“Govorun” supercomputer for the NICA megascience project

D.V. Podgainy

Laboratory of Information Technologies

Joint Institute for Nuclear Research

The Conference "RFBR Grants for NICA"

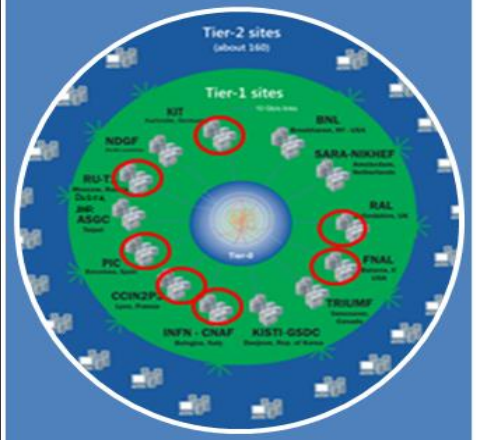
20-23 October 2020

RFBR grant (“Megascience – NICA”) № 18-02-40101

Adaptation of algorithms and frameworks for high-performance computing architectures, and development of new algorithms on the basis of machine learning approaches for drastic increase of performance and data processing and reconstruction efficiency in the NICA experiment.

One of the basic results of the project is development of a unified information-software environment for parallel processing of data at NICA. This approach allows combining various concepts and methods based on the heterogeneous computation paradigm. In order to provide efficient program and algorithm support of experiments in high energy physics, this environment should meet the following requirements: high performance; high reliability and availability; information security; scalability, developed software environment for different user groups.

Multifunctional Information and Computing Complex of JINR



Grid-Tier1:
10688 cores
10.85 PB disk
11.5+40 PB tape

Grid-Tier2
CICC:
4728 cores
2.7 PB disk

Cloud:
1872 CPU
8.142 TB RAM
1.3 PB disk

HybriLIT:
1.7 PFlops for single precision
860 TFlops for double precision
300 Gb/s Data input/output rate

https://micc.jinr.ru

MICC component: HybriLIT platform

HYBRILIT HETEROGENEOUS COMPUTING PLATFORM

Unified software and information environment

“GOVORUN” SUPERCOMPUTER

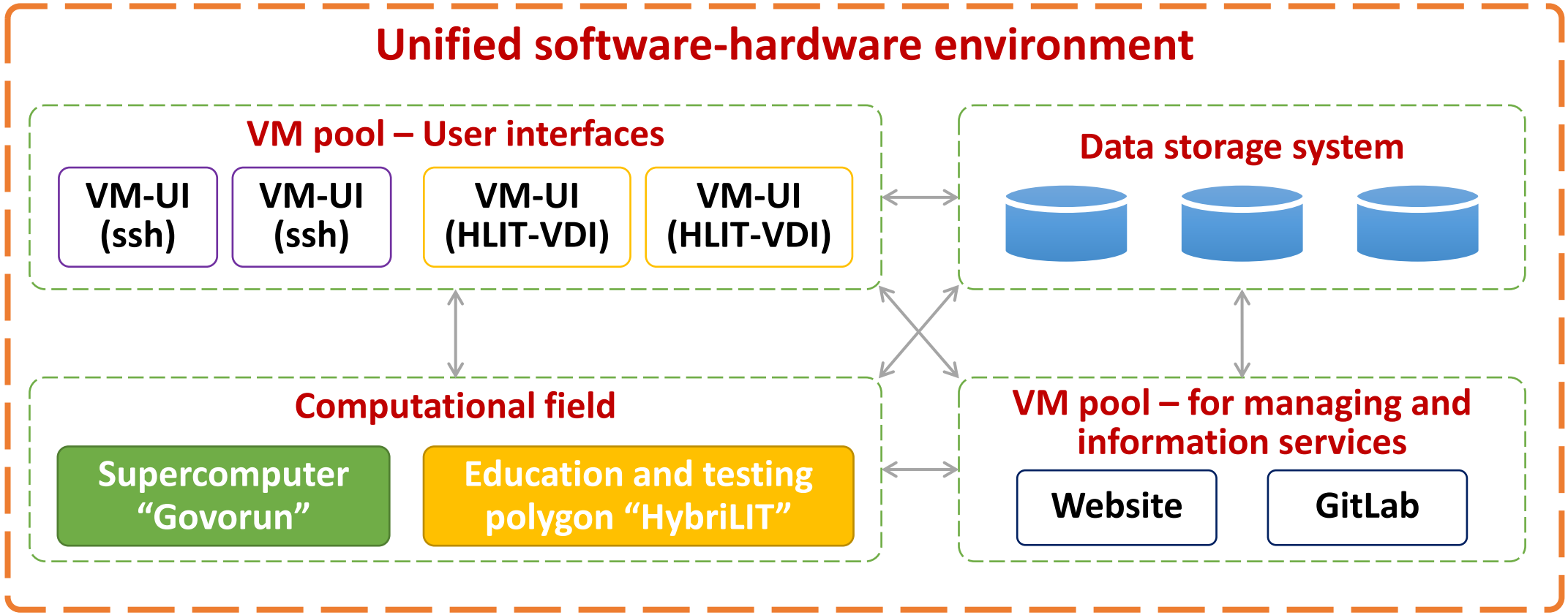
CPU-component
Intel® Xeon® Scalable gen 2,
Intel Xeon Phi (KNL), Intel Omni-Path

GPU-component
GPU DGX-1 Volta
(NVIDIA Tesla V100), Intel Omni-Path

HybriLIT education and testing polygon

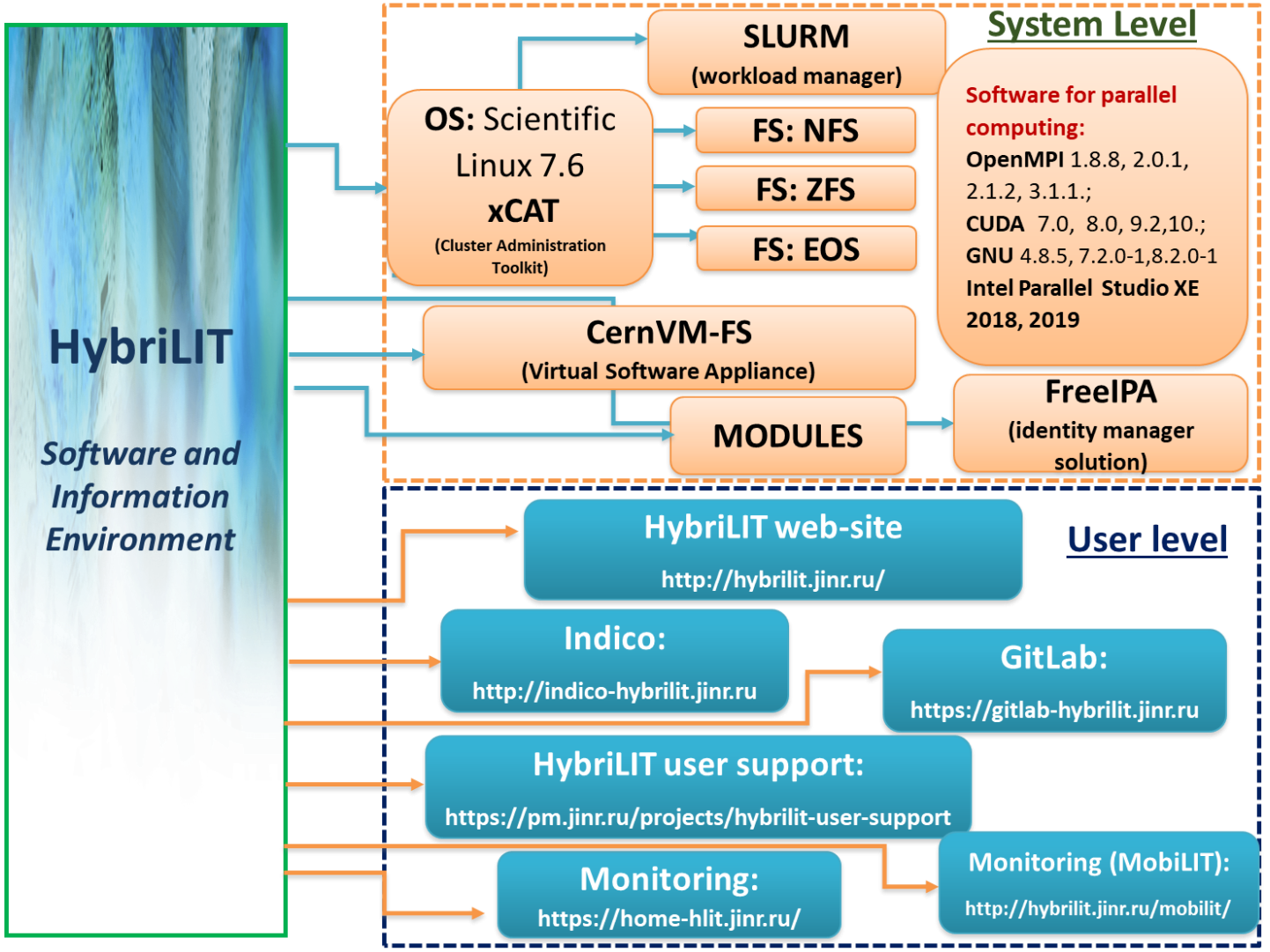
- Intel Xeon
- Intel Xeon Phi
- Nvidia Tesla K20
- Nvidia Tesla K40
- Nvidia Tesla K80

