LABORATORY OF INFORMATION TECHNOLOGIES

The main tasks of the Laboratory of Information Technologies (LIT) consist in the provision both with modern telecommunication, network, and information resources and with mathematical support of the theoretical and experimental studies conducted by JINR, Member-State institutes, and other scientific centres.

The LIT activity is focused on two directions, namely «Information, Computer, and Network Support of JINR's Activity» (topic 05-6-1048-2003/2007, headed by V. Ivanov, V. Korenkov, and P. Zrelov) and «Mathematical Support of Experimental and Theoretical Studies Conducted by JINR» (topic 05-6-1060-2005/2007, headed by V. Ivanov, Gh. Adam, and P. Zrelov). These directions are developed as part of the JINR general topic «Networks, Computing, and Computational Physics». The Laboratory staff participated in research work done at other JINR Laboratories within 15 topics at the project level and within 21 topics at the cooperation level. Main results of the investigations performed within these topics have been published in well-known journals, proceedings of scientific conferences, and preprints.

A number of scientific projects involving LIT staff members have been financed by grants afforded by the Commission of the European Community in the framework of the EU–Russia collaboration and INTAS. Ten grants were afforded by the Russian Foundation for Basic Research (RFBR). Among them, five RFBR projects were directed to the creation and development of the information, computing and telecommunication infrastructure, while the other five are scientific projects.

NETWORKING, COMPUTING, INFORMATION SUPPORT

The JINR network structure is a distributed hard- and software complex that uses a specialized software and multifunctional equipment. It serves as a basis for the JINR distributed information-computational infrastructure. Its purpose is integration of used information resources of the Institute in a unified structure; creation of a unified information and computing environment for all JINR users with application of Grid technologies, thus providing a way of data exchange between scientific laboratories and between administrative subdivisions; provision of remote access to Russian and foreign scientific networks; provision of remote access to the Institute's resources. To fulfil the above tasks, the network infrastructure should have such properties as highly effective protection, reliability, high speed of data transfer, simplicity in service, and scalability.

Main directions of LIT activities in the area of networking, computing, information support, and Grid include: provision of JINR and its Member States with high-speed telecommunication data links; creation of a high-speed, reliable and protected local area network (LAN) of JINR; creation and maintenance of the distributed high-performance computing infrastructure and mass storage resources; provision of information, algorithmic and software support of the JINR research-and-production activity; elaboration of the JINR Grid segment and its inclusion in European and global Grid infrastructure.

JINR Telecommunication Data Links. Development of external JINR computer communications includes: a) provision of the reliable operation of the 1 Gbps data link JINR–Moscow and step-by-step increase of its throughput; b) participation of JINR in the work on realization of the new-generation national and international computer networks (GLORIAD, GEANT2); c) integration with the scientific and educational network of Dubna.

At present, JINR leases 1 Gbps channel to Moscow from the Russian Satellite Communications Company (RSCC «Dubna») 2.5 Gbps channel. JINR has access to the Russian networks and information resources, as well as access to the international channels through shared RBNet+RUNNet Russian networks (Fig. 1).

The future development of the external communications is summarized in the following program: broadening the Dubna–Moscow channel up to 10 Gbps in 2007, 40 Gbps in 2010, and 100 Gbps in 2015; JINR's participation in the program devoted to the implementation of a new-generation research network; development of an international segment within projects GEANT2, GLORIAD, and increasing the throughput of the channels to 10 Gbps in 2007, 40 Gbps in 2010, and 100 Gbps in 2015; integration with the municipal educational network and its development following its transition to new technologies (10 Gbps).

Figure 2 shows the incoming and outgoing JINR traffic in 2005 and 2006. Total year incoming traffic was 82.71 TB (45.86 TB in 2005) and outgoing traffic — 78.01 TB (41.53 TB in 2005).

Table 1 shows the total year 2006 traffic distribution among the JINR divisions whose incoming traffic exeeded 1 TB.

