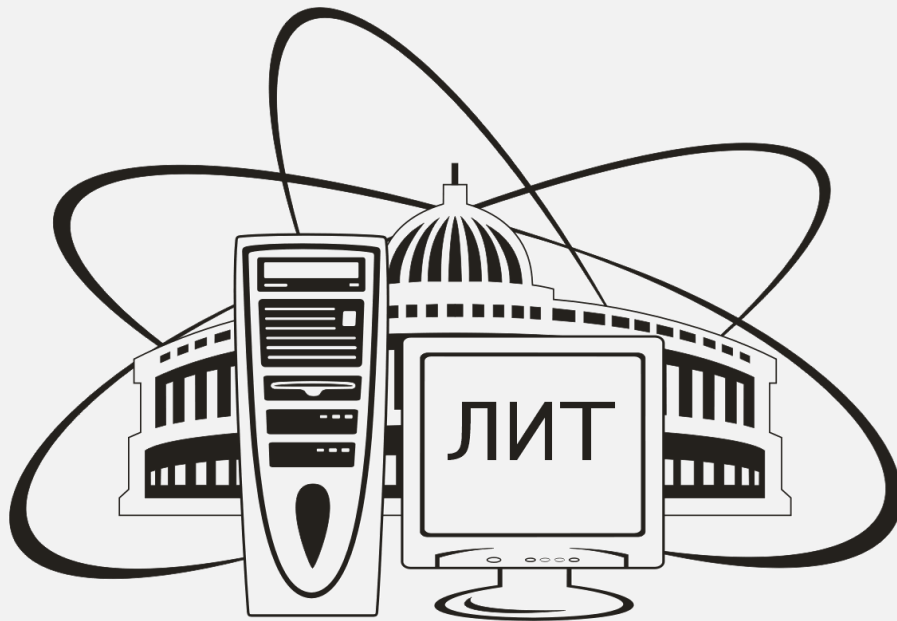


Laboratory of Information Technologies



Presented by :
Igor Pelevanyuk
engineer-developer



July 03, 2017

Here works:

~ 300 staff

It helps:

~ 4500 users

Provide:

- Services
- 10 Gb/s network
- Storage resources
- Computing resources

And wide range of scientific research are conducting here.

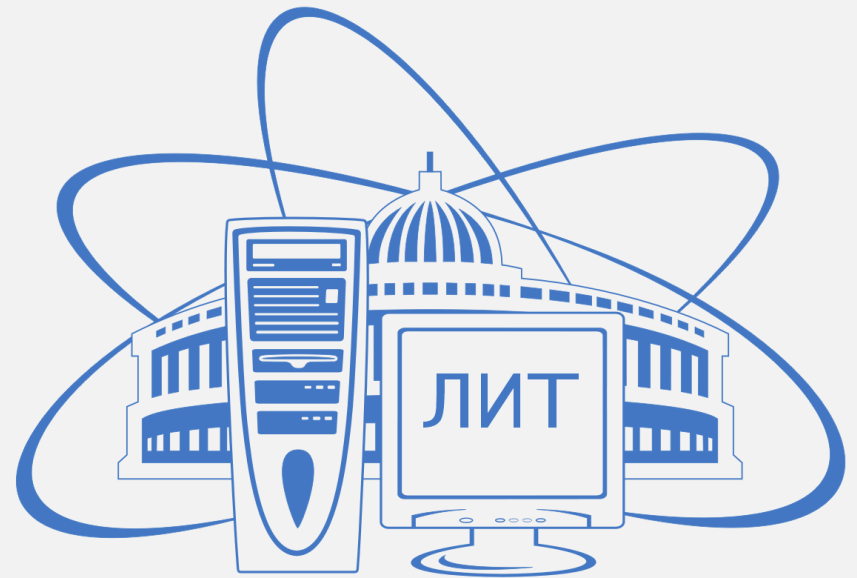




History

It is the performance of experimental information processing facilities that will eventually determine the “performance” of physical research

August 6, 1966





History

Laboratory of Information Technologies of the Joint Institute for Nuclear Research in Dubna was founded in August 1966.

The main directions of the activities at the Laboratory are connected with the provision of **networks**, **computer and information resources**, as well as **mathematical support** of a wide range of **research** at JINR in **high energy physics**, **nuclear physics**, **condensed matter physics**, etc.

Computing is an integral part of theory, experiment, and technology development

Many recent successes only possible because of significant community effort to develop and advance the necessary computing tools!



M.G. Mescheryakov



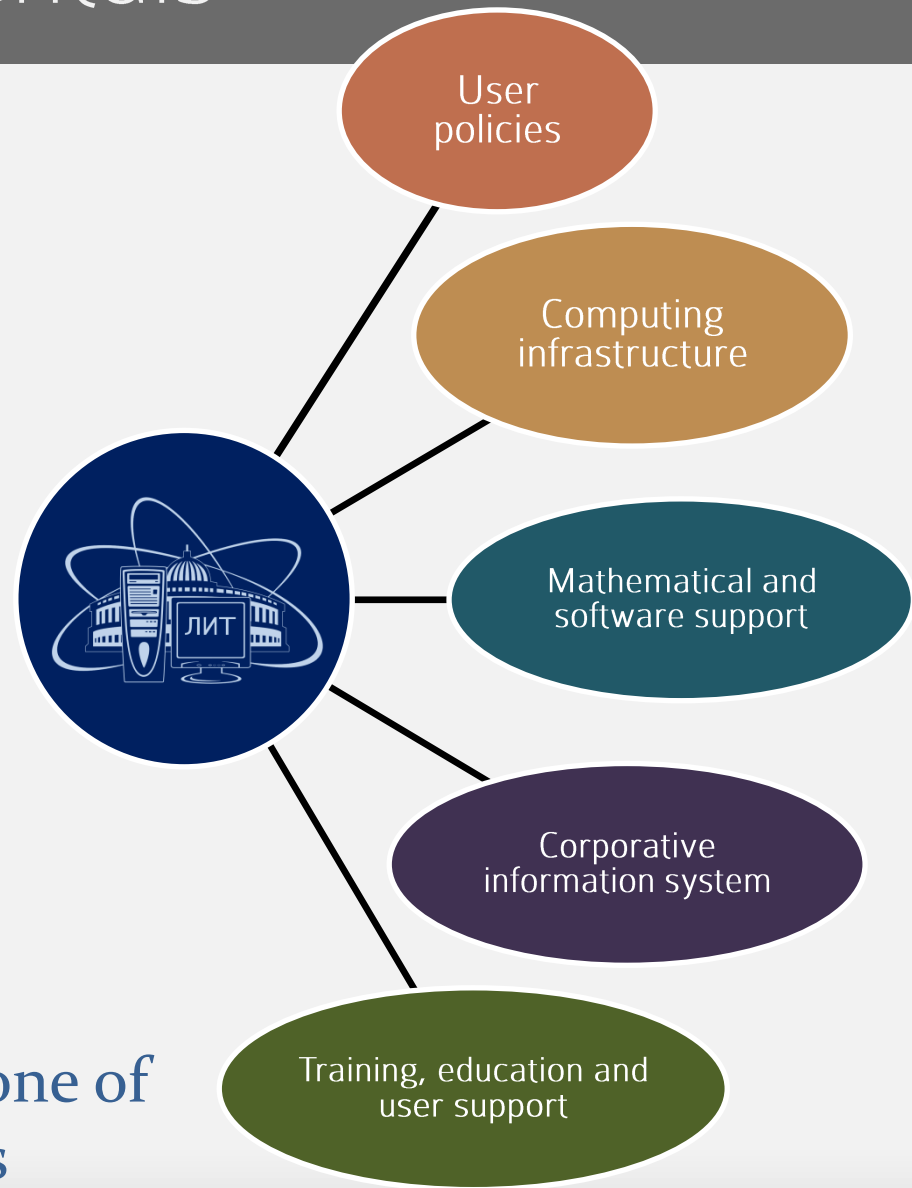
N.N. Govorun





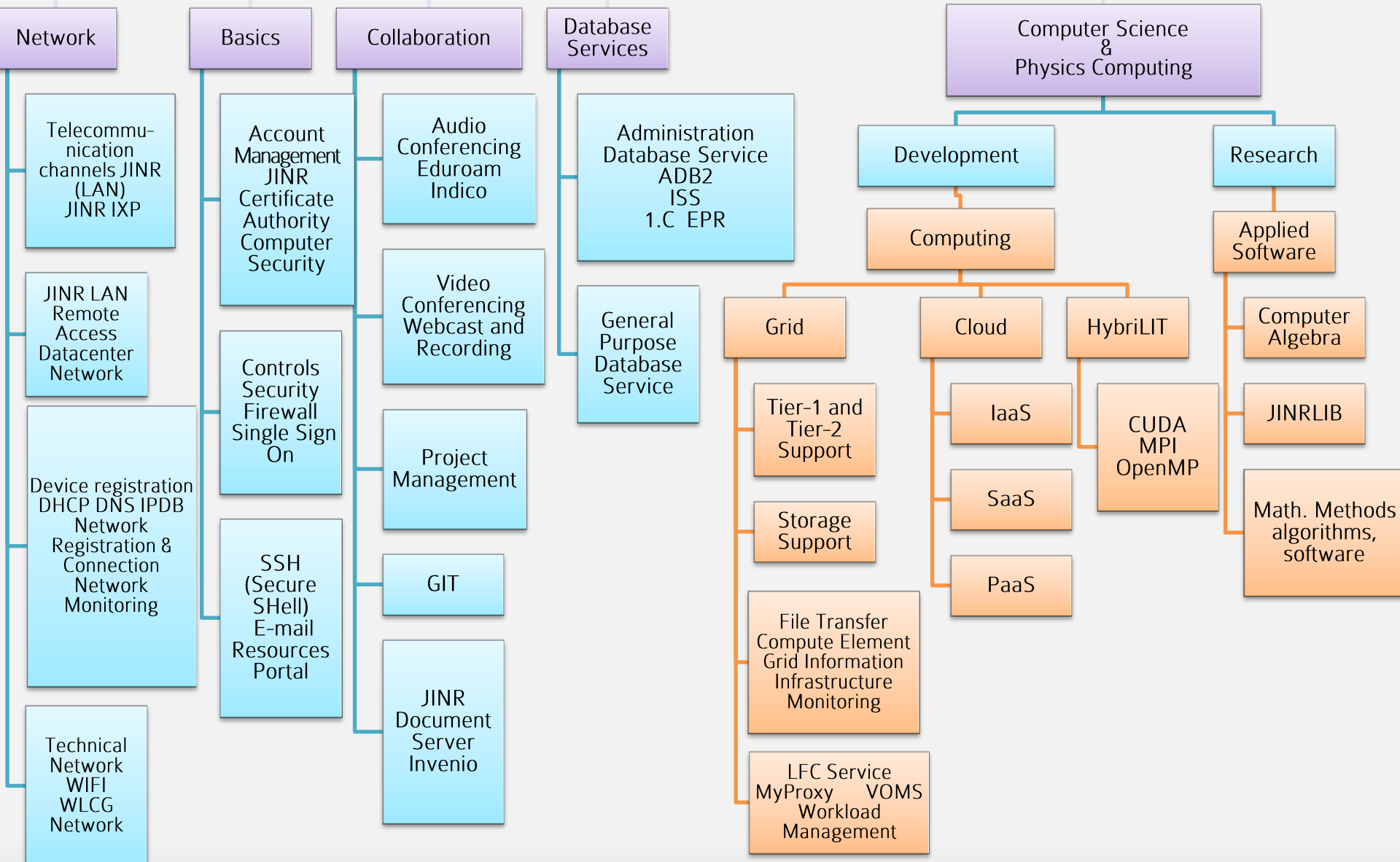
LIT fundamentals

- Provide IT services necessary for the fulfillment of the JINR Topical Plan on Research and International Cooperation in an efficient and effective manner
- Building world-class competence in IT and computational physics
- 24/7 support of computing infrastructure and services such availability is called nonstop service



IT-infrastructure is the one of JINR basic facilities

IT-services





Multifunctional Information and Computing Complex

- **LAN:** 10 Gbps
- **WAN:** 100 Gbps + 2x10 Gbps
- **Tier-1:** 3600 core, 56 kHS06, 4,5 PB disk, 8 PB tape
- **CICC/Tier-2:** 3500 core, 48 kHS06, 2PB disk
- **HybriLIT:** 252 CPU, 77184 GPU cores, 182 PHI-cores, 2.4 TB RAM, 57.6 TB HDD, 142 Tflops
- **Cloud:** 330 CPU, 840GB RAM

LIT IT-infrastructure is the one of JINR basic facilities



JINR grid sites of WLCG/EGI: Tier-1 for CMS
Tier-2 for ALICE, ATLAS, CMS, STAR, LHCb,
BES, biomed, fermilab



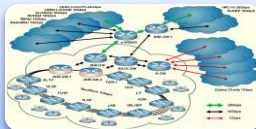
Cloud infrastructure



Heterogeneous(CPU + GPU)
computing cluster HybriLIT



Off-line cluster and storage system for BM@N, MPD,
SPD Storage and computing facilities for local users



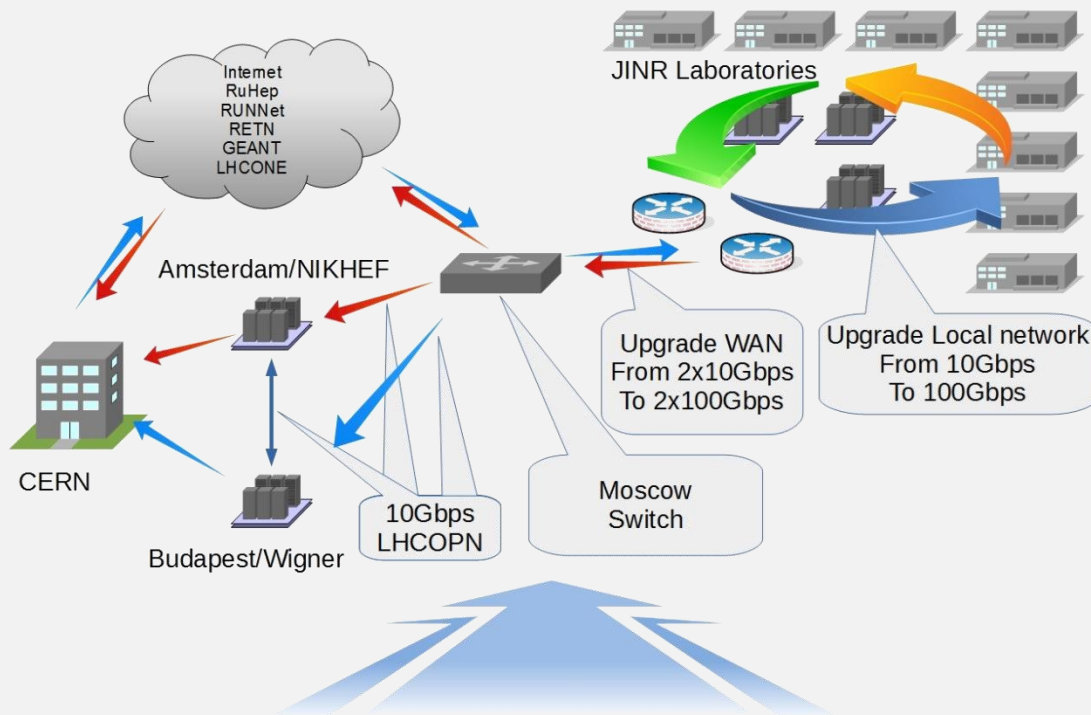
Network infrastructure



Engineering infrastructure



Network



Users – 4298

Network nodes – 7945

IP addresses – 13055

Remote access – 370

E-library – 1501

AFS – 367

VOIP – 127

E-mail – 2356

Local Area Network – 10Gbps, planned upgrade to 100Gbps

Wide Area Network – 2x10Gbp, 100Gbps – test mode

Upgrade WAN to 2x100Gbps planned



Grid technologies - success

On a festivity dedicated to receiving the Nobel Prize for discovery of Higgs boson, CERN Director professor Rolf Dieter Heuer directly called the **grid-technologies one of three pillars of success** (alongside with the LHC accelerator and physical installations).