Software and information environment of the HybriLIT



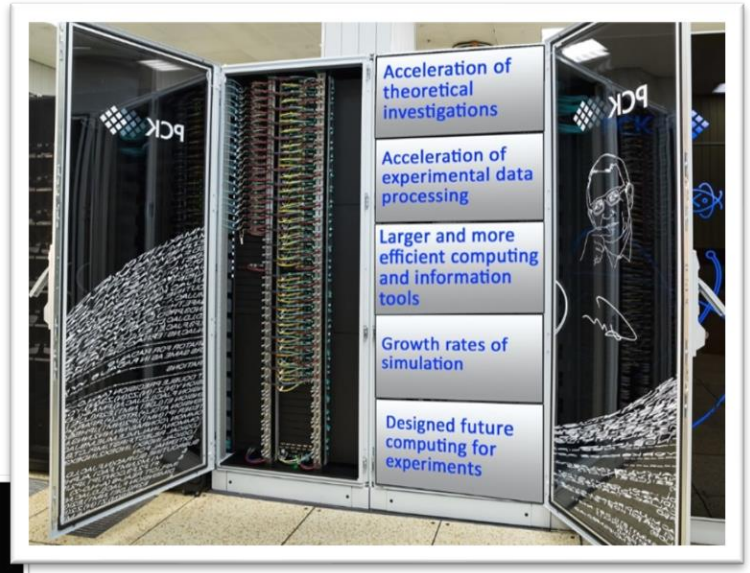
The unified software and information environment of the HybriLIT platform allows users to use the education and testing polygon is aimed at exploring the possibilities of novel computing architectures, IT-solutions, to develop and debug their applications, furthermore, carry out calculations on the supercomputer,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

Software and information environment of the HybriLIT



The unified software and information environment including the unified system level (the operation system, the job scheduler, file systems and software) as well as a set of services allowing users to quickly get the answers to their questions, jointly develop parallel applications, receive information about conferences, seminars and meetings dedicated to parallel programming technologies.

“Govorun” supercomputer



GPU-component
based on NVIDIA DGX-1 Volta

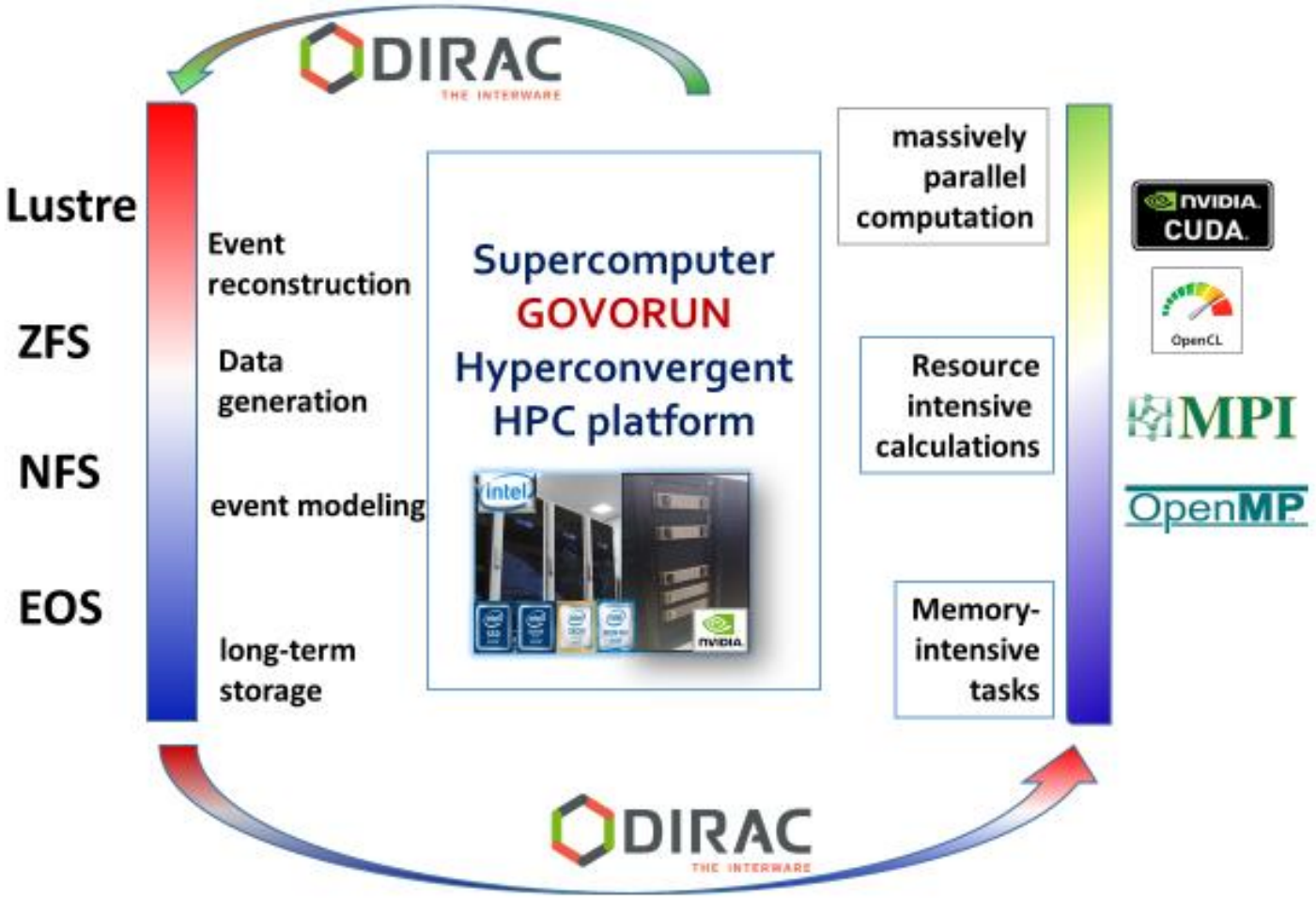
CPU-component
based on the newest Intel architectures: Intel Xeon Phi and Intel Skylake processors gen 2

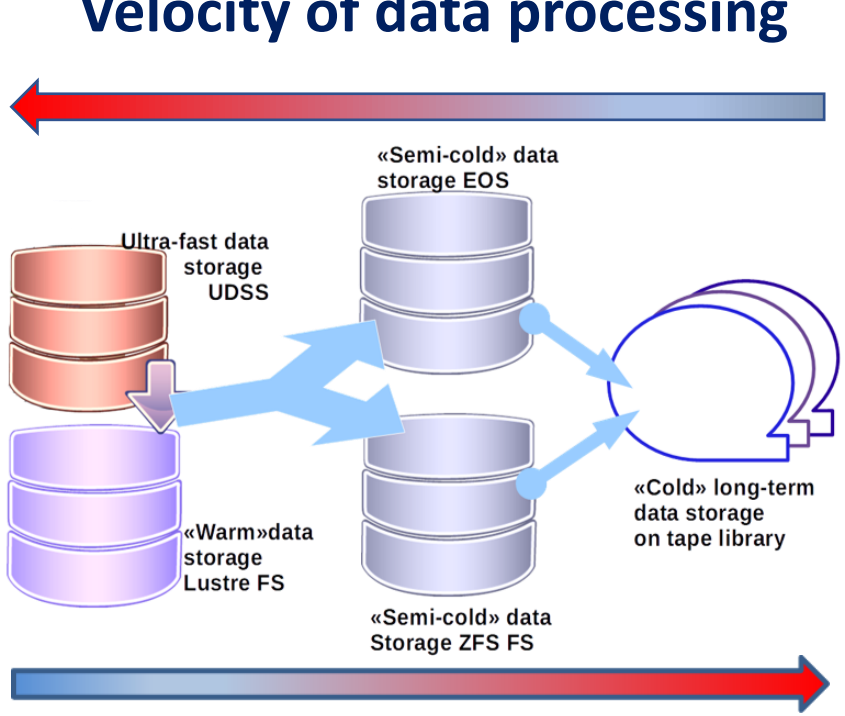
The “Govorun” supercomputer is a hyper-converged software-defined system, it has unique properties for the flexibility of customizing the user’s job, ensuring the most efficient use of the computing resources of the supercomputer.

The “Govorun” supercomputer is ranked on the **11th** place (CPU-component) and on the 21st place (GPU-component) in the current edition of the **TOP50** list, as well as on the **17th** place in the current edition of the **IO500** list (July 2020), and is the first in terms of the data processing rate among Russian supercomputers.