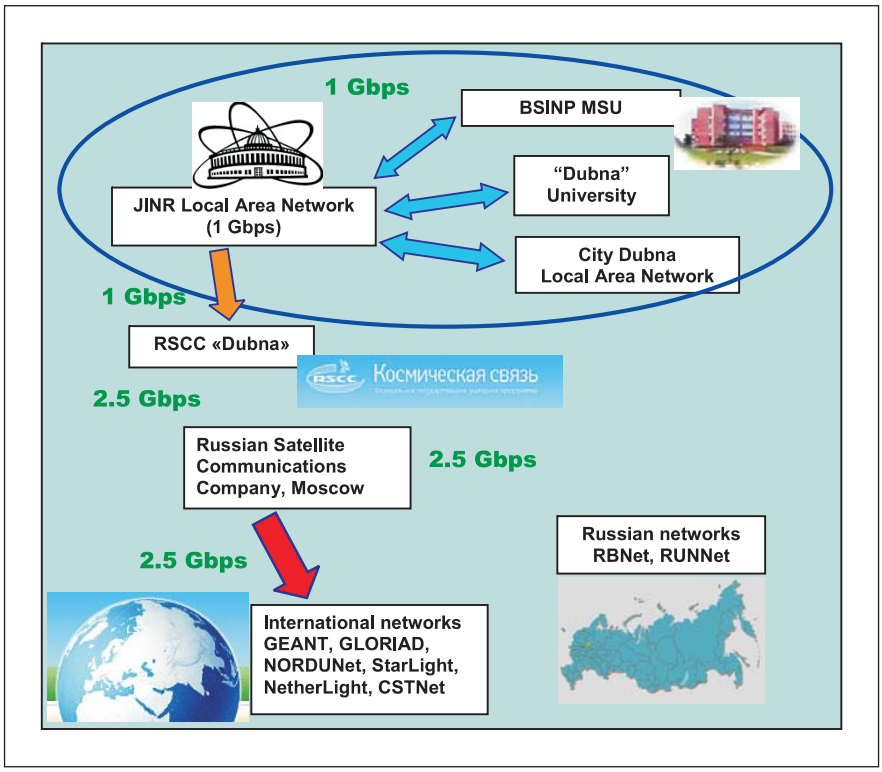

Fig. 1. The JINR telecommunication channels

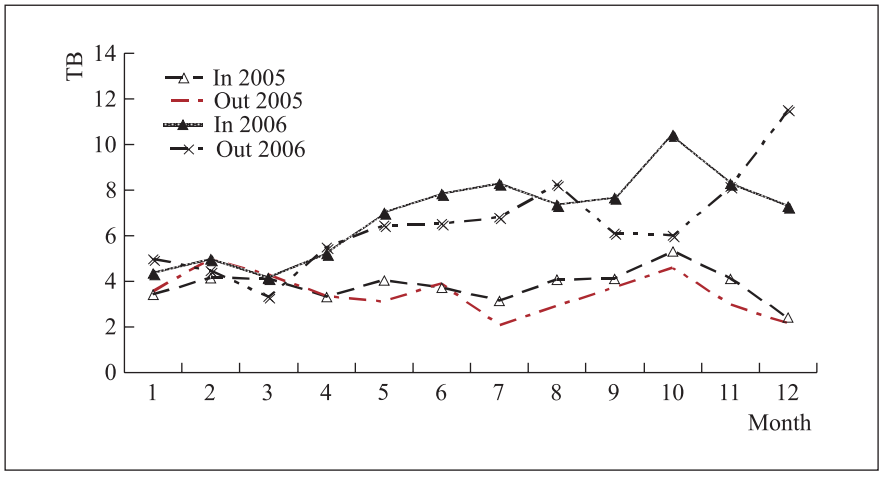

Fig. 2. Incoming and outgoing JINR traffic in 2005 and 2006

Table 1

JINR Laboratories	Incoming, TB	Outgoing, TB	Incoming, %	Outgoing, %
LIT*	32.22	14.21	38.96	18.21
DLNP	14.03	18.49	16.96	23.71
LPP	7.87	10.55	9.52	13.53
FLNR	6.7	2.52	8.1	3.23
VBLHE	5.42	4.06	6.55	5.2
FLNP	5.16	20.5	6.24	26.28
BLTP	3.63	2.07	4.39	2.65
Uni-Dubna	1.91	2.01	2.31	2.57
Adm.	1.49	0.66	1.8	0.82
Servers	1.38	2.39	1.67	3.06
Modem pool	1.34	0.26	1.61	0.32

*LIT traffic includes the total JINR Grid traffic.

JINR Local Area Network. Systematic work on the LAN management was performed by the LIT Network Operation Centre (NOC). At present the JINR LAN comprises 5681 computers and nodes (5335 in 2005). There are 3173 users, 863 modem pool users, and 339 JINR staff members use VPN connection.

In 2006 the specialists of the LIT NOC put into operation a software complex intended to scan in the local network the computers infected by Internet worms and to secure their subsequent blocking. As a result of the work carried out by the Network Service, the frequency of the occurrence of computers infected with such viruses in the JINR network has been reduced from 15–20 cases per week down to 3–5 cases per month.

To keep the JINR LAN as a full time working structure, we must perform LAN uninterrupted control and protection. With the extension of the network services towards secured remote access to JINR resources from home PC, and Internet access from Dubna hotels, security becomes a parameter of the greatest importance.

In 2006 the Central Communication Node modernization was performed (Fig. 3). The goals were to build a fail-proof core of the JINR LAN communication structure, to achieve an appropriate level of the network security, to have good data rate parameters and tools to control maintainability, accessibility, and reliability.

The new powerful switching & routing equipment Internet Cisco 7606 router (processor — Supervisor Engine 720, MSFC3, PFC3B Memory 1 GB, 48-port 10/ 100 /1000, Firewall security system), central switch Cisco Catalyst 6509E, and VPN router Cisco 7513 were put into operation in 2006.

Central Information and Computer Complex. The development of the JINR distributed high-performance computing infrastructure and mass storage resources is centered around the JINR Central Information and Computer Complex (CICC) as a core of the distributed infrastructure.

More than 500 staff members of JINR as well as other research centres are using the JINR Central Information and Computing Complex. Nowadays the JINR CICC comprises: an interactive cluster of common access; a common access computing farm for carrying out simulation and data processing for a number of physics experiments in which JINR participates, and for carrying out parallel calculations on the basis of the modern network technologies (Myrinet, SCI, etc.); LHC Computing Grid (LCG) farm for the tasks of the LHC experiments included into a worldwide LCG/EGEE (Enabling Grids for E-sciencE) infrastructure.

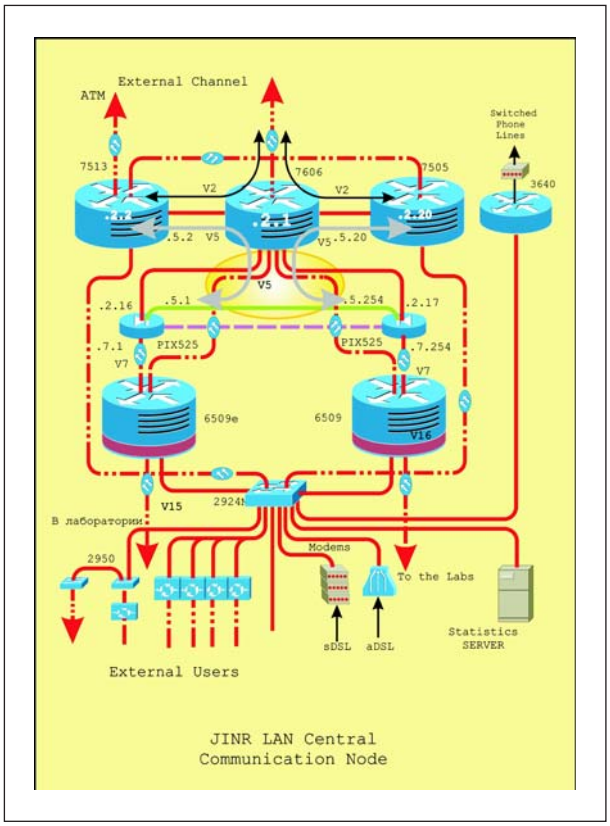

Fig. 3. JINR LAN Central Communication Node

With the last acquisitions, the JINR CICC comprises 160 CPUs and 56 TB (17 TB RAID-5, and 39 TB Certon100) disk memory. Total performance of the computer centre is now 100 kSI2K. JINR CICC fa-

cilities were used by the experiments E391A (KEK), COMPASS, D0, DIRAC, HARP, CMS, ALICE, ATLAS, HERAb, H1, NEMO, OPERA, HERMES, CBM, PANDA, etc., for mass event production, data simulation and analysis.