Without implementation of the **grid-infrastructure** on LHC it would be **impossible** to process and store enormous data coming from the collider and therefore to make discoveries.

Nowadays, every large-scale project will fail without using a distributed infrastructure for data processing.



Grid technologies - success



At the initiative of CERN, a project EU-dataGrid started up in January 2001 with the purpose of testing and developing advanced grid-technologies. JINR was involved with this project.

The LCG (LHC Computing Grid) project was a continuation of the project EU-dataGrid. The main task of the new project was to build a global infrastructure of regional centres for processing, storing and analysis of data of physical experiments on the Large Hadron Collider (LHC).

2003 – Russian Consortium RDIG – Russian Data Intensive Grid – was established to provide a full-scale participation of JINR and Russia in the implementation of the LCG/EGEE project.

2004 – The EGEE (Enabling Grid for E-Science) projects was started up. CERN is its head organization, and JINR is one of its executors.

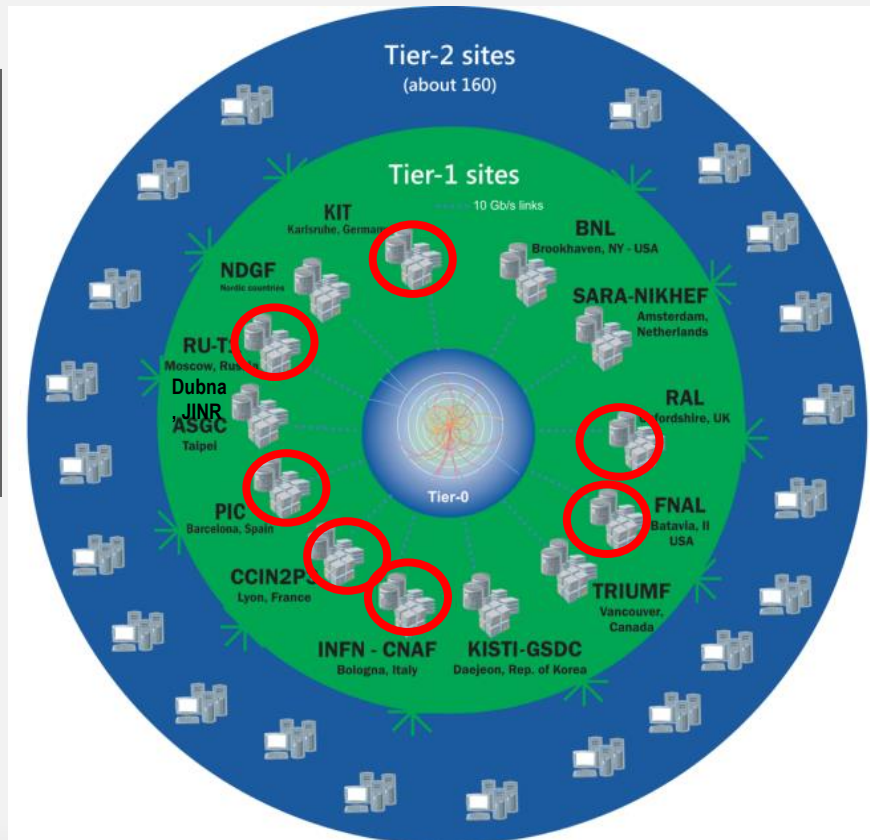
2010 – The EGI-InSPIRE project (Integrated Sustainable Pan-European Infrastructure for Researchers in Europe)



LHC computing model

The Worldwide LHC Computing Grid (WLCG):
Integrates computer centers globally to provide computing and storage resources into a single infrastructure accessible by all LHC physicists for data analysis

42 countries
~300,000 cores
Average
173 PB of storage
> 2 million
jobs/day
>10 Gb links



Tier-0 (CERN & Wigner, Budapest):

- Data recording
- Initial data reconstruction
- Data distribution

Tier-1 (11→14 centres):

- Permanent storage
- Re-processing
- Analysis
- Simulation

Tier-2 (>200 centres):

- Simulation
- End-user analysis

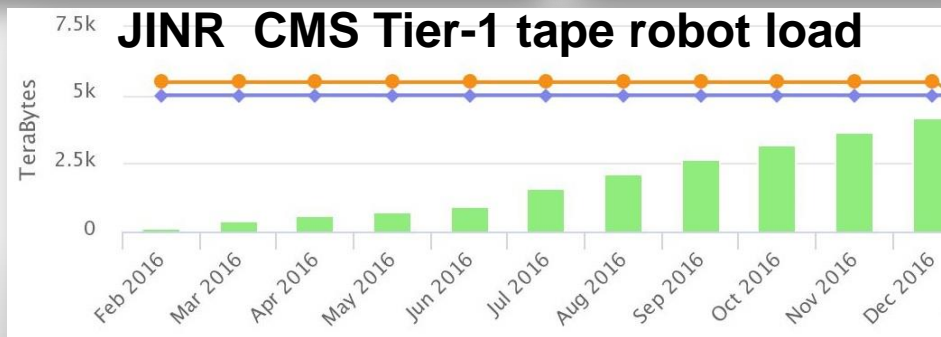
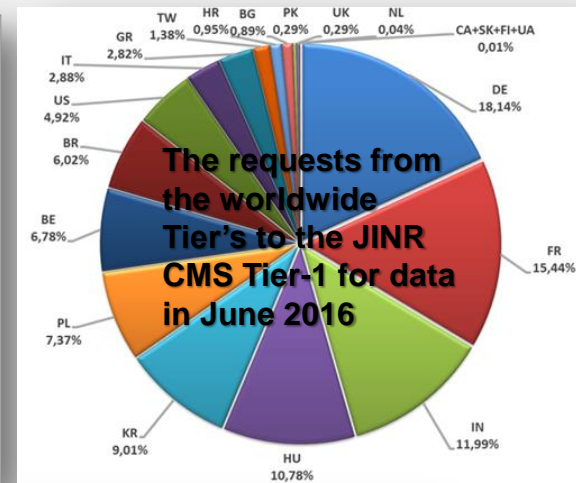
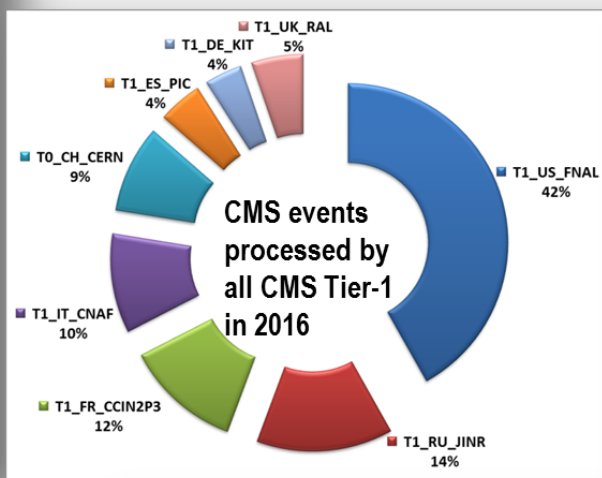


JINR Tier-1 center for CMS



Current configuration

- 3600 cores
- 8 PB tapes
- 4.5 PB disks
- 100% R/A
- 70 TB per day

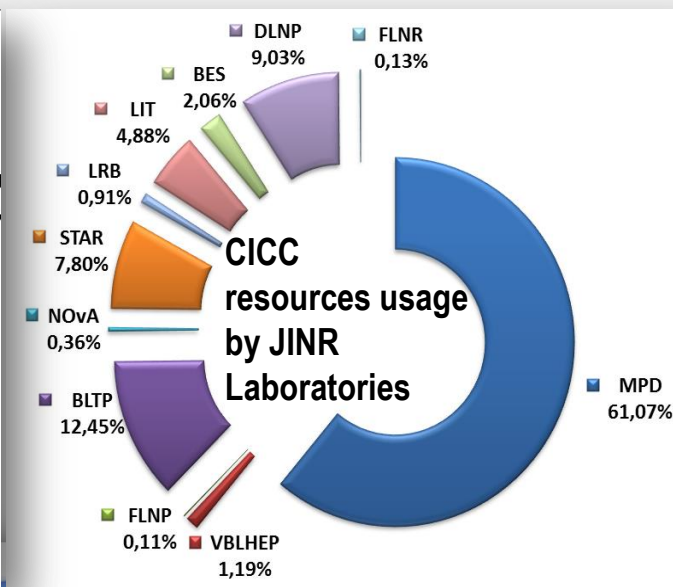
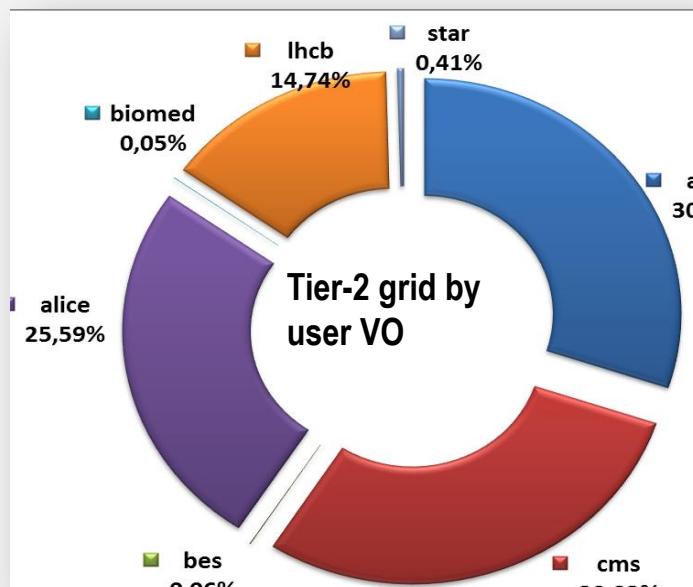




Tier-2 and CICC

Experiments

BM@N,
MPD,
CMS,
ATLAS,
ALICE,
LHCb,
COMPASS,
PANDA,
CBM,
STAR,
NOvA,
BESIII,
DIRAC,
OPERA
NEMO
Mu2e,
NUCLON,
HONE,
BIOMED



Tier-1 and Tier-2:
JINR in Worldwide LHC Computing Grid



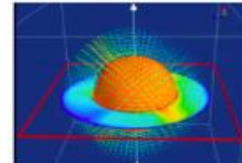
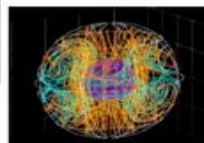
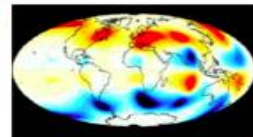
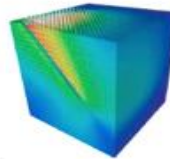
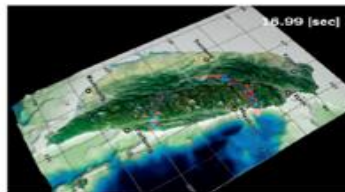
BigPanDA - Beyond ATLAS

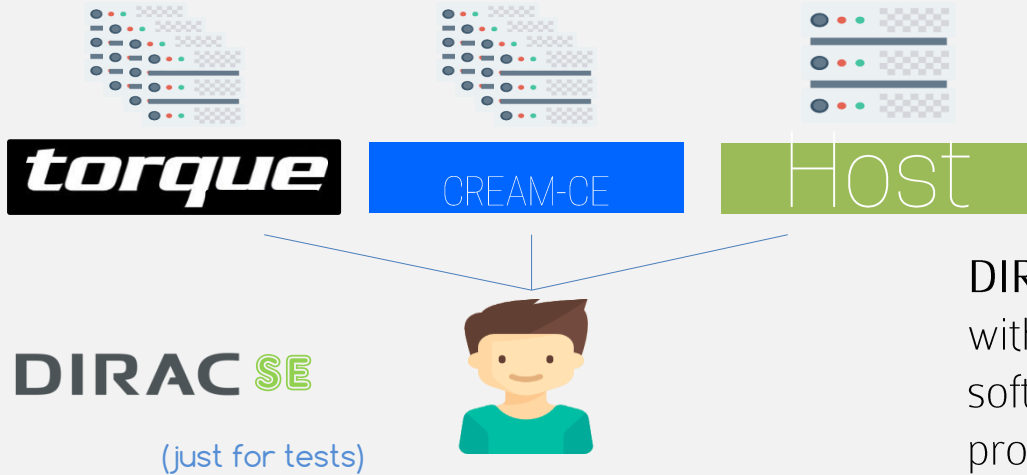


Google Cloud Platform

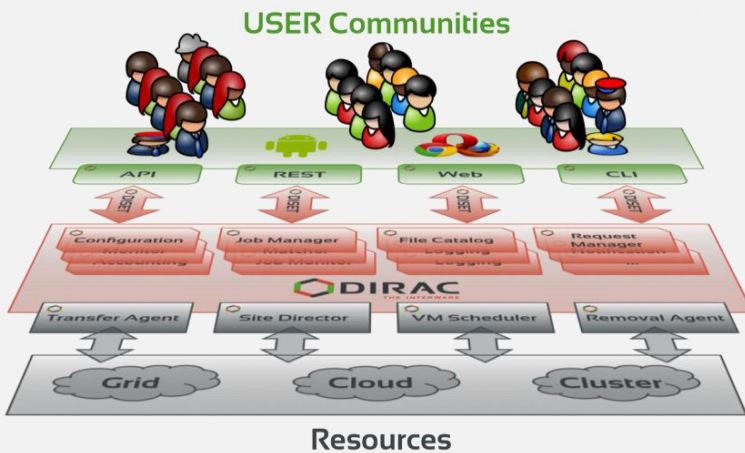


Titan System (Cray XK7)			
Peak Performance	27.1 PF 18,688 compute nodes	24.5 PF GPU	2.6 PF CPU
System memory	710 TB total memory		
Interconnect	Gen6 High Speed Interconnect	3D Torus	
Storage	Lustre Filesystem	32 PB	
Archive	High-Performance Storage System (HPSB)	29 PB	
I/O Nodes	512 Service and I/O nodes		





