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.

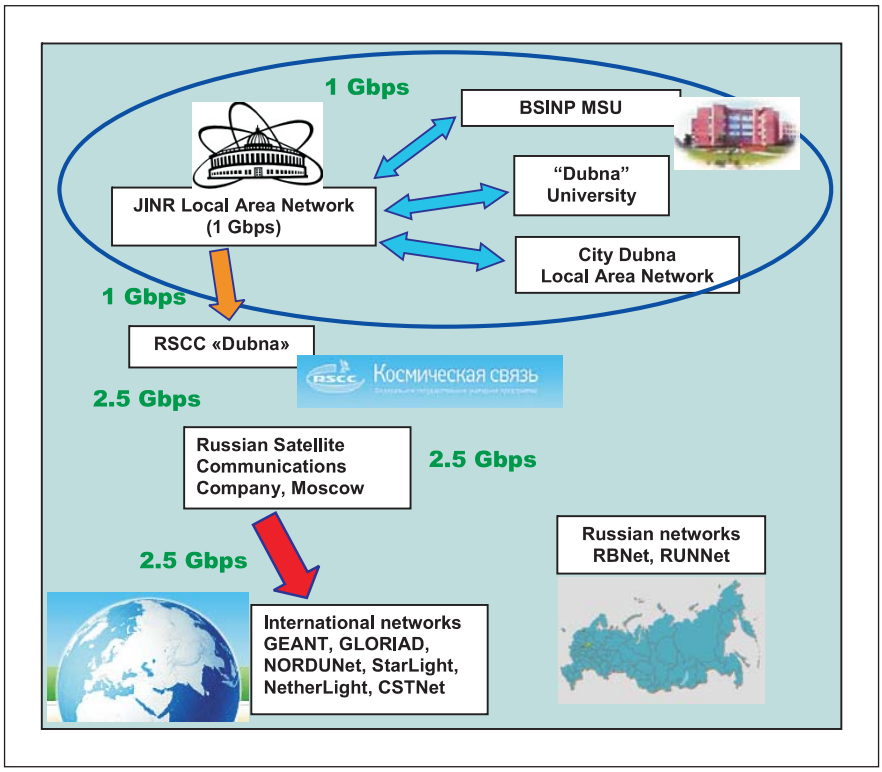

Fig. 1. The JINR telecommunication channels

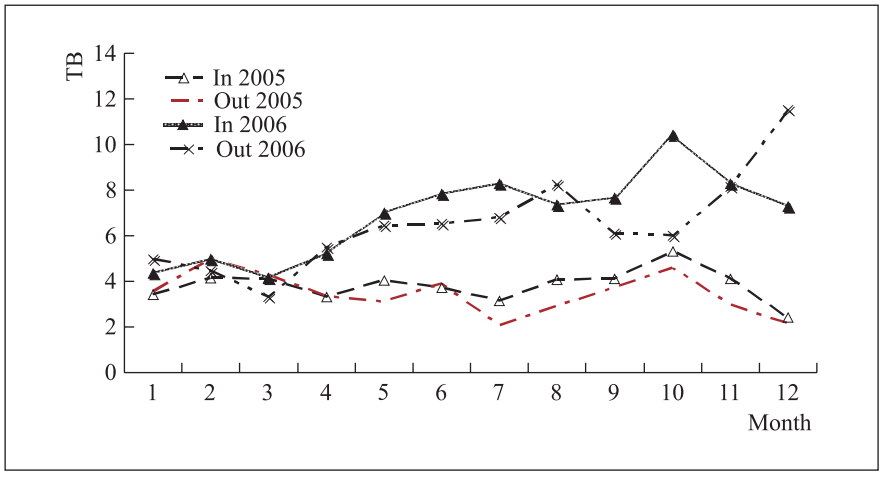

Fig. 2. Incoming and outgoing JINR traffic in 2005 and 2006

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.

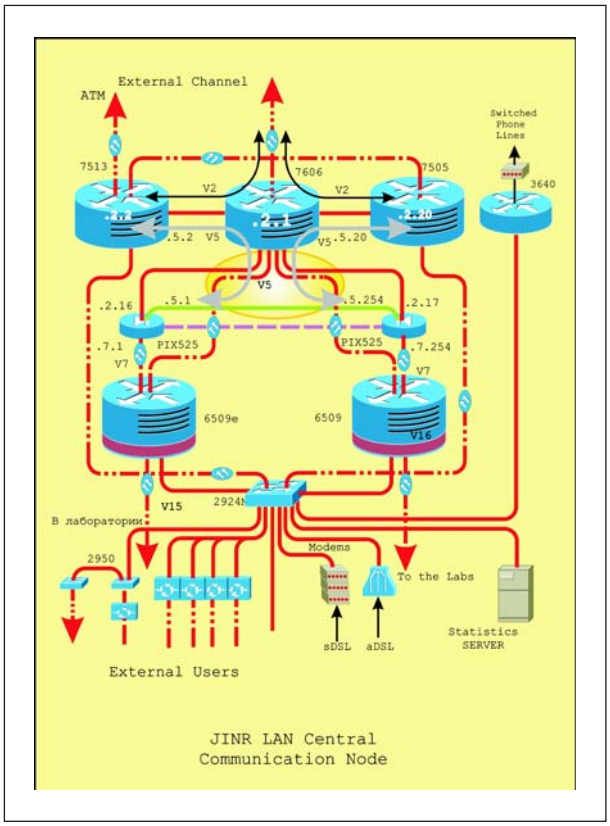

Fig. 3. JINR LAN Central Communication Node

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

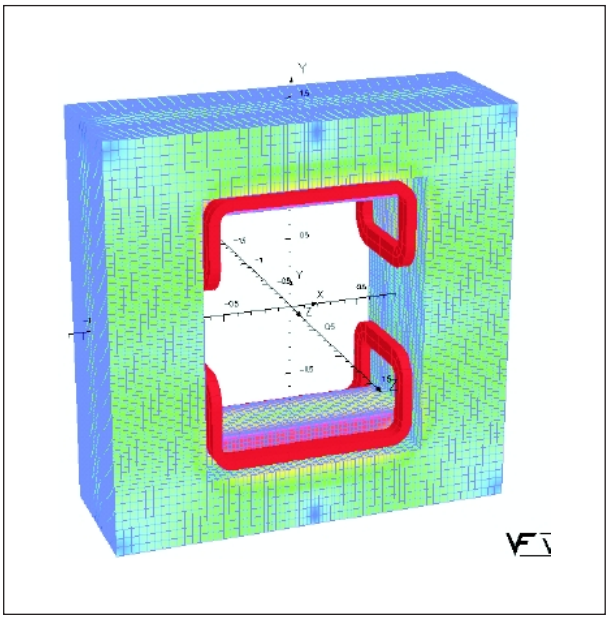

Fig. 4. The computer model of one variant of a superconducting dipole magnet for CBM experiment

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].