The JINR CICC users distributed over JINR divisions are presented in Table 2.

Table 3 shows the percentage of CPU time used by JINR Laboratories at CICC.

Table 2

LIT	DLNP	LPP	VBLHE	Non-JINR Grid users	FLNR	BLTP	FLNP	Adm.
182	120	60	48	33	28	15	12	9

Table 3

DLNP	VBLHE	LIT	BLTP	FLNR	LPP	Non-JINR
40.84 %	37.06 %	12.02 %	7.57 %	1.77 %	0.6 %	0.14 %

The future plans include the development of the JINR Central Information and Computing Complex as a core of the distributed Grid infrastructure: development of the CICC infrastructure meeting the needs of collaborations, JINR users, and JINR Member States; development of JINR's Grid segment with a fully functional set of services; participation in international, national, and regional projects of developing Grid technologies (LCG, EGEE, OSG, NorduGrid, Dubna-Grid, etc.); participation in developing technologies of application gridification that will allow applied software packages to be adapted to the Grid environment.

Grid Technologies and LCG Project. The work on creation of computing services and Grid-technology deployment in data processing was in progress. A good deal of work on this direction has been performed in the framework of JINR participation in LCG/EGEE projects: support and development of the JINR LCG segment within the global LCG infrastructure (installation of the last gLite version (3.02), and software for LHC experiments); LCG middleware testing/evaluation (gLite testing and deployment); monitoring the LCG infrastructure at JINR and others sites of the Russian Tier2 cluster; evaluation of new Grid technologies in the context of their usage in LCG (Globus Toolkit 4 testing & evaluation); re-design of JINR LCG/EGEE web-portal; participation in MCDB (Monte Carlo Databases) development; development of the server HEPWEB with Monte Carlo generators, and HEPWEB integration into the Dubna-Grid environment; participation in the ARDA project activities (testing AtCom/LEXOR usage for ATLAS; testing gLite-AMGA metadata service replication functionality and performance); participation in Data and Service Challenges for CMS, ATLAS and ALICE; organizing the courses for LCG administrators and ALICE users from Ukraine institutes; LCG training for ATLAS users; courses on gLite for participants of the second international conference «Distributed Computing and Grid Technologies in Science and Education». At present the JINR LCG infrastructure comprises site services (User Interface, Computing Element, Storage Element, Worker Nodes), basic services (Berkely DB Information Index, Proxy Server, Resource Broker), specific services (2 VOboxes for ALICE and CMS, ROCMON, MONbox), and PPS.

A package GridCom (Grid Commander) has been developed that represents a client part (GridCom) as a graphic shell for work of the user with problems and data in LCG and a program — the LEXOR inquiries executor.

In 2006 the investigation of the topic «Calibration of Forward Calorimeters with the Help of a Radioactive Source» was performed in the framework of research on RDMS CMS. As a result of this work, a database has been constructed, a data input procedure has been implemented, and the information system with a Web interface was realized.

In 2006 there were fulfilled JINR's obligations on participation in the on-line SW TDAQ ATLAS development: components of on-line SW Resource Manager and Event Dump are included in the structure of the on-line SW TDAQ release, prepared by TDAQ cooperation to start up in 2007 at a Dress Rehearsal stage. In the context of the participation in TDAQ ATLAS a test-bed has been assembled at LIT for installation of Data Quality Monitoring Framework Software.

At the end of 2006 within the Dubna-Grid project, a test-bed of the distributed meta-computing environment of Dubna city was created. More than 200 virtual nodes have been configured. Mass installation technologies and spreading software to all accessible nodes of the meta-cluster and monitoring system have been developed. The meta-cluster has been integrated with the JINR batch system. Integration of HEPWEB server in the Dubna-Grid environment is realized.

A Grid Laboratory, GridLab, is created at LIT. The aim of the Laboratory is to develop an educational program on Grid technologies for scientists from JINR and the Member States, students, PhD students and the teaching staff of Dubna higher schools. Technically, GridLab is a specialized segment of the Dubna-Grid project, consisting of a module of six working nodes and one server.

Information and Software Support. The traditional provision of information, algorithmic and software support of the JINR research-and-production activity included a large spectrum of activities at both LIT and JINR levels. Hard work was undertaken towards systematic development and maintenance of databases and information systems taking into account the user needs. The work was also in noticeable progress on the development of the WWW tools at the JINR and LIT main information servers: www.jinr.ru and lit.jinr.ru. Members of the LIT staff provided necessary work for JINR's STD AMS on the software and centralized support of the administrative databases. A regular actualization of the content of the central servers, their technical support and modernization of the software environment are performed in frames of supporting the JINR unified information environment on the basis of the central JINR site and LIT site. A new version of the LIT site, devoted to the 40th anniversary of LIT, has been developed and started up.

The consecutive development of the program library JINRLIB was in progress. The library is replenished with new programs created by JINR specialists. Six software packages were added in 2006. The Library programs were converted to double precision, the results of the work were checked up on computer platforms Unix and Windows. The maintenance of the program libraries developed by other research centres and organizations (CPCLIB, CERNLIB) and provision of the information and technical help to users continue. The full information on the JINR program libraries is available at the specialized WWW server http://www.jinr.ru/programs/ and in LIT News Bulletins.

