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LABORATORY OF INFORMATION TECHNOLOGIES
REPORT ON RESEARCH ACTIVITIES IN 2016

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The investigations performed in the Laboratory of information technologies during 2016 in frames of the JINR research field “Networks, Computing, and Computational Physics” were focused on two first priority themes, namely, "Information and Computing Infrastructure of JINR" and “Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data". The cooperation with other JINR laboratories involved the participation of the LIT staff in research work within 30 themes of the JINR Topical Plan for JINR research and international cooperation. The LIT activity is intended to provide a further development of the JINR network and information infrastructure, mathematical and software provision for research and production activity under way at JINR and its Member States on the base of advanced information and computer technologies.

For more than a decade, the development of the information and computing infrastructure of JINR created in LIT was done within the Central Information and Computing Complex (CICC) of JINR. In the last few years, in connection with work on the organization of the computing project for NICA, the commissioning of the grid-center Tier-1 for the CMS experiment, the implementations of a cloud computing structure and of a cluster for hybrid computing, the information-computing environment of JINR evolved in a set of stand-alone structures that have a common engineering infrastructure. Thus, it is possible to identify this structure as a Multifunctional Information and Computing Complex (MICC) of JINR, which currently has the following basic components:

- the Central Information and Computing Complex (CICC) of JINR with home built up compute elements (CE) and mass storage elements (SE),
- the grid-center Tier-2 site for experiments at the Large Hadron Collider (LHC) and other virtual organizations (VOs) in the grid environment,
- the grid-center Tier-1 for CMS experiment,
- the heterogeneous cluster "HybriLIT" for parallel computing,
- the cloud-based grid infrastructure,
- the training and research grid-cloud infrastructure.

The JINR MICC provides resources needed for different tasks, implied by many projects the JINR researchers take part in, namely: COMPASS, BESIII, DIRAC, HARP, CMS, ALICE, ATLAS, H1, NEMO, OPERA, PANDA, NoVA, STAR, LHCb etc. The JINR Tier-1 and Tier-2 are elements of the Russian Grid Segment used for LHC computing and other applications. The grid infrastructure at JINR is represented by CMS Tier-1 center and Tier-2 center for ALICE, ATLAS, LHCb and CMS. .

193 scientific papers were published by LIT researchers in referred journals and 47 reports were presented at international and Russian conferences in 2016.

Information and computing infrastructure of JINR

During 2016, the work related to the reliable operation and development of the JINR networking, informational and computing infrastructure was in progress. The key components of this infrastructure are the telecommunication data links, the JINR local area network (LAN), the CICC and the primary software, also on the basis of cloud-, grid- and hybrid technologies, integrating information resources of the Institute into a unified environment accessible to all users.

JINR telecommunication data links. In 2016, the reliable work of the high-speed computer communication channel Dubna-Moscow was secured. The connection with scientific networks and Internet used the following telecommunication links: LHCOPN/CERN (10 Gbps), RBnet (10 Gbps), E-arena and Russian scientific networks (10 Gbps), RUNet and international scientific networks (10 Gbps).

The throughput of the reserve data link was raised up to 10 Gbps and its reliability was improved at the expense of the addition of a supplementary router Cisco7606-S. The possibility of the gradual modernization of the external data link up to 100 Gbps has been studied and this work was finished at the end of 2016. The new Transmode equipment for this modernization was purchased and put into operation.

Table 1 shows the distribution of the incoming and outgoing traffics (more than 3TB incoming traffic) in 2016 over JINR subdivisions.

Table 1

Subdivision	Incoming (TB)	Outgoing (TB)
Laboratory of Nuclear Problems	125.98	154.99
Laboratory of High Energy Physics	102.43	90.68
General access servers	90.99	17.72
Laboratory of Information Technologies	62.13	34.79
Laboratory of Neutron Physics	49.2	63.15
University “Dubna”	48.98	38.43
Laboratory of Nuclear Reactions	37.6	18.18
JINR Management	26.82	58.2
JINR’s Hotel&Restaurant Complex	25.47	4.4
Node of remote access	24.05	5.74
Laboratory of Theoretical Physics	19.71	16.73
Joint Stock Company “Dedal”	10.78	5.97
Medical-Sanitary Unit-9	10.65	0.82
Laboratory of Radiation Biology	8.76	5.26
Resort Hotel Ratmino	7.77	2.08
Joint-Stock Company “Atom”	5.13	0.65
Procurement and Logistics Service	4.23	3.07
Chief Power Engineer’s Department	3.83	0.68

In 2016 the overall incoming JINR traffic, including the general access servers, Tier-1, Tier-2 and CICC amounted 14.2 PB (4.26 PB in 2015). The weights of the various incoming traffic categories are shown in Table 2.

Table 2

Scientific and educational networks	File exchange (p2p)	Web-resource	Social networks	Software
96.75%	2.32%	0.53 %	0.11%	0.29%

JINR local area network. In 2016, work was in progress on the further development and improvement of the JINR network IT-elements intended to increase the working efficiency of the JINR staff. The construction of the 10 GB network inside the laboratories was finished.

In frames of the user's computer environment support, the scheduled work has been done on enhancement of the IPDB, mail, webmail, proxy, e-lib and authorization services. For instance, work is carried out on the transition of the JINR subdivisions to the unified JINR mail service user@jinr.ru. An authorized WiFi has begun its operation on the JINR territory as well as services eduroam and VPN for remote work outside the JINR limits.

The JINR LAN includes 8222 network elements and 13364 IP addresses, 4301 users are registered at present within the network, 2341 users of mail.jinr.ru service as well as 1500 users of digital libraries and 371emote VPN users.

JINR Grid-environment. The Tier-1 center for CMS at JINR was put into a full-operation mode in March 2015. By the end of 2016 the JINR Tier1 resources comprise: a computing power of 55.16 kHS06, 3600 cores/slots (11 Supermicro Twin blades), a disk capacity of 4037 TB (30 Disk servers with hardware RAID6) and 521.88 TB used as a buffer for tape storage (8 Disk servers with hardware RAID6), a tape space of 5478.32 TB (IBM TS3500 tape library with 8 x FC8 links to 8 Disk servers). The network is configured as two redundant triangles shared with the NRC "Kurchatov institute" with 10 Gbit/sec LHCOPN connection.

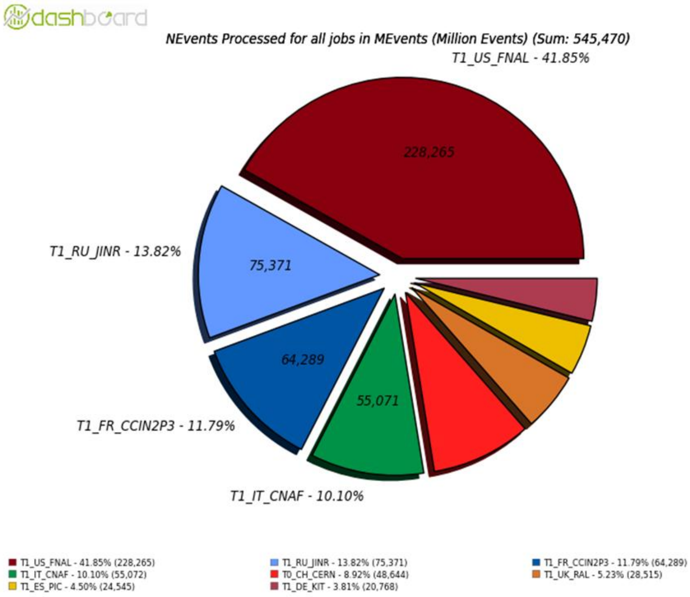

Fig.1. Number of events processed for all CMS Tier-1 in Million of Events in 2016

The mass storage systems are built on dCache and Enstore as a tape backend for dCache. Totally, 2 installations have now 4.PB of effective disk space, and the tape robot has a 5.4 PB of data storage capacity. To support the storage and access to data, 8 physical and 14 virtual machines have been installed.

