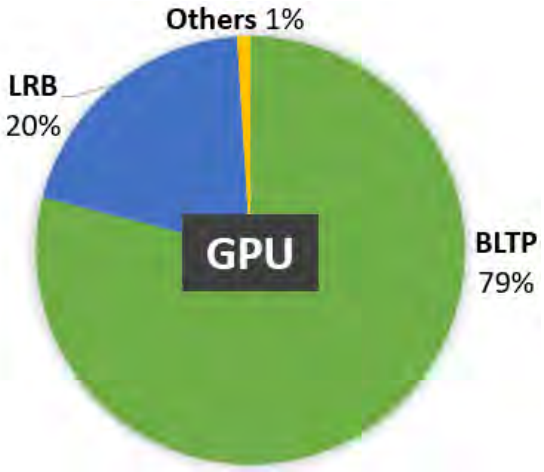


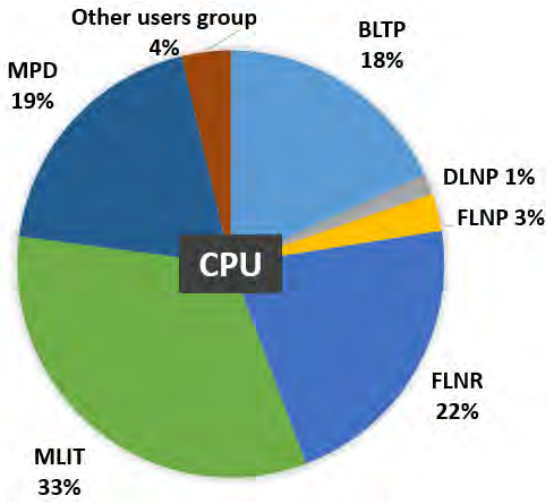
Key projects that use the resources of the “Govorun” supercomputer:

- NICA megaproject,
- calculations of lattice quantum chromodynamics,
- computations of the properties of atoms of superheavy elements,
- studies in the field of radiation biology,
- calculations of the radiation safety of JINR’s facilities.

Total number of users of the "Govorun" supercomputer: 323

Distribution of the GPU and CPU resources by user group





During February-August 2022, **555079** jobs were performed on the **CPU** component of the “Govorun” supercomputer, which corresponds to **~8M** core hours, and **455** jobs were carried out on its **GPU** component, which corresponds to **32890** GPU hours.

The average load of the CPU and GPU components amounted to 96.2% and 91.4% respectively.

“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 204 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