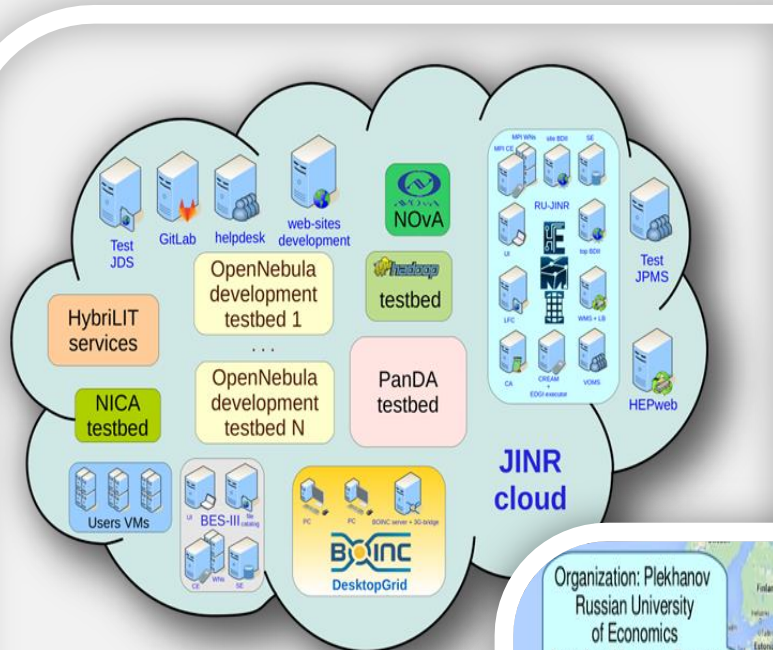
DIRAC (Distributed Infrastructure with Remote Agent Control) INTERWARE is a software framework for distributed computing providing a complete solution to one (or more) **user community** requiring access to **distributed resources**.



Tests for NICA were performed. MPD events were generated using MPD root and then saved storage. All done with DIRAC.



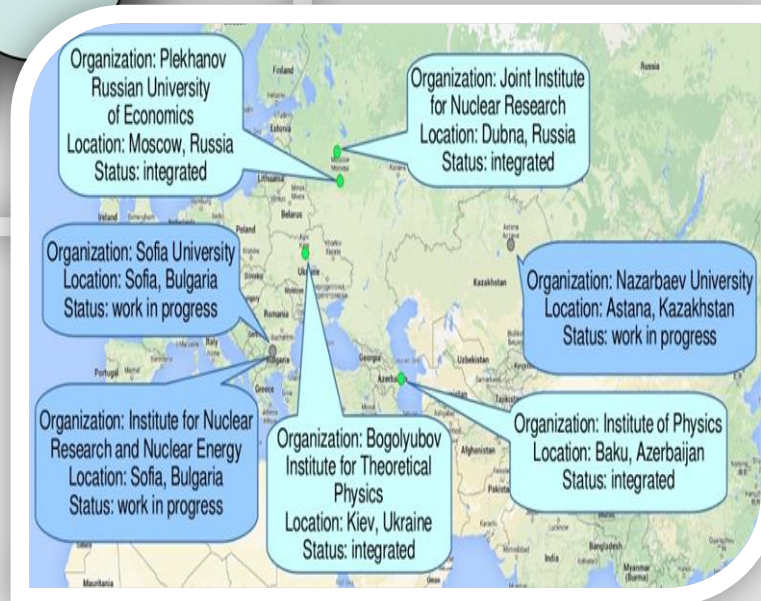
JINR Cloud



One of the most important trends in the cloud technologies is the development of method of integrating various cloud infrastructures.

In order to join the cloud resources of partner organizations from JINR Member State for solving common tasks as well as to distribute a peak load across them, a cloud bursting driver has been designed by the JINR cloud team. It allows one to integrate the JINR cloud with the partner clouds either OpenNebula-based one or any other cloud platform which supports Open Cloud Computing Interface (OCCI).

The geographical location of the partner's organizations from JINR Member States whose cloud resources are integrated into the JINR cloud following the so-called "cloud bursting" model.



Besides, the JINR cloud is integrated into EGI Federated cloud thus enabling a possibility to use part of the JINR computing resources by EGI FedCloud Virtual Organizations.



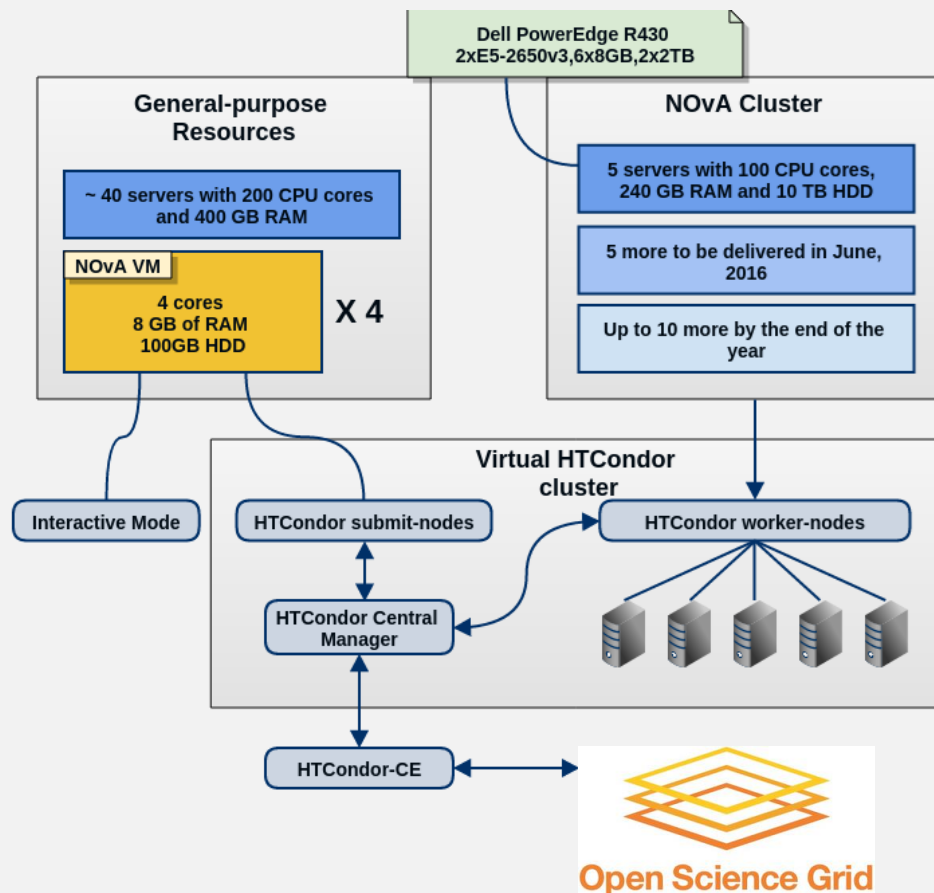
Neutrino computing support

NOvA (Fermilab, USA) is the first neutrino experiment actively using JINR Cloud:

- ✓ 4 VMs for interactive/batch processing used by local JINR NOvA team
- ✓ Virtual batch-cluster based on HTCondor and connected to OSG
- ✓ 100 CPU, 240 GB RAM and 10 TB HDD already available
- ✓ Up to 400 CPU, 1 TB RAM and 80 TB HDD by the end of the year
- ✓ Computing support team was formed including physicists and IT specialists

These resources may also be used by other future experiments at Fermilab, such as DUNE and mu2e.

Reactor neutrino experiments Daya Bay and JUNO also showed its interest in using JINR cloud resources. At the moment the experiments' tasks and required computing capacities are being discussed.





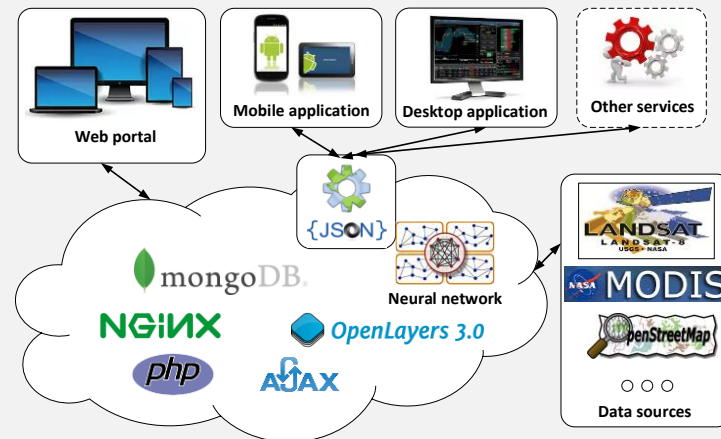
Environmental Monitoring

UNECE ICP Vegetation programme¹ is realized in 36 countries of Europe and Asia. Mosses are collected at thousands of sites across Europe and Asia.

The goal of this program is to identify the main polluted areas, produce regional maps and further develop the understanding of long-range transboundary pollution.

Since 2014 FLNP (Frank Laboratory of Neutron Physics) at the Joint Institute for Nuclear Research has been in charge of that part of the project which is related to the moss biomonitoring.

We propose a cloud platform for data management to facilitate IT-aspects of all biological monitoring stages starting from a choice of collection places and parameters of samples description and finishing with generation of pollution maps of a particular area or state-of-environment forecast in the long term.



HOME RESEARCH RESULT DETAIL LOGIN

Heavy Metals - Research

Activities

- European surveys of heavy metal accumulation in mosses
- Temporal trends in heavy metal accumulation in mosses (1990-2005)
- Studying heavy metal deposition to white clover
- Heavy metal deposition and potential contamination of food crops

Your datasets for project Tuxview 2011:

SITE NAME	SAMPLE DATE	LONGITUDE	LATITUDE	ALTITUDE (M)	OPERATIONS
5	2011-07-13	34.544625	60.10080278	53	Delete Edit Copy
			60.19776944	53	Delete Edit Copy
			59.75181389	53	Delete Edit Copy
			59.8333	53	Delete Edit Copy
			59.68491607	53	Delete Edit Copy
			59.69741607	53	Delete Edit Copy
			59.58608333	53	Delete Edit Copy

ELEMENT	RANGE	MD	± ST.DEV.	RP*	CF**	(GEO)***
Al	288 - 2630	665	530.31	0.008	2.31	0.62
As	0.067 - 0.21	0.1215	0.03	0.1	1.81	0.27
Cr	2.86 - 1610	17.2	263.35	1.5	6.01	2
Cu	2.42 - 2.47	7.43	0	10	1	0.48

1. United Nations Economic Commission for Europe International Cooperative Programme on Effects of Air Pollution on Natural Vegetation and Crops (<http://icpvegetation.ceh.ac.uk>)



Optimisation of Distributed Data Processing system for NICA BM@N Experiment by Using Simulation

2017 – second run of Baryonic Matter at Nuclotron (BM@N) experiment.

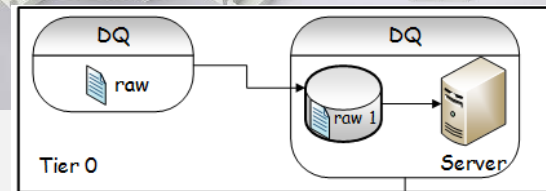
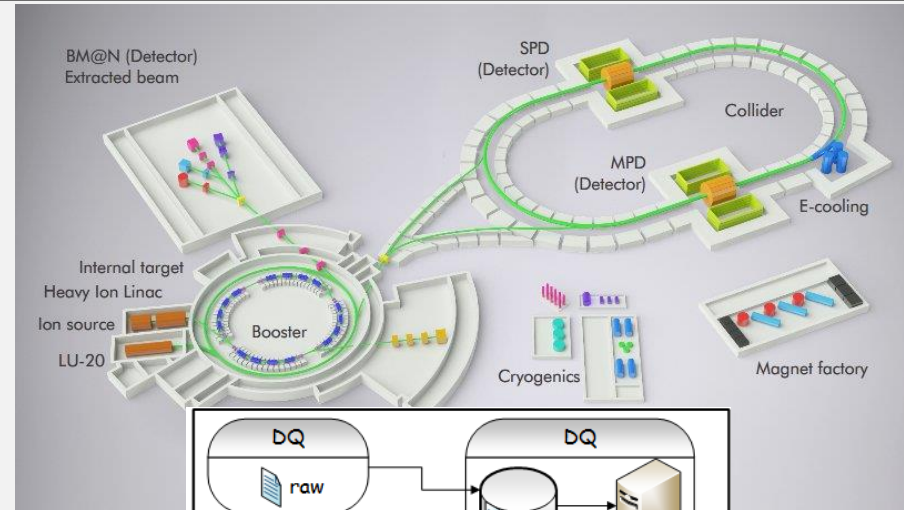
The run requires developing distributed computing system for BM@N data storing and processing.

A simulation is needed to: 1. optimize architecture and equipment. 2. define main parameters and structures of data processing system.