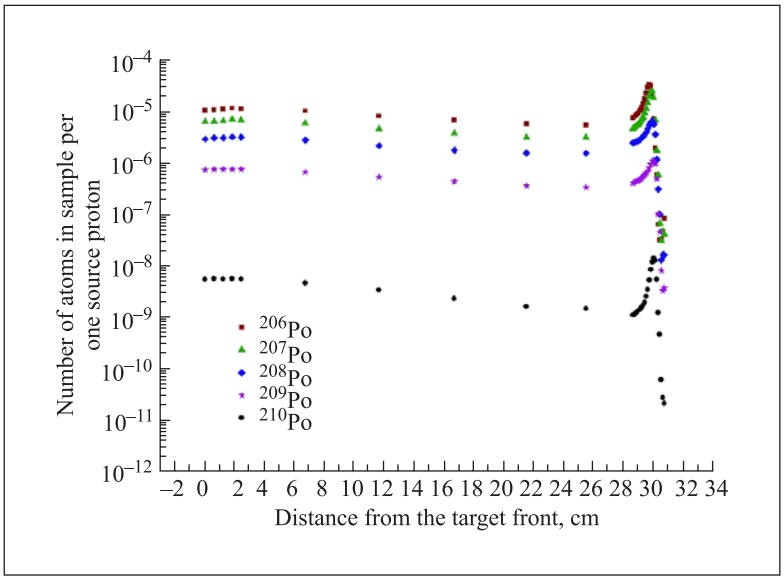

Fig. 5. Spatial distribution of speeds of producing polonium in the target

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

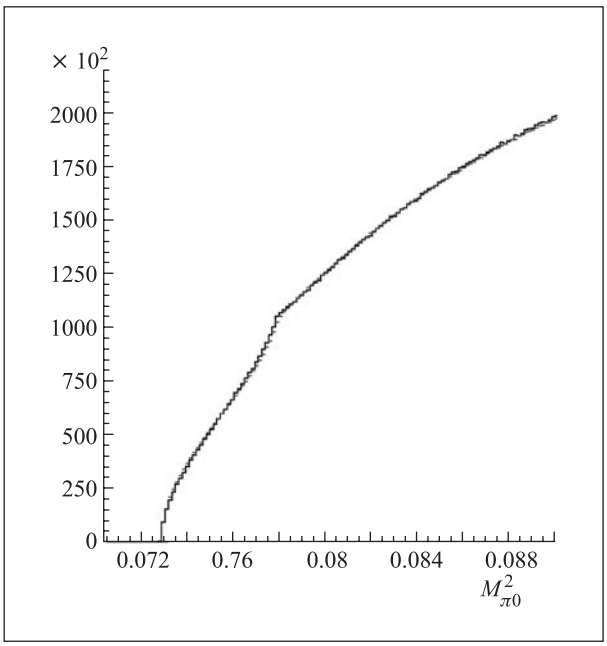

Fig. 6. The «cusp» effect in the $K^+ \to \pi^+\pi^0\pi^0$ decay. Comparison of the theoretical results (dashed line) with experiment (dotted line)

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.

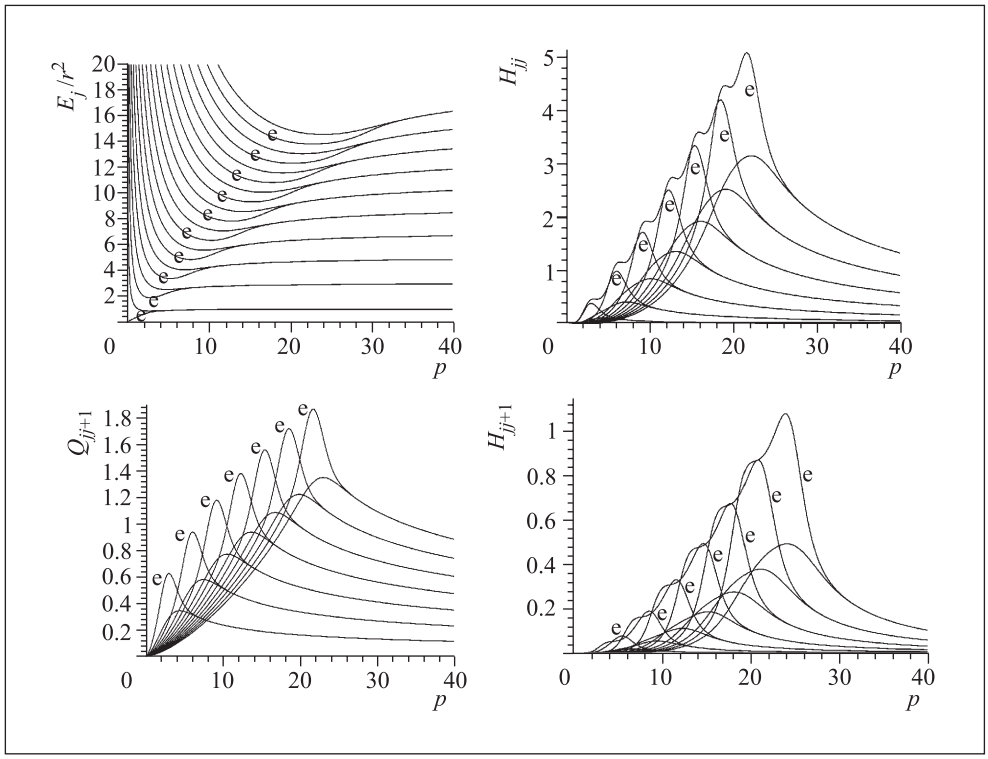

Fig. 7. Computed matrix elements $H_{ij}(r)$, $Q_{ij}(r)$ and potential curves $E_j(r)/r^2$ depending on parameter $p = \gamma r^2/2$ for even («e») and odd states of a hydrogen atom for $|m| = 0$ and $\gamma = 1$

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].

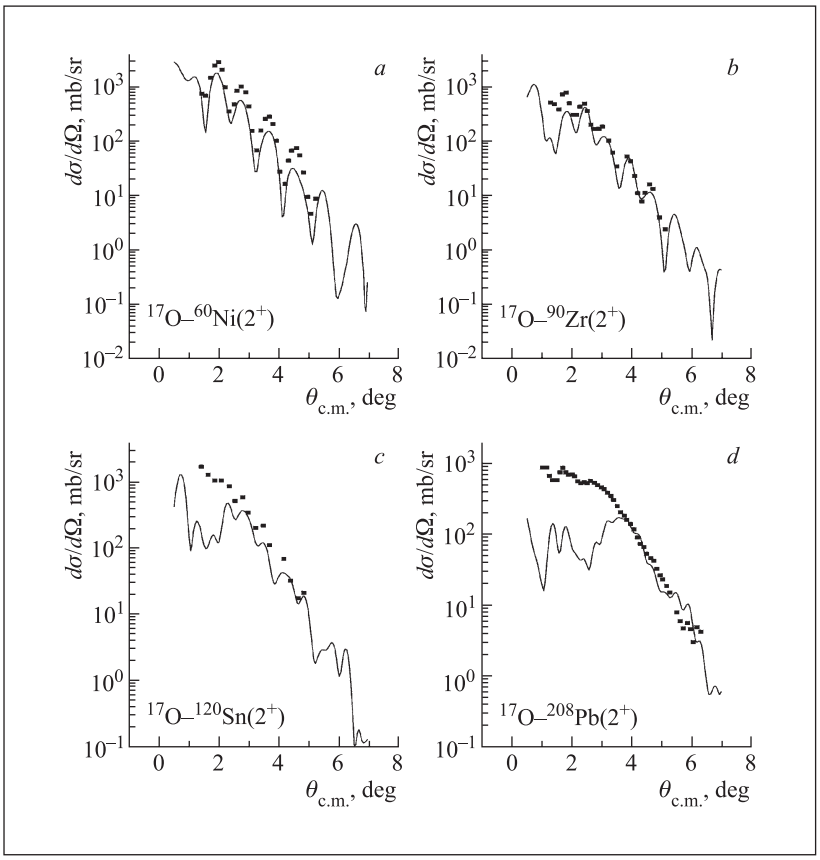

Fig. 8. Comparison of the calculated inelastic scattering differential cross-sections with the experimental data

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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LABORATORY OF RADIATION BIOLOGY

The research programme of the Laboratory of Radiation Biology (LRB) determined by the first priority theme was concentrated in 2006 on the following main directions: fundamental radiobiological and radiation genetic research with heavy charged particle beams, investigation of molecular photo- and radiobiological processes in eye structures, research in the field of molecular dynamics, radiation research and radiation protection at the basic nuclear facilities of JINR and its environment. Special attention was devoted to participation of young researchers, students and postgraduates in current LRB events and also in conferences and seminars in which LRB took part.