Torque/Maui is used as a scheduler. The standard WLCG software stack was used for computing: 2 x CREAM, 4 x ARGUS, BDII top, BDII site, APEL parsers, APEL publisher, EMI-UI, 220 x EMI-WN + gLExec-wn, 4 x FTS3, LFC, WMS, L&B, glite-proxyrenewal.

The JINR CMS Tier-1 has shown its stable state for the whole period after putting it into the full-operation mode [1]. During 2016, this center performed 8 257 163 tasks, using a normalized CPU time of 237 346 520 hours in HEPSpec06 units. Figure 1 gives the contribution of the Tier-1 global centers to the CMS experimental data processing (in MEvents) for the year of 2016. The JINR Site takes one of the leading ranks in the world as to its productivity.

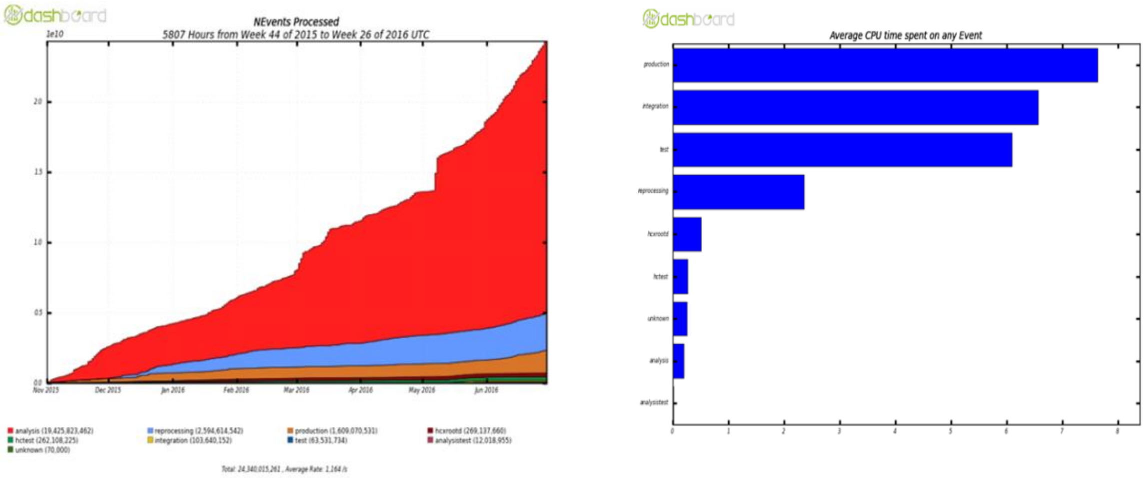

Fig.2. Number of events processed at the JINR CMS Tier-1 in June 2016 by the CMS activities (production, integration, reprocessing, analysis, etc.)

Figure 2 shows the number of events processed at the JINR CMS Tier-1 in June 2016 by the CMS activities (production, reprocessing, analysis, etc.)

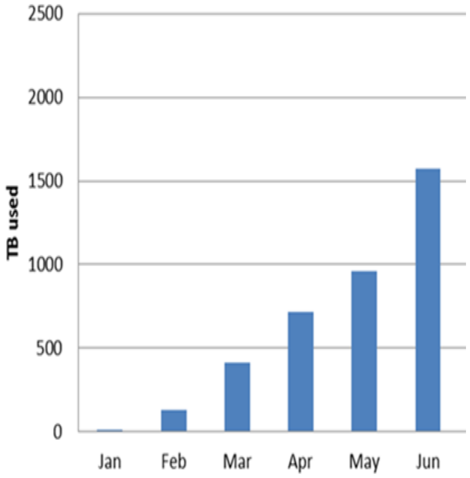

Fig. 3: JINR Tier-1 CMS tape robot load

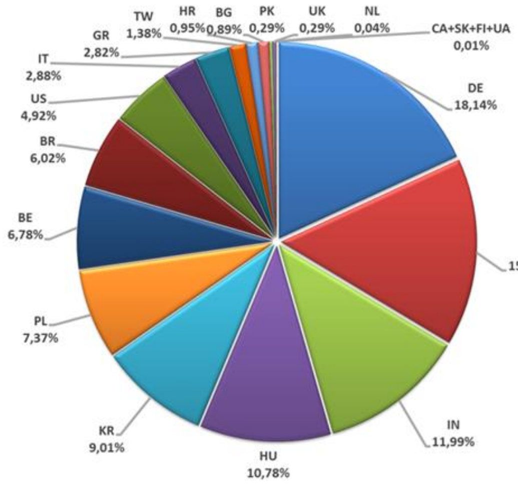

Fig.4. The requests from the Tier-1 and Tier-2 centres to the JINR CMS Tier-1 for data in June 2016

One of the main functions of the Tier-1 centres is the archival storage of raw experimental and simulated data. Figure 3 shows the load of our tape robot during 2016. Figure 4 illustrates the requests from the Tier-1 and Tier-2 centres worldwide to the JINR CMS Tier-1 for data in June

2016. The average rate for RAW data transfers to the JINR CMS Tier-1 site is 250-300 MB/s, more than 1 TB/hour was transferred.

The JINR Tier-2 center supports a number of Virtual Organizations, in particular, ALICE, ATLAS, BES, BIOMED, CMS, HONE, FUSION, LHCB, MPD, NOVA, STAR. The JINR Tier-2 computing resources comprise 2470 cores/slots, 46.72 kHS06; disk capacity: 587.46 TB for ALICE, 641.87 TB for ATLAS, 659.31 TB for CMS.

We are working on integration of OSG type Computing Element - HT-CONDOR in our WLCG Tier-2 infrastructure. At the moment it is for STAR VO mainly, but can be extended for support other VOs in the future.

The main users of the JINR grid-resources are virtual organizations of all LHC experiments [2]. In 2016 this site executed 4 185 956 jobs (3 912 779 for LHC), CPU time being 186 711 011 hours in HEPSpec06 units. Figure 5 summarizes data on using the grid-site JINR-LCG2 by the virtual organizations within the RDIG/WLCG/EGI community in 2016.

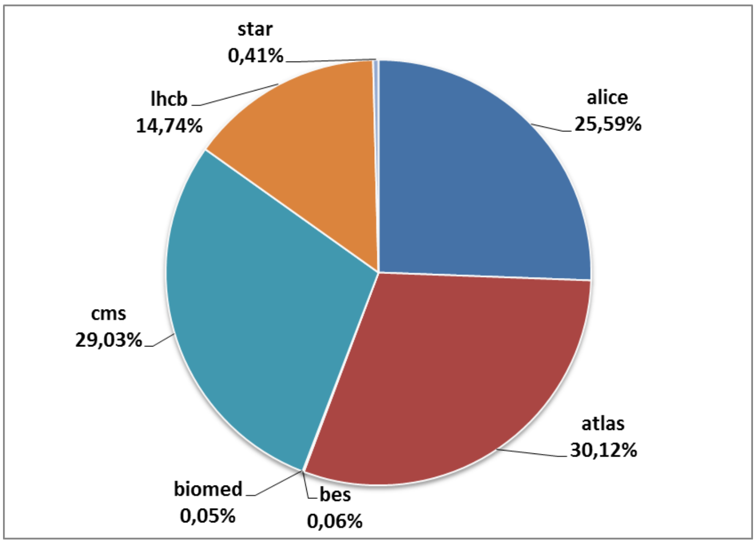

Fig.5. Using the JINR-LCG2 grid-site by virtual organizations within RDIG/WLCG/EGI