Total peak performance:
1.7 PFlops for single precision
860 TFlops for double precision
300 Gb/s Data input/output rate

TECHNOLOGIES for STORING, PROCESSING and ANALYZING EXPERIMENTAL DATA in the NICA MEGASCIENCE PROJECT





High-performance data processing and storage system on the “Govorun” supercomputer

Virtual Institute for I/O

You are here: Virtual Institute for I/O » IO-500

Lists | Call for Submission | News | Radar Chart | Submission

IO-500

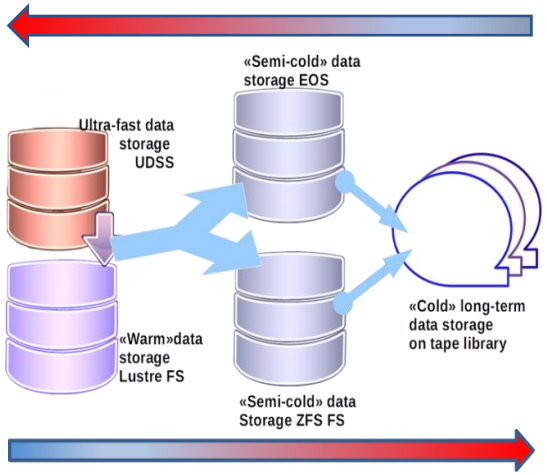
This is the official list from ISC-HPC 2018. The list shows the best result for a given combination of system/institution/filesystem.

#	information						io500		
	system	institution	filesystem	storage vendor	client nodes	data	score	bw	md
								GiB/s	kIOP/s
1	Oakforest-PACS	JCAHPC	IME	DDN	2048	zip	137.78	560.10	33.89
2	ShaheenII	KAUST	DataWarp	Cray	1024	zip	77.37	496.81	12.05
3	ShaheenII	KAUST	Lustre	Cray	1000		41.00*	54.17	31.03*
4	JURON	JSC	BeeGFS	ThinkparQ	8		35.77*	14.24	89.81*
5	Mistral	DKRZ	Lustre2	Seagate	100		32.15	22.77	45.39
6	Sonasad	IBM	Spectrum Scale	IBM	10	zip	24.24	4.57	128.61
7	Seislab	Fraunhofer	BeeGFS	ThinkparQ	24		16.96	5.13	56.14
8	Mistral	DKRZ	Lustre1	Seagate	100	zip	15.47	12.68	18.88
9	Govorun	Joint Institute for Nuclear Research	Lustre	RSC	24	zip	12.08	3.34	43.65
10	EMSL Cascade	PNNL	Lustre		126		11.12	4.88	25.33
11	Serrano	SNL	Spectrum Scale	IBM	16		4.25*	0.65	27.98*
12	Jasmin/Lotus	STFC	PanFS	Panasas	64	zip	2.33	0.26	20.93

Values with indicate that a value for the computation was missing.*

Further lists with more deta

Velocity of data processing



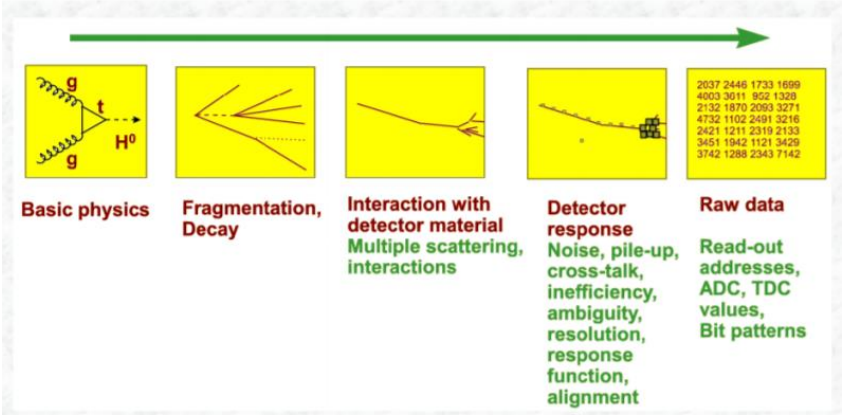
Volume of data storage

#	Institution	System	io500		
			Score	BW GiB/s	MD kIOP/s
1	Intel	Wolf	1792.98	371.67	8649.57
2	WekaIO	WekaIO on AWS	938.95	174.74	5045.33
3	TACC	Frontera	763.80	78.31	7449.56
4	Argonne National Laboratory	Presque	537.31	108.19	2668.57
5	National Supercomputing Center in Changsha	Tianhe-2E	453.68	209.43	982.78
17	JINR	Govorun	90.87	35.61	231.88
22	SPbPU	Polytechnic RSC Tornado	64.29	21.56	191.73

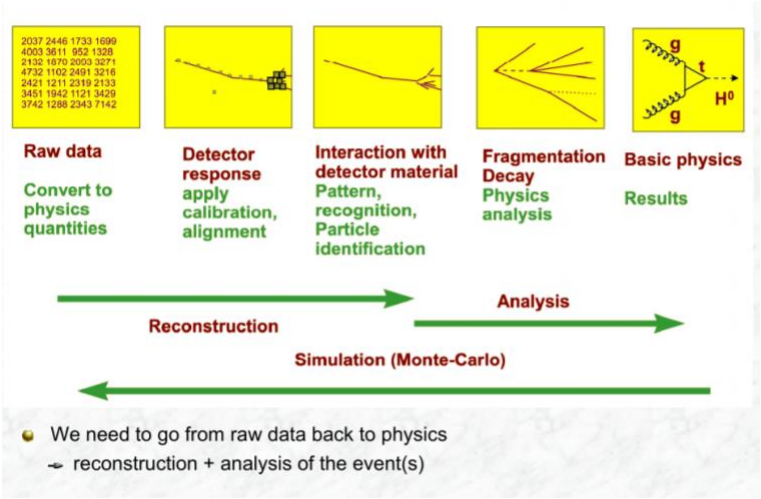
The “Govorun” supercomputer is ranked on the 17th place in the current edition of the IO500 list (July 2020) and is the first in terms of the data processing rate among Russian supercomputers. The second fastest Russian supercomputer “Polytechnic – RSC Tornado”, which is located in SPbPU, takes the 22nd place in the IO500 list.