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

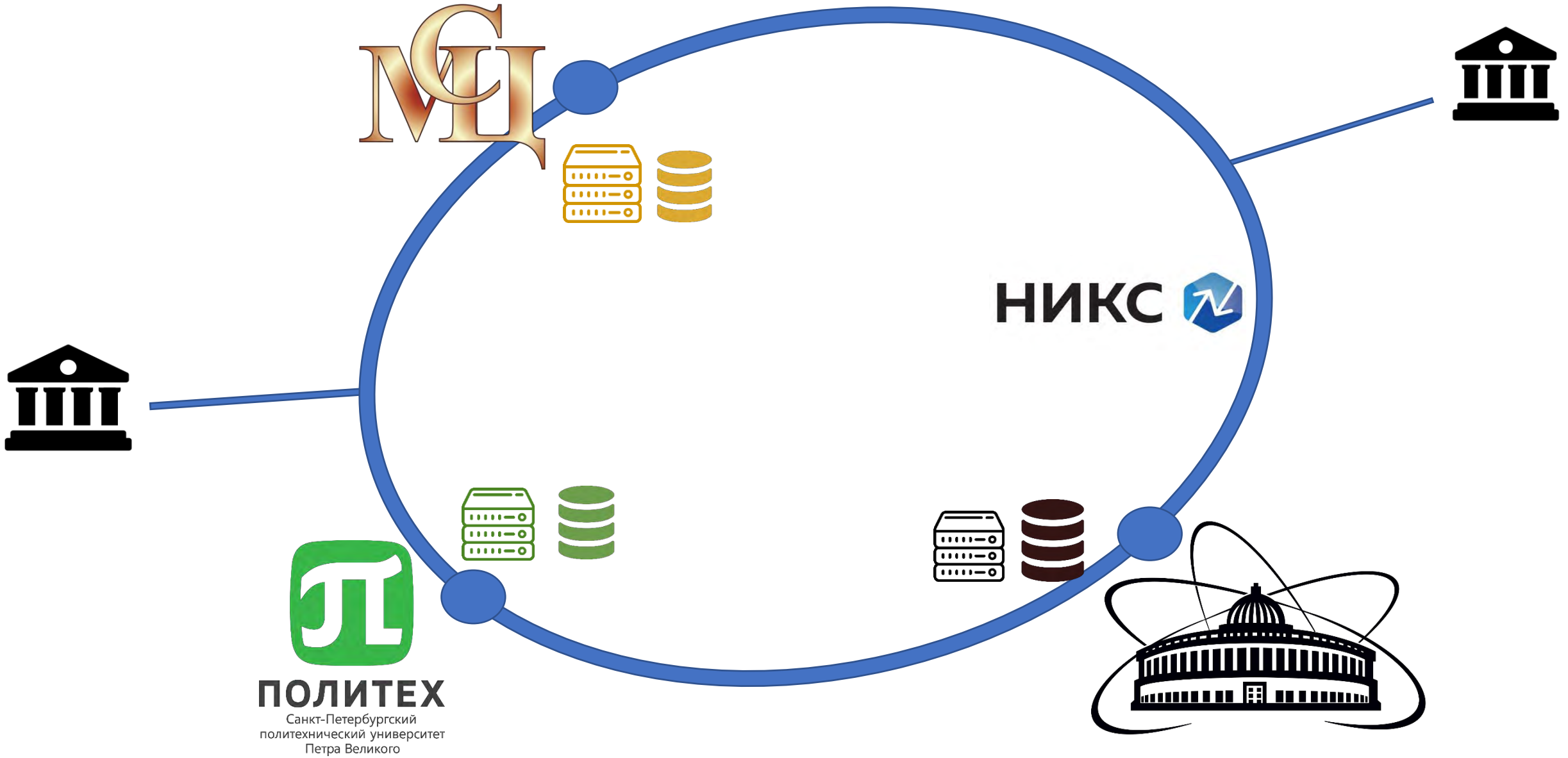
Director of the Meshcheryakov Laboratory of Information Technologies JINR Vladimir Korenkov

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.

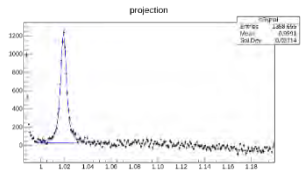
Unified supercomputer network of Russia

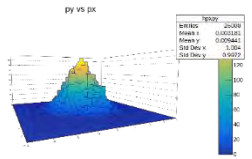


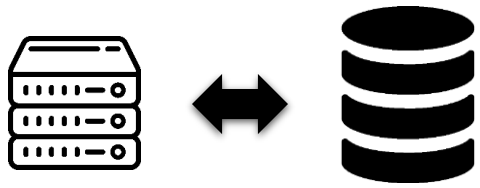
Unified supercomputer network of Russia for the NICA

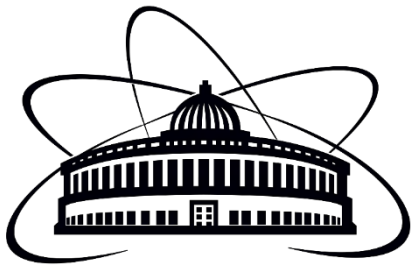
Based on the integration of supercomputers from JINR, the Interdepartmental Supercomputing Center of the Russian Academy of Sciences and St. Petersburg Polytechnic University, a scalable research infrastructure of a new level has been created. Such an infrastructure is in demand for the tasks of NICA megascience.

