LABORATORY OF INFORMATION TECHNOLOGIES

The investigations performed at the Laboratory of Information Technologies in 2010 in frames of the JINR general topic «Networks, Computing, and Computational Physics» were focused on two first priority themes, namely, «Information, Computer and Network Support of the JINR's Activity» and «Mathematical Support of Experimental and Theoretical Studies Conducted by JINR». The LIT staff participated in research work within 20 themes of the «Topical Plan for JINR research and international cooperation».

The computing power of the JINR Central Information Computer Centre (CICC) added 400 kSI2K and reached 2800 kSI2K, the capacity of the data storage system added 500 TB and is 1068 TB at present. The effective organization of the JINR grid-site operation has allowed it to take its place in the first ten among more than 160 sites of the second level of the global grid-infrastructure within the project WLCG (Worldwide LHC Computing Grid). The JINR contribution to solving tasks in the framework of the Russian Grid for intensive operations with data integrating the JINR grid-segments and 16 resource centers in the Russian institutes and the JINR Member States has exceeded 40%.

NETWORKING, COMPUTING, INFORMATION SUPPORT

In 2010, the work on the provision of reliable operation and development of the JINR networking and informational infrastructure was in progress. The key components of this infrastructure comprise telecommunication data links, JINR local area network, CICC and base software responsible for integration of the Institute's information resources in a unified environment accessible to all users and with the use of grid-technologies.

JINR Telecommunication Data Links. In 2010, the reliable work of the high-speed computer communication channel Dubna–Moscow was supported. To provide connection with scientific networks and Internet, the JINR network infrastructure used the following communication lines: with CERN (10 Gbps), RBnet (10 Gbps), GEANT (12.4 Gbps), Moscow scientific networks (10 Gbps), RASnet (10 Gbps), RadioMSU (10 Gbps), GLORIAD (1 Gbps), E-arena (10 Gbps).

In 2010, the Dubna-IX node was maintained to provide a remote access of the JINR employees via VPN from the town networks «Lanpolis», «Contact», TMPK and carrying out a network-to-network peering between the town networks.

Figure 1 gives the distribution of the incoming and outgoing JINR traffic in 2003–2010. Sharp growth of the traffic in 2010 is explained by activation of work on the LHC experiments.

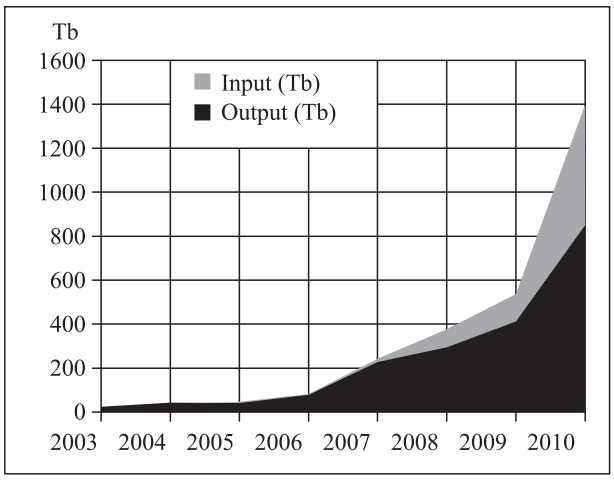

Fig. 1. Distribution of the incoming and outgoing JINR traffic since 2003

Table 1 shows the distribution of the incoming traffic among the JINR subdivisions in 2010 (exceeding on the income traffic 1 TB).

Table 1

JINR subdivision	Incoming, TB	Outgoing, TB
VBLHEP	45.74	87.73
LIT	45.53	39.38
DLNP	42.71	66.45
FLNP	28.18	49.04
BLTP	15.97	16.82
VPN	10.72	3.04
Adm.	8.89	7.35
FLNR	6.42	2.9
LRB	5.71	1.59
Uni-Dubna	3.98	5.78
SCAR	2.62	5.17
UNC	2.18	0.91

In 2010, the total incoming JINR traffic, including the general access servers and CICC, amounted 1399,02 TB (536,15 TB in 2009). A percentage distribution of the incoming traffic on categories can be seen in Table 2.

JINR Network. The regular work at LIT is directed both at a constant perfection and increase of fault tolerance of the node of the telecommunication structure of the JINR LAN and at provision of essential increase in information streams and its security level. In 2010, alongside with the modification and optimization of the external data link and the JINR Backbone, work was conducted on granting in a test mode of a centralized wireless access in JINR, centralized services VoIP and Video Conferencing. A first stage of transition of the JINR Backbone to a data transfer rate of 10 Gbps has been realized. Three JINR laboratories — LIT, LHE, and DLNP — were transferred to the mentioned rate in 2010.

The JINR LAN includes 6988 computers and computing nodes. In 2009, 3726 users were registered within the network, more than 1500 users of mail.jinr.ru service and about 1300 remote VPN users. The LIT specialists continued modernization and support of the in-house software complex IPDB — a network database with multiple functions of monitoring and control based on IP-address. The IPDB became the main tool for the network and system administrators to fulfill their administration tasks.