PanDA, production and distributed analysis system, manages jobs for ATLAS since 2005. Since that time the system has grown up and in 2013 the BigPanDA project started, aiming to prepare packets of PanDA which can be used by outside the LHC. One of the experiments to which production management PanDA is being applied, is COMPASS at CERN. The workflow of the experiment has to be changed to enable Grid for production and user jobs. Lots of the infrastructure work should be performed. PanDA job definition replaces native batch system job definition, automatic submission to Condor computing elements comes in place of console job submission, Grid user certificates identify job submitters instead of AFS user names, Grid storage elements substitute local directories on AFS and EOS. Production software moves from private directory of production account to CVMFS. Also, a virtual organization with role management has to be established for the experiment. In this year the JINR as a computing site for COMPASS was connected through PanDA, i.e., allocate the space and define PanDA queue at JINR's computing infrastructure; define PanDA queues in other participating in COMPASS institutes and make their data analysis distributed [3].

The JINR MICC monitoring system provides real-time information about: work nodes, disk servers, network equipment, uninterruptable power supply elements, and cooling system. It also can be used for creating network maps and network equipment load maps, for drawing state tables and different plots. Special Control room was equipped for operators of the MICC (Fig.6).

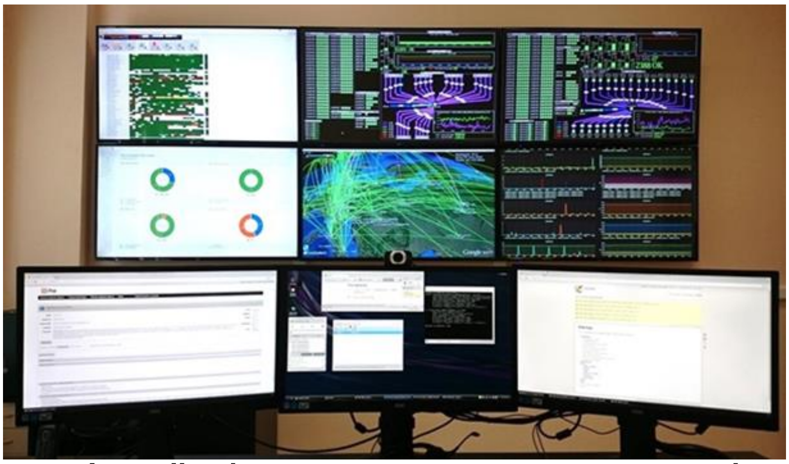

Fig.6. Video Wall with HappyFace monitoring system at Control Room

HappyFace monitoring system was installed and configured for the purposes of JINR Tier-1. It is a product developed in KIT for monitoring grid sites of CMS and ATLAS experiments. Currently it is one of the key elements of JINR Tier-1 services monitoring (http://happyface.jinr.ru).

Development of the new service monitoring system for CMS Tier-1 in JINR was initiated. The system has modular structure. The next modules was developed: Job Status – to determine the number of executed and aborted jobs; SSB Status – to collect monitoring results performed by WLCG Dashboard; PhedexQuality – to determine transfers quality from other grid-sites and T1_RU_JINR; PhedexErrors – to determine Phedex errors connected to T1_RU_JINR. The test version of the service monitoring system was lunched at lcgsens01o.jinr.ru. Now it aggregates and displays on the web page data related to Phedex, dCache and WLCG monitoring [4]. The system is developing as a general purpose tool which could lately be adapted for other Tier-1 centers and experiments.

High-performance computer system. The multipurpose information complex in LIT provides carrying out computations, including the parallel ones, outside the grid-environment. They are asked both by the experiments NoVA, PANDA, BES, NICA/MPD, etc. and the local users of the JINR Laboratories. The JINR users and the grid users have access to all the computer facilities via a unified batch processing system. Figure 7 gives the time distribution of the tasks executed on the computing cluster by the JINR subdivisions and the user groups. The main user of these resources is NICA/MPD (61.07% of astronomic time and 55.53% of processor time).

Systems of storage and access to data dCache and XROOTD ensure work with the data both for local JINR users and for the WLCG users and collaborations. Two dCache installations are supported: dCache-1 for experiments CMS and ATLAS; dCache-2 for local users, groups of users and international projects NICA/MPD, HONE, FUSION, BIOMED, COMPASS. Two installations of the XROOTD data access arrangement maintain work with data of three international collaborations: ALICE, PANDA and CBM. All the storage systems are constructed under the hardware data protection mechanism RAID6.

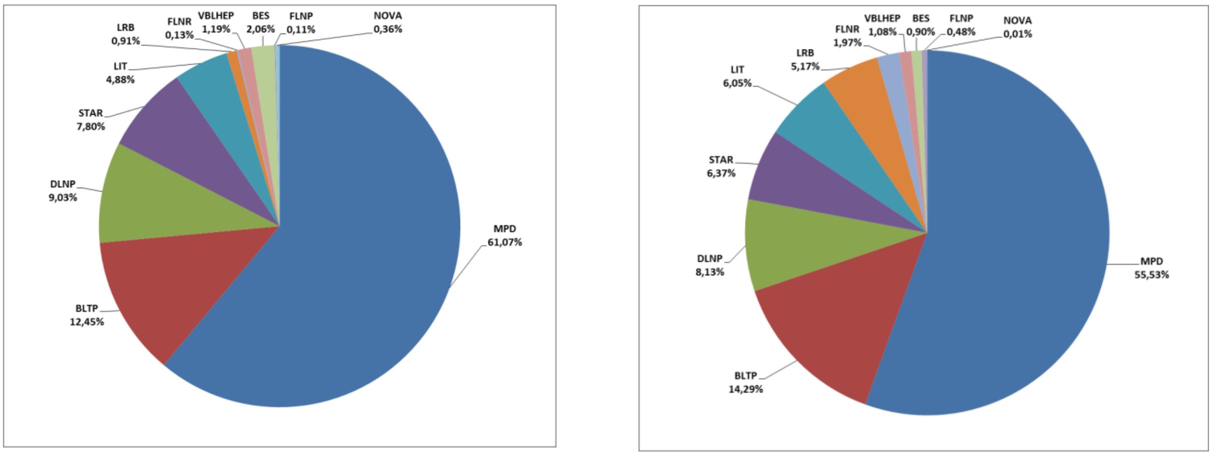

Fig.7. Statistics of using astronomic (left) and processor time (right) of the computing cluster by the subdivisions and experiments of JINR without grid users

A system for grid and cloud services simulation of contemporary HENP experiments of the Big Data scale was developed. This simulation system is focused on improving the efficiency of the grid/cloud structures development by using the work quality indicators of some real system. This system is intended to improve the efficiency of the design and development of a wide class of grid-cloud structures by using the work quality indicators of some real system to design and predict its evolution. For these purposes the simulation program is combined with a real monitoring system of the grid-cloud service through a special database (DB). The DB accomplishes acquisition and analysis of monitoring data to carry out dynamical corrections of the simulation. Such an approach allows us to construct a general model pattern which should not depend on a specific simulated object, while the parameters describing this object can be used as input to run the pattern. The development of such kind software is very important for making a new grid/cloud infrastructure for such big scientific experiments like the NICA/MPD/SPD Tier-0/Tier-1 distributed computing [5,6]. The NICA includes the BM@N experiment first run of which is planned to be performed in 2017. Therefore, it is necessary to develop a computing system for distributed data storing and processing for the experiment. The simulation program SyMSim is used to choose a proper architecture of the BM@N computing system infrastructure. SyMSim facilitates making a decision regarding a required equipment [7].