Participation of a group of best LIT specialists in preparation and carrying out of the XXXIII International Conference on High Energy Physics (ICHEP'06) that took place in Moscow on 26 July – 2 August 2006 in the building housing the Russian Academy of Sciences, deserves particular attention. JINR Directorate and Conference Organizing Committee made LIT responsible for information and technical support of ICHEP'06. In the framework of this activity, a specialized information system «ICHEP'06 Conference» integrated with the Conference Web site has been created. The technical support was provided in cooperation with the «COMSTAR — United TeleSystems» and included expansion of a local computer network, provision of wireless access to the Internet, telephone links for the Organizing Committee and Conference attendees (IP telephony), Internet translation of plenary sessions, as well as organization of the Internet Hall equipped with plenty of stationary computers, free sockets for notebooks of the participants and wireless communications.

In progress was the maintenance and development of the interactive information environment for operative access to scientific and technical information in the Internet that allows efficient work of the Institute's scientific staff with bibliographic and factual data. It includes references to encyclopedias, directories, databases on particle and nuclear physics, Internet book-shops, provides access to text-through journals of Russian and foreign publishing houses, etc. It is available at http://dbserv.jinr.ru/~genis/Infpublish.htm. The work was done in cooperation with the specialists of the JINR Science and Technology Library.

MATHEMATICAL SUPPORT OF EXPERIMENTAL AND THEORETICAL STUDIES

The main tasks of these LIT activities are the mathematical, algorithmic and programming support of experimental and theoretical research under way at JINR. More than 100 scientific publications and proceedings of conferences were published in 2006. More than 40 reports were presented at international conferences.

Mathematical Methods for Elementary Particle Physics and Relativistic Nuclear Physics. The problem of optimization of the 2D magnetic field of a 4 T dipole magnet with the aperture diameter 100–110 mm for a fast-cycling synchrotron is considered. A single-layer coil is made of hollow superconducting NbTi cable designed at an operating current of 30 kA. The description of mathematical method developed for minimization of higher harmonic of the magnetic field by variation of the coil current loops angular position is given. The numerical simulation results for 2D magnetic fields are presented [1].

A study of the equation-of-state of high compressed nuclear matter is the aim of the CBM collaboration. It is assumed to carry out the investigation at the future GSI accelerator on the event-by-event analysis base. In 2006, the computer modeling of various variants of a superconducting dipole magnet for CBM experiment was carried out (Fig. 4). On the basis of a multivariate spline approximation, differentiated approximations of the magnetic field in the working area of the magnet have been constructed. The modeling of the magnetic systems of the accelerator complex GSI SIS100 was performed, too.

Non-homogeneous magnetic field and large multiplicity of produced particles make the reconstruction of events extremely complicated. For solving the problem, one needs finding and fitting particle tracks in various parts of the setup (STS, TRD, RICH, TOF, ECAL), recognition of rings in RICH, reconstruction of primary and secondary vertices, and so on. The CBM group of

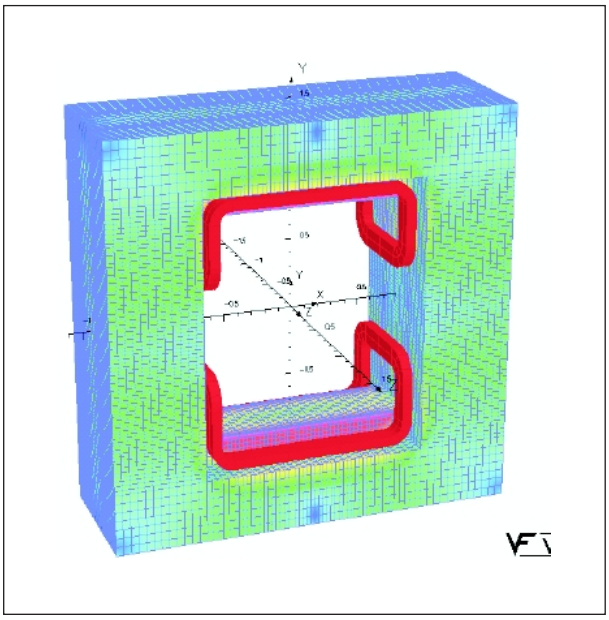

Fig. 4. The computer model of one variant of a superconducting dipole magnet for CBM experiment

JINR LIT has proposed a set of effective methods for event reconstruction and has created corresponding computer codes which are either implemented in the CBM computational system or tested and trialed now. In particular, two algorithms of track reconstruction in the region of STS detector have been presented, two approaches for Cherenkov ring finding in RICH have been proposed, methods for charged particle momentum determination have been developed, and so on. This interesting and useful work is in progress [2].

A method of internal alignment of HERA-B OTR PC chambers is discussed. The method is based on simultaneous fit of the track and alignment parameters using Millepede matrix reduction and singular value decomposition. Software which implements this idea has been developed, the method has been studied on Monte Carlo models with different levels of simulation. A method generalization for the case of track nonlinear model has been proposed [3]. The method was applied to studies using real data taken by HERA-B in a 2002–2003 run period [4].

The research work on the autotracking of knots for piecewise cubic approximation carried out at LIT gives an algorithmic solution to the segment approximation problem that is important for applications and very difficult from a theoretical viewpoint. An original method and an algorithm for automatic tracking of a cubic segment of a curve have been developed on the basis of the criterion of uniformity of the third derivative of the cubic model and a recurrent calculation of estimates of this derivative. A real time oriented adaptive algorithm for knot detection has been developed. The algorithm is simple and stable to errors. On the basis of the algorithm, MS Visual C# components and Windows application APCA (Autotracking Piecewise Cubic Approximation) were developed. The efficiency of the algorithm is confirmed by the results of its application to the approximation of complex curves and real data [5].

Computations have been done on studying speeds of forming polonium isotopes in bismuth foils placed into a massive lead target exposed to a 660 MeV proton beam. The calculation was performed by two methods: first, the isotope yield was computed with the help of the MCNPX program. Then the MCNPX code was used only to calculate a proton spectrum in various points of the target, and then the calculated spectrum was compared with experimental data on the cross-sections of obtaining polonium in reaction $\mathrm{Bi}(p, xN + g)\mathrm{Po}$ (Fig. 5) [6].