Table 2

Scientific & educational networks	File exchange (torrent, ftp)	Web-resources	Social_Net	Software	Multimedia	Dubna-net
89.24	8.63	1.45	0.25	0.21	0.17	0.05

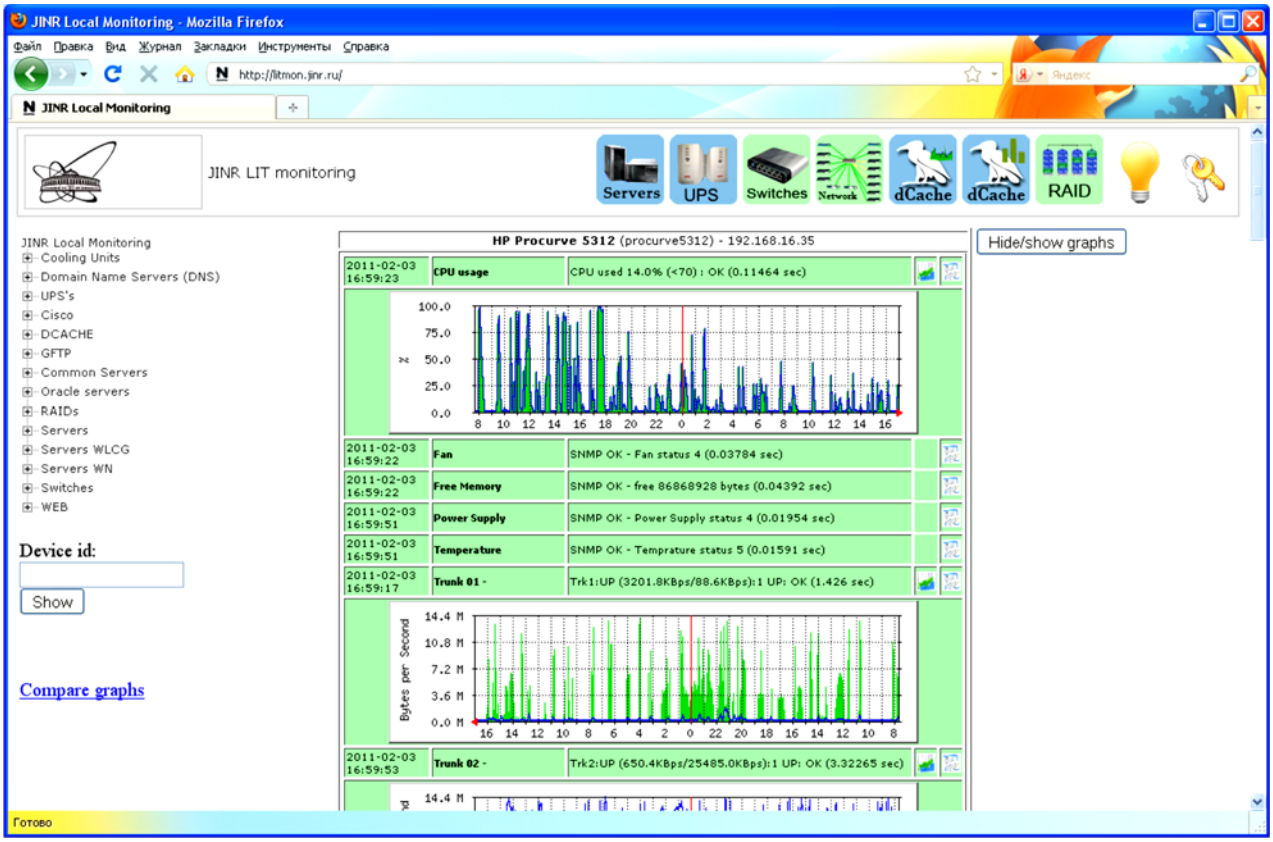

Fig. 2. JINR LIT monitoring main web-page

The monitoring of the JINR LAN infrastructure is one of the major tasks in the provision of a reliable functioning of the whole infrastructure. A first version of the local monitoring system (NMIS) with a graphic web-interface (Fig. 2) has been developed and put into operation. This system provides a real time monitoring of the main network elements: routers, network switches, climatic installations, uninterrupted power supply (UPS), DNS servers, dCache servers, database servers, RAIDs, WLCG servers, computing nodes, etc. More than 350 network nodes are in round-the-clock control in the NMIS system.

JINR Central Information and Computing Complex. The growth of the performance and the data storage of the JINR CICC based on a distributed model of data storing and data processing was continued in 2010. The CICC is organized as a unified informational-computational resource intended for provision of all directions of JINR's activity. The accounting and data storage resources are managed by a base software (BS). The options of the CICC BS provide optimum use of accounting resources and support of the most universal and protected methods of access to the data storages. Distribution and account of computing resources is realized on the basis of the batch system *torque* and the resource scheduler *maui*.

At present, the CICC computing farm comprises 1104 64-bit central processors. All the computing nodes are accessible to the CICC users and users of the grid-environment through a unified batch system. A new climate control system was put into operation in the CICC in 2010.

Five interactive machines were included in the CICC structure to provide access to the CICC resources for JINR users. There are some servers supporting the work of users and services of JINR: batch, WWW, DB mysql and Oracle; e-mail; DNS, etc.