RADIOBIOLOGICAL AND RADIATION GENETIC RESEARCH

The study of molecular damages in peripheral human blood lymphocytes after irradiation with γ-rays and accelerated heavy ions was continued. The regularities of induction and reparation of double-strand breaks (DSB) in cells irradiated with ^{60}Co γ-rays and lithium ions (^{7}Li and ^{11}B, linear energy transfer 20 and 40 keV/μm) by using comet assay analysis were studied. The histograms of cell distribution on the level of their DNA violation after γ-ray and heavy ion irradiation were obtained. It was shown that in control samples the value of «tail moment» is negligible but its distributions are revealed with growing of the irradiation dose. The distribution is shifted to the larger values of the «tail moment». The relationships between DSB yield and the dose of used types of radiation were built on the basis of obtained results. The linear dose–effect dependences were revealed for γ-rays and heavy ions (Fig. 1). The analysis of the results demonstrates that heavy ions are more effective on the induction of DSB in comparison with γ-rays. The coefficient of relative biological effectiveness of accelerated lithium ions is 1.6 ± 0.1.

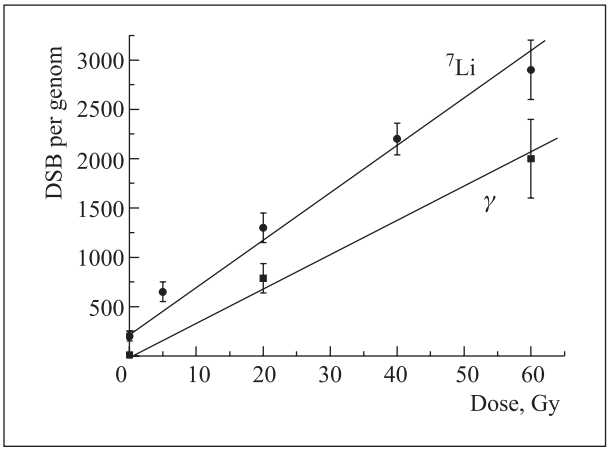

Fig. 1. Induction of DSB in DNA of human blood lymphocytes irradiated with γ-rays of ^{60}Co and lithium ions ^{7}Li

The regularities of induction and reparation of DSB under influence of inhibitors of DNA synthesis arabinofuranosyl cytosine (Ara C) and hydroxyurea (HU) in γ-irradiated cells were studied. The combination of these agents blocks not only the replicative but also the reparative synthesis of DNA. As was shown, the short gaps in DNA transform to the enzymatic DSB, as a result of the S_1-endonuclease impacts of the opposite strand of DNA. It was established that in comparison with the normal conditions the number of DSB increases up to ~ 3 times after 2 h in irradiated cells under Ara C + HU influence. The difference in DSB number in irradiated cells under normal conditions and under Ara C + HU after 5 h reaches 7 (Fig. 2). This explains the effective DSB repair in cells under normal conditions and transformations of single-strand gaps into enzymatic DSB under inhibitors of DNA repair synthesis. In the following experiments with heavy ions when mainly direct DSB will be formed in DNA it is planned to study the influence of DNA synthesis inhibitors on the yield of DSB and kinetics of their repair.

The investigations in the range of low doses of ionizing radiation were extended. Additional data confirming nonlinearity of dependence of chromosome aberration frequencies on the dose in human peripheral blood lymphocytes were obtained. Namely, irradiated cells

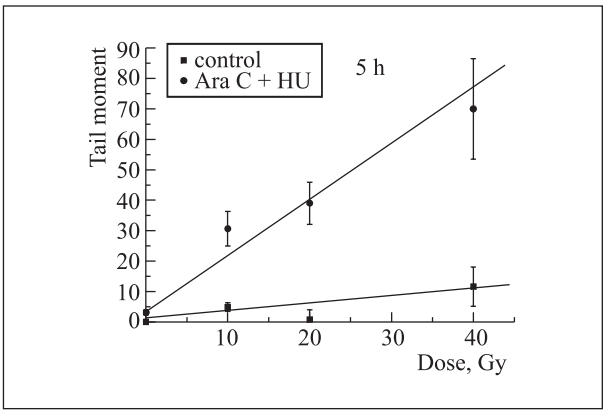

Fig. 2. The differences in DSB number in irradiated cells under normal conditions and under Ara C + HU inhibitors after 5 h

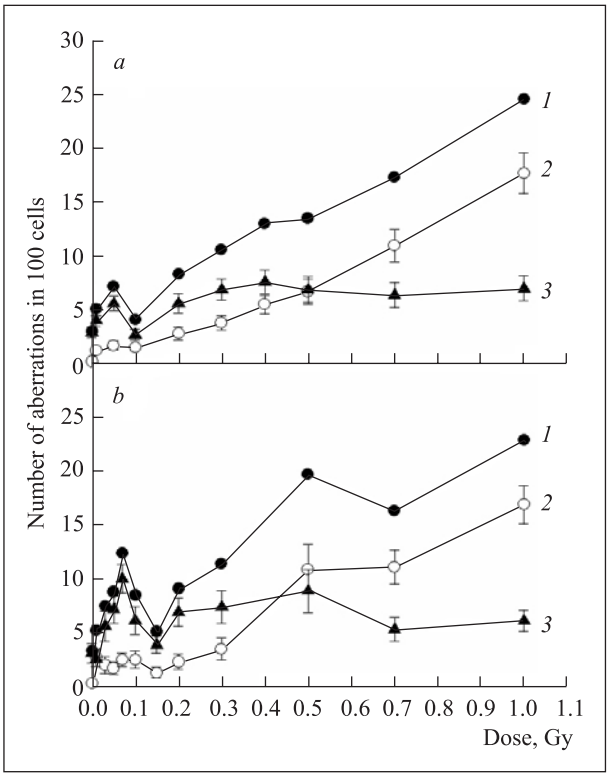

Fig. 3. The dependence of the number of chromosome aberrations on γ-ray doses in human blood lymphocytes

displayed hyper radiosensitivity (HRS) at very low doses with a peak around 5–7 cGy determined by chromatid type of aberrations. With the subsequent increase of the dose to 10–15 cGy, the aberration yield decreased significantly and demonstrated an inverse dependence on the dose. At $\geqslant 50$ cGy the dose–effect curve became linear with a less steep slope as compared to the initial one (increased radioresistance, IRR) [10]. Analysis of literature data concerning the mechanisms of low dose action allowed one to hypothesize about possible cellular processes underlying HRS and IRR. The most probable cause of highest aberration yield in the region of extremely low doses is radiation-induced drastic elevation of generated endogenous reactive oxygen species (ROS). At the same time, the ensuing decrease of aberration frequency may be caused by activation of cytoprotective signaling pathways (mostly Erk protein kinase) that is aimed at reduction of oxidative stress [11, 12]. In order to verify this hypothesis the work was started with human mammary carcinoma cells cal51, allowing one to apply a variety of inhibitors and activators of cellular processes that are supposed to be involved in realization of atypical phenomena of low-dose radiation.