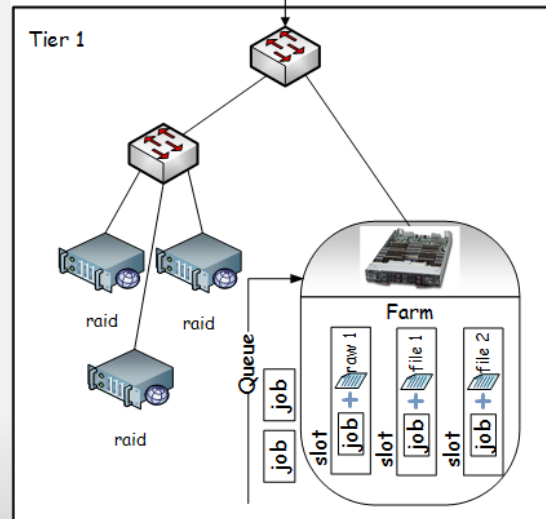
The simulation program SyMSim (Synthesis of Monitoring and Simulation) was developed at LIT-JINR.

SyMSim was used to model and optimize the infrastructure of the CMS JINR Tier1 center and NICA project computing system infrastructure

Now SyMSim is used to choose a proper architecture of the BM@N computing system infrastructure.



Data flow: about 1 PB per run



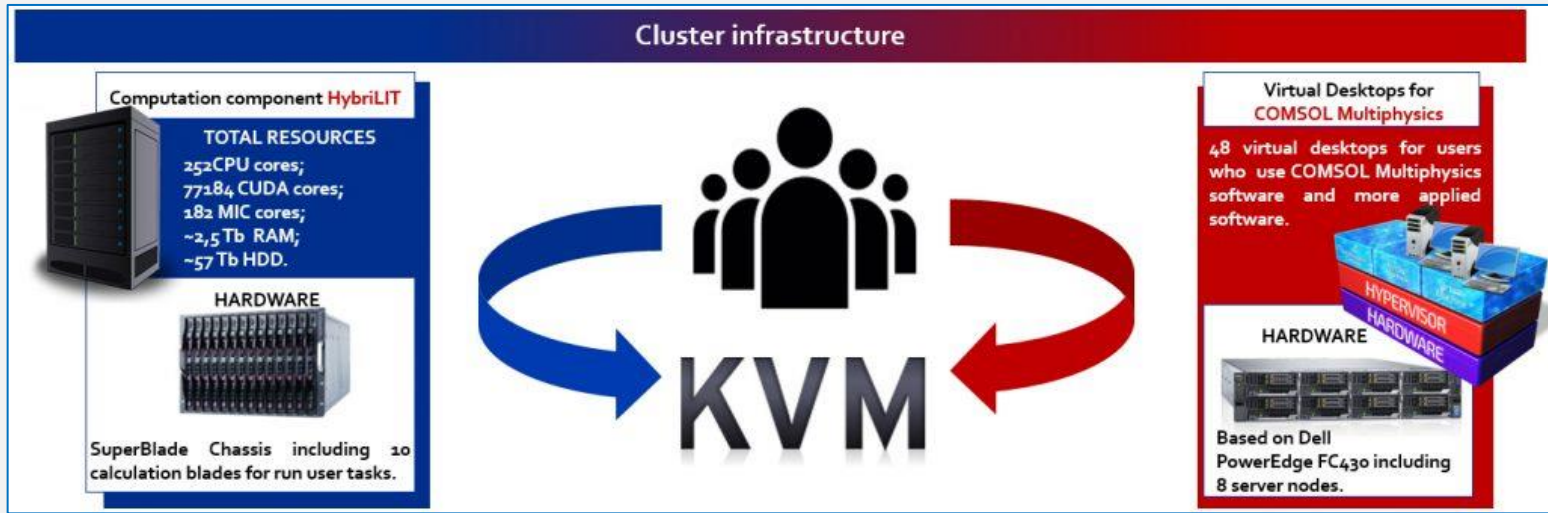
Scheme of the Data Processing System



HYBRILIT IN 2016: NEW POSSIBILITIES AND SERVICES



New **possibilities** for carrying out computations: component for using COMSOL Multiphysics



New **services** providing a more convenient workspace computations: <http://hybrilit.jinr.ru>

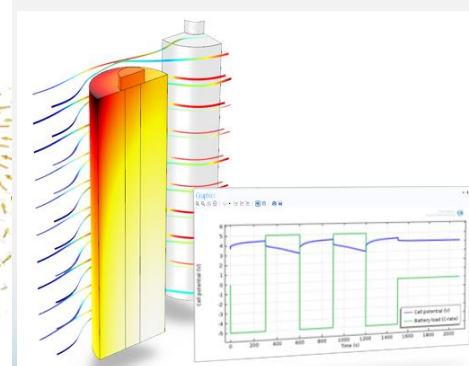
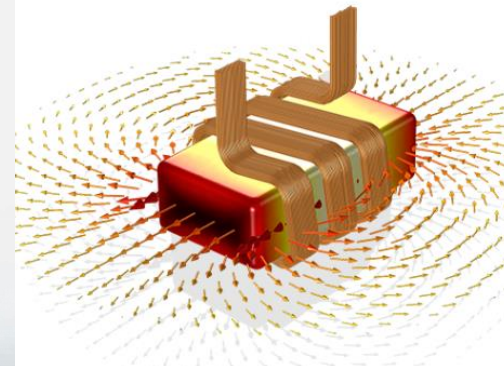


MobiLiT – is a native Android mobile application for users of the HybriLiT HPC cluster.

Author: [Alexej I. Streltsov](#) (Heidelberg, Germany), developed with support from HybriLiT team.

We are on Google Play Store with the name "MobiLiT@HPC" available.

Computations with COMSOL Multiphysics – new possibilities for physics and engineering applications

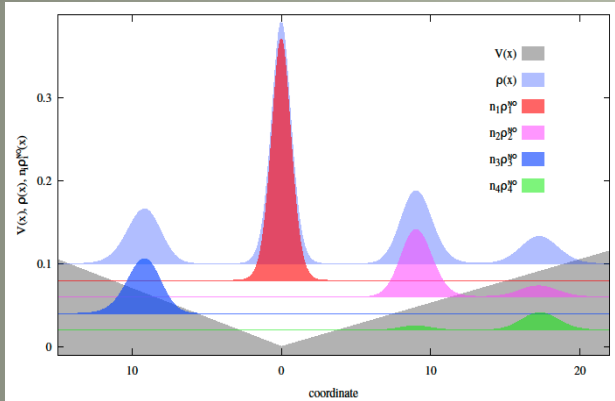


Parallel computing on HybriLIT

Parallel computing for QCD problems:

F. Burger (IP, HU, Berlin,),
M. Müller-Preussker (IP HU, Berlin, Germany),
E.-M. Ilgenfritz (BLTP& VBLHEP, JINR),
A. M. Trunin (BLTP JINR)

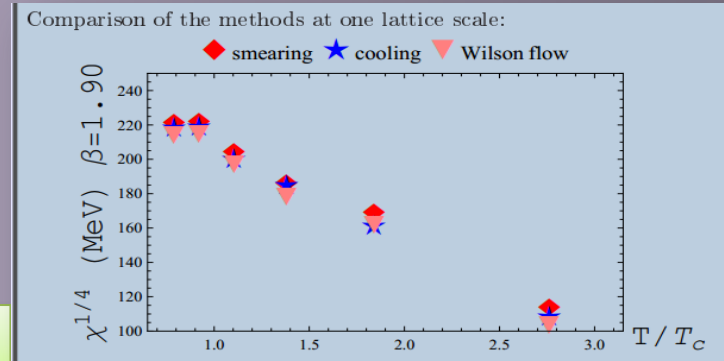
<http://theor.jinr.ru/~diastp/summer14/program.html#posters>



Parallel computing for investigation of Bose-systems:

Alexej I. Streltsov (“Many-Body Theory of Bosons” group at CQD, Heidelberg University, Germany),
Oksana I. Streltsova (LIT JINR)

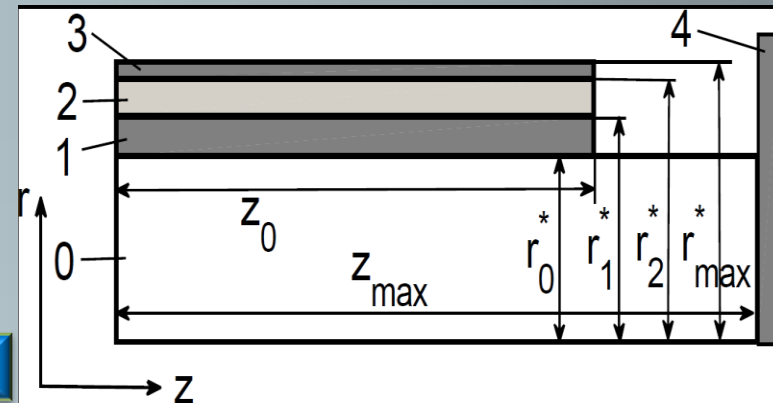
<http://MCTDHB.org>



Parallel computing for Technical problems:

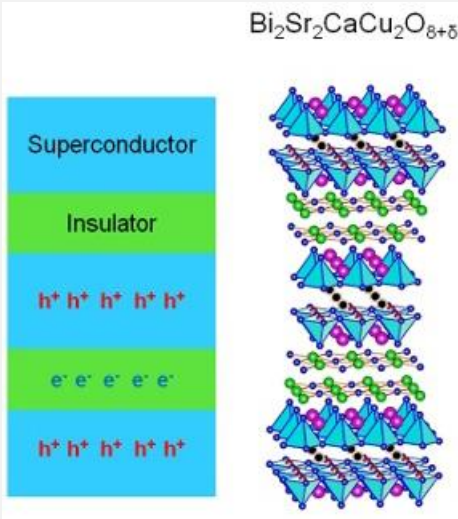
A. Ayriyan (LIT JINR), J. Busa Jr. (TU of Kőcsice, Slovakia),
E.E. Donets (VBLHEP, JINR),
H. Grigorian (LIT JINR,; Yerevan State University, Armenia),
J. Pribis (LIT JINR; TU of Kőcsice, Slovakia)

[arXiv:1408.5853](https://arxiv.org/abs/1408.5853)



Standing Wave Solutions Corresponding to the Cavity Resonances in BSCCO Intrinsic Josephson Junctions

Hybrid MPI+OpenMP Parallelization of a Leapfrog Algorithm for Solving Systems of 2D Sine-Gordon Equations

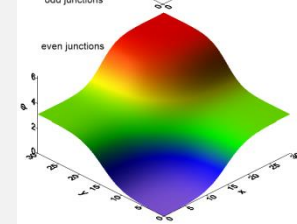
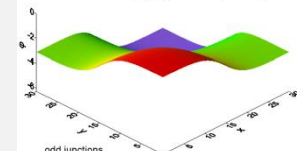


The Intrinsic Josephson Junctions in BSCCO crystals (IJ-BSCO) are a strong source of THz radiation.

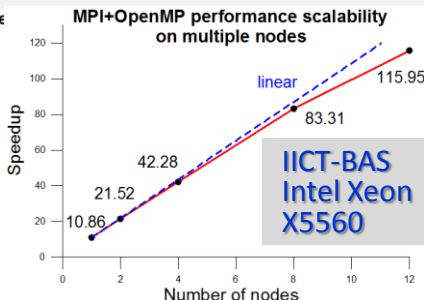
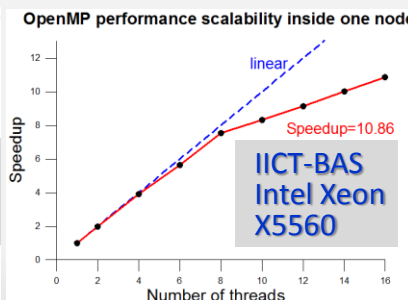
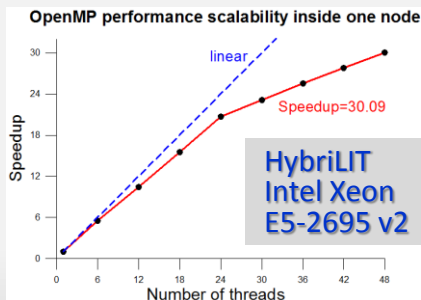
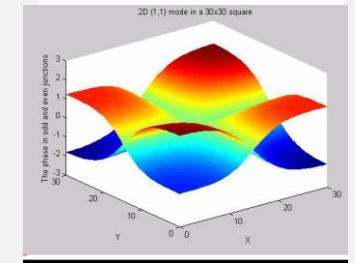
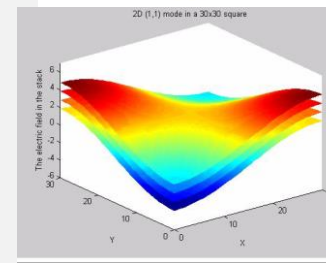
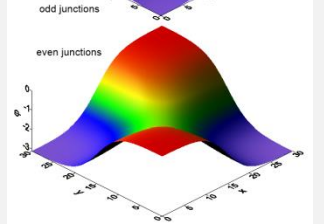
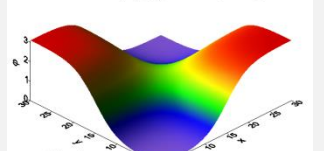
The phase dynamics of the IJ-BSCO is described by a system of **perturbed 2D Sine-Gordon equations**.

Computational challenges in solving this system: Discretization of the 2D domain may ask for 10⁶–10⁸ mesh points. Stable integration scheme with respect to the time variable depends on problem parameters and may ask for 10⁸–10⁹ time steps.