Reconstruction,
Physical analysis

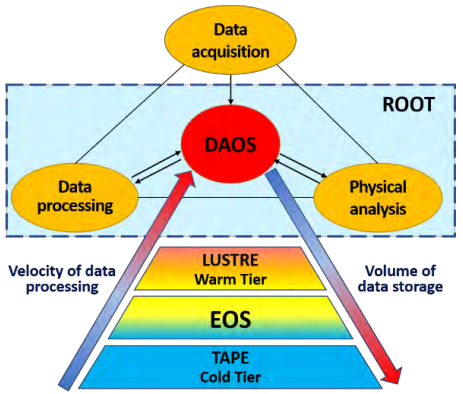








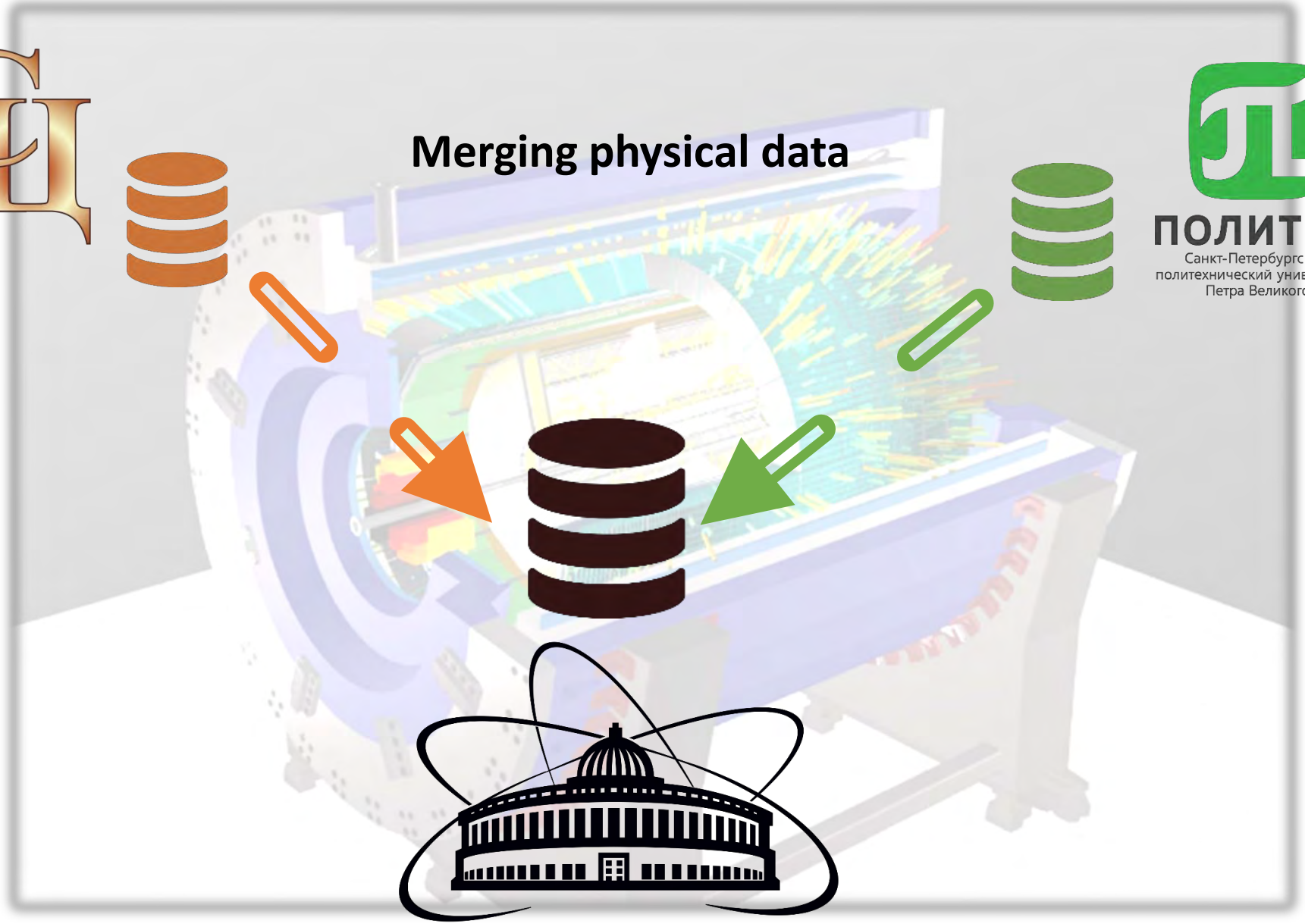
ПОЛИТЕХ
Санкт-Петербургский политехнический университет Петра Великого