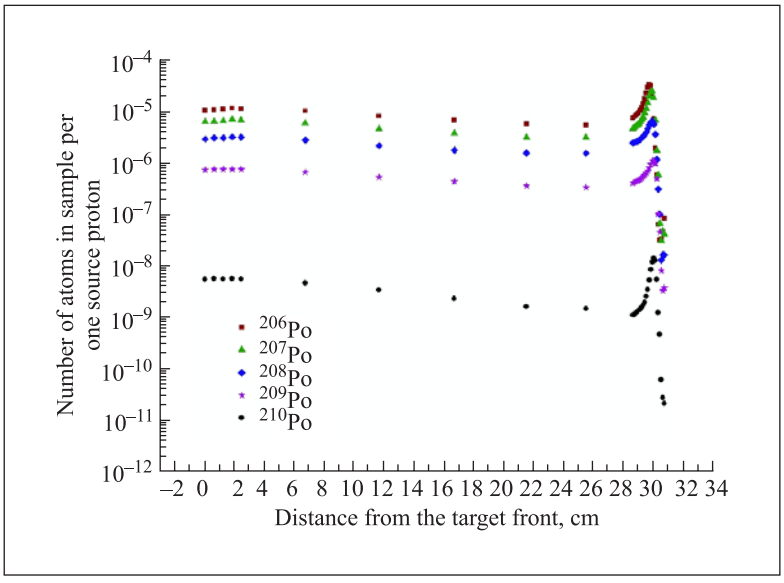

Fig. 5. Spatial distribution of speeds of producing polonium in the target

The quarkonium production in a field-theoretical setting was reconsidered. It is shown that the lowest-order mechanism for heavy-quarkonium production receives in general contributions from two different cuts. The first one corresponds to the usual colour-singlet mechanism. The second one has not been considered so far. It was treated in a gauge-invariant manner, introduced were new 4-point vertices, suggestive of the colour-octet mechanism. These new objects enable one to go beyond the static approximation. It was shown that the contribution of the new cut can be as large as the usual colour-singlet mechanism at high transverse momentum for J/ψ. In the ψ' case, theoretical uncertainties are shown to be large, and agreement with data is possible [7].

The theory of the lepton pair production in nucleus–nucleus collisions has been developed at high energies beyond the frames of Born approximation [8]. A Watson representation has been obtained for the amplitude of process $Z_1 + Z_2 \to Z_1 + Z_2 + e^+e^-$ and a resummation procedure of Watson series has been developed on the basis of the hypothesis of the infrared stability of the amplitude of this process. An explicit expression was found for the first two terms of decomposition of the amplitude $Z_1 + Z_2 \to Z_1 + Z_2 + e^+e^-$ on infrared-stable complexes up to the items of order $(Z_1 Z_2 \alpha^2)^4$. The obtained results are of particular importance for the analysis of experiments on RHIC and LHC.

Work was in progress on providing of theoretical support for the experiments DIRAC and NA48/2 (CERN). Closed expressions have been obtained for the form factor transition between the bound states of dimesoatoms and conditions of a continuous spectrum of meson pairs characterized by certain values of the size and direction with respect to a relative pulse [9]. The form factors are expressed as a superposition of the finite number of items with a simple analytical structure and can be calculated with any degree of accuracy. The obtained results are important for calculation of spectra of products of dimesoatom ionization, measured in the DIRAC experiment.

In the framework of the quantum-mechanical approach, a «cusp» effect discovered in the NA48/2 experiment, has been analyzed [10]. An expression for $K^+ \to \pi^+\pi^0\pi^0$ decay amplitude was obtained that generalizes N. Cabibbo's result on all orders over the scattering lengths (T). Further generalization of N.Cabbibo's amplitude is given to include electromagnetic effects T_c. The results of theoretical calculations (Fig. 6, dashed line) are compared with experimental data (Fig. 6, dotted line), satisfactory agreement is reached. The obtained results allow one to describe in a new manner the threshold anomalies that have been found in the NA48/2 experiment.

In order to investigate the problem of initial singularity and asymptotical isotropization as well as early inflation and late time accelerated mode of evolution of the Universe, a system of interacting nonlinear spinor and scalar fields within the scope of a Bianchi type-I (BI) cosmological model in the presence of a perfect fluid and a cosmological constant (Λ term) has been studied and solutions to the corresponding field equations are obtained. Role of the spinor field nonlinearity and the Λ term in generating both initial inflation and late-time acceleration has been analyzed. Some modified models of dark energy that enable one to generate oscillatory mode of expansion are proposed. A system with time varying gravitational (G) and cosmological (Λ) constants is also studied to some extent, as well as the system with magneto-fluid [11].

Within the framework of Bianchi type-I space-time, the Bel–Robinson tensor and its impact on the evolution of the Universe have been studied [12]. The nature of cosmological solutions for a homogeneous, anisotropic Universe given by a BI model in the presence of a cosmological constant Λ is investigated by taking into account dissipative process due to viscosity. The model is thoroughly studied both analytically and numerically. It is shown that the viscosity, as well as the Λ term, exhibits essential influence on the nature of the solutions [13].