2D static kinks, (1,1) mode $\gamma=1.14, \alpha=0.13$



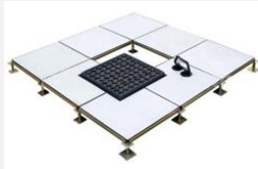
2D static kinks, (1,1) mode $\gamma=1.14, \alpha=0.13$





MICC Engineering Infrastructure

Raised Flooring System



Fibre Optic & Data Structured Cabling System



Diesel generator set



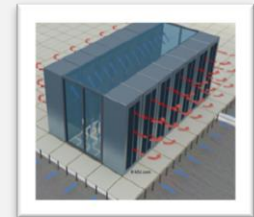
Uninterruptible power supply



Computer Room Air Conditioner



High Density Heat Containment System



Water Detection System



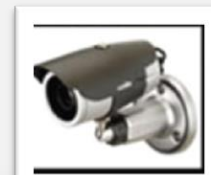
MICC Monitoring System



Biometric Access System



Fire Suppression System



Surveillance System



VESDA (Very Early Smoke Detection Apparatus)



Data storage, processing, analysis



During three years more than **15 million** tasks have been carried out at the Computing center of JINR

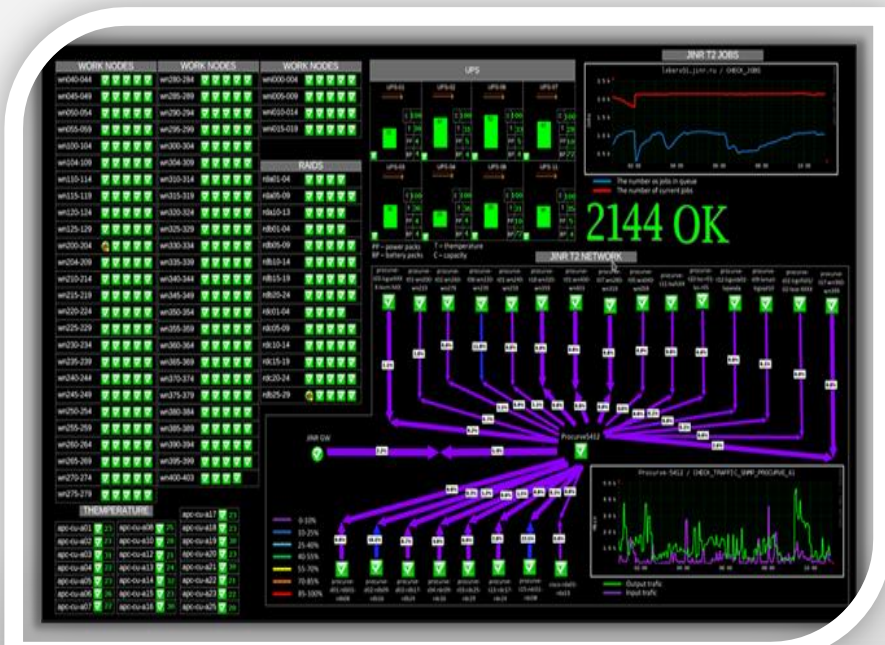


MICC Control Room

The monitoring system of the JINR Computing Complex has been developed and put into exploitation.

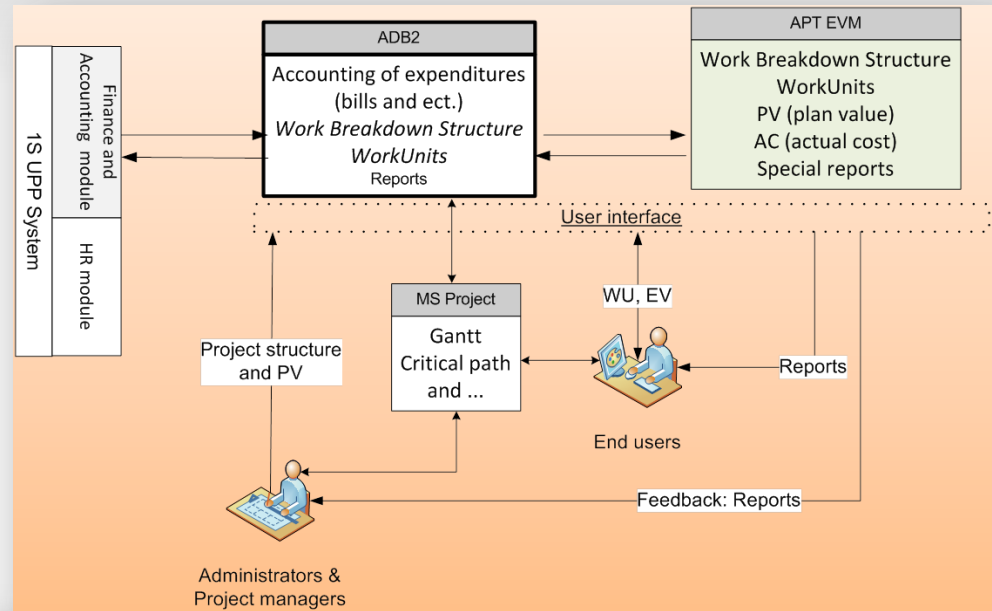
System allows one, in a real time mode, to observe the whole computing complex state and send the system alerts to users via e-mail, sms, etc.

690 elements are under observation
3497 checks in real time



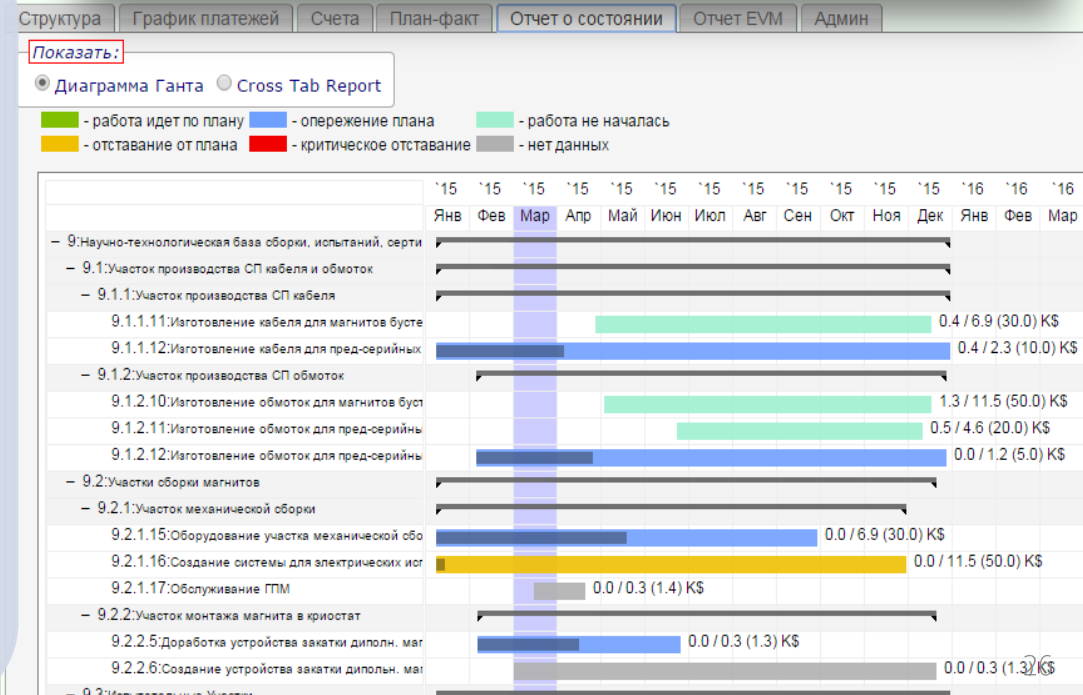
NICA Project Management Information System

A flexible instrument was created by extending the existing PMIS system ADB2 for the needs of the NICA project developed in the process of system APT EVM. In addition, the project plan is to further expand the PMIS NICA for the implementation of ADB2 integration with MS Project.Prof.



NICA PMIS has the following features:

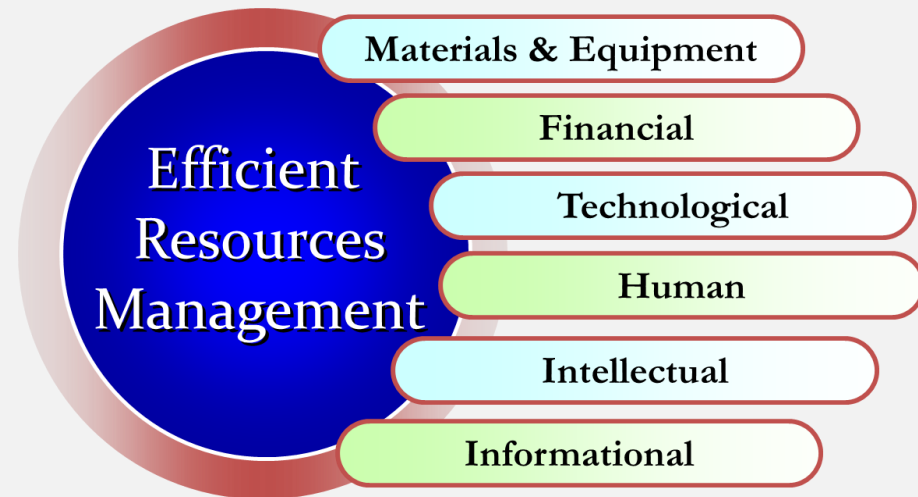
- Control over the project structure (WBS);
- Planning and replanning the project work;
- Versions of the project plans (baselines);
- Monitoring of the project in terms of AC (actual payments) and EV (earned value);
- System alerts users via e-mail (for the timely report on the progress of the work);
- Charts by the method of EVM (PV, AC, EV).





JINR Corporative Information System

- ❑ General 1C:Enterprise platform intended for automation of everyday tasks of economic and management activity,
- ❑ APT EVM system (Activity Planning Tool Earned Value Management) for NICA and future projects management,
- ❑ Electronic document handling system EDH «Dubna»
- ❑ JINR Document Server – electronic open archive-repository of scientific publications and documents,
- ❑ JINR and JINR Member-states access to e-library,
- ❑ PIN – JINR staff personal information,
- ❑ JINR video portal





Electronic document handling system EDH "Dubna"



Continued development and maintenance of an electronic document management system EDH "Dubna".

Processed more than 1000 documents

Developed variety of specialized reports

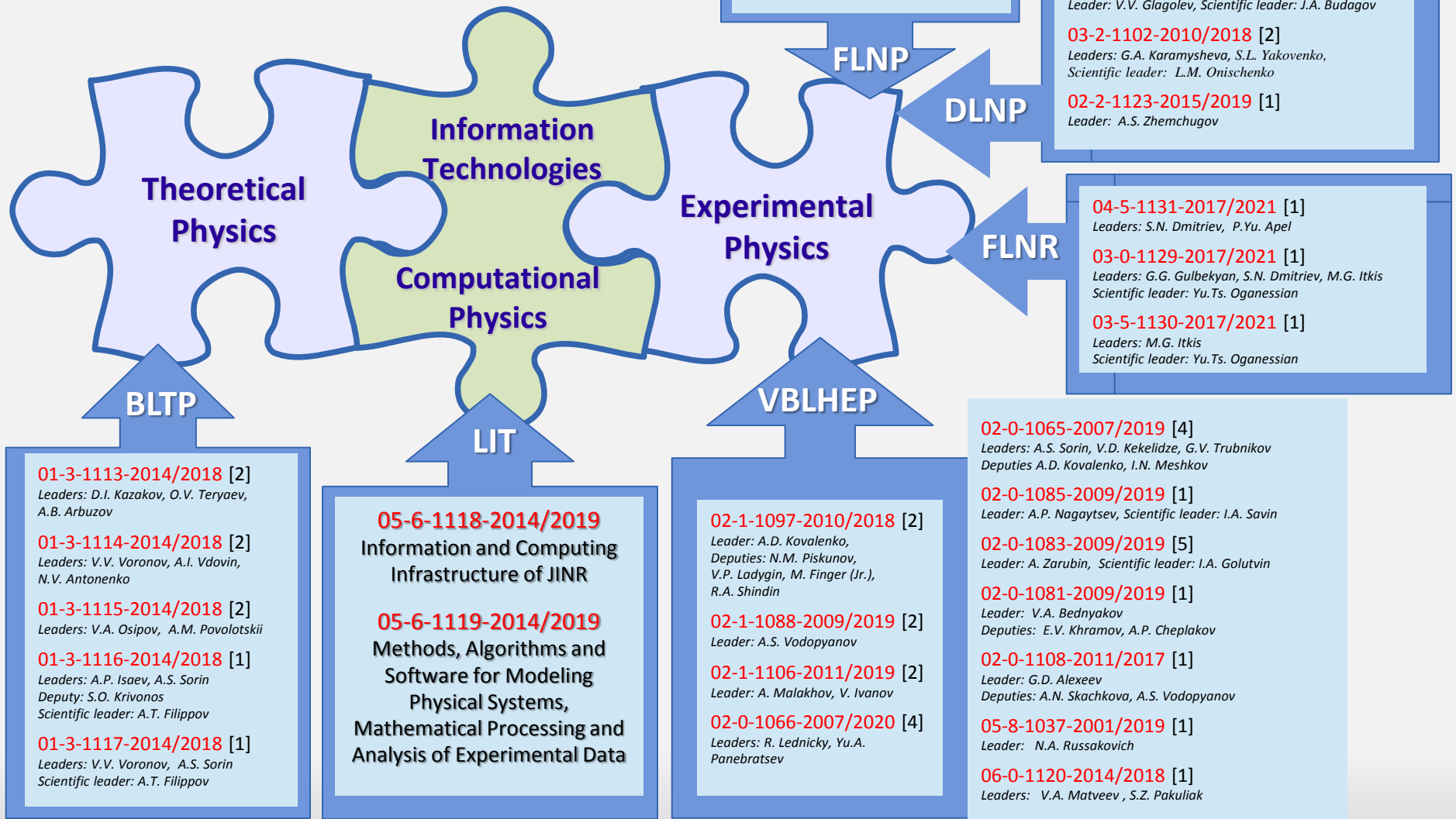
In the year 2017 substantial increase in the number of documents processed in EDH "Dubna" was planned.