The investigations of high LET radiation-induced chromosomal aberrations DNA-proportional deviations distribution in individual variability were continued in collaboration with the biophysical group of the Institute of Biology (Keltce, Poland).

In all published studies concerning individual radiosensitivity the lymphocytes were exposed only to low LET radiation (Fig. 3). Our studies showed that the inter-donor variability acts as a potential source of mistakes at absorbed dose quantification. Choosing chromosome 2 for analysis, one could minimize this error. Moreover, the present results support the point of view that the ratio of centric/dicentric rings (F ratio) could be a signpost to estimate to high LET exposure.

A series of experiments on whole blood samples irradiated with heavy ions ^{11}B, ^{17}Li and ^{20}Ne have been done. The frequency of dicentric + centric rings in the first post-irradiation metaphases and PCC excess fragments of human peripheral blood lymphocytes of several donors has been studied. The obtained results are in agreement with previous studies data.

Together with the Institute of Biochemical Physics of RAS, the investigation for item «New Experimental and Theoretical Approaches for Study of Biophysical and Molecule-Cytogenetical Chromosome Instability Mechanisms Induced by Radiation with Different LET for Prognosis of Radiation Cancerogenic Risks» has been performed. The obtained data allow us to estimate the possible mechanisms of chromosome instability for the human and mammalian cells and show the ways of investigating such problems.

A new method was developed to detect hidden defects in membranes of human blood erythrocytes. The method consists in membrane electroporation application for detection of hidden disorders of membrane electrodynamics characteristics of erythrocytes. A possibility was shown to use the method for detection of damaging action of radiation on the membranes. Research of laws of gamma ray action in a wide range of radiation doses on membranes of human blood erythrocytes has been continued.

Several lines of genetic research were developed in 2006. One of them is an induction of different types of mutations from ionizing radiation with yeast *Saccharomyces cerevisiae* as model system of eukaryotic cells.

We continued to use tester strain systems for detecting various types of mutations:

• Large deletions on plasmid model [2, 5]. UV-light and gamma-irradiation efficiently induced deletions. Mutation *rad53* decreased a frequency of induced mutations [7].

• Intergenic mutations — a forward mutation rate assay that detects all mutations inactivating the *CAN1* gene. As shown, a linear dependence of induced mutations is up to $3 \cdot 10^{-6}$ (survival 0.2%) after UV irradiation [4].

• Base-single deletions — frame shift assays detecting mutations that revert 4-base insertion in the *LYS2* gene or +1T insertion in a stretch of 6T's in *HOM3* gene [4]. The rate of spontaneous *lys2*-revertion was $4 \cdot 10^{-8}$ and of *hom3*-revertion — $3 \cdot 10^{-8}$. The UV-light induced frame shift mutations more effectively. For dose 134.4 J/m^2 frequency of frame shift mutations for revertion to Lys$^+$ is $2 \cdot 10^{-5}$ and for revertion to Hom$^+$ is $7 \cdot 10^{-6}$. Dose dependence curves of frame shift mutation induction were linear for survival up to 0.2%.

• Tester system for base substitution is based on critical requirements for cycteine at position 22 of iso-1-cytochrome encoded by *CYC1* gene [4]. In order to restore codon 22 and revert to wild type the defined substitution is necessary. All possible base-pair substitutions — 2 transitions and 4 transvertions — can be monitored. The curve of survival for all haploid and diploid strains after UV-light exposures is obtained. They are linear and sigmoidal, respectively. The base pair substitution — transversion AT–TA induced by UV-light and neon ions with LET values 120 keV/μm was characterized. The shape of curves for diploids is similar and may be fitted by a linear-quadratic function in the case of UV-light exposure.

• Gross rearrangements of genome [8]. We study a gross rearrangement including a recombination and a loss of chromosome VII by disomic strain under ionizing radiation and UV-light. A linear-quadratic curve of induction of these rearrangements was shown.

We continned to study genetic control of genetic stability, particularly genetic control of repair and checkpoint control [1, 3, 6, 9].

The studies of structure and functional elements of human and yeast kinases were continued. 3D structure of yeast kinase was built on the base of crystal structure of human kinase. Phenotypes of different *cdc28* mutations were compared with structural rearrangements. A correlation was shown between phenotypes (radiosensitivity, generation time and mitochondrial mutability) and rearrangements [16, 18, 19].

DNA mismatch repair (MMR) plays a major role in the recognition and correction of the mispaired base, increasing radioresistance, replication fidelity and maintaining genome integrity. Defects in MMR are the underlying cause for cancer susceptibility syndrome called HNPCC and account for 20% of sporadic cancers. High mutability and likelihood of cancer can be caused by mutations that reduce MMR or by external factors that directly inhibit MMR. Identifying such factors has important implications for understanding the role of the environment in genome stability. Cadmium (Cd^{2+}) is a known human carcinogen — ubiquitous metal with unknown biological function that can come into human's organisms mainly through environmental contamination and cigarette smoking. It is shown that Cd^{2+} inactivates the DNA mismatch repair (MMR) pathway.

MMR is a complex reaction that involves multiple proteins, that recognizes the mismatch, excises the DNA containing the error and resynthesizes the correct DNA sequence. In yeast, several genes have been identified, particularly MSH2, MSH3 and MSH6, which are homologues of MutS in *Escherichia coli*. Homologues of *E. coli* MutS have been found nearly in all organisms. Prokaryotic MutS proteins are encoded by a single gene and homodimer form. Eukaryotic MutS proteins are heterodimeric. The initial recognition of mispair (a critical step in the pathway) is carried out by two protein complexes: the Msh2–Msh6 heterodimer, which recognizes base–base mismatches and frameshift (± 1 bp) mispair, and the Msh2–Msh3 heterodimer, which recognizes frameshifts and large insertion deletion mispairs (2–4 bp).

All members of the MutS family possess a conserved ATPase activity (Fig. 4). Both mismatch recognition and the ATPase activities of MutS are essential for MMR even though each activity is independently detectable. ATP binding and hydrolysis by the dimeric Msh protein complexes is a critical factor of MMR and can modify the interactions of Msh2–Msh6 and Msh2–Msh3 with the mismatched DNA and other downstream factors. Cd^{2+} inhibits both Msh2–Msh6- and Msh2–Msh3-dependent human MMR activity *in vitro* and is less inhibitory to its DNA mismatch binding activity and more mismatched duplexes. The inhibition of ATPase activity by Cd^{2+} is prevented by cysteine and histidine, suggesting that these residues are essential for the ATPase activity and are targeted by Cd^{2+}. Cysteine inhibits the ATP coupling and hydrolysis through the Msh2–Msh6 complex and inhibits the DNA coupling to some extent. The interactions of cadmium with Msh2 and/or Msh6 that are responsible for inhibition are unknown.

Two structures of MutS complexes have already been reported, the *Thermus aquaticus* (TAQ) and *E. coli* enzymes and its complex with heteroduplex DNA. A MutS subunit consists of five structural domains arranged in the shape of a comma. The globular domain I and domain IV are involved in DNA binding. Domain V contains the ATPase activity. Domains II, III and V retain similar structures in the presence or absence of DNA. MutS forms a stable dimer due to the extensive interactions between the ATPase domains.