Heterogeneous computing cluster HybriLIT. During 2016 the total performance of the HybriLIT cluster increased 1.8 times. At the moment, the computing component of the cluster contains four nodes with NVIDIA Tesla K80 graphical processors and four nodes with NVIDIA Tesla K40 accelerators, a node with Intel Xeon Phi7120P coprocessors and a node with two types of computing accelerators NVIDIA Tesla K20x and Intel Xeon Phi 5110P. All the nodes have two multi-core processors Intel Xeon. Overall, the cluster contains 252 CPU cores, 77184 GPU cores, 182 PHI-cores, it has 2.4 TB RAM and 57.6 TB HDD, and its total capacity is 142 Tflops for operations with single precision and 50 TFlops for double precision.

In 2016, a new component was included in the cluster structure - a virtual desktop system to support users work with applied packages. Deployed was a polygon of eight servers where on the basis of KVM (Kernel-based Virtual Machine) virtual desktops with remote access to the package COMSOL Multiphysics for user groups have been designed. The developed new cluster's component allows the users to effectively utilize the cluster's resources conducting intensive calculations from the applied software packages on the computing nodes of the cluster (Figure 8).

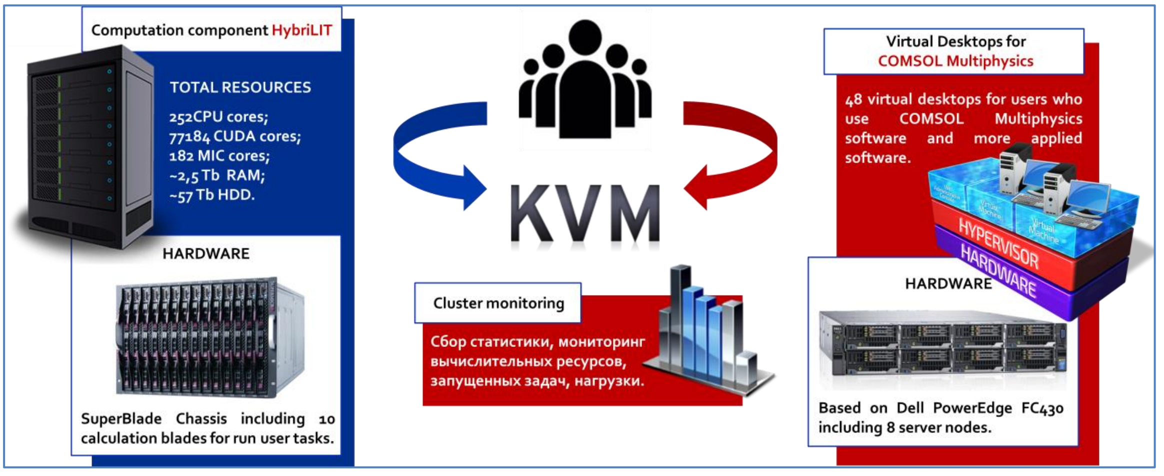

Fig.8.The new component of the cluster to work with applied packages.

In 2016, the software and information environment of the cluster was actively maintained and developed allowing its users to develop software applications, to perform calculations with the help of the latest computational architectures. The total number of its users is 450 people from the JINR laboratories and the JINR Member States. In particular, the cluster resources are used for calculations in the field of quantum chromodynamics, quantum mechanics and molecular dynamics. In addition, software PandaRoot, MpdRoot installed on the cluster allows one to perform calculations in high energy physics.

The heterogeneous cluster HybriLIT is used both to perform massively parallel computations and to learn how to use applied software packages and parallel programming technologies. During 2016, over 20 training courses were held which were attended by over 200 specialists from various departments of the Institute, young scientists from the JINR Member States and Russia universities.

The tutorials were dedicated to using applied packages MCTDHB-Lab, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), VMD (Visual Molecular Dynamics) and parallel programming technologies CUDA, OpenMP, OpenCL, and MPI. Tutorials and master classes were held in frames of the 7th International conference "Distributed Computing and Grid-technologies in Science and Education" (GRID'2016) and the JINR-CERN School "Grid and Advanced Information Systems".

Cloud environment. In 2016, the JINR cloud infrastructure [8] has been developing due to the following directions: increasing a number of resources its users have access to; increasing a number of tasks it is used for; re-implementing an aggregation and visualization statistics on the cloud resources utilization using InfluxDB and Grafana software. The amount of the resources available for the JINR cloud users has been increased due to 1) maintaining additional servers as cloud nodes and 2) integration of part of computing resources of partner's organizations clouds.

At present, the total number of CPU cores available for users in the JINR cloud is 330 (200 in 2015) and the total RAM is 840 GB (400 GB in 2015). The spectrum of the task solved with the help of the JINR increases. For this purpose, the following components have been installed on this infrastructure:

- PanDA testbed was deployed for PanDA software validation and extensions development for ATLAS and COMPASS experiments;
- DIRAC-based testbed (it is used for monitoring tools development for BESIII experiment distributed computing infrastructure as well as its computing facility);
- a set of VMs of NOvA experiment users for analysis and software development;
- NICA testbed for grid middleware evaluation for NICA computing model development;
- EOS testbed for research on heterogeneous cyber-infrastructures, computing federation prototype creation and development based on high performance computing, cloud computing and supercomputing for Big Data storage, processing and analysis;
- a standalone Spark instance for Machine Learning and BigData analysis.

At present, one of the most important trends in the cloud technologies is the development of method of integrating various cloud infrastructures [9]. 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 (and in this case it is possible to enable real time external cloud resources monitoring) or any other cloud platform which supports Open Cloud Computing Interface (OCCI). The clouds of the following partner organizations from JINR Member States are integrated with the JINR cloud:

Institute of Physics of Azerbaijan National Academy of Sciences (Baku, Azerbaijan); Bogoliubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine (Kiev, Ukraine); Plekhanov Russian University of Economics – PRUE (Moscow, Russia). The geographical location of the organizations from JINR Member States whose cloud resources are integrated into the JINR cloud following the so-called "cloud bursting" model, are shown on Figure 9.

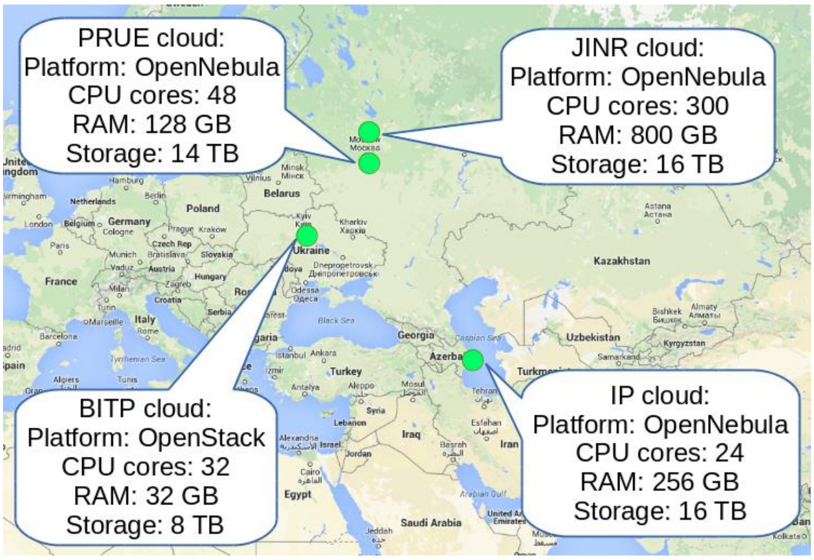

Fig. 9.Geographical locations of the partner cloud infrastructures from JINR Member States which provide part of their computational resources being integrated into the JINR cloud.