HEP experiments data flow

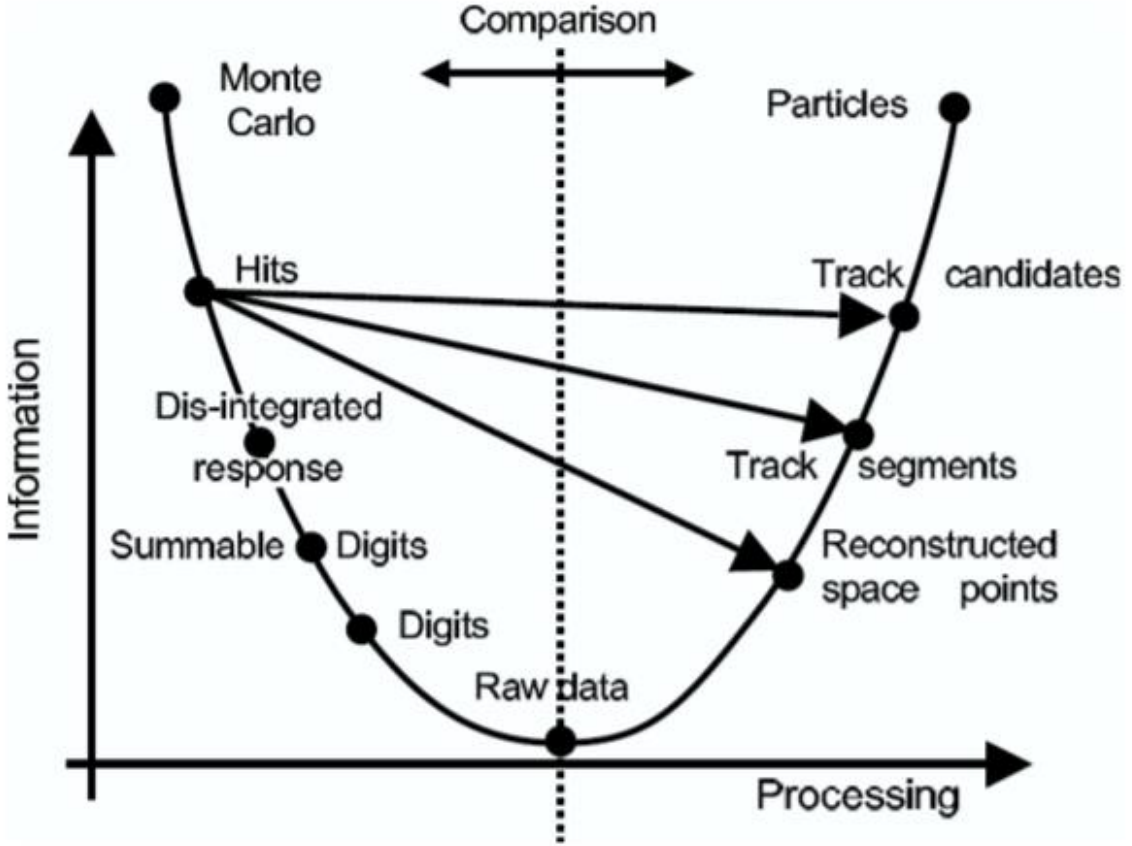
From Physics to raw data



From raw data to Physics

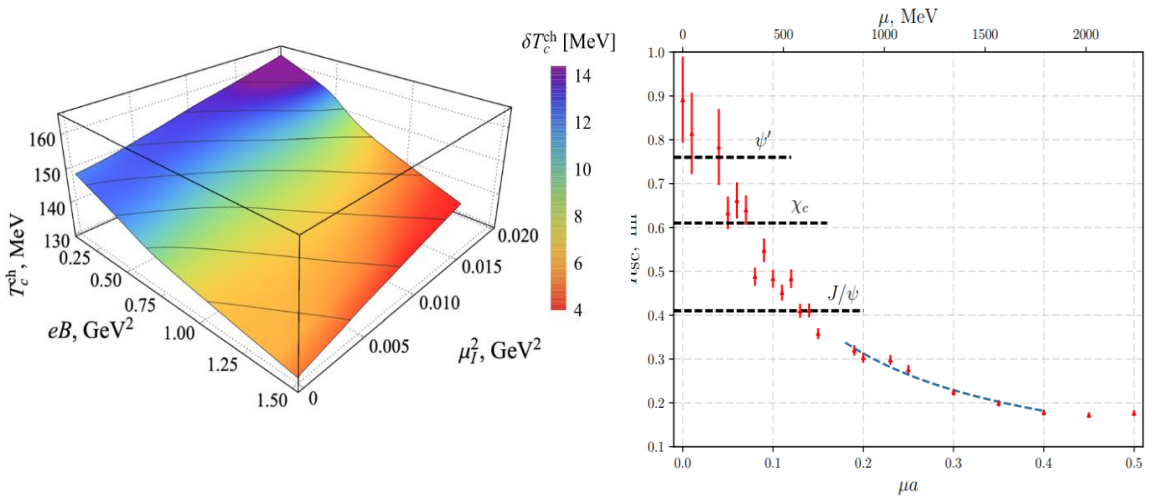


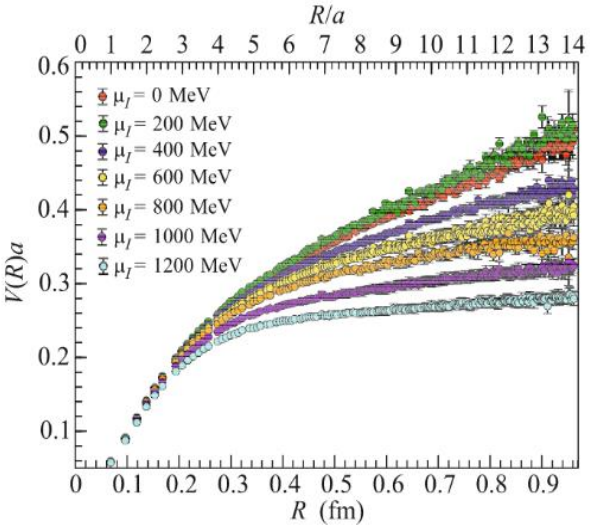
- We need to go from raw data back to physics
  - reconstruction + analysis of the event(s)

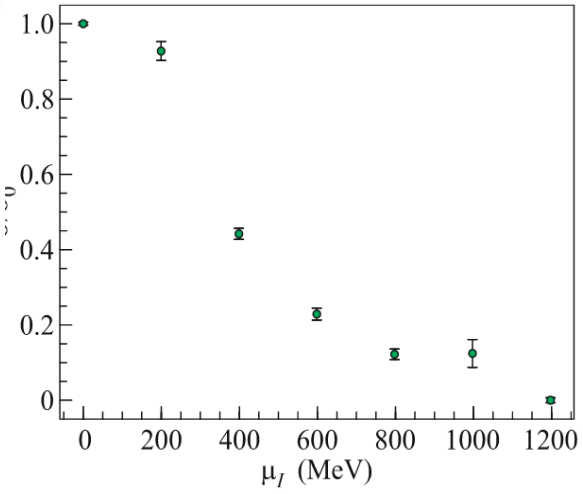


Slide courtesy of O.V. Rogachevsky, VBLHEP JINR

“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.

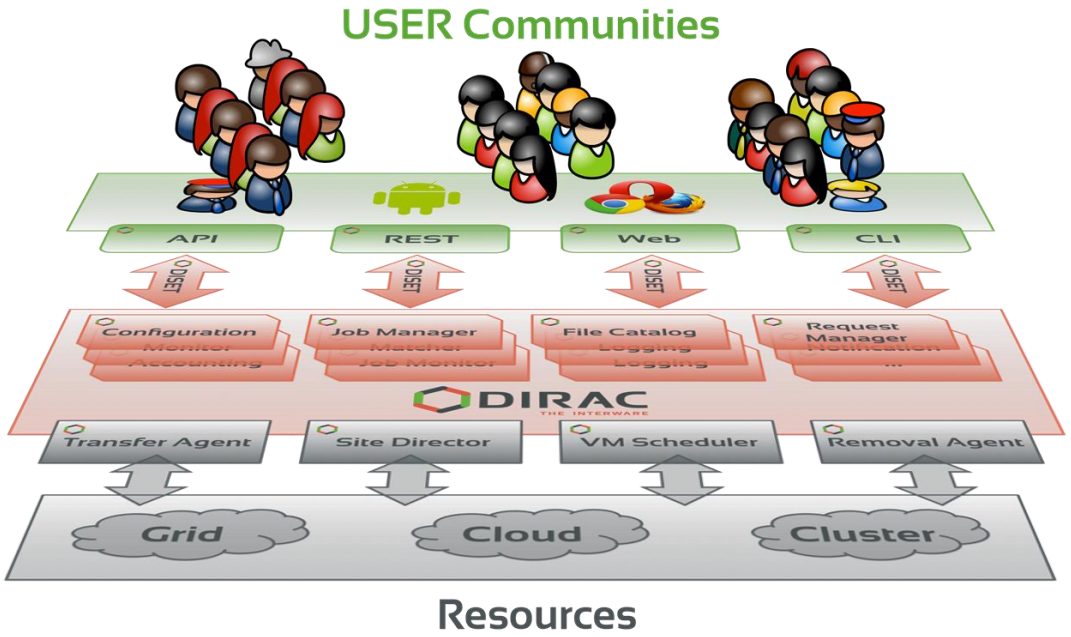
- The influence of the external magnetic field on the electromagnetic conductivity of quark-gluon plasma was investigated.

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

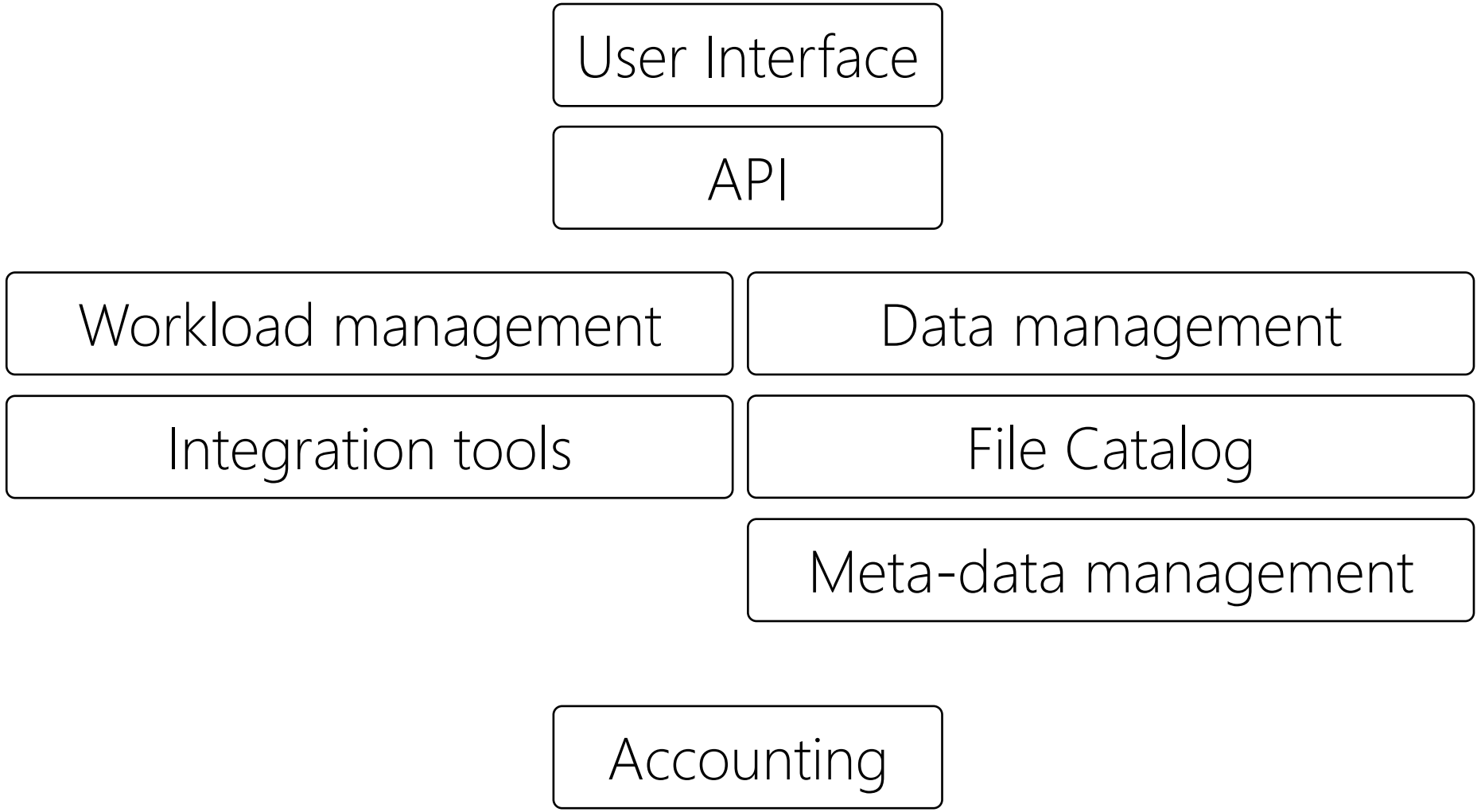
DIRAC INTERWARE

DIRAC provides all the necessary components to build ad-hoc grid infrastructures **interconnecting** computing resources of different types, allowing **interoperability** and simplifying **interfaces**.