A software complex has been designed to calculate wave functions of discrete and continuous spectra of multidimensional quantum systems by Kantarovich method [14–16]. The obtained eigenvalue problems for the systems of ordinary differential equations are solved by a finite element method. The efficiency and convergence of this algorithm is demonstrated using two-dimensional exactly solvable models. The algorithm [14] is applied to an exactly solvable «benchmark» model of three one-dimensional particles on a

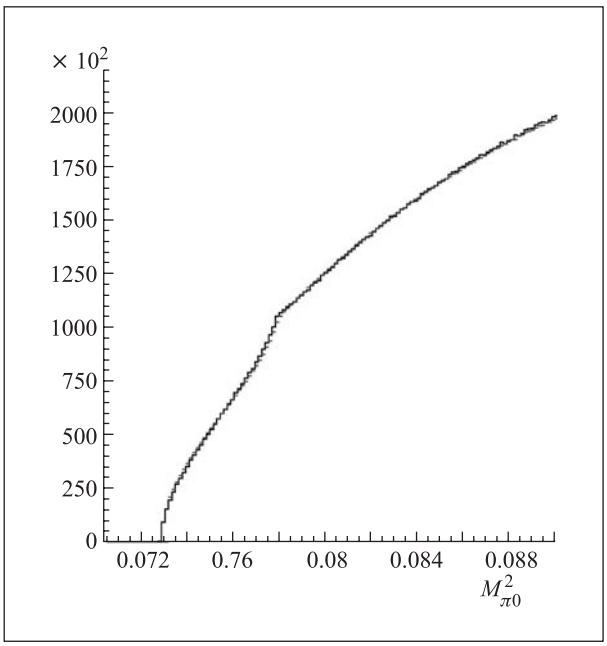

Fig. 6. The «cusp» effect in the $K^+ \to \pi^+\pi^0\pi^0$ decay. Comparison of the theoretical results (dashed line) with experiment (dotted line)

line. The Kantarovich method is used to compute wave functions of discrete and continuous spectra of hydrogen atom in a magnetic field [15], which are required to calculate the rate of forced recombination under effect of laser impulses and finally to determine the conditions under which the yield of recombining atoms will be the largest. The cross-sections of photoionization of hydrogen in the basic state have been computed.

The Kantarovich method was used also to solve a time-dependent Schrödinger equation [16] (Fig. 7). With the help of a unitary Pade decomposition of evolution operator, sixth-order accuracy numerical schemes have been obtained with respect to the time step. The efficiency and convergence of the algorithm is shown by an example of a hydrogen-like atom in a magnetic field and in impulse electric laser field approximated in form of a delta-impulse order.

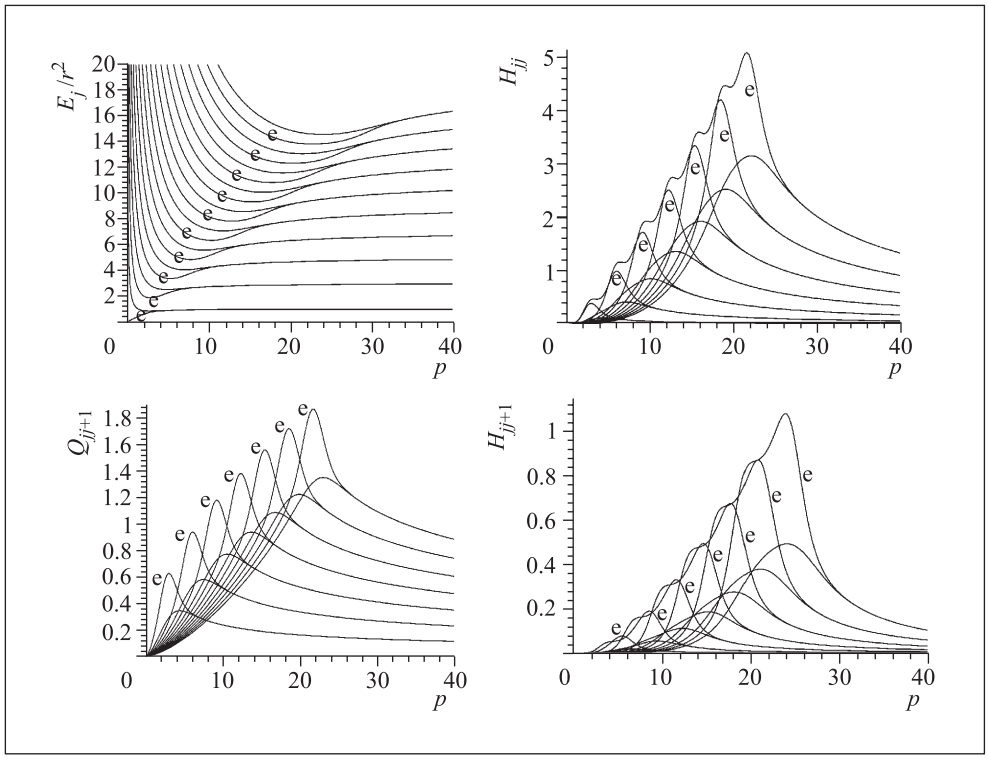

Fig. 7. Computed matrix elements $H_{ij}(r)$, $Q_{ij}(r)$ and potential curves $E_j(r)/r^2$ depending on parameter $p = \gamma r^2/2$ for even («e») and odd states of a hydrogen atom for $|m| = 0$ and $\gamma = 1$

Special variational wave functions of the basic state of helium atom have been constructed to compute theoretical estimates of the cross-section of single and double ionization for description of present-day $(e, 2e)$ and $(e, 3-1e)$ experiments [17]. Wave functions of a helium atom were constructed for a main state on an exponential basis, which satisfy a Kato condition (in both weak and strong senses). Their advantage is in decreasing divisibility of integrals used for calculation of ionization cross-sections.

Mathematical Methods for Nuclear Physics and Condensed Matter Physics. In the framework of high-energy approach and a double-folding method, a model of elastic nucleus–nucleus interactions [18], as well as inelastic interactions, has been developed in view of collective nucleon excitations [19]. Methodical calculations with Woods–Saxon phenomenological potential are presented that confirm applicability of this approach to the modelling of inelastic nucleus–nucleus interactions in the energy range from 10 up to 100 MeV per nucleon. The model has been generalized for a case of the microscopic transition double-folding potential. A comparison is made of the differential cross-sections of elastic and inelastic scattering calculated in the microscopic approach with experimental data (Fig. 8).

Experimental data on total reaction cross-sections of neutron-rich isotopes of helium and lithium with silicon have been analyzed on the basis of the microscopic model that integrates the double-folding method for calculation of real part of nucleus-nucleus potential and the high-energy approximation for calculation of imaginary part. The microscopic double folding Coulomb potential has been calculated and its effect on cross-sections is compared with traditional Coulomb potential of the uniform charge distribution. Semi-microscopic potentials are constructed on a basis of renormalized microscopic potentials and their derivatives to take into account the collective motion effects and to improve an agreement with experimental data [20].