Information technologies – expected results in 2017 – 2023

- Creation of a JINR Multifunctional Information and Computing Complex (MICC) of a global level for the development of advanced information technology
- Development of a territorially distributed research environment to provide the use of the Complex capacities by the JINR and cooperating centres worldwide
- Research in the field of intensive operations with mass data in the distributed systems (Big Data), development of corresponding tools and methods of visualization, including 3D
- Research on issues of optimizing the processes of using the existing capacities, in particular supercomputers, for data processing in distributed environment and their integration into a unified distributed computing system
- Creation of a software technological complex providing introduction of cloud technologies for organization of research by distributed user groups, introduction of intellectual methods of new generation grid-cloud structures management
- Research in the field of the global monitoring of the distributed computing systems
- Development of new parallel applications, cross-platform and multi-algorithm software complexes in a heterogeneous computing environment that allow one to expand a spectrum of computationally intensive solved fundamental scientific problems

LIT participates in 48 projects of 30 JINR topics of the 2017 Topical Plan of JINR



04-4-1122-2015/2017 [1]
Leaders: S.A. Kulikov, V.I. Prikhodko

03-4-1128-2017/2019 [1]
Leader: V.N. Shvetsov,
Deputies: Yu.N. Kopatch, E.V. Lychagin,
P.V. Sedyshev

04-4-1121-2015/2017 [1]
Leaders: D.P. Kozlenko, V.L. Aksenov,
A.M. Balagurov

02-2-1099-2010/2018 [1]
Leaders: D.V. Naumov, A.G. Olshevskiy

02-2-1125-2015/2017 [2]
Leader: L.G. Tkatchev, Deputy: V.M. Grebenyuk

03-2-1101-2010/2017 [2]
Leader: A.V. Kulikov, Deputy: Z.Tsamalaidze

02-2-1124-2015/2017 [1]
Leader: V.V. Glagolev, Scientific leader: J.A. Budagov

03-2-1102-2010/2018 [2]
Leaders: G.A. Karamysheva, S.L. Yakovenko,
Scientific leader: L.M. Onischenko

02-2-1123-2015/2019 [1]
Leader: A.S. Zhemchugov

04-5-1131-2017/2021 [1]
Leaders: S.N. Dmitriev, P.Yu. Apel

03-0-1129-2017/2021 [1]
Leaders: G.G. Gulbekyan, S.N. Dmitriev, M.G. Itkis
Scientific leader: Yu.Ts. Oganessian

03-5-1130-2017/2021 [1]
Leaders: M.G. Itkis
Scientific leader: Yu.Ts. Oganessian

02-0-1065-2007/2019 [4]
Leaders: A.S. Sorin, V.D. Kekelidze, G.V. Trubnikov
Deputies A.D. Kovalenko, I.N. Meshkov

02-0-1085-2009/2019 [1]
Leader: A.P. Nagaytsev, Scientific leader: I.A. Savin

02-0-1083-2009/2019 [5]
Leader: A. Zarubin, Scientific leader: I.A. Golutvin

02-0-1081-2009/2019 [1]
Leader: V.A. Bednyakov
Deputies: E.V. Khramov, A.P. Cheplakov

02-0-1108-2011/2017 [1]
Leader: G.D. Alexeev
Deputies: A.N. Skachkova, A.S. Vodopyanov

05-8-1037-2001/2019 [1]
Leader: N.A. Russakovich

06-0-1120-2014/2018 [1]
Leaders: V.A. Matveev, S.Z. Pakuliak

01-3-1113-2014/2018 [2]
Leaders: D.I. Kazakov, O.V. Teryaev,
A.B. Arbuzov

01-3-1114-2014/2018 [2]
Leaders: V.V. Voronov, A.I. Vdovin,
N.V. Antonenko

01-3-1115-2014/2018 [2]
Leaders: V.A. Osipov, A.M. Povolotskii

01-3-1116-2014/2018 [1]
Leaders: A.P. Isaev, A.S. Sorin
Deputy: S.O. Krivonos
Scientific leader: A.T. Filippov

01-3-1117-2014/2018 [1]
Leaders: V.V. Voronov, A.S. Sorin
Scientific leader: A.T. Filippov

05-6-1118-2014/2019
Information and Computing
Infrastructure of JINR

05-6-1119-2014/2019
Methods, Algorithms and
Software for Modeling
Physical Systems,
Mathematical Processing and
Analysis of Experimental Data

02-1-1097-2010/2018 [2]
Leader: A.D. Kovalenko,
Deputies: N.M. Piskunov,
V.P. Ladygin, M. Finger (Jr.),
R.A. Shindin

02-1-1088-2009/2019 [2]
Leader: A.S. Vodopyanov

02-1-1106-2011/2019 [2]
Leader: A. Malakhov, V. Ivanov

02-0-1066-2007/2020 [4]
Leaders: R. Lednickiy, Yu.A.
Panebratsev

Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data

Theme 1119

- Software development and realization of mathematical support of experiments conducted on the JINR basic facilities and in the frameworks of international collaboration;
- Development of numerical methods, algorithms and software packages for modelling complex physical systems:
 - interactions inside hot and dense nuclear matter
 - physicochemical processes in materials exposed to heavy ions
 - evolution of localized nanostructures in open dissipative systems
 - properties of atoms in magnetic optical traps
 - electromagnetic response of nanoparticles and optical properties of nanomaterials
 - evolution of quantum systems in external fields
 - astrophysical studies
- Development of methods and algorithms of computer algebra for simulation and research of quantum computations and information processes
- Development of symbolic-numerical methods, algorithms and software packages for the analysis of low-dimensional compound quantum systems in molecular, atomic and nuclear physics



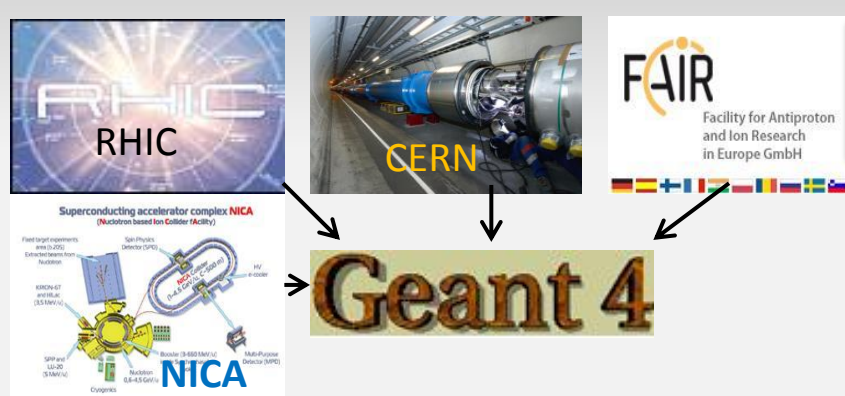
Software development

Parallel software will be the mainstream since it enables substantial reduction of CPU time

- Development and support of **program libraries** of general and special purpose
- Creation and support of program libraries and software complexes implemented with **parallel programming techniques** CUDA, OpenCL, MPI+CUDA, OpenMP, etc.
- Support and development of a **specialized service-oriented environment** for modeling experimental installations and processes and experimental data processing
- **Tools and methods** for software development
 - flexible, platform-independent simulation tools
 - self-adaptive (data-driven) simulation development software

Improvement of QGSp in Geant4

Now FTFP_BERT Physics List is a favorite Physics List of Geant4
 Physics List – QGSp_BERT used by ATLAS and CMS



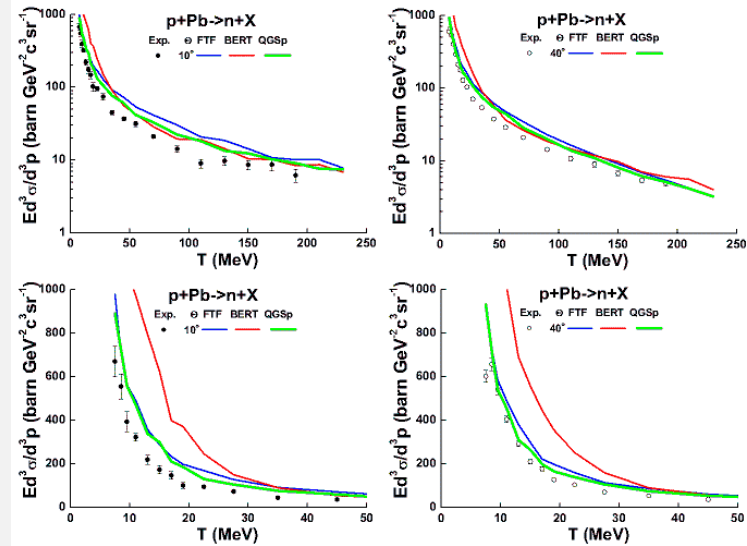
Geant 4

Geant4 – toolkit for simulating particle passage through matter.
Areas of application: high energy, nuclear and accelerator physics, medical and space science.
Main task – Simulation of hadronic interactions and electromagnetic showers.
Main yield of LIT: Development of Fritiof (FTF) hadronic model; Simulation of interactions: (1) π , K , p , n , Λ , Nucleus+Nucleus (2) Anti-proton, Anti-Nucleus+Nucleus
Specific tasks solved:

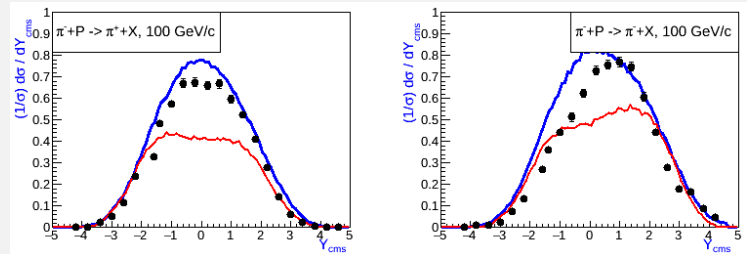
- Improvement of string fragmentation;
- Improvements of processes cross sections;
- Inclusion of the Reggeon cascading for correct description of nucleus breakups;
- Improvement of parton momenta sampling

Future tasks:

- Contribution to code parallelization within Geant 4 modules



Slow neutron production, ITEP experimental data (1983)
 [Shower shape improvement]



πP interactions at 100 GeV/c
 Red lines – old QGSp Blue lines – new QGSp

The [present status of Geant4](https://arxiv.org/abs/1608.08811) was defined with the important co-authorships of A. Galoyan (VBLHEP) and V.V. Uzhinsky (LIT). See, Nuclear Instruments and Methods, A835 (2016) 186–225, DOI: [10.1016/j.nima.2016.06.125](https://doi.org/10.1016/j.nima.2016.06.125)

● Dedicated Support for Experimental Data Processing and Analysis

– Automation upgrade of on-line data acquisition and processing

[Instance: ●● For the future modernizations of YUMO spectrometer at IBR2]

– Reliable statistical inferences under low statistics and incomplete observation

[Instance: ●● This is a permanent problem asked for scrutiny by the low-statistics experiments]

– New mathematical methods and emerging software for reliable data acquisition

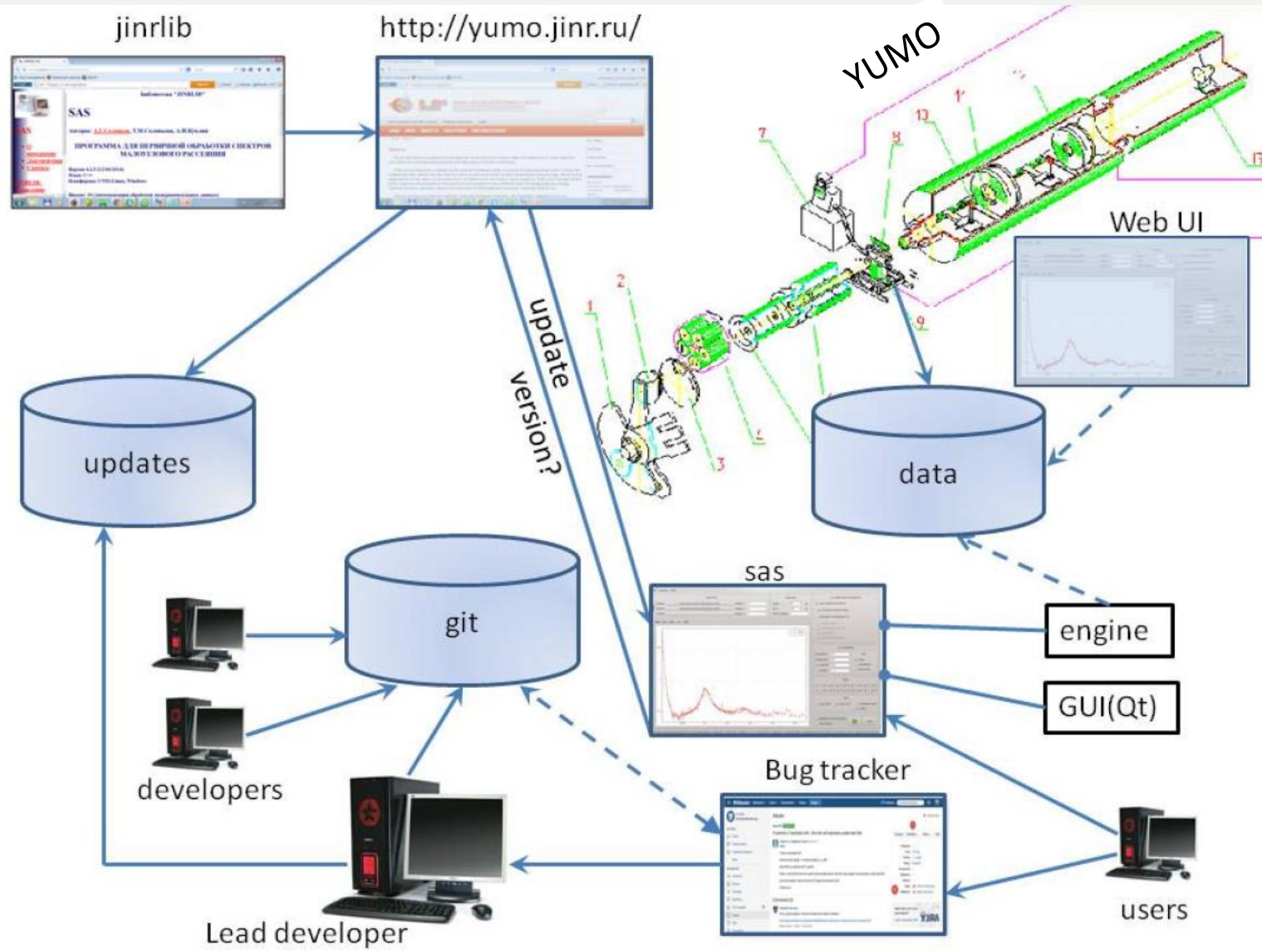
[Instances: ●● Methods for dynamical image recognition under neutron diffraction on poly-crystals enabling analysis of crystalline matter concerning crystallographic symmetry analysis, microstructural analysis, investigation of the kinetics of the matter processes at **FLNP detectors**;

●● Methods for solving problems of the high "intellectuality" pattern recognition serving to the elaboration of new software for the automatic calibration of multi-detector systems in **FLNR**;

●● Methods for solving ill-posed problems which emerge in the analysis of multidimensional distributions enabling elaboration of new software for the determination of times of decay by scintillators using an autocorrelation delayed coincidence time spectrometer in **DLNP**]

– New segment building algorithm for the Cathode Strip Chamber (CSC) of the CMS facility