The basic system to store enormous data volumes in CICC is the hard- and software complex dCache. It comprises 32 data storage systems of the total capacity of ~ 600 TB. A system of real time monitoring of the data storage has been put into operation which allows one to obtain rapid information on using the disk space by users. Several CICC user groups utilize a system of access to remote information XROOTD. For the functioning of the XROOTD system to be maintained, a hard- and software complex of a total capacity of ~ 175 TB has been designed. All the storage systems of a total capacity of 1 Petabyte are constructed with the help of a RAID6 hardware mechanism. The total accessible capacity of the system is ~ 800 TB.

In order to maintain the JINR WLCG site, 24 servers under the gLite system have been installed. In line with the functions of supporting the operation of the site JINR-LCG2, a part of the servers provides services and realizes functions of support of the Russian segment of projects WLCG and EGI.

The central CICC network router is connected to the main border router of the JINR network with a rate of 10 Gb Ethernet. Aggregation of several 1 Gb Ethernet connections in the uniform virtual channel (TRUNK) with an increased throughput from 4 up to 8 Gb Ethernet is applied with the purpose to provide a high throughput of the CICC network and a minimal time of access to data and files.

Table 3 shows the distribution of batch jobs over the Institute's subdivisions and user groups excluding the participants of grid-projects in 2010.

JINR Grid-Environment. JINR actively participates in large-scale global grid-projects: «World-wide LHC Computing Grid» (WLCG project, http://lcg.web.cern.ch/LCG/), and «Enabling Grids for E-science» (EGEE, http://www.eu-egee.org/) and its continuation — project «European Grid-Infrastructure» (EGI-InSPIRE — Integrated Sustainable Pan-European Infrastructure for Researchers in Europe, http://www.egi.eu/projects/egi-inspire/).

Participation in the mentioned projects includes support and development of the JINR grid-infrastructure in accordance with the requirements of the experiments for the LHC running phase, participation in WLCG middleware testing/evaluation software, grid-monitoring tools development, development of a database of simulated physical events, training of users of the grid-infrastructure, support of the JINR-participating countries in their WLCG activity, etc.

Since 2004, the JINR CICC has been a component of the global computing grid-infrastructure in frames of the Russian grid-infrastructure for intensive operations with data (RDIG). In 2010, about 40% of the total CPU time, spent within the Russian grid-infrastructure for the LHC tasks, was provided by the JINR grid-site JINR-LCG2. Our site is one of the most effective sites of the Tier2 level of the WLCG infrastructure and on a regular basis takes (by results of independent monitoring) its deserved place in the top ten of more than 160 Tier2 sites.

In 2010, enormous work was done on data receiving and processing for experiments ALICE, ATLAS, and CMS at JINR. Table 4 presents the results on using the JINR CICC grid-infrastructure by the virtual organizations (VO) within RDIG/WLCG/EGI in 2010.

Table 3

Laboratory/Group	LIT	BLTP	DLNP	FLNP	MPD	VBLHEP	CBM	PANDA	FLNP
CPU time, kSi2K · h	459733.92	207786.00	166082.38	84794.83	35793.66	4395.21	316.51	6.34	4.4
Number of jobs	2013	1688	106	716	10764	1090	123	704	13
Astronomical time, kSi2K · h	370271.94	210619.64	3591.58	35639.36	38132.28	4509.36	394.62	436.38	0.92

Table 4

VO	CPU time, kSi2K · h	Jobs
ATLAS	5204619.87	777996
ALICE	2949151.97	234057
CMS	2472183.90	479948
LHCb	1955205.91	68707
Fusion	497976.03	9108
BioMed	156795.87	26142
HONE	89959.07	7702
ops	2655.99	66217
dteam	16.22	6595
Total	13328564.84	1676472

The monitoring and accounting system of using the resources of the RDIG infrastructure developed and maintained at JINR, has been advanced (http://rocmon.jinr.ru:8080).

The JINR specialists make a noticeable contribution to the development of the monitoring system for the LHC virtual organizations (Dashboard) developed and supported by the Information Technologies Division at CERN [1]. This system allows one to obtain data used for visualization of the grid-infrastructure operation (static information on grid-sites with their coordinates, number of sent and completed tasks on the site, number of problems computed at the moment and information on data transmission in the grid-environment).

Now the JINR grid-site is the best of all RDIG sites. Our 2010 contribution to the job processing of experiments ALICE, ATLAS, and CMS is resulted on the diagrams of Fig. 3.

Development and support of the database of modeled events for the project LCG — LCG MCDB (LCG Monte-Carlo Events Data Base) was progressing. At present it is actively used by the CMS experiment. A specialized language HepML has been developed on the basis of the XML language for automation of the simulation process [2].

In 2010, in cooperation with CERN, work was continued on the development of one of the central services of the data management system for the experiment ATLAS (DQ2) — the Deletion Service which is intended for centralized deletion of data of the ATLAS experiment on sites Tier0–Tier1–Tier2. The use of web-service technologies has allowed one to build a scalable system as well as to provide integration of the Deletion Service with other DQ2 services. Service monitoring subsystems and an interface of viewing and searching errors have been implemented. Since November 2010, all sites of the Tier0–Tier1–Tier2 level of the ATLAS experiment have been served by an updated Deletion Service. About 1000000 files of the total volume of 300 TB are deleted per day within the whole ATLAS Grid infrastructure.