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.

Currently, one of the most important directions of the JINR cloud development is a re-implementation of an aggregation and visualization statistics on resources utilization. Initially it was done by JINR cloud team as an additional item in a menu of OpenNebula graphical web-interface (which is called "Sunstone"). However, a drawback of the implementation was a necessity to check a compatibility of that aggregation and visualization add-on against each new release of OpenNebula because its web-interface might be changed. It was needed to adopt the code of visualization module for the new Sunstone in case of its incompatibility. So in order to avoid such extra steps before software update on the JINR cloud as well as to store a collecting metrics in a database for further analysis against their changes over time and to obtain the dynamics for the selected period it was decided to implement aggregation and visualization statistics on JINR cloud resources utilization using such tools as InfluxDB and Grafana software [10].

Information and software support. A traditional direction of LIT activity in 2016 is the development and the support of the program library JINRLIB as well as support of the program libraries (CERNLIB, CPC Program Library) developed by other research centres and organizations. The JINRLIB web-site was renovated. A special section for parallel programs was added together with educational programs on parallel programming (MPI). The H-Utils package that is being developed in LIT for the HybriLIT users was included in the JINRLIB (http://wwwinfo.jinr.ru/programs/jinrlib/h-utils/index.html). This package contains a number of libraries and is aimed at help in solving general difficulties that the developers often faced while creating software complexes for solving problems in the field of physics, chemistry, biology, etc. on high performance computational platforms.

In frames of the development of the JINR corporate information systems (CIS) [11], a subsystem of the electronic coordination of orders on the basic activity has been developed and put into operation in the structure of the system “Base of JINR documents”, a universal gateway for data exchange between different CIS subsystems 1C, EDH “Dubna”, ADB2, ISS, PIN was implemented in 2016; work was in progress on enhancing the functionality of the information system of the NICA project management based on base of ADB system, implementation of functionality on the formation of Cost Book for the NICA project, realization of functionality on the formation of various consolidated reports on the project [12]; the development of the unified system 1C 8.2 UPP was in progress, a regular support of the end-users of the system also continued in 2016.

In 2016, the functioning of the system of electronic document handling (EDH "Dubna") created in LIT in 2015, continued. During the year, more than 1000 documents were processed by the system. The system has proved its working capacity and efficiency. Simultaneously with the operation, the system was intensively developed and adapted to the specific requirements of JINR. Developed was a series of specialized reports, documents "Supply Agreement", "Paid Services Agreement", "Agreement on performance of research work" as well as "Supplementary Agreement" to these contracts have been prepared to run. To achieve the successful development of the system with minimal expenses of the human and material resources was possible due to applying the principles of a flexible development methodology ("agile software development") as well as due to the use of the experinece accumulated at JINR in the field of the development of information systems. It is planned to significantly increase the number of documents processed in the system EDH "Dubna" in 2017.

In 2016, the improvement of the software for the JINR Document Server (JDS) was in progress, namely, tools have been developed to speed up data entry, improved was the quality of the content and efficient data re-use. The work is carried out on the test server jds-test3 (http://jds-test3.jinr.ru) deployed in the cloud infrastructures of LIT JINR.

METHODS, ALGORITHMS AND SOFTWARE FOR MODELING PHYSICAL SYSTEM, MATHEMATICAL PROCESSING AND ANALYSIS OF EXPERIMENTAL DATA

One of the main directions of the research activity at LIT is to provide a mathematical, algorithmic and software support of the experimental and theoretical research underway at JINR. Below there is a brief report on some results.

Event reconstruction is one of the most important problems in high energy physics experiments. It consists of track finding and track fitting procedures in the experiment tracking detectors. This requires a tremendous search of detector responses belonging to each track aimed at obtaining the so-called “seeds”', i.e. the initial approximations of track parameters of charged particles.

BM@N (Baryonic Matter at Nuclotron) is a fixed target experiment at the Nuclotron to study *A+A* collisions by measuring a variety of observables. The proposed setup for this experiment is shown in Figure 10.

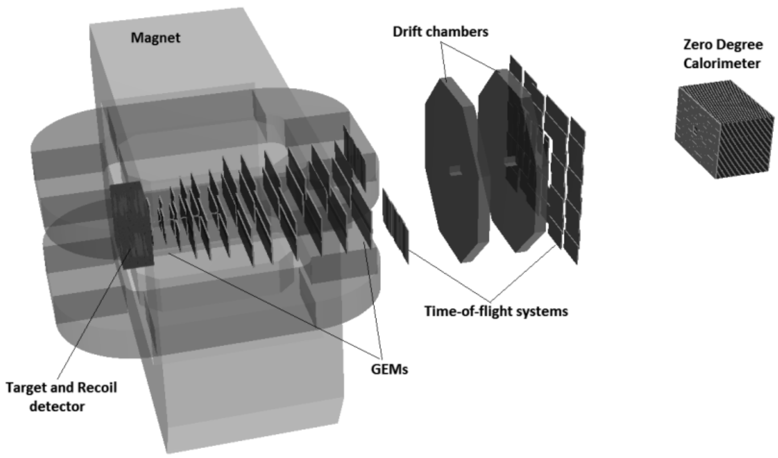

Fig. 10. Setup of the BM@N experiment

The event reconstruction for the BM@N experiment consists in finding track seeds in the GEM detectors and then their extrapolation by Kalman filter to other detectors. As one can see from the left image of the Figure 11, the seed finding problem is really a hard and time consuming one on any projection due to overcrowding the area of search by hits (*hit* is an reconstructed spatial point of crossing track and sub-detector system).

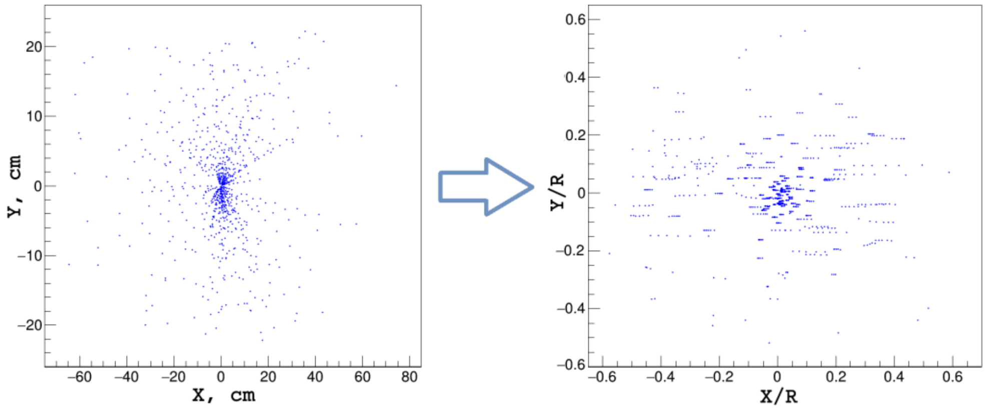

Fig. 11. Left: XY view of a simulated data for the BM@N facility; right: representation of the same tracks after using proposed transformation

To find a seed from the set of hits registered by a tracking detector, one should classify somehow those hits by their closeness to particle trajectories. There are several methods which are used to achieve that, namely, Hough transform, elastic tracking, cellular automaton, etc, with their advantages and shortcomings. We propose here a new transformation of the coordinate system:

$$\{X, Y\} \rightarrow \{\frac{X}{R}, \frac{Y}{R}\},$$

where $R = \sqrt{x^2 + y^2 + z^2}$.