Automation of on-line data storage on modernized YUMO spectrometer

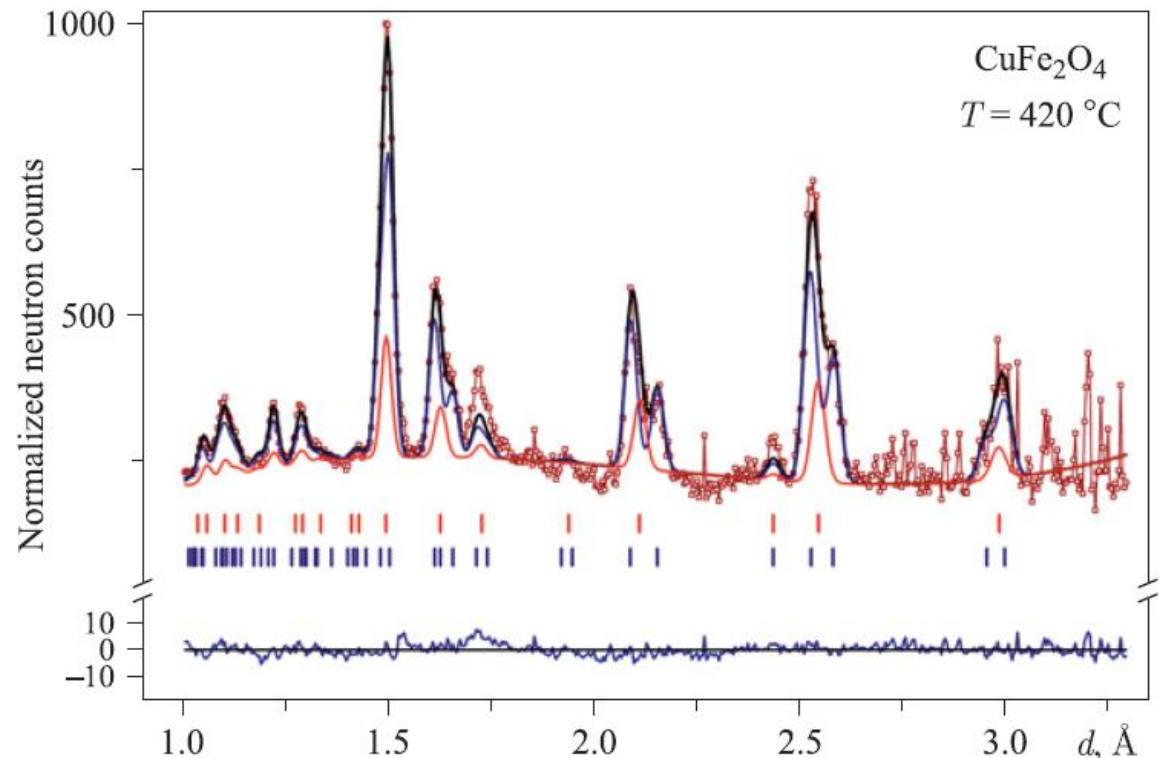


Real-Time Visualization and Analysis of Neutron Diffraction Data

Packages **MAPS** and **SPEVA** were developed for preliminary analysis and final mathematical processing of *large neutron diffraction data* got in studies of transition processes in crystals. They secure *automatic visualization* of 2D data obtained at HRFD-diffractometer with time of flight scanning, respectively analysis of *atomic structure changes* during transition processes

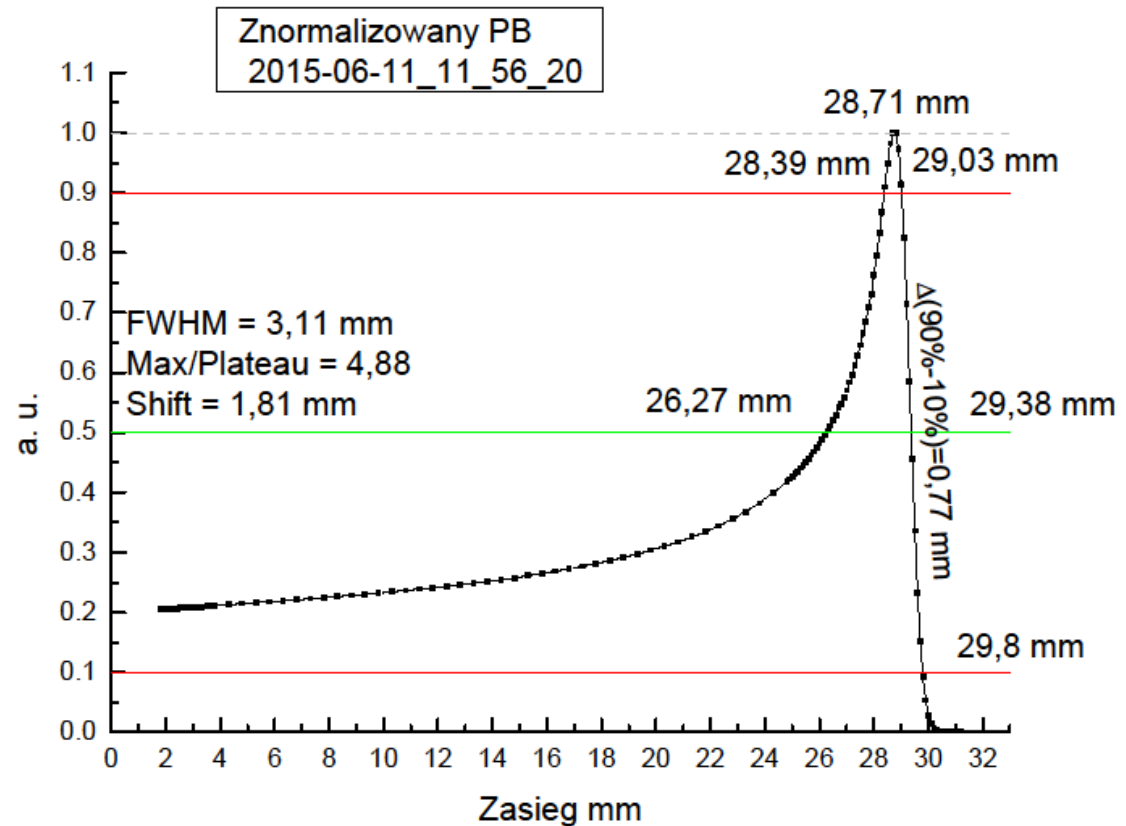
An instance:

Structural phase transition between **cubic** (in red) and **tetragonal** (in blue) phases resolved in the diffraction spectrum of CuFe_2O_4 at the temperature $T = 420^\circ\text{C}$



Strength of the mathematical modeling in the performance increase of the AIC-144 cyclotron

The development of mathematical models [LIT&DLNP] for the *creation of the main operation mode of the AIC-144 isochronous cyclotron*, located in the Institute of Nuclear Physics of the Polish Academy of Sciences, Krakow, Poland. [As a result of the successful simulation, AIC-144 was launched in the main operation mode, for the **proton therapy of eye melanoma**. The extracted proton beam shows the *best world rating* (smallest length of trailing edge of the Bragg peak). The JINR second prize in 2014]

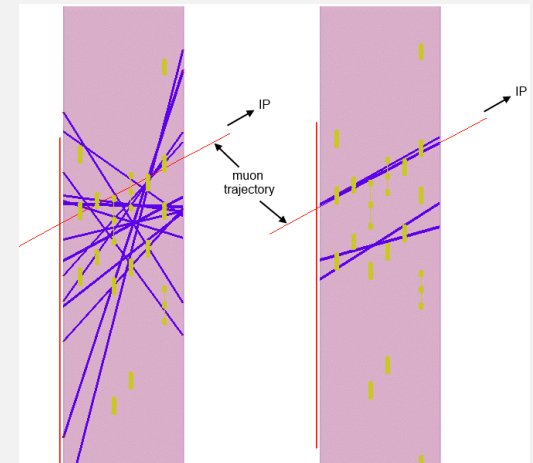
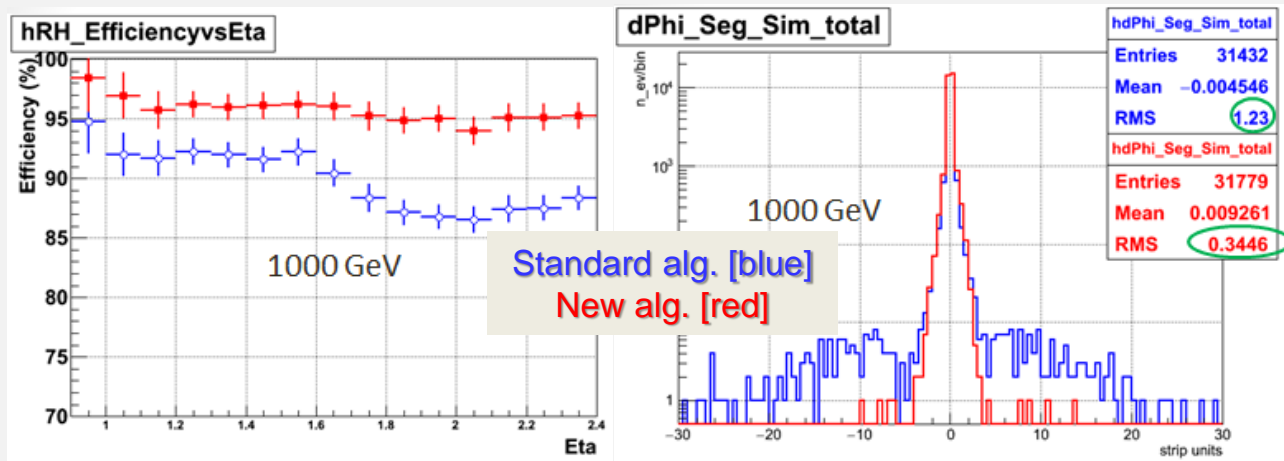


The Bragg peak in the case of run of protons in water for the AIC-144 main operation mode

New segment building algorithm for the Cathode Strip Chamber (CSC) of the CMS facility

Purpose: to improve the reconstruction for high hit rate and big backgrounds due to luminosity increase
 The **new algorithm** was implemented in the **official CMS software package** in July, 2016, extensive testing period until end of January 2017. It proved to be **effective, stable and robust**.

Future: Further reconstruction procedure refinements, its use as reconstruction algorithm for the new GEM detectors that will be included in the experimental setup for the next major upgrade.

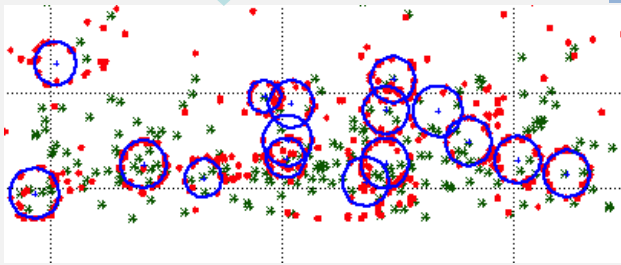
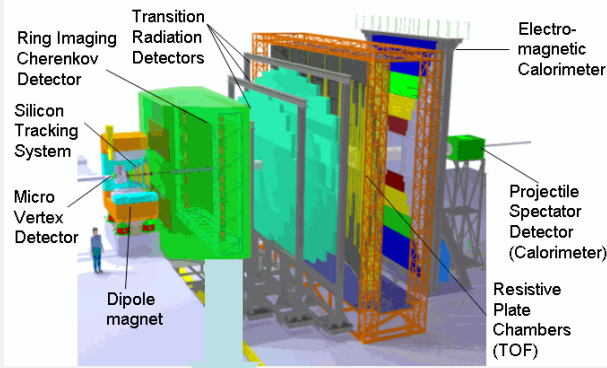


Reconstruction efficiency vs. pseudorapidity (new alg. efficiency is **high** and **almost constant**, standard alg. eff. decreases with the increase of the pseudorapidity)

Distance in strip units between the reconstructed and the simulated segment (**3.5 times signal improvement**)

Example of a high hit multiplicity event reconstruction (standard alg. – left, new alg. – right) [**# of fake segments: is considerably reduced**]

CBM (GSI) – Methods, Algorithms & Software for Fast Event Reconstruction



Event reconstruction algorithms:

- 1) Tracking: Kalman filter and track following;
- 2) Ring reconstruction: Hough Transform, COP, ellipse fitting;
- 3) Electron identification in RICH: ANN and cuts.

Modern technologies for parallelization:

- 1) Vectorization (SIMD - Single Instruction Multiple Data);
- 2) Multithreading (many cores CPU).

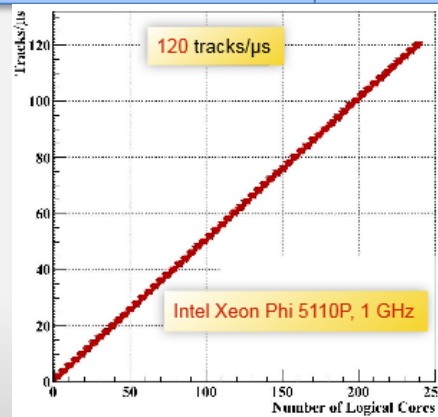
Results:

- 1) High efficiency of track and ring reconstruction (93-95%);
- 2) Very fast algorithms (few ms per event).