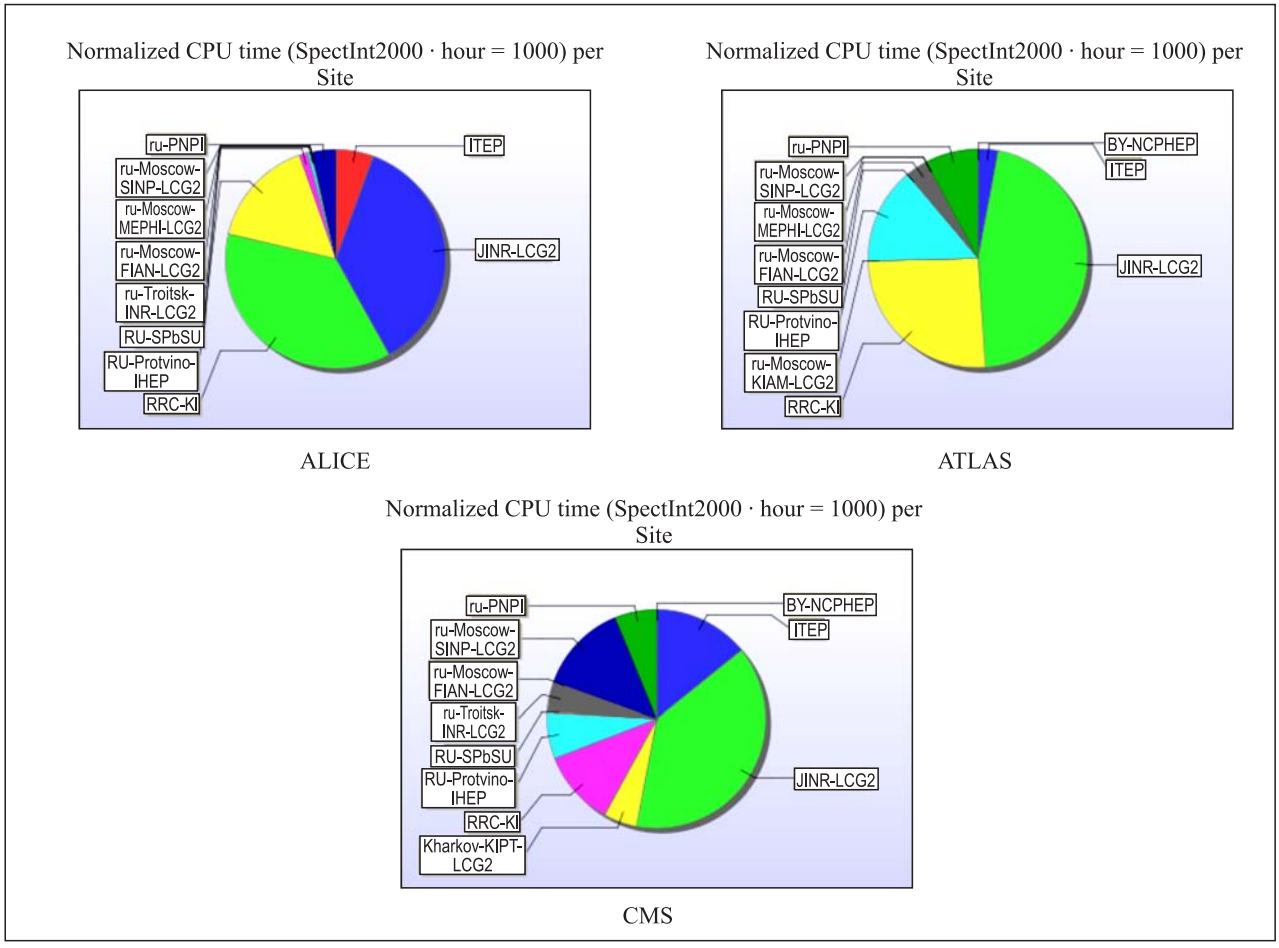

Fig. 3. Normalized CPU time per RDIG sites for ALICE, ATLAS and CMS in 2010

The development and start-up of the prototype system of the real time remote access to monitor the data gathering and processing in the ATLAS Control Room is a result of the long-term JINR–CERN cooperation under the TDAQ ATLAS project. This system represents unique opportunities on its use in the future as a hardware–software platform for engineering systems of modeling in real operating conditions of the computer complex in a distributed environment.

In addition to the experiments on the LHC, JINR grid-site serves six more virtual organizations within the RDIG infrastructure.

At the end of 2010, a first session of mass event modeling for experiment CBM (FAIR) in frames of CBMGRID on sites of JINR and GSI was successfully carried out. The modeling of 5000000 events (35A GeV Au-Au) was performed within the UrQMD program.

In cooperation with nine resource centers in different regions of Russia, JINR participates in the project GridNNN (Grid National Nanotechnological Network) which is carried out within the federal programme «Development of a Nanoindustry Infrastructure in the Russian Federation for 2008–2010». In this project the JINR's tasks are as follows: monitoring and accounting, support of the registration system of grid-services and sites, support of virtual organizations.

For training users and system administrators to work within the grid-environment, an educational infrastructure has been launched at LIT (http://gridedu.jinr.ru) that allows users to gain an experience in working with the modern Grid middleware. At present this distributed infrastructure integrates 8 sites in the JINR participating countries. It is a first step towards creation of the integrated grid-infrastructure of the JINR participating countries.