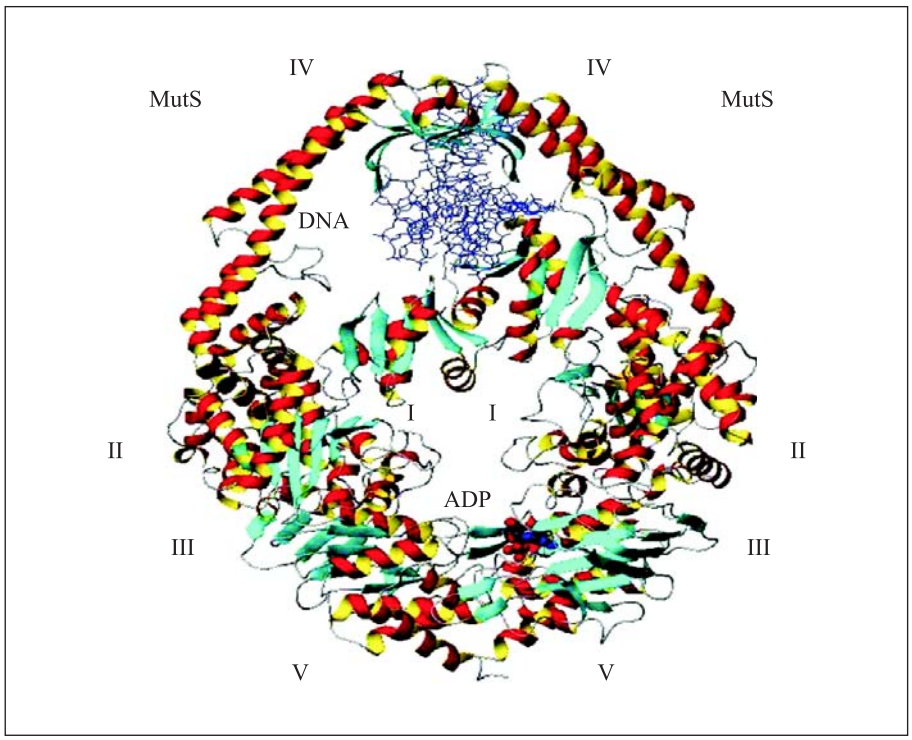

Fig. 4. Overview of the MutS–DNA complex of *E. coli*. The MutS is drawn by ribbons, DNA is line, the ADP molecule is shown as spherical balls

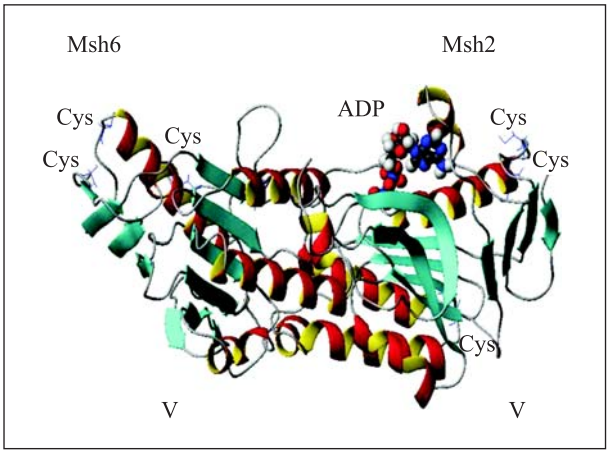

Fig. 5. Molecular modeling of the Cys localization in yeast Msh2–Msh6 complex. The ADP molecule is drawn as spherical balls

The molecular modeling for the Msh2–Msh6 complex of yeast *Saccharomyces cerevisiae* was performed using MODELLER, based on the template structure of *E. coli* (the PDB file: 1E3M). The secondary-structure prediction algorithms and sequence alignment methods were implied. Since we are interested in studying the influence of ions Cd^{2+}, we modeled only the fifth domain-fragment (residues 543–765). MODELLER generates the three-dimensional structure that relies on structure prediction and sequence alignment results followed by energy minimization using CHARMM force field. The ribbon structures were created with MOLMOL. Ribbon diagram of the Msh2–Msh6 nucleotide-binding sites and associated dimer interface is shown in Fig. 5.

In this case the basic structure of domain V of yeast Msh2–Msh6 complex was identified using homology modeling approach. Further from the MMR mechanism the Cd^{2+}-inhibition activity can be analyzed using the computationally generated structures.

PHOTORADIOBIOLOGICAL RESEARCH

Based on computer simulation approach, a molecular dynamics of dark-adapted state of the visual rhodopsin has been investigated [17]. The analysis has been provided for the interactions of chromophore group, 11-*cis* [14] retinal and surrounding amino acid residues in the Schiff base region. It was shown (Fig. 6) that interaction of protonated Schiff base linkage with negative charged Glu113 is most likely not simple classical electrostatic one between two opposite charged groups. One can propose that not only Glu113, but also Glu181 and Ser186 take part in the protonated Schiff base linkage stabilization. In accordance with our cal-