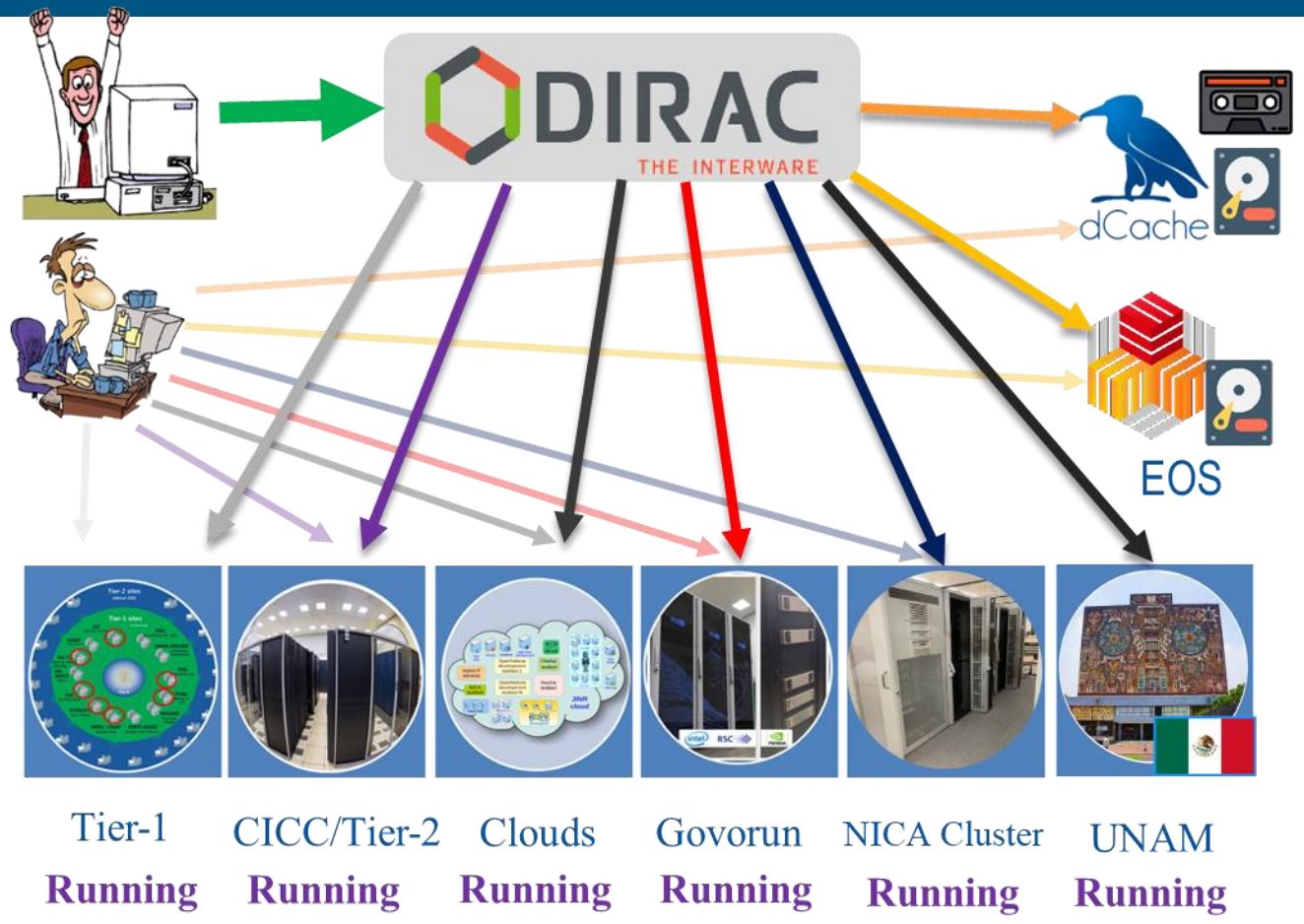


- Web
- CLI
- API
- REST

DIRAC PROVIDES

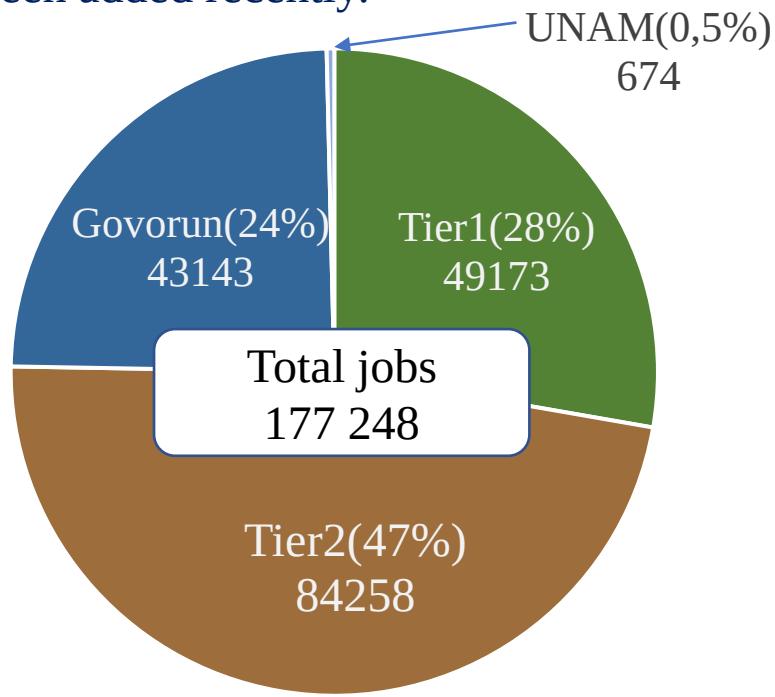


JINR COMPUTING RESOURCES INTEGRATION for the MPD EXPERIMENT



The computing resources of the JINR Multifunctional Information and Computing Complex (**Tier1/Tier2**, **"Govorun"** supercomputer, **storage** resources) were combined using the DIRAC Interware. **Cloud resources** of JINR and its Member States were tested and are ready to accept jobs. The **NICA Cluster** is the next on the list.