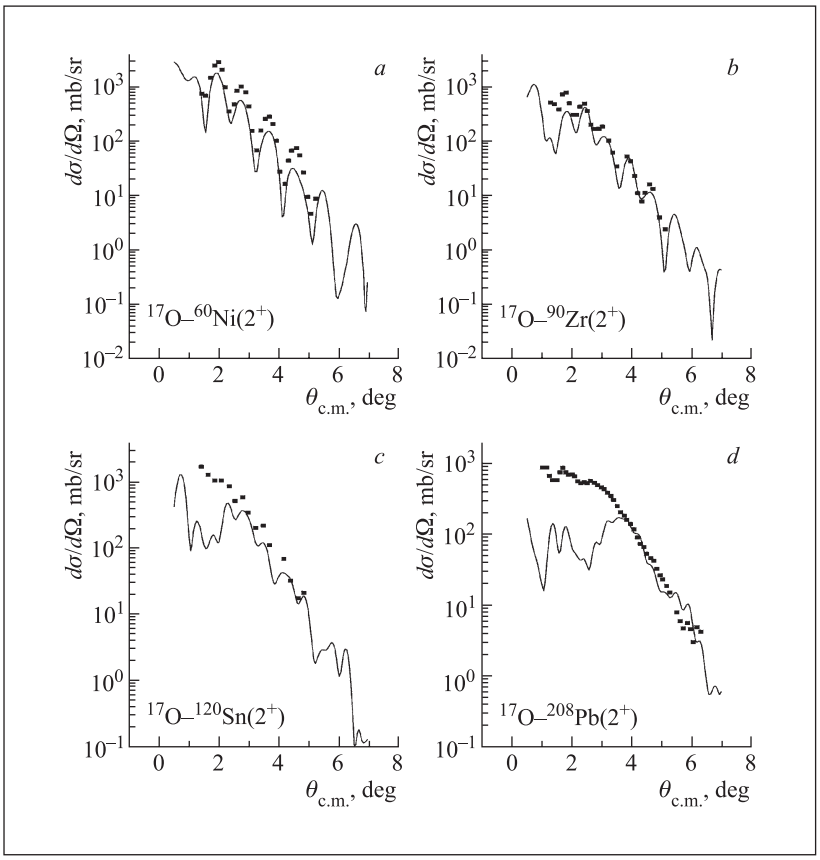

Fig. 8. Comparison of the calculated inelastic scattering differential cross-sections with the experimental data

A nonlinear system of equations for electron gas and lattice around and along the trajectory of a 700 MeV uranium heavy ion in nickel at the constants of heat capacity and heat conductivity taken at room temperature was solved numerically in the cylindric axial-symmetric coordinate system. Based on the temperature dependence upon radius and depth around the ion trajectory, one can conclude that the ionizing energy loss is enough for the melting and evaporation processes in the target. The maximal sizes of radius and depth in target where the melting and evaporation processes can take place have been estimated [21].

The results of sputtering coefficient measurements for pure metals, alloys, amorphous alloys, semiconductors, and highly oriented pyrolytic graphite under irradiation with high-energy ions were considered. The possible mechanisms of strong sputtering of materials with high defect concentrations were discussed. The three-dimensional thermal spike model («hot ion track») with the temperature dependence of thermodynamic parameters (specific heat thermal conductivity) was formulated for single-layer mono- and polycrystals and multilayer systems (materials). The results of a numerical solution to the introduced system of partial differential equations were considered for the lattice and electronic subsystem temperatures around and along the fast heavy ion trajectory as a function of the time t, as well as radial r and longitudinal z coordinates, taking into account possible phase transitions such as melting and evaporation [22].

Partial critical dependences of the form current–magnetic field in a two-layered symmetric Josephson junction were modeled. A numerical experiment showed that, for the zero interaction coefficient between the layers of the junction, jumps of the critical currents corresponding to different distributions of the magnetic fluxes in the layers may appear on the critical curves. This fact allows a mathematical interpretation of the results of some recent experimental results for two-layered junctions as a consequence of discontinuities of partial critical curves [23].

Based on the method of molecular field dominated by magnetic component, it was shown that a homogeneous magnetically aligned nematic liquid crystal can respond to a circularly polarized optical field by transverse nemato-magnetic wave in which velocity of incompressible flow and director undergo coupled oscillations slowly traveling along the axis of magneto-optical anisotropy. The effect may be of practical interest for the magnetically controlled information processing and storage [24].

It is argued that in the long wavelength limit of electromagnetic, far infrared, field optical response of an ultrafine metal particle threaded by uniform magnetic field can be properly modeled by equations of

semiclassical electron theory in terms of the surface inertial wave–like oscillations of free electrons driven by Lorentz restoring force. The detailed calculation of the frequency of size-independent gyromagnetic plasmon resonances computed as a function of multipole degree of electron cyclotron oscillations was presented [25].

A system of traps was considered, each containing a large number of Bose-condensed atoms. It was found that when the frequency of the modulating field was in resonance with the transition frequency between two different topological coherent modes, each trap became an analog of a finite-level resonant atom. A method was suggested for regulating entanglement production in such a system of multitrap and multimode Bose–Einstein condensates coupled through a common resonant modulating field. Several regimes of evolutional entanglement production, regulated by manipulating the external field, were illustrated by numerical calculations. The suggested method can be used for information processing and quantum computing [26].