An information Internet portal "Grid at JINR" (http://grid.jinr.ru) was developed in 2010. It reflects JINR's activity in the field of grid-technologies.

Information and Software Support. The information, software and algorithmic support of the research-and-production activity of JINR is a traditional direction of research performed at LIT. In particular, it includes the development and support of information WWW/FTP/DBMS servers of JINR and LIT, creation and storage of electronic documents related to the Institute's scientific and administrative activities. The programme environment has been upgraded, the administrative databases are maintained and modernized on a regular basis in cooperation with STD AMS of JINR.

In 2010, work was conducted on creation and support of various information sites, sites of conferences, workshops, symposia organized by JINR Laboratories in 2010–2011 (at their requests). In particular, such work was done for the 18th International Seminar on Interaction of Neutrons with Nuclei, Dubna, 26–29 May, 2010 (http://isinn.jinr.ru), the Crimea Conference (of a series of international conferences on modern problems of genetics, radiobiology, radioecology and evolution), Alushta, Ukraine, October 9–14, 2010 (http://lrb.jinr.ru/Timofeeff/Alushta / Menu / Menu Set_r_10.htm), IV International Pontecorvo School on Neutrino Physics, Alushta, Ukraine, September 26 – October 6, 2010 (http:// pontecorvosch.jinr.ru / index.html), 4th International Conference on Physics and Chemistry of Transactinide Elements, Sochi, Russia, 5–11 September, 2011 (http://tan11.jinr.ru), 4th International Conference «Distributed Computing and Grid-Technologies in Science and Education» GRID'2010, Dubna, June 28 – July 3, 2010 (http://grid2010.jinr.ru), 5th International Symposium on *in situ* Nuclear Metrology as a Tool for Radioecology, Dubna, Russia, October 20–23, 2010 (http://insinume2010.jinr.ru), etc.

A system of electronic document circulation DoctorDoc, developed for internal paperless document circulation in LIT, has been put into trial operation. The system has a process-oriented structure and possesses a number of advantages over existing service-oriented systems. The technical base of the system has been upgraded and the opportunities of the information system are expanded.

Work was in progress on the maintenance and modernizations of the portal of the journals «Physics of Elementary Particles and Atomic Nuclei» and «Part. Nucl. Letters».

In 2010, LIT released its regular Bulletin. The electronic version of the bulletin is available on the LIT site http://lit.jinr.ru/Inf_Bul_5/.

Another traditional direction of LIT activity is the development and support of the program library JINRLIB as well as support of program libraries (CERNLIB, CPC Program Library) developed by other research centres and organizations as well as information and technical support of users. The information on the JINR program libraries is available on a specialized web-server http://www.jinr.ru/programs/. In 2010, the JINRLIB was stocked by new in-house software, namely SLIPM — a software complex in language MAPLE for a numerical solving of Sturm–Liouville partial problem on the basis of the continuous analogue of Newton's method; BioDosimetry — a computer program for processing and analysis of data of radiation biological dosimetry and automatic calculation of radiation dozes; a new versions of SAS — a program for primary processing of the small-angle scattering spectra, FITTER — a program of fitting a chosen theoretical multiparameter function through a set of data points, and Gluplot — a data plotting package.

The research on using the parallel computation technologies (MPI, OpenMP, GPU) for paralleling big computing programs was progressing. Methodical instructions for work with MPI on the CICC/JINR computing cluster have been prepared and published in the LIT Bulletin and on the LIT site (http://lit.jinr.ru/view.php?lang=lat&var1=comp&var2=ccic&file=ccic/recom/compilat&menu=ccic/menu).

Agreements have been concluded between JINR and Autodesk and Siemens PLM companies for purchasing a licensed software. The network and single-user licenses for program products Autodesk Inventor Suite 2010/2011 and Autodesk Inventor Professional 2010/2011 (Russian, English versions and versions for educational institutions) were purchased for JINR Laboratories. The network licenses are available at a server of licenses iis1.jinr.ru. Training courses Autodesk Inventor were organized for beginners and advanced users.

MATHEMATICAL SUPPORT OF EXPERIMENTAL AND THEORETICAL STUDIES

The main objective of this research field at LIT is to provide the mathematical, algorithmic and software support of the experimental and theoretical research underway at JINR. In 2010, the obtained results were reported in more than 200 papers, 89 works being published in the leading journals. More than 90 reports were presented at international conferences. Below there is a brief report about some results.

An algorithm has been proposed to build an estimate of the half-life of a «daughter» nucleus in case when it is not known what nucleus is its «mother» [3]. This method can be applied to experiments with nuclear reactions of full fusion induced by heavy ions if sequences of rare decays recoil-alpha (and/or spontaneous fission) are detected and thus more than one statistically significant recoil-candidate for such events is observed.

Calculations are made of the $K^+ + {}^{12}C$, ${}^{40}Ca$ differential elastic scattering cross sections at the beam momenta 0.635, 0.715, and 0.8 GeV/c. The microscopic optical potential derived in the high-energy approximation was used where existing data on the kaon-nucleon amplitude and on the point-like density distributions of target-nuclei were utilized. The effect of different methods of relativization was studied and shown to play an important role. A good agreement with the experimental data on differential elastic cross sections was obtained [4].