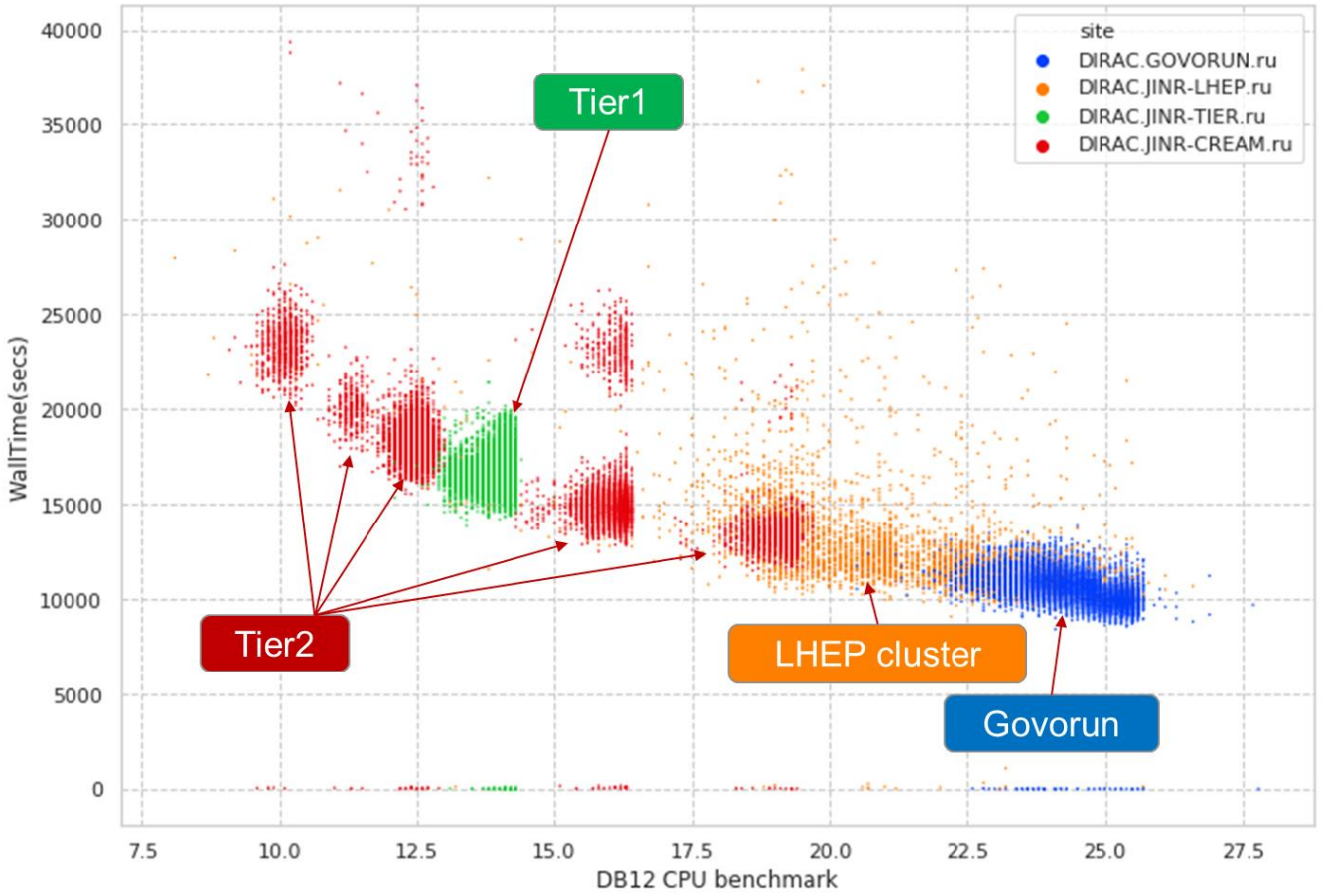
More than 175,000 jobs were performed on the Tier1/Tier2 components and the "Govorun" supercomputer using the DIRAC platform in the framework of Monte-Carlo data simulation for the MPD experiment. A new UNAM cluster has been added recently.



Distribution of simulation jobs by the computing resources via DIRAC

Computing for the NICA megaproject “Govorun” supercomputer for MPD tasks

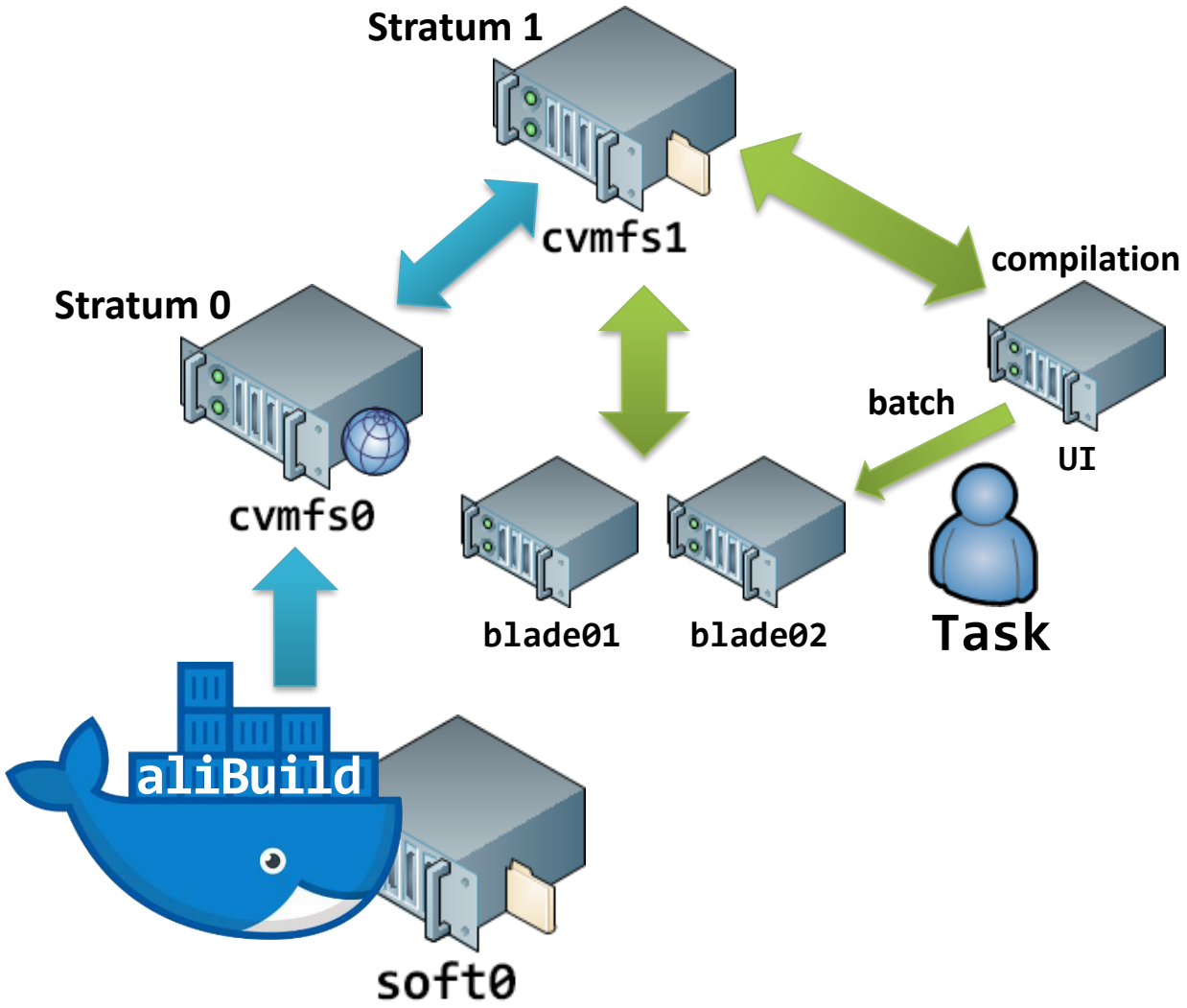
The experience of using different computing resources of JINR and other institutes of the MPD collaboration has shown that at the moment **the use of the computing resources of the “Govorun” supercomputer is the most efficient.**



The use of only 270 computing cores (such a limited resource is related to the insufficient resources and high load of the supercomputer) provides data processing equivalent to the use of 450-500 cores on the other available computing resources, such as Tier1, Tier2 and the NICA computing cluster of the Laboratory of High Energy Physics (VBLHEP). On the computing resources of JINR and the National Autonomous University of Mexico, over **50 million** events were modeled and processed by the MPD collaboration for 2020, and a quarter of these events were performed directly on the “Govorun” supercomputer.

The unique equipment of the “Govorun” supercomputer, which comprises an ultrafast data access system and computing nodes with a large volume of RAM (3 TB per node), made it possible to process on almost half the number of computing cores the same number of events as on the other available computing resources.