The main directions of development of the created infrastructure are :

- consolidation of supercomputer resources into an integrated geographically distributed network;
- creation of an ecosystem of a professional community of users of supercomputer resources;
- joint development of storage and processing of large amounts of data;
- creation of cloud digital services for access to supercomputer resources;
- creation of machine learning and big data analytics services, distributed data marts for users of scientific and educational organizations.

Unified supercomputer network of Russia for the NICA



Объединенная географически распределенная суперкомпьютерная инфраструктура для мегапроекта NICA

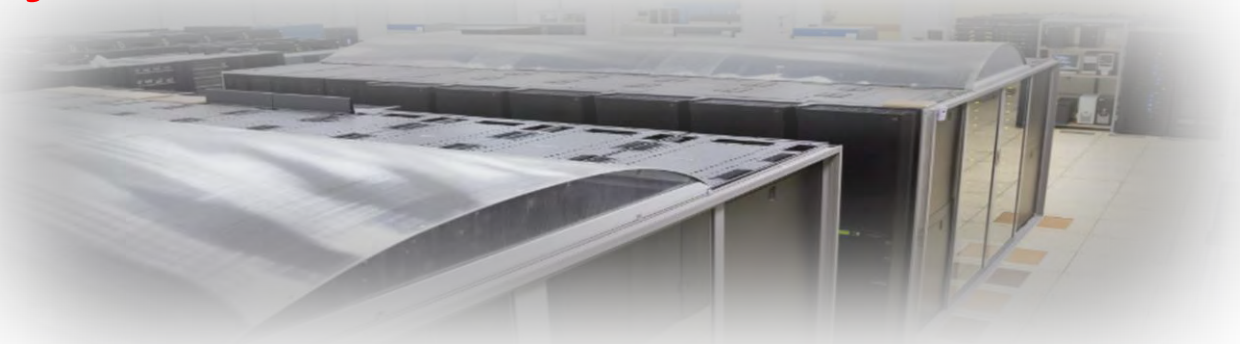
In January 2022, the first joint experiment on the use of a single supercomputer infrastructure for the tasks of the NICA mega-science project was successfully completed. :

- ✓ 3000 data generation tasks were run for the MPD experiment;
- ✓ about 3 million events were generated;
- ✓ the obtained data were transferred to the SC “Govorun” for further processing and physical analysis.

The main features of the SC "Govorun"

1. A hyperconverged architecture for compute nodes of a supercomputer has been created and implemented for the first time worldwide. The hyperconvergence of compute nodes allows orchestrating computing resources and data storage elements, as well as creating computing systems on demand, using the RSC BasIS software. In addition to increasing the efficiency of solving user tasks of different types, this feature allows one to enhance the level of confidentiality of working with data and avoid system errors that occur when crossing the resources for different user tasks.
2. A hierarchical data processing and storage system, which is a single centrally controlled system divided into several layers of data storage, namely, very hot data, hot data and warm data, has been developed and implemented. The implementation of the hierarchical data processing and storage system enables a significant increase in the efficiency of working with large data arrays, including for the NICA project.
3. The flexible architecture of the “Govorun” supercomputer allows one not only to carry out calculations, but also to use the supercomputer as a research polygon for developing software-hardware and IT solutions for tasks underway at JINR. This feature made it possible to integrate the resources of the “Govorun” supercomputer into a single heterogeneous environment based on the DIRAC platform for the NICA project and utilize its resources to implement the program of runs of data mass modeling within the MPD experiment. It is noteworthy that some tasks for modeling MPD experiment data can only be performed on the resources of the “Govorun” supercomputer.

Thank you for your attention

HYBRILIT HETEROGENEOUS PLATFORM at MLIT JINR:

http://hlit.jinr.ru