The ${}^{6}He + {}^{12}C$ elastic scattering data at $E = 3, 38.3,$ and 41.6 MeV/nucleon have been studied using microscopic optical potentials (OP). The depths of the real, imaginary and surface parts of microscopic OP were taken for fitting parameters. The problem of the ambiguity of the adjusted OP was resolved by imposing the condition that the computed values of some characteristic volume integrals agree with their experimentally determined dependences at the collision energy. The structure of microscopic OP, the role of the in-medium effects, interconnection between the surface term and the breakup processes are discussed [5].

A fast algorithm of the global track reconstruction for the CBM experiment (Compressed Baryonic Matter) at the FAIR accelerator in Darmstadt has been developed. The global track reconstruction procedure is based on track following and Kalman Filter methods. The track reconstruction efficiency for central $Au + Au$ collisions at $25A$ GeV beam energy using events from the UrQMD model is at the level of 93–95% [6]. The parallel implementation of the algorithm using some advantages of the present-day processor architecture and a multiple-stream property, have allowed one to get almost a 500-multiple decrease of the one event processing time as compared to the traditional processing methods (from 730 to 1.5 ms/event) for two-core processors Intel Core i7 (2.66 GHz) [7].

Algorithms and approaches have been developed for solving problems of electron identification and pion suppression with the Transition Radiation Detector (TRD) of the CBM experiment. The characteristic properties of the energy losses of electrons and pions in the TRD layers and peculiarities of applying artificial neural networks and statistical methods for the solving of the formulated problem were analyzed [8].

A generalization of the few-body quantum scattering theory is given for the case of the Coulomb interaction. A recipe for regularizing integrals (eliminating divergences), which describe the terms of a perturbation theory series for different perturbing potentials, is formulated. As an example, the general theory is applied to the calculations of differential cross sections for a quasi-elastic electron-impact ionization reaction on atomic hydrogen [9].

A probability of decaying kaons into pions, neutrino and lepton atom has been computed. The obtained results are used to estimate the background in the NA-62 experiment on research of the K-meson decay into π meson and neutrino-antineutrino pair [10].

With the aim of finding an appropriate description of the state of an ejected electron from a linear three-centre molecular target, a wave function is constructed in a closed analytical form by solving the Schroedinger equation of an unbound electron in a Coulomb field of three fixed charged nuclei. It is employed, in the frame of a perturbative first Born three-centre procedure, to the determination of the multiply differential cross sections (MDCS) of the $(e, 2e)$ simple ionization

of the valence $1\pi_g$ level of CO_2, for which experimental results were given recently (Fig. 4). The ionization of the inner $1\pi_u$ and $3\sigma_u$ levels of CO_2 are also investigated [11]. The study of the variation of the MDCS with the direction of the scattered electron and the ejected electron in the case of oriented three-centre targets shows interference patterns similar to those created by the diffraction of light by three apertures.

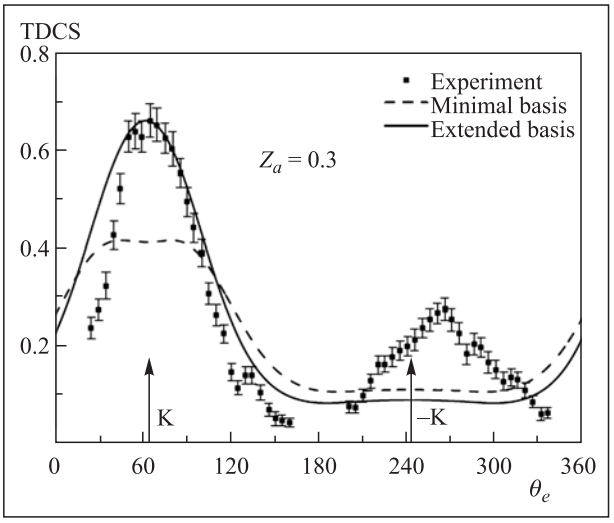

Fig. 4. Variation of the TDCS in terms of the ejection angle θ_e of the $(e, 2e)$ ionization of the $1\pi_g$ level of CO_2 for parameter $Z_a = 0.3$. The experimental cross section is from paper (*Lahmam-Bennani A., Staicu Casagrande E. M., Naja A.* // J. Phys. B. 2009. V. 42. P. 235205–1–7) at energies of the ejected electron $E_e = 37$ eV and scattered electron $E_s = 500$ eV. Full line: the extended basis set $(1s, 2s, 2p, 3d)$. Dashed line: the minimal basis set $(1s, 2s, 2p)$

For the numerical simulation of the processes when heavy ions pass condensed matters, the time of passing the ion from the irradiated surface to its full stop in the target is of particular importance. The performed calculations have shown that the time of passage by a uranium ion with the energy of 700 MeV in a nickel target is $\Delta t \approx 4 \cdot 10^{-12}$ s. In the previous investigations, the motion of an ion in a material was not considered and a source with the action time $\Delta t \approx 10^{-14}$ s was used. A thermal spike model with a new source considering the motion of an ion within a material has been proposed. Some results of calculations are given for nickel exposed to 700 MeV uranium ions. A comparative analysis with the previous results, where the ion motion in a material was not considered, has been also performed [12].