Workflow with CernVM-FS and aliBuild



https://dberzano.github.io/alice/alibuild/
https://www.docker.com/

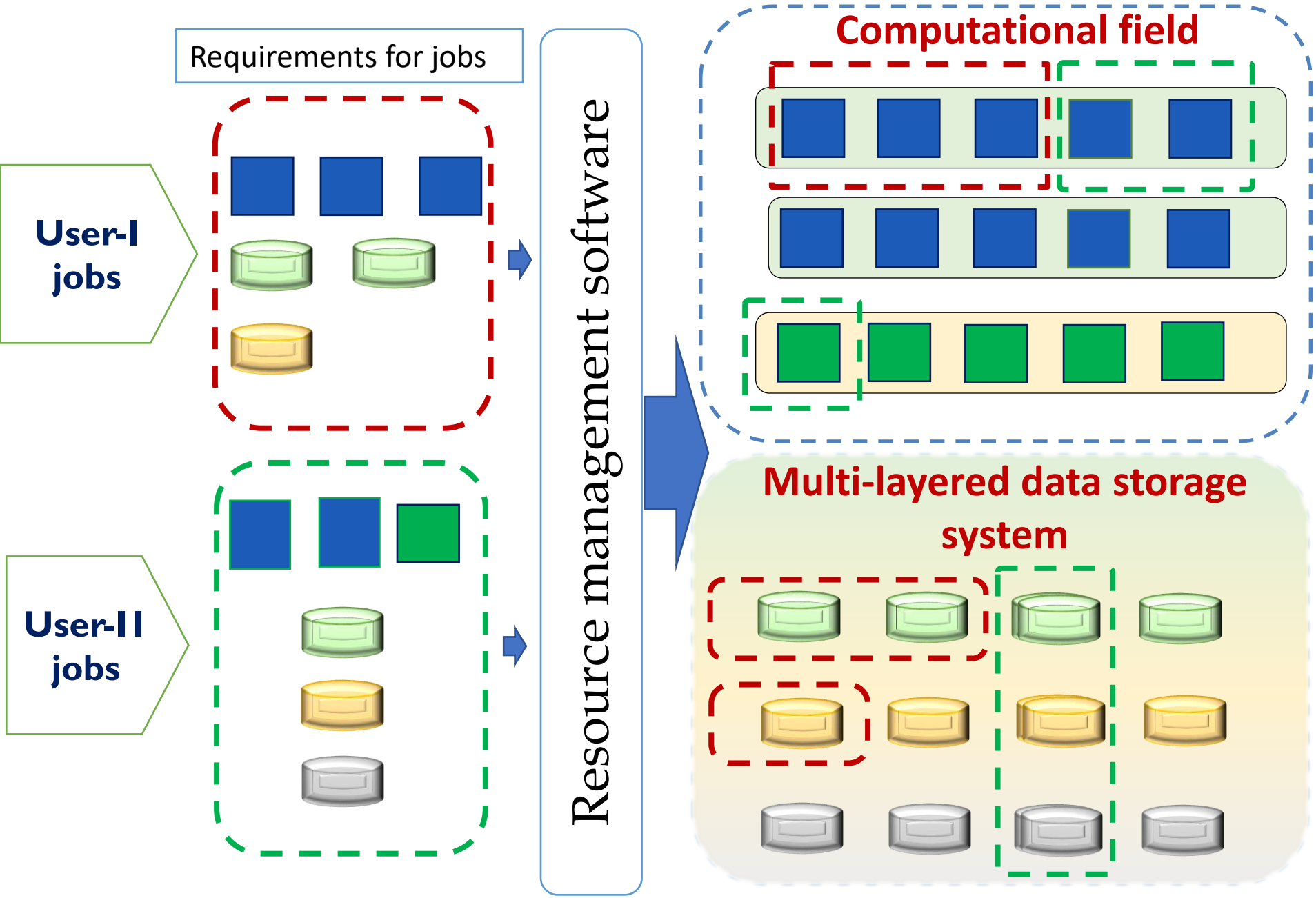
NICA experiment
FairRoot/v18.2.0
FairRoot/v18.2.1
FairSoft/june19p1
FairSoft/june19p2
FLAIR/v2.3.0
FLUKA/v2011.2x

SMASH/v1.8

...

Full list
Execute
$ module avail
on **hydra.jinr.ru**

Orchestration and hyperconvergence on the “Govorun” supercomputer

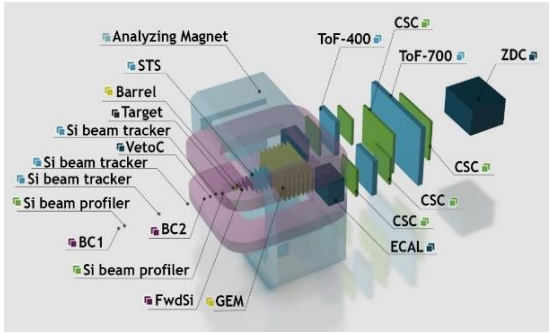


The “Govorun” supercomputer is a hyper-converged software-defined system, it has unique properties for the flexibility of customizing the user’s job.

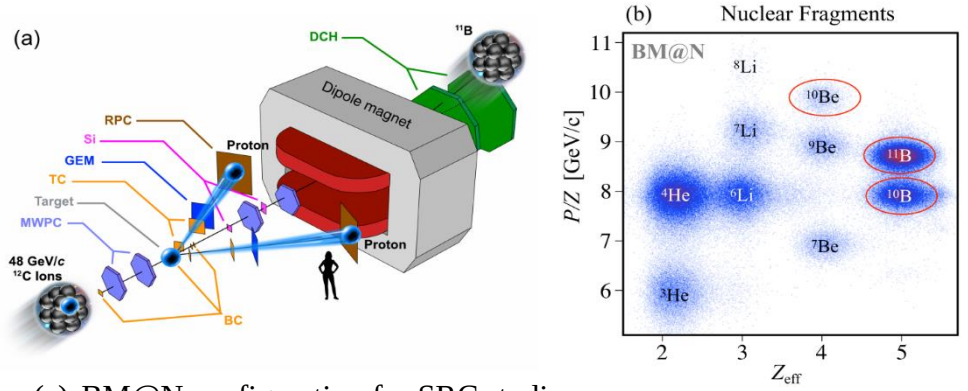
For his job the user can allocate the required number and type of computing nodes and the required volume and type of data storage systems.

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

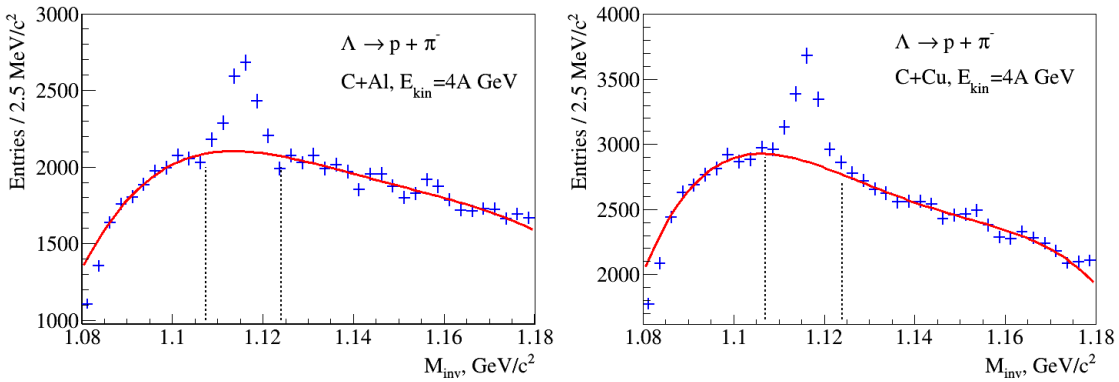
Computing for the NICA megaproject “Govorun” supercomputer for BM@N tasks



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.

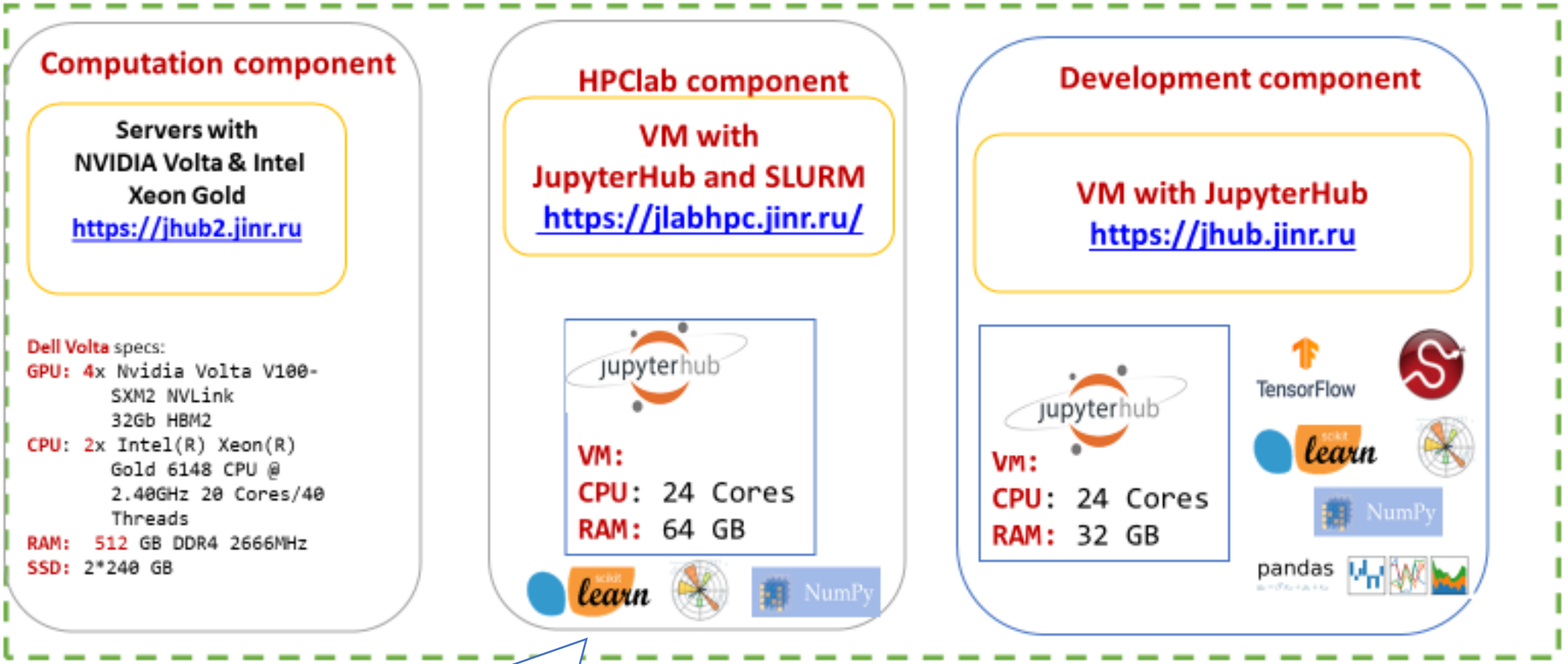


Signals of Λ-hyperons in the spectra of invariant masses (p,π-) measured in C+Al and C+Cu interactions.