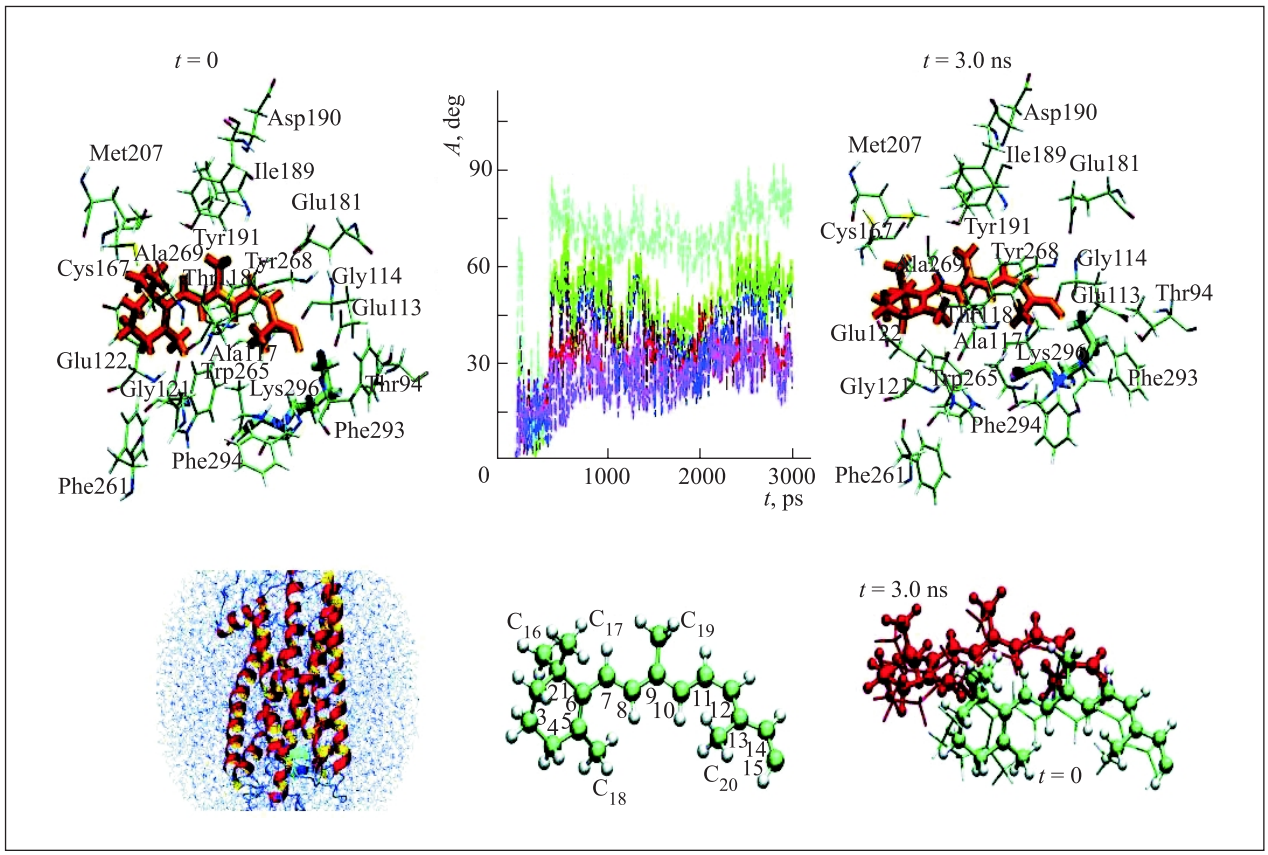

Fig. 6. Molecular dynamics of 11-*cis*-retinal in the rhodopsin chromophore center at the initial ($t = 0$) and final ($t = 3$ ns) simulation states are presented along with the torsion rotation angles of five methyl groups (C_{16}–C_{20}) (top). The positions of the 11-*cis*-retinal atoms during the 3 ns dynamical changes are separately displayed (bottom). (View from the side of the rhodopsin molecule)

culations Glu181 as a counterion interacts with Schiff base linkage through Ser186.

It was shown that UV irradiation causes a covalent modification of α-crystallins. But an aggregation of damaged molecules does not occur. It confirms a high stability of α-crystallins. UV irradiation causes a covalent modification of β-crystallins, which is accompanied with protein aggregation and precipitation. UV irradiation of α- and β-crystallins mixture does not cause protein aggregation. We developed a new method for separation of protein damage and aggregation. Using this method it was shown that molecular mechanism of α-crystallin chaperone-like function protection is not connected with stable complex formation [21].

It was shown that α-crystallin decreases the thermostability of rabbit muscle GAPD, which is connected to protein oligomeric structure [22].

COMPUTER MOLECULAR MODELING OF BIOPHYSICAL SYSTEMS

In 2006 the staff of CMM sector performed the scientific research and educational activity within the following topics:

• Molecular dynamics of chromophore 11-*cis* retinal and surrounding amino acid residues in the chromophore binding pocket at physiological regeneration of visual pigment rhodopsin: computer simulation. Molecular dynamics calculations were performed for the time interval from $t = 0$ to 3000 ps, so that the configuration states of rhodopsin and free opsin were analyzed and compared. It was demonstrated that the adaptation of the chromophore retinal in the opsin site causes a considerable influence on its protein binding pocket, as well as on conformations of the cytoplasmic part, but the extracellular part of the protein shows a comparably small changes. On the basis of the simulation results we discuss some molecular mechanisms for the rhodopsin protein function as a G-protein-coupled receptor in the dark state, i.e., for the chromophore retinal as a ligand-agonist stabilizing the inactive conformation of the rhodopsin (Fig. 7).

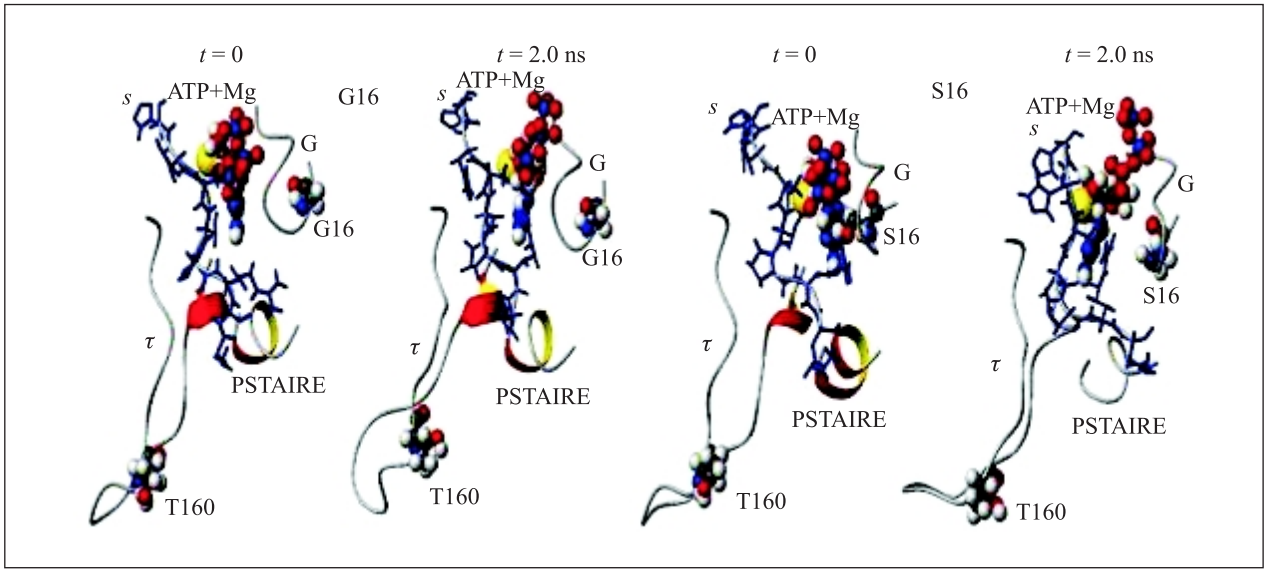

Fig. 7. Orientation of ATP complex relative to magnesium ion in the finite state ($t = 2$ ns) for G16 and S16 complexes

• Analysis of the bonds between the ATP and catalytic subunit of kinases (wild and mutant) using MD simulations of the active cdk2 crystal lattice.

• Molecular-dynamics simulations of mechanism of SOS mutagenesis in *Escherichia coli*, based on the studies of the conformation behavior of lexa and proteins involved in the formation of single- and double-stranded DNA structure. Nanoseconds long MD simulations of the cyclin-dependent proteinkinases (CDK) with ATP complex were performed [16, 19]. The central role that CDKs play in the timing of cell division and repair and the high incidence of genetic alteration or deregulation of CDK inhibitors in a number of cancers make CDC28 of yeast *Saccharomyces cerevisiae* very attractive model for studies of mechanisms of CDK regulation. The crystal structure of the human CDK2 has served as a model for the catalytic core of other CDKs, including CDC28. MD simulations of substitution CDK2-G16S in conserved G-loop show an important change of this amino acid and a conformational change of CDK2 structure resulting in the moving of the G-loop away from ATP and a new rearrangement of amino acids in the T-loop.

• Application of the methods of quantum information theory to the visual information processing in retina [15].

• Application of genetic algorithms for simulation of proteins 3D structure.

• Application of wavelet transform for eliminating divergences in solution of stochastic differential equations and quantum field theory problems [12, 13].

It was proposed that information processing in brain, and in retina in particular, is most likely performed by means similar to hypothetic quantum computers, but at the presence of dissipation. Quantum mechanical tunneling effects are suggested to be responsible for the visual signal processing by bipolar cells in retina.

The results of the research performed by the staff of the CMM sector were presented at all-Russian and international conferences, symposiums and seminars, as well as published in the domestic and foreign journals.

RADIATION RESEARCH

The main radiation component of the radiation fields at the working accelerators is neutrons with very wide energy range. The neutron spectra behind the JINR nuclear facilities are very differing depending on the accelerated particle energies, shielding materials, source–shield geometry, and so on. The following tasks were done in 2006.

• The systematization of the neutron spectra at the JINR accelerators and reactor was done for determination of the neutron ambient dose dependence on the shape of neutron spectrum. It is necessary for definition of the real range of the normalization coefficients at the area radiation monitoring.