The effective two-band two-dimensional Hubbard model of the high-Tc superconductivity in cuprates, as recently modified to include appropriately the zero doping limit, is rigorously solved within the generalized mean field approximation of the equation of motion of the Green function matrix. The energy spectra, derived both for the normal state and the superconducting state, are finite over the whole available range of the doping, irrespective of the kind of doping (with holes or with electrons) of the cuprate system. The hopping-induced hybridization of the normal state energy levels is found to preserve the centre of gravity of the unhybridized levels. However, the hopping-induced hybridization of the superconducting state energy levels at a given momentum q inside the Brillouin zone displaces the centre of gravity of the hybridized normal levels. This is consistent with the overall displacement of the energy spectrum of the superconducting state as found from very precise optical measurements [13].

A computational scheme for solving elliptic boundary value problems with axially symmetric confining potentials using different sets of one-parameter basis functions is presented. The efficiency of the proposed symbolic-numerical algorithms implemented in Maple is shown by examples of spheroidal quantum dot models, for which energy spectra and eigenfunctions versus the spheroid aspect ratio were calculated within the conventional effective mass approximation. Critical values of the aspect ratio, at which the discrete spectrum of models with finitewall potentials is transformed into a continuous one in a strong dimensional quantization mode, were revealed by using exact and adiabatic classifications [14].

Efficient algorithms for disjoint triangular decomposing systems of nonlinear partial differential equations into involutive subsystems were developed and implemented in Maple. Such a decomposition allows in finitely many steps to verify compatibility of equations in the system (i.e., existence of their common solutions), and make easier construction of their solutions either analytically, when it is possible, or numerically. In addition, as a result of the indicated collaboration, a new algorithmic approach to verification weather a discretization of linear partial differential equation systems approximate their solution was developed in [15].

A self-consistent system of interacting spinor and scalar fields in Bianchi type VI (B-VI) cosmology is studied in the presence of a cosmological constant. Exact solutions to the spinor, scalar and gravitational field equations are obtained for some special choice of the spinor field nonlinearity. It is shown that introduction of a positive cosmological constant, which is often used to model dark energy, results in a rapid growth of the universe, while negative cosmological constant gives rise to an oscillatory or nonperiodic mode of expansion. If the metric functions a and b are taken to be inverse to each other $(ab = 1)$, one gets a singularity-free universe independently of the sign of cosmological constant [16].

The cornerstone of quantum computing and theory of quantum information is an extraordinary quantum phenomenon — the so-called «entanglement» of composite quantum states, and the main challenging problem is to identify, classify, and quantify the entanglement and thus understand the nonlocalities exposing by

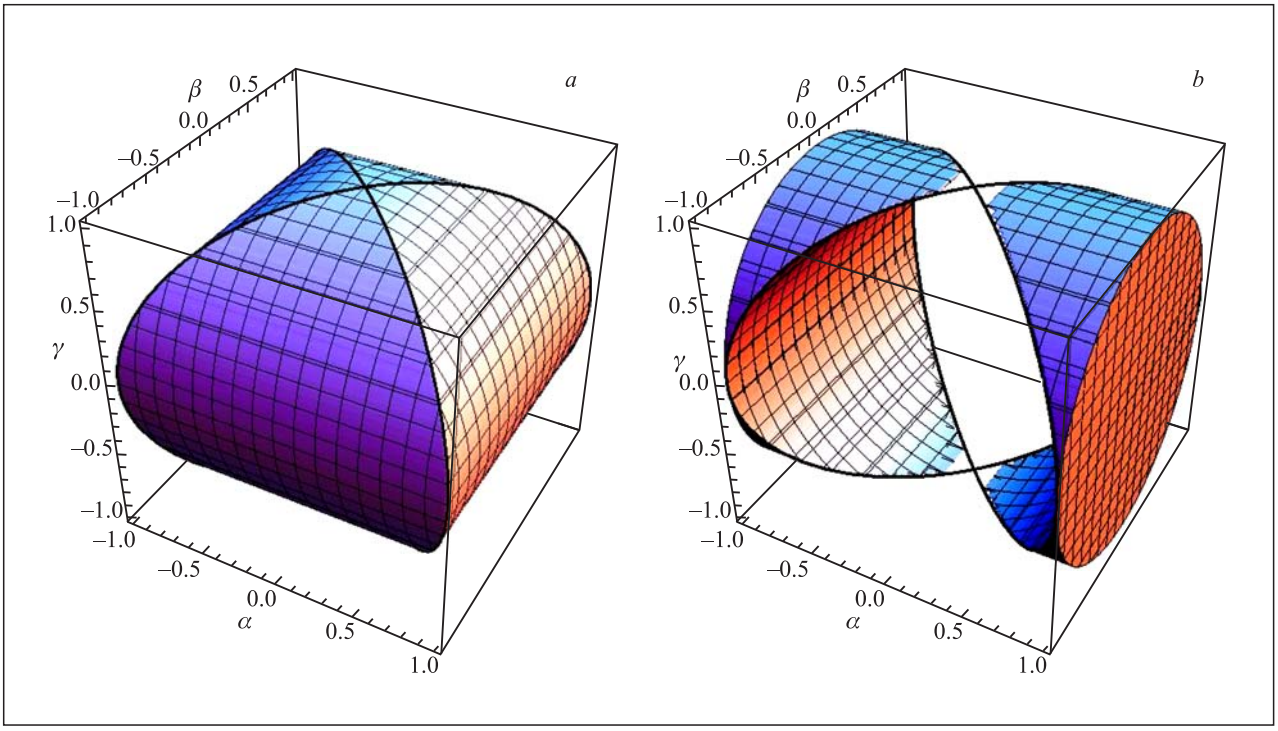

Fig. 5. Separated (*a*) and entangled (*b*) domains for a 3-parametric family of density matrices

entangled systems. In [17] the exact algebraic conditions on a density matrix for a generic two-qubit quantum system were obtain, They allow one to determine easily whether the given state is entangled or not. An example of separated and entangled domains for a 3-parametric family of density matrices is shown in Fig. 5.