This transformation converts experimental data into a space of normalized coordinates where the hits corresponding to one track are grouped more compact (the right image, Figure 11) and almost horizontally.

An appropriate algorithm of the fast horizontal histogramming for track-candidate search has been proposed in order to find track-candidates as groups of closed hits satisfying to special acceptance criteria. The found track-candidates are approximated by Archimedean spirals to estimate the required track parameters (momentum, charge, vertex, etc.). The proposed algorithm of horizontal histogramming reveals an opportunity to be parallelized on modern computers.

Distribution of the efficiency and the percentage of the ghost-tracks and clones is shown on the left pad of the Figure 12. A momentum distribution is presented on the right pad of Figure 12.

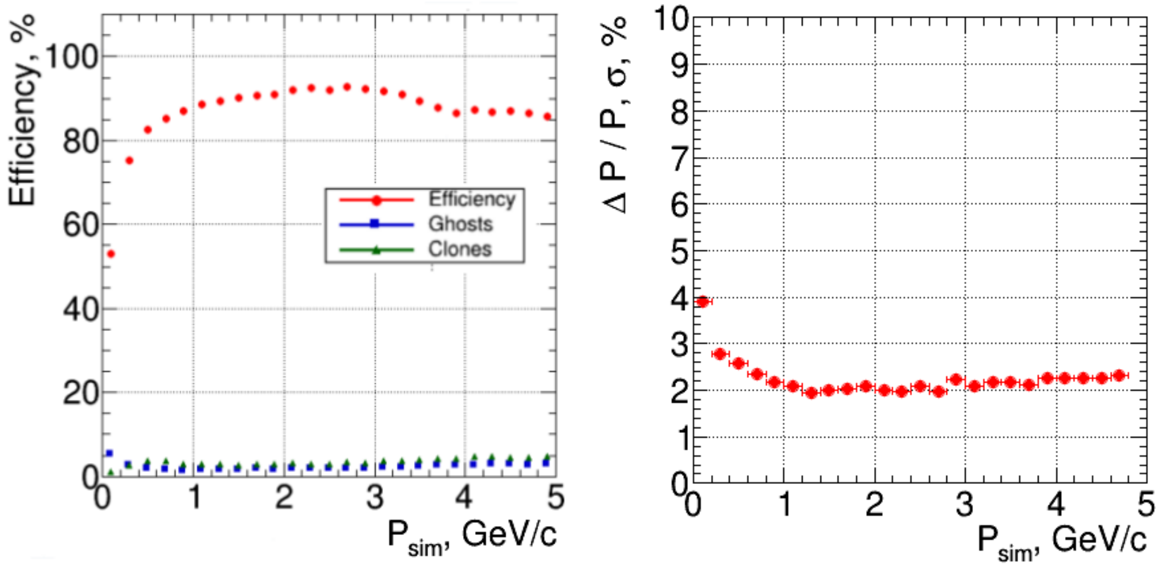

Fig. 12. BM@N track reconstruction efficiency and momentum resolution for Au+Au collision

In case of high multiplicity, the problem of the fake hits gets extremely important. We proposed a new approach with applying Lorenz potential to reject the fake hits [13].

A computer program of the Glauber calculations for the NICA experiments has been proposed. It should be noted that all contemporary experiments with relativistic nuclear beams (RHIC, LHC, NICA, CBM) use and will use various methods of determining the geometrical properties of interactions, especially collision impact parameter. No impact parameter can be measured directly. That is why the experimental observable quantities are connected, in one or another manner, with the geometrical properties calculated within the Glauber approach. However, the existing methods of the Glauber calculations do not met modern requirements. The proposed approach allows one to calculate the geometrical properties of interactions of gold nuclei with gold nuclei at RHIC and NICA energies (5 – 10 GeV in the center of mass of NN collisions) and to improve the result on 5 – 7 % as compared to the currently used software. The changes of the physical characteristics of NICA collisions can be related to changing the interaction physics [14].

A new segment building algorithm for the cathode-strip chambers has been developed. There were obtained results of comparison of the standard and new algorithm for various types of simulated data. Track-segments are reconstructed with higher precision and efficiency using the new algorithm, especially for high luminosity on the LHC and high transverse momentum of particles passing through the muon endcap system. In July 2016, the algorithm was implemented in the official CMS reconstruction software package [15].

Effects of vector interaction in Nambu-Jona-Lasinio model with Polyakov loop have been studied in combination with entanglement interaction between quark and pure gauge sector. Investigated was the QCD phase diagram. It has been found find that the first-order chiral phase transition at the finite baryon chemical potentials and its critical point disappear at sufficiently large values of the vector interaction constant G_V. The presence of entanglement interaction between the quark and pure gauge sector leads to the increasing of value G_V when the first-order phase transition in the thermodynamic system disappears. The influence of non-zero G_V on the curvature of the crossover boundary in the $T - \mu$ plane nearby $\mu = 0$ is also examine for the cases of the additional quark-gluon interaction and without it [16].

The Asynchronous Differential Evolution (ADE) method is applied to research on the drug delivery Phospholipid Transport Nano System (PTNS) in frames of the Separated Form Factor model. Basic parameters of PTNS unilamellar vesicles are fitted to experimental data of the small angle synchrotron X-ray scattering. The structure of PTNS nano-particles has been analyzed depending on the maltose concentration in water. Numerical results confirm the efficiency of parallel MPI-implementation and the preference of the ADE-based global minimization in comparison to other popular optimizing procedures [17].

A new approach is proposed to the high-order polynomial approximation (smoothing) based on the basic elements method (BEM.) The design of the BEM-polynomial is built on a three-point grid and depends on the control parameters $x_0, \alpha = x_\alpha - x_0,\ \beta = x_\beta - x_0$ related to the independent variable $\tau = x - x_0$ by a cross-ratio rule. The n^{th}-degree BEM-polynomial is expressed using four basic elements given on the three-point grid: $x_0 + \alpha < x_0 < x_0 + \beta,\ \alpha\beta < 0$. Formulas were obtained for calculating the coefficients of the 12-th order polynomial model depending on the interval length, the parameters α, β and the derivatives $f^{(m)}(x_0 + \nu),\ \nu = \alpha, \beta, 0,\ m = \overline{0,3}$. Application of the high degree BEM-polynomials for piecewise polynomial approximation of functions and data smoothing enhances the stability and accuracy of calculations when increasing the grid step and reduces the computing complexity as well [18].

Two conceptual developments in the Bayesian automatic adaptive quadrature approach to the numerical solution of one-dimensional Riemann integrals [Gh. Adam, S. Adam, Springer LNCS 7125, 1–16 (2012)] are reported. First, it is shown that the numerical quadrature which avoids the overcomputing and minimizes the hidden floating point loss of precision asks for the consideration of three classes of integration domain lengths endowed with specific quadrature sums: microscopic (trapezoidal rule), mesoscopic (Simpson rule), and macroscopic (quadrature sums of high algebraic degrees of precision). Second, sensitive diagnostic tools for the Bayesian inference on macroscopic ranges, coming from the use of Clenshaw-Curtis quadrature, are derived [19].