• Calculations of different types of radiation shields for mobile and stationary installations for identification of hidden explosive and narcotic substances were performed.

• The calculation of the local shields of two electron accelerator scrapers for the IREN project was done.

• In the framework of the participation in the planet surface research programme, the calculation and the

experimental study of the collimated neutron detector characteristics for the Moon spacecraft was carried out.

• Support of the biological experiments with the blood lymphocytes, plant cells and laboratory mouse irradiation by the carbon ^{12}C ions with energies 200 and 500 MeV/amu was provided at the VBLHE Nuclotron. A series of radiobiological experiments were carried out with the neon, lithium and boron ion beams at the FLNR U-400M.

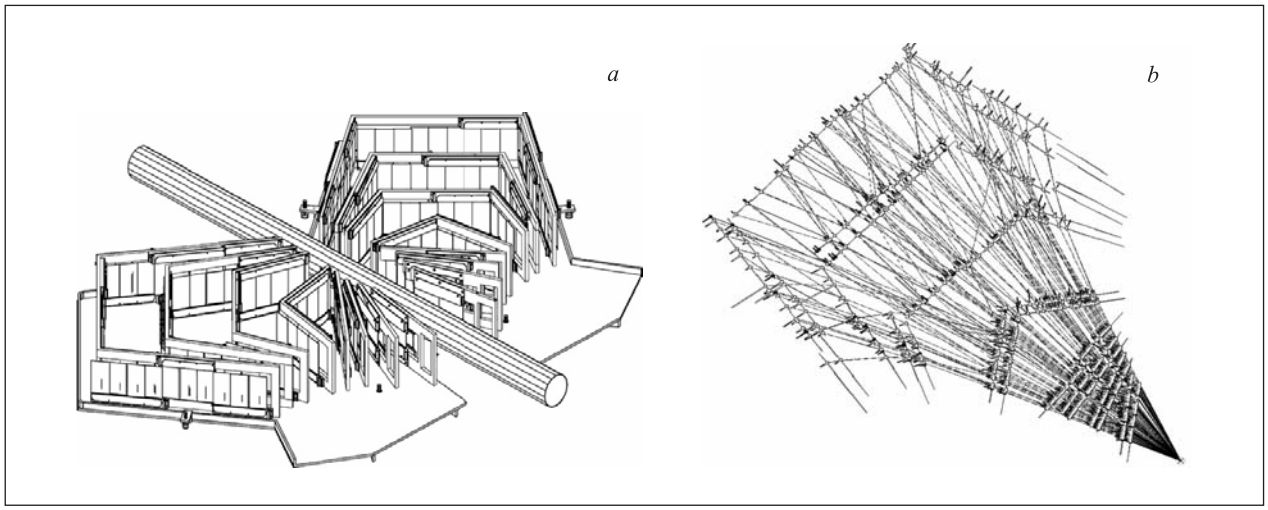

Fig. 8. Schematic sketch of PHOBOS silicon detector (*a*) and example of real event track reconstruction on the left arm of the spectrometer (more than 150 tracks) (*b*)

The particle track reconstruction based on new String Banana Template Method (SBTM) was developed for the PHOBOS setup (RHIC/BNL) [23]. The main idea of the method is based on the features of ensembles of tracks selected by three-fold coincidences. The SBTM provides a narrower search window than other methods by exploiting the features of such ensembles: it deals with particular «branches» in the Multiple Scattering (MS) «tree». A two-step track model with additional parameters to account for MS is used. The SBTM uses stored template fields generated by precise Monte Carlo (MC) simulation. SBTM capabilities in terms of track parameter resolution are demonstrated for a model spectrometer.

SCIENTIFIC MEETINGS AND EDUCATIONAL ACTIVITY

On 5–9 June the 4th International Workshop on Space Radiation Research and 17th Annual NASA Space Radiation Health Investigators' Workshop was held in Moscow and St. Petersburg. The major role in the organization of this meeting is shared by the JINR Laboratory of Radiation Biology and the Institute for Biomedical Problems of RAS. The modern problems of classical and space radiobiology, space radiation protection, dosimetry, etc., were discussed at the workshops. Special attention was given to Moon exploration programme, Mars manned flight programme and to study of possible application of obtained data to medicine, biology and radiation protection as well. More than 100 scientists from Russia, USA, Germany, Italy, Japan, and JINR took part in the workshops.

On 18–21 September the 2nd international conference «Molecular Simulation Studies in Material and Biological Sciences» (MSSMBS'06) was held at JINR. The main topics of the conference were the molecular simulation studies of nano- and biostructures. For the purposes the organizers invited the key experts from universities and institutes of Japan, Russia, Armenia, Denmark, and Ukraine.

In the middle of November at the autumn JINR meeting of the Programme Advisory Committee for Condensed Matter Physics special appreciation was obtained for the poster session of LRB young scientists. Over 15 reports of young scientists and students from Russia, Germany, Poland, Slovakia, and Bulgaria were presented at the meeting.

The education process at the chair of Biophysics of the International University «Dubna» was continued. A total of 69 students are studying on the specialty «Radiation Protection of People and Environment» now. Nineteen new students were admitted in 2006 to the chair. The second graduation of the chair yielded eight new scientists in 2006.

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UNIVERSITY CENTRE

The results of the JINR Education Programme were discussed at the University Centre (the UC) Council session held on December 13, 2006. It was pointed out by the JINR Director Prof. A. N. Sissakian that the UC successfully fulfilled its duties in 2006 regarding organizing, running, and supporting the education process at JINR. In addition to the UC's traditional activities (graduate and postgraduate studies, international actions, and work with secondary school pupils), a new task was started in 2006: the establishment of the UC's student laboratories.

Student Laboratories — a New Structure within the UC

In 2006, a new structure emerged within the UC: the student laboratories. An important contribution to the acquisition of equipment was made by Dubna University.

The UC laboratories will first be used for the students of the JINR-based Departments performing the general physics practicum exercises. In the future, special practicum equipment is planned to be installed there, which will be interesting to graduate students of the JINR Member States.

By 2007, the laboratories of thermodynamics and molecular physics, optics, and atomic physics have been equipped; a nuclear physics laboratory has been founded.

International Cooperation and the Summer Student Practice

The key mission of the JINR Education Programme and the UC's activities is to attract the youth of the JINR Member States to the Institute. With this aim, short-term actions are carried out for the youth of the Member States that help them to know JINR better and, possibly, to find their prospective scientific supervisors at JINR.

The UC organizes international student schools and practices, as well as acquaintance visits for secondary school pupils, students, and postgraduates of Member States. The visit programmes include excursions to the JINR Laboratories, seeing the Institute's basic research facilities, studies at the laboratories, and performing the physics practicum exercises.

On July 2–22, 2006, the UC hosted the Third International Summer Student Practice in JINR Fields of Research. It was remarkable for a record high number of its participants: 51 students came from higher education institutions of the Czech Republic, Poland, Romania, and Slovakia. There were more applications for attending the practice than planned; so the organizers had to select the participants. This points to the growing publicity of this Practice. The largest group — 20 students — was the Polish one; it was made up by students of the universities of Gdansk, Krakow, Lodz, Lublin, Poznan, Szczecin, and Wroclaw. The second largest group came from the Czech Republic (14 students). The number of the Romanian and Slovak participants has also grown (nine and eight, respectively).