INTERNATIONAL COOPERATION

The research work at the Laboratory is carried out in a close cooperation with scientists and specialists of the JINR Member States as well as a number of research centers of other countries. Some examples of such cooperation should be particularly noted.

In cooperation with the University of Cape Town, the particle-like excitations of nonlinear dispersion matter have been studied in the frame of models of condensed matter theory and nonlinear optics based on the nonlinear Schrödinger equation (NLS). A region of damping and driving parameters, where different classes of stable localized structures: stationary two-soliton complexes, temporally periodic two-soliton structures, quasi-periodic complexes coexist, has been obtained and studied. A number of stable periodic two-soliton complexes in the region of large damping coefficients were discovered [18].

A mathematical modeling of static magnetic flux distributions in long Josephson junctions (JJ) taking into account a second harmonic in the Fourier decomposition of the Josephson current has been conducted at LIT in cooperation with the researchers of BLTP and Sofia University «St. Kliment Ohridski». The stability analysis is based on a numerical solution to the spectral Sturm–Liouville problem formulated for each distribution. In this approach the nullification of the minimal eigenvalue of this problem indicates a bifurcation point in one of parameters. At each step of numerical continuation in parameters of the model, a corresponding nonlinear boundary problem is solved on the basis of the continuous analog of Newton's method using a spline-collocation scheme for linearized problems at each Newtonian iteration. Main solutions of the double sine-Gordon equation have been found and the stability of the magnetic flux distributions has been investigated. Numerical results are compared with the results of the standard JJ model of a superconductor-isolator-superconductor type [19].

In the paper «Using GPU for Scientific Computations» an OpenCL (Open Computing Language) implementation of the algorithm of calculating an accessible surface area and volume of a macromolecule taking into account the intramolecular cavities, performed in cooperation with the Technical University of Košice, Slovak Republic, has been presented. The developed program is intended for solving problems arising in the molecular simulations and is based on modification of the original algorithm in order to utilize the parallelization possibilities of OpenCL. An advantage of the created program is its universality: computations can be performed on all the machines within the OpenCL standard. Earlier this algorithm, using a stereographic designing of spheres on a plane, was realized in FORTRAN. A comparison of these two realizations of the algorithm has been provided. The efficiency of computations with the help of the new realization on NVIDIA GeForce GTX285 GPU has been demonstrated [20].

In September 2010, in frames of the international cooperation the JINR University Center organized a cycle of classes for students from the Republic of South Africa on the hands-on learning of the MPI technology on the UC computers and on the CICC/JINR computing cluster.

WORKSHOPS, CONFERENCES

On January 25-30, 2010 the Laboratory of Information Technologies hosted the 17th International Conference «Mathematics. Computer. Education». More than 350 attendees from the remote corners of Russia and the near abroad gathered together in Dubna to discuss their professional issues and present-day problems in various areas of mathematics and education, in the sphere of using information technologies, simulations of complex biological systems and economic processes. The Conference included the following sections: mathematical theories, computational methods and mathematical simulations, analysis of complex biological systems; experiment and models, mathematical methods in economy (econophysics), analysis and modelling of economic and social processes, humanitarian and natural-science education.

An International Conference «Distributed Computing and Grid-Technologies in Science and Education» was held on 28 June – 3 July, 2010 at the Laboratory of Information Technologies. The Conference was devoted to the 80th anniversary of the birthday of N. N. Govorun, an outstanding scientist, a corresponding member of the USSR Academy of Sciences and a former Deputy Director and Director of the Laboratory of Computing Techniques and Automation. It was the fourth conference on this topic held by LIT under support of the Russian Foundation for Basic Research every two years. The Conference programme included issues related to the creation and exploitation of grid-structures and grid-applications as well as theoretical and practical aspects of using distributed computing complexes, distributed data processing, etc. The representatives of sponsoring companies «Niagara» and «SuperMicro» acquainted the conference participants with new solutions in the information technologies. The Conference was attended by 252 participants from 21 countries. Russia was presented by participants from 56 universities and research centers.

The conference included 8 sections: WLCG — Worldwide LHC Computing Grid, grid-applications, grid in business, distributed computing and grid-technologies in education, GridNNN — Grid of the National Nanotechnology Network, methods and algorithms for distributed computing, grid-infrastructure and «cloud» computing. In frames of the Conference, round tables were organized on using grid-technologies in business and on training in grid-technologies and their application in education. A training course was held on the integrated infrastructure, tools and methods for support of the scientific applications development in Grid and the systems of voluntary distributed computing.

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