A research work was in progress at LIT on the problem of mathematical description of quantum correlations in composite systems. A problem of classification and correlations in systems being in so-called X-states was studied within the mathematical framework of the classical theory of invariants by means of advanced methods of computer algebra. Quantum entanglement properties of a mixed two-qubit system in mixed X-states were analyzed in terms of local unitary invariant polynomials in the elements of the density matrix [20]. The structure of the ring of invariant polynomials was studied, and it is shown that for the X-states there is an injective ring homomorphism of the quotient ring of SU (2) × SU (2)-invariant polynomials modulo its syzygy ideal and SO(2) × SO(2)-invariant ring freely generated by five homogeneous polynomials of degrees 1, 1, 1, 2, 2. The separable mixed 2-qubit X-states are classified in accordance with degeneracies in the spectrum of density matrices [21].

APPLIED RESEARCH

The aim of the UNECE ICP Vegetation program is to identify the main polluted areas, produce regional maps and further develop the understanding of the long-range transboundary pollution. Since January 2014, the coordination of moss surveys in 36 European and Asian countries has been conducted from the JINR in Russia. The ICP Vegetation programme is very important project, but it has a serious weakness related to its weak adoption of modern informational technologies. There are dozens of respondents in the existing monitoring network and their number is increasing, but information on collecting and pro-cessing of samples is carried out manually or with minimum automation. Data mostly stored in xls files and aggregated manually by the coordinator. Files from respondents are usually passed to the coordinator by email or by ordinary mail. There are no common standards in data transfer, storing and processing software. Such situation does not meet the modern standards for quality, effectiveness and speed of research. Lack of a single web-platform that provides comprehensive solution of biological monitoring and forecasting tasks is a major problem for research.

To optimize the whole procedure of data management, it is proposed to build a unified platform consisting of a set of interconnected services and tools to be developed, deployed and hosted in the JINR cloud. Sampling results from the contributors are saved at MongoDB that was designed for ease of development and scaling. The portal back-end is based on Nginx and developed with PHP and AJAX. Basic statics and indicator calculation is done with PHP. OpenLayers is used for regional and global maps representation. The general architecture of the platform and technologies used are depicted in Figure 13.

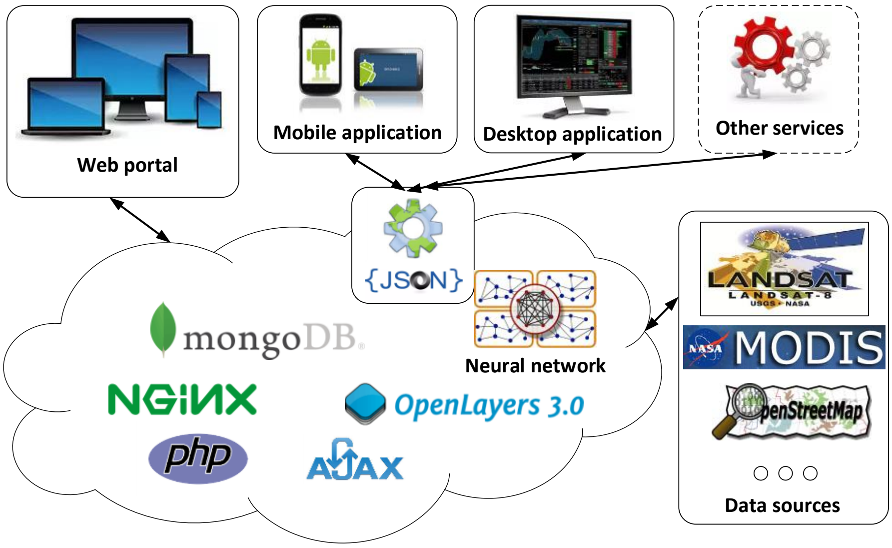

Fig. 13. General architecture of the platform and technologies used

The web-portal with responsive design that adjusts to different screen sizes is the main interface of the platform. The portal allows multilevel access to the data and has advanced data processing and reporting mechanisms. There are two parts of the portal – public and private ones. A general information about the project and the platform is presented in the public part. The private part can be accessed only by authorized contributors. Users can manage the project/regions and data samples in the private part. Data samples can be added manually or imported from xls files. Users can get statistical information about their datasets and build distribution or graduated symbol maps. Some screenshots of web-portal interface are shown on the Figure 14.

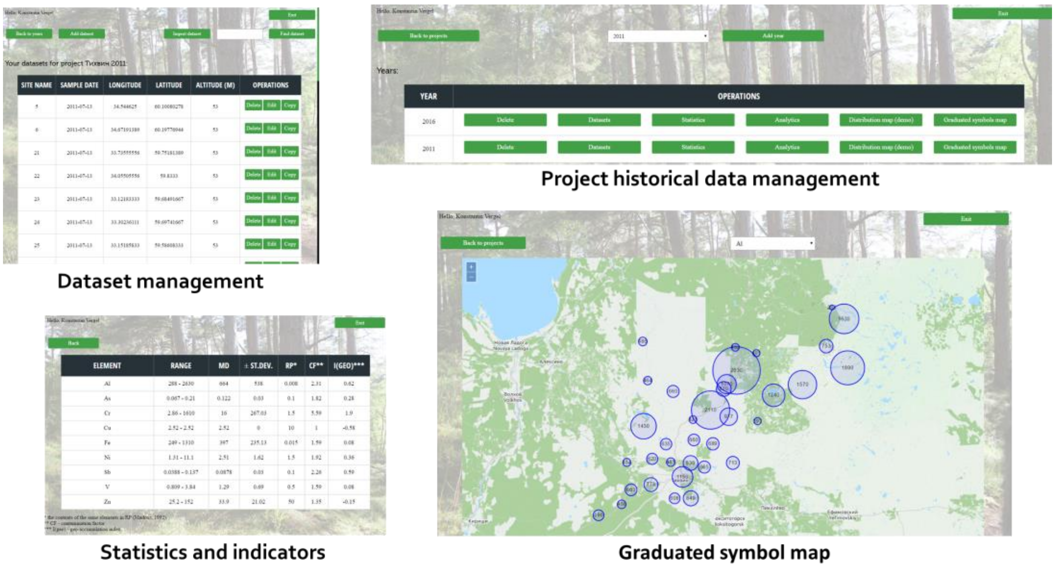

Fig. 14. Web-portal interfaces. Top-left – public part of the portal. Top-right – dataset management interface. Bottom-left – Statistics, factors and indexes calculation for dataset. Bottom-right – graduated symbol map for dataset

Prediction is an important step of the data analysis of any ecological survey. Application of prediction methods enables mapping of estimate values. Maps in their turn provide visualization of spatial variability of data and can be used for visual analysis so that ecological hazards can be identified. We propose to use neural network together with satellite spectroradiometer products, as surface reflectance, land surface, temperature, land cover, vegetation indices, land use to model the statistical relations between element concentrations in moss and potential explanatory variables. This approach has been already tried on the modeled data. A result was a nice concentration map with quite law discrepancy. LANDSAT, MODIS and OpenSteetMap are considered as source of the satellite and GIS data. Currently the work on import of the satellite spectroradiometer and other useful for neural network data is in progress. Another actual task is determination of the correlated parameters for concentration distribution and integration of the neural network program and the portal [22].

LIT researchers in cooperation with VBLHEP scientists conduct research on the behavior of the solution to the nonlinear boundary-value magnetostatic problem in a vicinity of the "corner point" (the intersection of two environments-vacuum/iron) of ferromagnet The upper estimate for the acceptable growth of the magnetic field in the vacuum region near the corner point of the ferromagnet has been obtained. It is shown that under certain conditions imposed on the magnetic permeability, the magnetic field within the vacuum region in the vicinity of the corner points is limited. An algorithm of thickening differential grid near the corner point has been developed. It allows one to significantly reduce the computation time and simultaneously to increase the accuracy of the solution of the boundary value problem. The results of modeling the magnetic system containing corner points are presented. The problems of creating a homogeneous map of the field of possible solenoid-type magnetic systems of the NICA installation are analyzed. The computations were performed with the help of two software products, i.e. TOSCA and MFC (Magnetic Field Calculation) developed by the authors [23].