Tasks:

- global track reconstruction;
- event reconstruction in RICH;
- electron identification in TRD;
- clustering in MVD, STS and MUCH;
- participation in FLES (First Level Event Selection);
- development of the Concept of CBM Databases;
- magnetic field calculations;
- beam time data analysis of RICH and TRD prototypes;
- contribution to the CBMROOT development;
- D_0^- , vector mesons, $J/\psi \rightarrow e^+e^-$ and $J/\psi \rightarrow \mu^+\mu^-$ reconstruction;

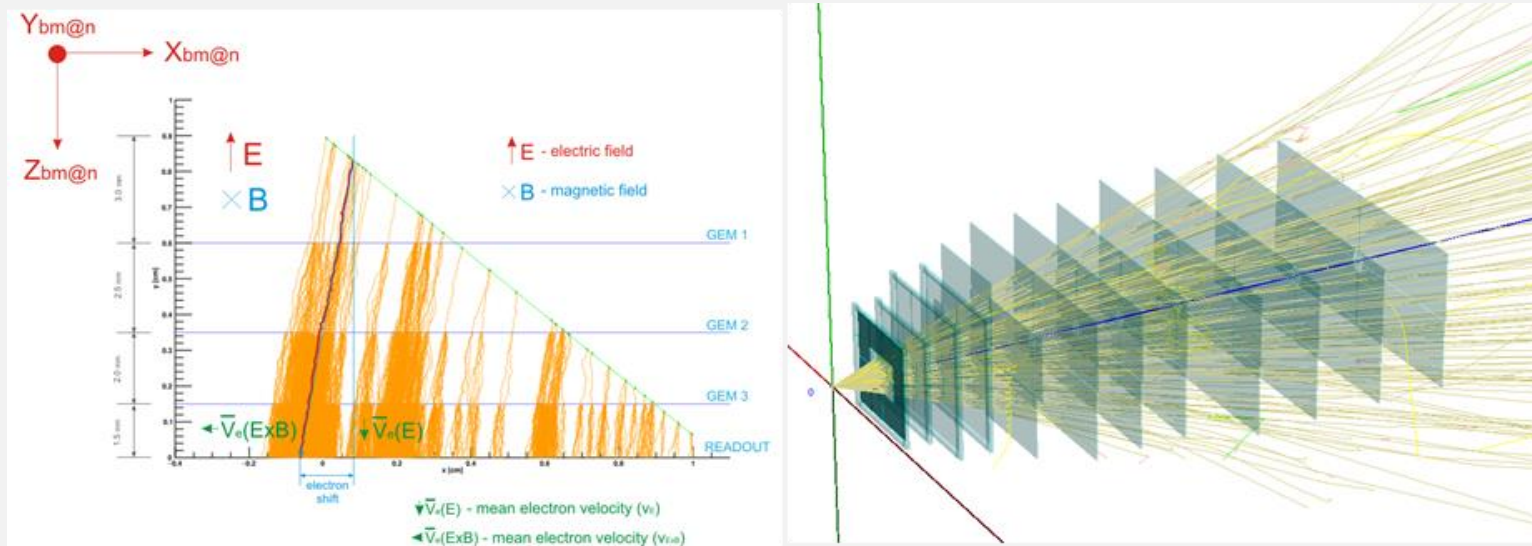
Task	Initial Time [ms/event]	Parallel Time [ms/event]	Speedup
Tracking	730	1.5	487
Ring reconstruction	375	2.5	143



Fast parallel algorithms were developed for event reconstruction in the CBM

Software for BM@N GEM (Gas Electron Multiplier) tracker

- Realistic Simulation of GEM detector needs development of data generation algorithms which take into account features controlling the actual data in the GEM chamber: the signal deviation under external magnetic fields and the influence of the angular deviation of the flying particle from the beam axes to the shape and the size of the strip cluster (signal). (See left figure)
- The hit reconstruction algorithms restore the coordinates of the particle trajectories across the detector planes (hits). The hits serve as inputs to track finding methods.



Left: Garfield++ modeling of the process of formation of **avalanches of electrons** (signal) inside the GEM chamber. The **green line** denotes the track of the particle traversing the GEM chamber. The **orange color** marks electron trajectories provoking avalanches. The avalanche signal is registered by the readout plane.

Right: Realistic version of the complete GEM detector configuration in the BM@N experiment

Intensive work is underway!

● **Developments in Computer Algebra and Quantum Computing**

– **New approaches to the derivation of involutive Groebner bases**

- [Tasks: ●● Down-up approach to the derivation of compact bases;
●● Parallel algorithms for the construction of compact involutive bases;
●● Generation of finite difference schemes inheriting the algebraic properties of the ancestor partial differential equations;
●● Numerical algorithm applications to the analysis of low dimensional nanostructures and other composite quantum systems in molecular, atomic and nuclear physics]

– **Modeling and control of quantum information processes**

- [Tasks: ●● Entanglement description in systems of qubits as the main resource in quantum information and communication;
●● Study of systems of charged particles under strong laser radiation;
●● Modelling quantum dynamics of elementary particles and nuclei interacting with strong laser radiation. Proposals for the European project “Extreme Light Infrastructure (ELI)”, Prague (Czech Republic) and Măgurele (Romania)]

– **Design of algorithmic methods of discrete quantum mechanics**

- [Tasks: ●● Description of quantum gates;
●● Applications to quantum information processes]

Symbolic-numeric simulation of slender structures (rods, fibers, cilia, flagella, etc.)

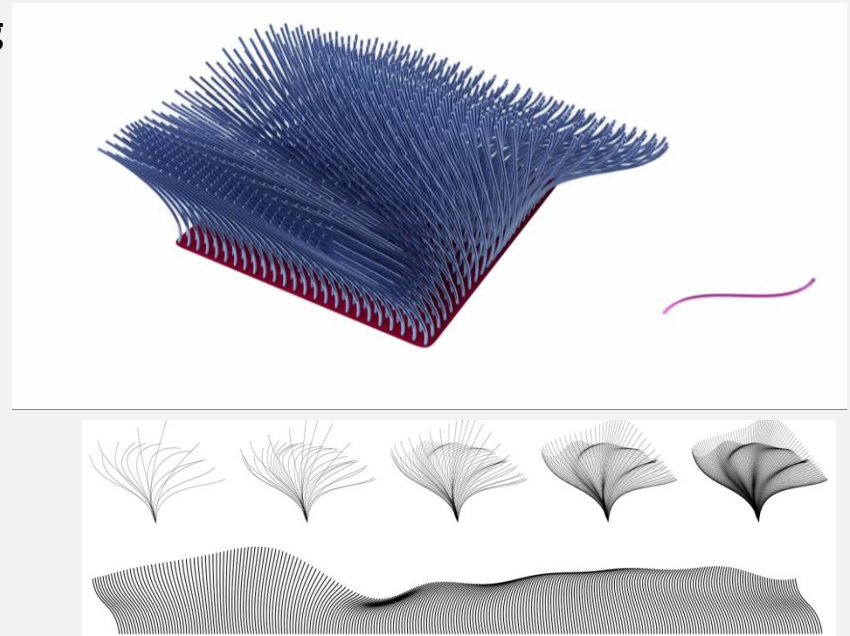
Governing system of 12 nonlinear **very stiff** partial differential-algebraic equations:

$$\rho A \partial_t \vec{v} = \partial_s \vec{n} + \vec{f}, \quad \rho I \partial_t \vec{\omega} = \partial_s \vec{m} + \text{adiag}(1, -1) \vec{n} + \vec{l}, \quad \partial_t \vec{\kappa} = \partial_s \vec{\omega}, \quad \partial_s \vec{v} = \text{adiag}(1, -1) \vec{\omega}, \quad \vec{\omega} \text{ adiang}(1, -1) \vec{\kappa}^T = 0, \quad \vec{v} \text{ adiang}(1, -1) \vec{\kappa}^T = 0$$

To obviate stiffness, the solution derived by the authors from LIT JINR and HMTI-BAS (Minsk) **combined computer algebra and numerical methods**: analytical solution of the parameter-free part of the system and numerical for the remaining

Demonstration: simulation of the beating pattern of a cilium (of interest in the context of simulations in biology and biophysics, e.g., cilia carpets in the interior of the lung are responsible for the mucus transport).

As compared to a pure numerical solution, the step size can be increased by three orders of magnitude, which leads to two orders of magnitude decrease of CPU time.



Simulation of a cilia carpet (top) composed of multiple cilia beating in a meta-chronal rhythm (middle) produces the appearance of a wave.

LIT traditional conferences

**GRID
2016**



**Distributed Computing and Grid-technologies
in Science and Education**

MMCP'2017
The International Conference
**MATHEMATICAL MODELING AND
COMPUTATIONAL PHYSICS**
Satellite event: students' school
Mathematical modeling for NICA
July 3-7, 2017 — Dubna

Methods, Mathematics, Modeling, Data, Computer, Physics, Algebra, CUDA, MPI, NICA, Distributed, Complex, Systems, Parallel, Processing, Energy, Applications, Particle, BigData, Engineering, Technology.



NEC'2017
26th International Symposium
on Nuclear Electronics & Computing

The 2nd International School on
Heterogeneous Computing
Infrastructure **NEC' 2017**

LIT schools

Mathematics. Computing. Education



**DIGITAL LIBRARIES:
ADVANCED METHODS AND TECHNOLOGIES
DIGITAL COLLECTIONS**



JINR / CERN

GRID AND ADVANCED INFORMATION SYSTEMS

International Conference-School for Young Scientists
"Modern Problems of Applied Mathematics &
Computer Science"

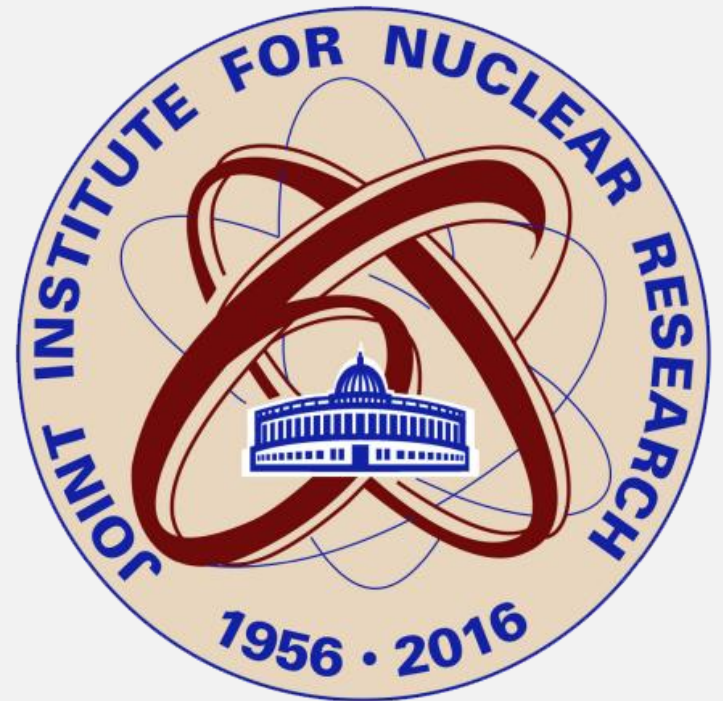
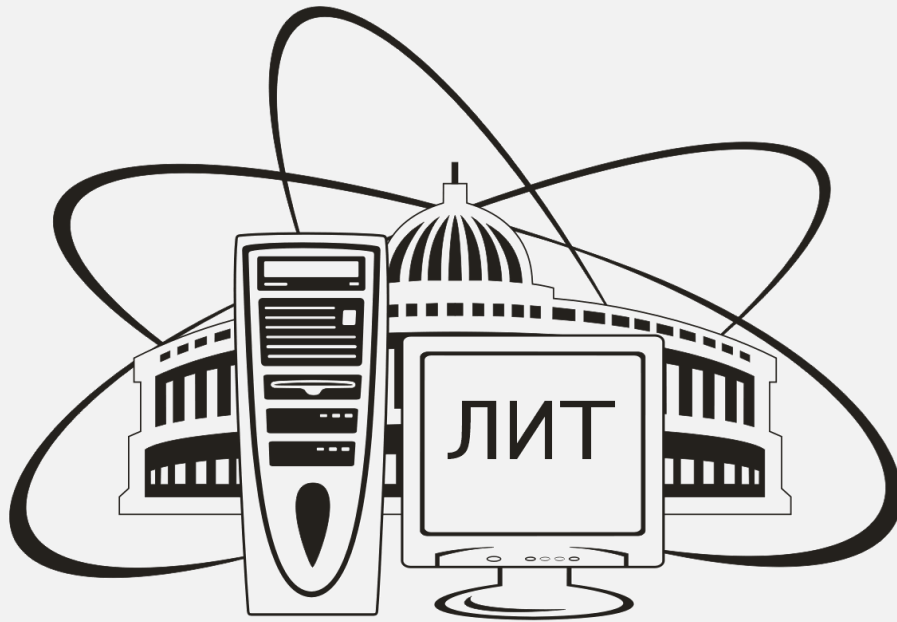
August 22 - 27, 2012, Dubna, Russia



MPAMCS 2012

INFORMATION

Thank you for attention!



HybriLIT: heterogeneous computation cluster

Summary of current version

252 CPU-cores, 77184 GPU-cores,
182 PHI-cores; 2.4 TB RAM; 55.2 TB HDD

Peak performance:

with single precision **142 TFlops**;

with double precision **50 TFlops**

Dell PowerEdge

- 2x Intel Xeon CPU E5-2695v3; - 4x NVIDIA TESLA K80

Supermicro SuperBlade Chassis

-2x Intel Xeon
CPU E5-2695v3
-2x NVIDIA TESLA K80

- 2x Intel Xeon
CPU E5-2695v2
3x NVIDIA TESLA K40

- 2x Intel Xeon
CPU E5-2695v2
- 6x HDD 1.2 TB

- 2x Intel Xeon
CPU E5-2695v2
- NVIDIA TESLA K20X
- Intel Xeon Phi
Coproprocessor 5110P

-2x Intel Xeon
CPU E5-2695v2
- 2x Intel Xeon Phi
Coproprocessor 7120P



HybriLIT: heterogeneous computation cluster

The cluster contains 10 computational nodes with graphical accelerators NVIDIA Tesla K20X, K40, K80, Intel Xeon Phi 7120P, 5110 coprocessors. All computational nodes include two Intel Xeon E5-2695v2 and V3 processors each.

Computation component **HybriLIT**

TOTAL RESOURCES

252 CPU cores;
77184 CUDA cores;
182 MIC cores;
~2,5 Tb RAM;
~57 Tb HDD.

HARDWARE



SuperBlade Chassis including 10 calculation blades for run user tasks.

7 blades include specific **GPU accelerator** sets. Driven by **NVIDIA CUDA** software.

1 blade includes **2 PHI accelerators**. Driven by **Intel MPSS** software.

1 blade includes **1 PHI and 1 GPU accelerators**. Mixed **NVIDIA CUDA** and **Intel MPSS** software.

1 blade includes **2 multi-core CPU processors**. Large ~7 Tb storage area



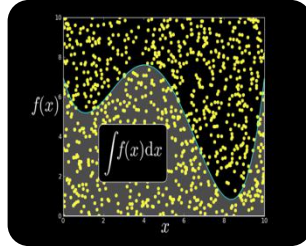
hYBRI



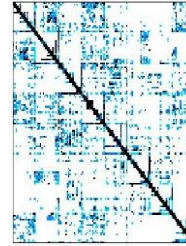
Some GPU-accelerated Libraries



NVIDIA cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE



NVIDIA NPP

GPU VSIPL

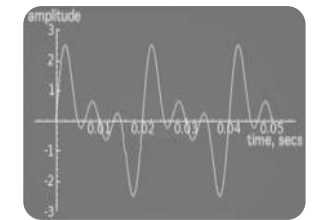
Vector Signal
Image Processing

CULA | tools

GPU Accelerated
Linear Algebra



Matrix Algebra
on GPU and
Multicore



NVIDIA cuFFT

ROGUE WAVE
SOFTWARE
IMSL Library



ArrayFire Matrix
Computations

CUSP

Sparse Linear
Algebra



C++ STL
Features for
CUDA