Distributions of phosphate backbone-produced electrostatic potentials around several tRNAs were calculated by solving the nonlinear Poisson–Boltzmann equation. The tRNAs were either free or bound to the proteins involved in translation: aminoacyl-tRNA and elongation factor EF-Tu identified several regions of strong negative potential related to typical structural patterns of tRNA and invariant throughout the tRNAs. The patterns are conserved upon binding of tRNAs to the synthetase and the EF-Tu. Variation of tRNA charge in our theoretical calculations of electrostatic potential-mediated pK shifts of pH-dependent labels attached to tRNA, compared to experimentally observed pK shifts for those labels, shows that the total charge of tRNA is large, within the interval from –40 to –70 proton charges. The electrostatic field of tRNA is sufficient to cause ionization of histidine residues of ARSase, causing additional free energy of ARSase-tRNA interaction of at least several kcal/mol. This may discriminate proteins with respect to the particular tRNA at large distances. Two types of tRNA-protein electrostatic recognition mechanisms were discussed. One, more specific, involves charges induced on protein by the large electrostatic potential of tRNA, while the other, less specific, does not involve induced charges [27].

At present, after 120 years of the theoretical and experimental works, the issue of the genome macroarchitecture as the highest level of interphase chromosome organization in somatic cell nuclei remains still unresolved. The problem of the spatial arrangement of interphase chromosomes in haploid germ cells has never even been studied. A 3D simulation of packaging of the entire second chromosome in Drosophila mature sperms has been performed by using mathematical approaches and visualization methods to present macromolecular structure data. For the account of a degree of spatial affinity and visualization of chromosomal loops, modern 3D-modeling methods with application of splines, libraries OpenGL, language Delphi, program Gmax were used [28].

COMPUTER ALGEBRA AND QUANTUM COMPUTING

Dynamics of cellular automata with symmetric local rules has been studied [29]. These rules act on lattices with high degree of symmetry under permutation of their cells. Analysis of such cellular automata can be used in simulation of such trivalent structures as fullerens and graphemes which are currently considered as potential basis of future nanotechnologies.

Algorithm was designed and implemented in Maple for automatic generation of finite difference schemes for linear partial differential equations with two independent variables and for uniform and orthogonal grids. The algorithm is based on construction of difference Gröbner bases [30].

A new parametrization of the $SU(3)$ group manifold was found which can be considered as a generalization of the classical parametrization of group $SU(2)$ by the Euler angles. The new parametrization can be used, in particular, for Hamiltonian reduction of gauge field theories with $SU(3)$ symmetry and for quantum computation based on the use of qutrits — quantum particles with three classical states [31].

A numerical and analytical algorithm for reconstructing the two-dimensional discrete elliptic equation of a part of spectrum and prescribed symmetry conditions was developed. The right problem is solved in the rectangle $M \times N$ with the zero-boundary conditions. If the given symmetry conditions are satisfied, the eigenfunctions can be prolonged from the rectangle to the whole plane with reserving continuity of the first derivatives. The problem is reduced to reconstruction of a symmetric five-diagonal matrix. It is proved that when the prescribed symmetry conditions are satisfied, the considered block three-diagonal matrix and all its blocks are persymmetric. This matrix has $L < MN$ different elements and can be reconstructed of L given eigenvalues. Numerical experiments were produced. The polynomial systems were derived and solved by using CAS REDUCE [32].

The specialists of LIT and the Institute of Cybernetics of Georgia conduct joint research in the field of quantum mechanics and quantum computations. Using a method of transformation of soluble time-independent

problems of quantum mechanics into time-dependent ones, periodic potentials with a complex dependence on time and coordinate variables are employed. The problem of evolution of spins of a particle in a heterogeneous T periodic magnetic field, a special case of which is a dynamics of spin states in a homogeneous magnetic field, is under study. The matrices of the evolution obtained in an explicit form are used to construct a universal set of gates needed for quantum computations. Non-adiabatic geometrical phases are determined in terms of the cyclic solutions found. In the suggested approach, the geometrical phase effect at construction of one-cubit gates is naturally taken into account. A way of obtaining entangling operators is discussed, too [33].

The interwining operator technique was applied to the generalized Schrödinger equation with an additional functional dependence $h(r)$ in the right-hand side of the equation [34]. The suggested generalized transformations turn into the Darboux transformations for both fixed and variable values of energy and angular momentum. A relation between the Darboux transformation and supersymmetry was considered.

CONFERENCES

On 17–23 January 2006 LIT hosted the XIII interdisciplinary conference «Mathematics. Computer. Education». The purpose of the conferences is to get acquainted with new achievements of modern Russian and world science. Most of the participants are higher school lecturers simultaneously involved in pedagogical and research work.

The 10th Workshop on Computer Algebra was organized on 23–24 May 2006. Attending were more than 30 scientists from Linz (Austria), Turku (Finland), Moscow, St. Petersburg, Belgorod, Samara, Saratov, Tambov, Tver and Dubna. The main goal of the workshop 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.

The second international conference «Distributed Computing and Grid Technologies in Science and Education» was held at LIT from 26–30 June 2006. The conference was attended by more than 200 specialists from 17 countries and from 46 universities and research centres of Russia. Representatives of commercial enterprises, in particular Cisco Systems and Kraftway, took part at the conference. The scientific programme of the conference, which included 96 reports and presentations, covered the following topics: creation and operating experience of Grid infrastructures in various areas of science and education; methods and technologies of distributed computing; architecture, algorithms; distributed processing and data storage; organization of the network infrastructure for distributed data processing; algorithms and methods of solving applied problems in distributed computing environments; theory, models and methods of distributed data processing; distributed computing within LHC projects; technologies of designing and experience of using distributed information Grid systems.

The international conference «Mathematical Modeling and Computational Physics» (MMCP-2006) devoted to the 50th anniversary of the Joint Institute for Nuclear Research was held in High Tatras Mountains, Slovakia, on 28 August – 1 September 2006. The organizers of the Conference were the JINR Laboratory of Information Technologies, the Institute of Experimental Physics of the Slovak Academy of Sciences (Košice) and the Technical University, Košice. The Conference was the fourth one organized by LIT under this name. On the initiative of the Slovak colleagues, it was for the first time organized outside JINR. The Conference was attended by known specialists in the field of mathematical simulation and computational physics from many countries. The Conference highlighted the role of the mathematical modeling and computing methods as an integrating factor in the present-day scientific research in various fields of knowledge: particle physics, physics of solids, hydrodynamics, biology, biochemistry, material studies, quantum computations, economy, computer science, etc.

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