The Practice programme included lectures on special subjects by JINR's leading scientists, lecture presentations of the JINR Laboratories; and traditional exercises at the basic research facilities of the Flerov Laboratory of Nuclear Reactions (FLNR), Frank Laboratory of Neutron Physics (FLNP), Veksler and Baldin Laboratory of High Energies (VBLHE), Dzhelepov Laboratory of Nuclear Problems (DLNP), and Laboratory of Radiation Biology (LRB).

For the first time the lecture programme of the Practice included the presentations of the JINR Laboratories.

The topics of the laboratory exercises — the key part of the Practice — were announced in advance; therefore, when registering at the UC Internet site for participating in the Practice, the applicants, besides specifying their scientific interests in general, chose laboratory exercises from the list published at the site. The exercises were provided by FLNR, FLNP, VBLHE,

DLNP, and LRB. The widest range of topics was provided by FLNR and FLNP. For example, six exercises were arranged at FLNR's facilities, including «Studying Nuclei at the Stability Border», «Studying Micro-Objects Using an Electronic Microscope», and «Studying Radiation Properties of Materials». FLNP organized ten laboratory exercises reflecting all the main fields of its research (nuclear physics, condensed matter physics, and neutron activation analysis). Students of JINR Member States show great interest in laboratory work on applying nuclear methods in biology and medicine. Therefore, LRB was involved in 2006 in the Practice; the Laboratory provided the following exercises: «Instrumental Methods of Radiation Safety», «Cytology», «Microbiology», and «Molecular Biology».

The Practice became possible thanks to the financial support by the grants from the Plenipotentiaries of the Czech Republic, Poland, and Slovakia, and to the programme of cooperation between JINR and Romania. Remarkably, great help was given by W. Chmielowski (Poland), A. Constantinescu (Romania), A.-S. Dubnickova (Slovakia), and I. Stekl (the Czech Republic).

JINR Graduate Studies

On the basis of JINR, graduate programmes in physics reflecting the main fields of the Institute's research (nuclear physics, elementary particle physics, and condensed matter physics) are offered. The programmes begin either with the first year of studies (for the students of the Dubna branch of Moscow Institute of Radio Engineering, Electronics, and Automatics (MIREEA); and the departments of Dubna International University of Nature, Society, and Man) or with the graduate years (for physics students coming from Moscow State University (MSU), Moscow Engineering Physics Institute (MEPI), Moscow Institute of Physics and Technology (MIPT), and higher education institutions of JINR Member States).

In 2006, more that 500 students attended courses at the JINR Laboratories, including 34 students of MSU, nine of MEPI, 15 of MIPT, more than 200 students of Dubna University, and 120 of other higher education institutions of the following JINR Member States: Armenia, Belarus, the Czech Republic, Poland, Ukraine, and Uzbekistan.

One of the UC's functions is creating and supporting additional special advanced courses for graduate students delivered by JINR staff members. The program of the courses is based upon the recommendations and requests of the JINR-based departments of higher education institutions. The following courses were given at the UC in 2006: Telecommunications and World Information Resources (V. V. Korenkov); Database Management Systems (V. V. Korenkov); Database Management Systems (practice, I. A. Filozova); Statistical Physics (G. G. Adamian); Selected Topics of the Elementary Particle Physics (seminar, Ye. A. Strokovsky); Elementary Particle Physics Methodology (Ye. A. Strokovsky); Computer Modelling of Physics Processes in Detectors Using the GEANT4 Software Package (A. S. Zhemchugov, A. Demichev); C++ (V. G. Olshevsky); Introduction to the Object-Oriented Analysis of Data Using the ROOT Software Package (T. M. Solovyova); Introduction to the Theory of Accelerators (G. V. Trubnikov).

Besides offering lectures on certain subjects, the UC participates in working out the education programmes in specific disciplines comprising lecture courses and seminar classes and supports them. In 2006, the Large Hadron Collider (LHC) special programme continued at the UC. The programme was initiated by Prof. I. A. Golutvin to train staff for the LHC experiments in which JINR participates. The programme was attended by students of MSU, MIPT, Voronezh University, Kostroma University, and MIREEA.

JINR Postgraduate Studies

In 2006, the UC did a great job of preparing the documents for the prolongation of its license to offer postgraduate programmes. JINR offers postgraduate programmes in ten specialties.

In 2006, JINR's total postgraduate enrolment was 67. Table 1 shows the distribution of the postgraduates over the JINR Laboratories in 2006.

Table 1

Laboratory	Number of postgraduates
Laboratory of Theoretical Physics	20
Laboratory of Nuclear Problems	21
Laboratory of Nuclear Reactions	5
Laboratory of High Energies	6
Laboratory of Neutron Physics	4
Laboratory of Particle Physics	1
University Centre	1
Laboratory of Information Technologies	7
Laboratory of Radiation Biology	2
Total	67

Table 2 shows the total enrolment distribution over all JINR's postgraduate specialties in 2006.

In 2006, 18 applicants were accepted in the postgraduate studies.

It is certainly interesting to examine from which higher education institutions postgraduates came to JINR. About half of those accepted graduated from Moscow's elite institutions (four came from MSU and four from MIPT); others graduated from institutions of JINR Member States (mostly from Russian ones). In 2006, JINR's total postgraduate enrolment from its Member States was 16, including seven from Armenia,

five from Belarus, three from Ukraine, and one from Uzbekistan.

Table 2

Specialty	Number of postgraduates
Nuclear and Elementary Particle Physics (01.04.16)	26
Theoretical Physics (01.04.02)	19
Charged Particle Beam Physics and Accelerator Techniques (01.04.20)	3
Solid State Physics (01.04.07)	3
Physics Experiment Techniques, Instrument Physics, and Physics Research Automation (01.04.01)	5
Mathematical and Software Support of Computers, Computational Complexes, and Networks (05.13.11)	1
Mathematical Modelling, Numerical Methods, and Software Complexes (05.13.18)	7
High Energy Physics (01.04.23)	—
Radiobiology (03.00.01)	3

Pre-University Studies

In the modern world the formation of a prospective physicist actually begins before the person enters a university. Besides, the choice of a career by a secondary school pupil depends on his or her mental outlook and interests. Therefore, the UC attaches great importance to its activity aimed at secondary school pupils of JINR Member States to raise their interest in physics and research carried out at JINR.

In 2006, the UC was visited by eight secondary school pupils and their two teachers from Poland (the cities of Leszno, Poznan, Swinoujscie, and Tarnowskie Gory), ten students of Opole University (Poland), and 15 school pupils from Berlin.

Throughout 2006, the UC was offering an optional physics course for the 10th and 11th-year school pupils of Dubna, which included lectures and laboratory work.

In March 2006, the UC and Dubna University held together an Open Scientific Conference on Physics and Mathematics for Moscow Region's School Pupils. The conference was attended by more than 50 secondary school pupils of Russia, Ukraine, and Belarus.

Staff Training and Retraining and Qualification Improvement

In 2006, the UC continued the training, retraining, and improvement of the qualifications of its working staff and specialists. JINR's ten staff were trained in an allied profession; ten, in a second profession.

At the JINR courses training personnel for operating facilities that are within the jurisdiction of the Federal Technical Inspection 60 JINR's staff were trained; 86 JINR's staff were trained and certified to operate and maintain machines, mechanisms, and pressurized vessels.

Fifty JINR's management staff and leading specialists were trained and certified according to the standards and regulations on using atomic energy. JINR's seven staff improved their qualifications at different seminars held by education institutions of Moscow, Obninsk, and Dubna.

Information Support of the UC's Activities

In January 2007, the UC opens its new Internet site. It will meet the requirements to modern sites and is designed so as to let the UC's potential partners in the JINR Member States learn about the JINR education programmes and the UC's activities.