INTERNATIONAL COOPERATION

In cooperation with scientists from South Africa, the inclusive reaction 59Co(p,α) at an incident energy of 100 MeV has been studied. A theoretical analysis based on a statistical multistep mechanism indicates that the terminal step leading to emission of an α-particle can be a pickup or knockout process, in which both are very prominent. This is a conclusion which is in agreement with an earlier study of the 93Nb(p,α) reaction. This inspires an investigation of the reason why a mixture of knockout and pickup is present at incident energy of 100 MeV, whereas at both higher and lower incident energies knockout appears to dominate for the target nucleus 93Nb. It has been found that the different dynamics of the two competing reaction mechanisms provides explanation for the observed phenomenon. It is speculated that for 59Co at both lower and higher incident energies the trend is likely to besimilar to that of 93Nb [24].

In collaboration with scientists from research centers of the USA, the development of the workflows management system PanDA (Production and Data Analysis) has been proposed which allows one to send tasks to supercomputing computing platforms. This development was tested on the Titan supercomputer (Oak Ridge Leadership Computing Facility, USA), supercomputer of the National Research Center "Kurchatov Institute", supercomputer IT4 (Ostrava, Czech Republic) and others. The testing has shown a possibility of using the modified PanDA WMS as a portal, independent of a computing infrastructure which can be used not only for solving intensive tasks of high energy physics and nuclear physics, but also in other fields such as bioinformatics and astrophysics [25].

In 2016, in collaboration with colleagues from China and France work was in progress on the creation of a distributed computing environment for the experiment BES-III which currently joins 12 resource centers from China, USA, Italy, JINR, and providing access to more than 3000 CPU cores and 0.5 PB disk space. In the current year, more than half a million tasks were executed in this distributed system. To date, the distributed data processing system of the BES-III experiment is reliable, it is a significant part of the computing power for experimental data processing [26].

CONFERENCES, WORKSHOPS

On January 25-30, 2016 LIT hosted the XXIII International conference «Mathematics. Computer. Education». The Conference has been held since 1993 and manifested itself as a productive form of exchanging experience between specialists in various scientific directions including mathematicians, biologists, economists, teachers. 250 scientists from the JINR-participating countries and 32 cities of Russia, Ukraine, Belarus, and Kazakhstan attended the Conference. A symposium "Biophysics of complex systems. Molecular modeling. System biology" was organized in the framework of the conference. Some sessions on mathematics, mathematical simulation and computing methods, biology, economy and pedagogy included oral and poster reports. Alongside with the traditional round tables 11 maser-classes were organized to get acquainted with the basics of the modern high-level programming languages and their applications to modeling in solving research problems. The conference was traditionally brought to an end with a discussion of the work of the sections and awarding young participants with certificates for the best reports.

A traditional 19-th two-day Workshop on Computer Algebra was held at the Laboratory of Information Technologies (JINR) on May 24-25, 2016. More than 40 scientists from universities and scientific institutes of Bucharest (Romania), St. George's (Grenada), Tbilisi (Georgia), Turku

(Finland), Moscow, Petrozavodsk, St. Petersburg, Saratov, Tambov and Dubna took part in this Workshop. 24 reports were presented. The main goal of these workshops is to provide a forum for researchers on computer algebra methods, algorithms and software and for those who use this tool in theoretical, mathematical and experimental physics. A number of new promising results on the development of algorithms for investigating and solving systems of algebraic, differential and difference equations, on symbolic-numeric simulation of quantum-mechanical systems as well as on computation of multiloop Feynman integrals by computer algebra methods and on various computer algebra applications to physics and mathematics were presented.

On 4 - 9 July, the Laboratory of information technologies hosted the seventh international conference "Distributed computing and grid-technologies in science and education" (GRID'2016). The conference is held every two years and is traditional for the Laboratory. This year the conference was dedicated to the 60th anniversary of JINR and the 50th anniversary of LCTA/LIT. Note that the GRID’2016 conference is a unique platform for discussing a wide range of issues related to the use and development of distributed grid-technology, heterogeneous and cloud computing in various fields of science, education, industry and business. The conference attracted a large community of Russian and foreign specialists ready to discuss emerging challenges and prospects of the development of advanced information technology. The conference was attended by more than 250 scientists from the research centers of Azerbaijan, Belarus, Bulgaria, Germany, Georgia, China, Moldova, Mongolia, Romania, Slovakia, Czech Republic, Chile, France, Sweden, etc. Russia was represented by participants from more than 30 universities and scientific research centers. The conference was organized in ten sections which discussed the issues related to the development of grid technologies, heterogeneous computing, volunteer computing, cloud computing, big data analytics. Also, in frames of the conference organized was a school for young scientists, postgraduates and students, where tutorials were conducted on heterogeneous and cloud computing. In total, the conference participants heard 35 plenary, more than 120 oral and 43 poster reports. 40 students and young scientists from Mongolia, Romania and the Russian universities (MEPhI, St. Petersburg State University and University "Dubna") attended the School.

On 24 – 28 October, the Seventh School on information technologies "Grid and Advanced Information Systems" organized by the Joint Institute for Nuclear Research and the European Organization for Nuclear Research (CERN) and supported by the National Research Nuclear University "MEPHI" and the Plekhanov Russian University of Economics was held at LIT. The School was attended by over 90 students as well as masters and post-graduates from Russia and Kazakhstan. The students attended lectures on modern information technologies delivered by the leading specialists of CERN and JINR. On the basis of the materials of the lectures organized were trainings and competitions, the winners were awarded with prizes.

On September 16, 2016 the House of Culture "MIR" hosted a ceremonial meeting of the staff of the JINR Laboratory of Information Technologies (LIT) which celebrated the 50th anniversary of its foundation. The decision on establishing a new laboratory, called the Laboratory of Computing Techniques and Automation (LCTA,) was adopted at the twentieth session of the JINR Scientific Council in 1966. Its first director was appointed a corresponding member of the USSR Academy of Sciences M. G. Mescheryakov. The main tasks the LCTA faced were the creation and development of a measuring and computing complex, mathematical methods for theoretical and experimental research, coordination of joint research work of the laboratories and JINR member States on the methods of measurement and processing of experimental data. The new laboratory was launched on the base of the Computing Centre located at the Laboratory of Theoretical Physics. In 2000, the LCTA was renamed into the Laboratory of information technologies, LIT.

The official part of the meeting ended with awarding the well-deserved LIT employees and veterans with the honorary diplomas and commendation certificates of the Joint Institute for Nuclear Research. In the exhibition hall and in the foyer presented were releases of the very popular in good times wall newspaper "Impulse". Two books have been published on the occasion of the anniversary of the Laboratory: a collection of memories of the LCTA/LIT employees (compiled by L. Kalmykova) and a collection of materials based on the wall newspaper "Impulse" (author-compiler A. Rastorguev). Numerous LIT veterans will be interesting to look through the pages of these books and to remember their friends and colleagues, who all together laid the foundation for the subsequent successful development of the Laboratory, the achievements of which have rightly provided its high rank among the computing centers worldwide.

The organizers of the ceremonial meeting express their gratitude to the Director of the House of Culture "MIR" S. G. Ferdzhulyan, deputy director L. N. Orelovich and all the staff-members for their friendly attitude and help in organizing the event.

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