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.

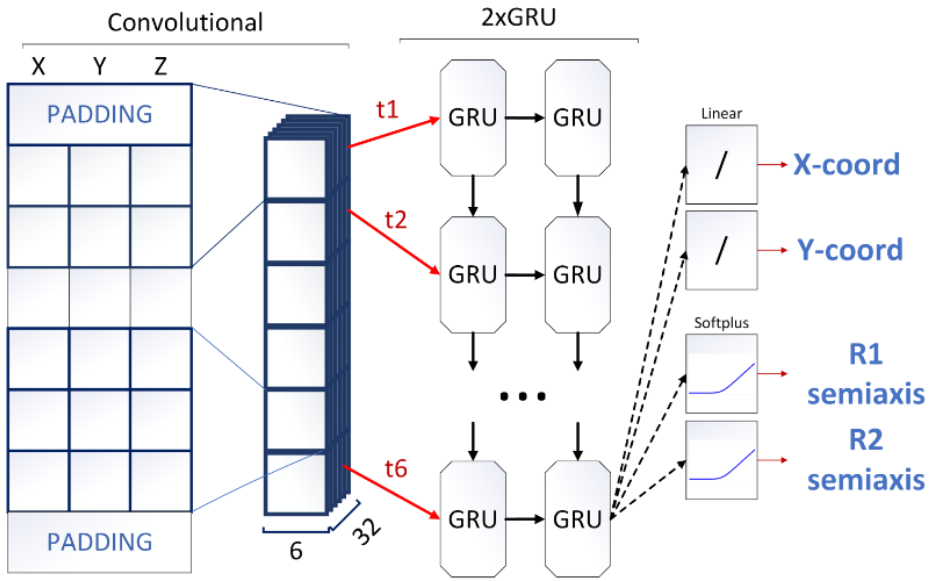
Ecosystem for HPC and ML/DL tasks



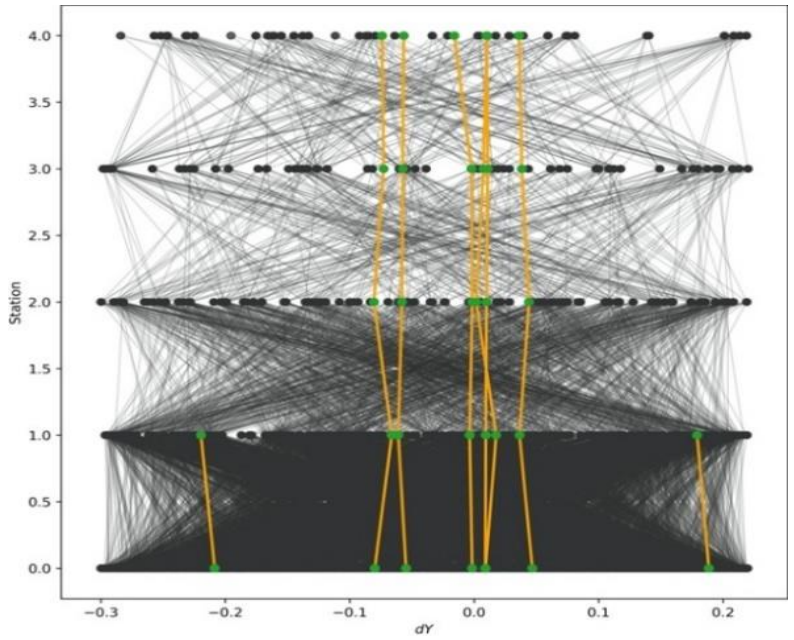
Calculations on "Govorun"
Application development, scientific visualization, working with data ...

Computing for the NICA megaproject
Machine learning for tracking tasks

The global detection of tracks among noises is performed immediately over the entire picture of the event. The GraphNet program is based on the use of graph neural networks for tracking. An event is represented as a graph with counts as nodes, then this graph is inverted into a linear orggraph, when the edges are represented by nodes, and the nodes of the original graph are represented by edges. In this case, the information about the curvature of track segments is embedded in the edges of the graph, which simplifies the detection of tracks among fakes and noises.



TrackNETv2 neural network diagram

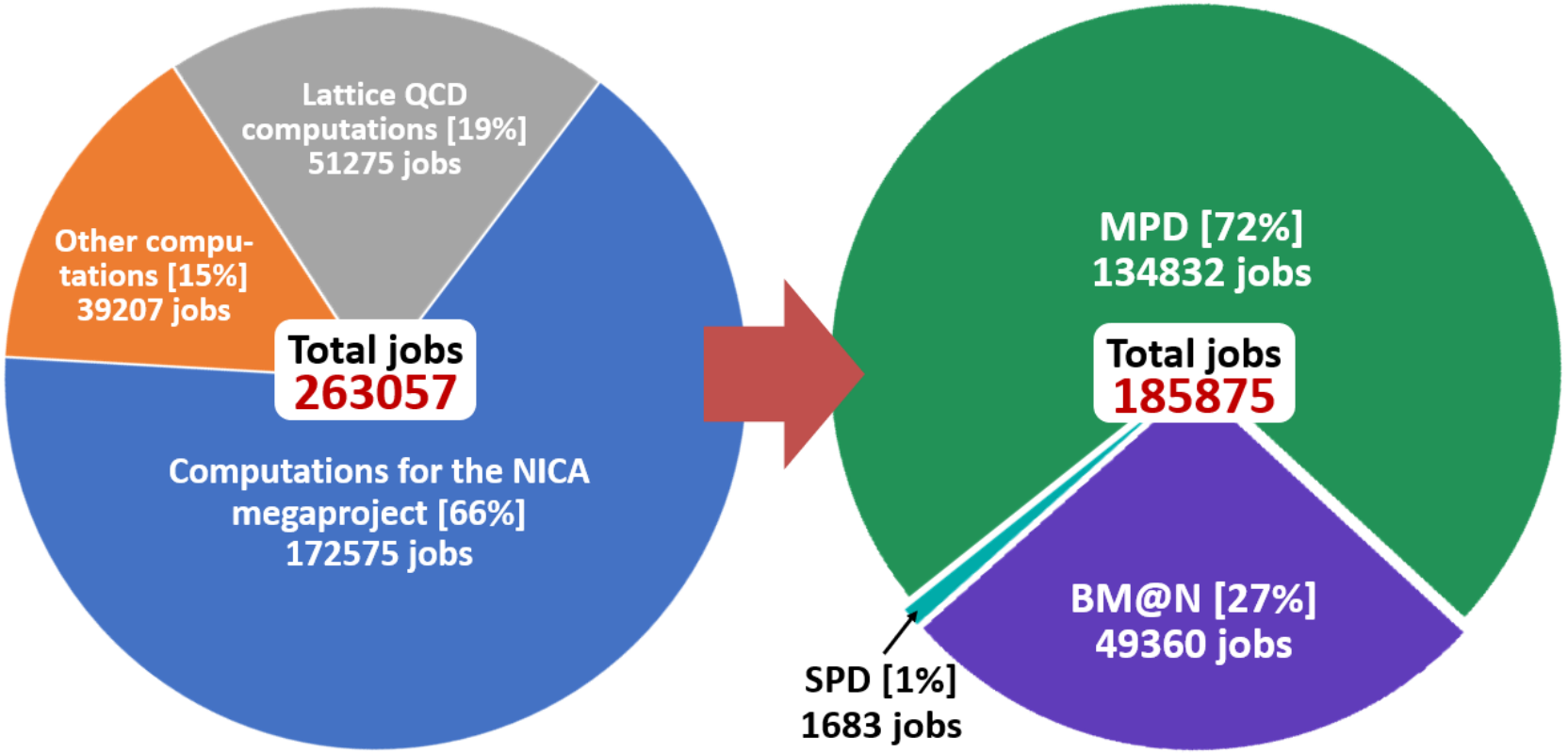


Graphical representation of the C+C 4 GeV event of the BM@N experiment. The black nodes and the edges correspond to fakes, the green nodes and the yellow edges correspond to found tracks.

The results of the test run on the "Govorun" supercomputer also allow one to roughly estimate the rate of processing one event of the future detector HL-LHC or NICA with 10,000 tracks at a reasonable level of 3 microseconds.

P. Goncharov, G. Ososkov, D. Baranov, https://doi.org/10.1063/1.5130102,
P. Goncharov, E. Shchavelev, G. Ososkov, D. Baranov, http://ceur-ws.org/Vol-2507/280-284-paper-50.pdf

“Govorun” supercomputer for the NICA project



The “Govorun” supercomputer, being a hyper-converged software-defined system, has unique properties for the flexibility of customizing the user’s job, which allows one to effectively solve different tasks, **i.e. it makes the “Govorun” supercomputer a unique tool for computing of the NICA megascience project**.

Thank you for your attention

HYBRILIT HETEROGENEOUS PLATFORM at LIT JINR:

http://hlit.jinr.ru