LABORATORY OF INFORMATION TECHNOLOGIES

In 2003, the scientific programme of the Laboratory of Information Technologies (LIT) covered three first-priority topics of the Topical Plan for JINR Research and International Cooperation in 2003. The Laboratory staff participated in 13 more topics of the Topical Plan in collaboration with other JINR Laboratories on the project level and in 17 topics on the level of cooperation.

The main aim of the Laboratory is the performance of work in the framework of the topics «Information, Computer, and Network Support of JINR's Activity», 09-6-1048-2003/2007 (leaders V. V. Ivanov and V. V. Korenkov) and «Computer Physics for Theoretical and Experimental Research», 09-6-1041-2002/2004 (leaders I. V. Puzynin and A. Polanski). Main results of the investigations performed within these topics have been published in the well-known journals, proceedings of scientific conferences and preprints.

In the year 2003, a number of scientific projects with the LIT participation received grants of the Commission of the European Community in the framework of the EU–Russia collaboration, INTAS, and 12 grants of the Russian Foundation for Basic Research (RFBR). Seven RFBR projects are devoted to the creation and development of information, computing and telecommunication resources, and the remaining five are initiative scientific projects.

In 2003, LIT was an organizer of two conferences: the Focus Symposium «Quantum Physics and Communication» (Dubna, 29 July – 2 August) and the XIX International Symposium on Nuclear Electronics & Computing (NEC'2003) (Varna, Bulgaria, September 15–20).

Second «Information Bulletin of LIT» (JINR, 4-8160. Dubna, 2003; http: //lit.jinr.ru/Inf_Bul_2/) was published which contains information for users of the JINR networking, computing and information resources.

EXTERNAL TELECOMMUNICATION SYSTEMS

At present, JINR leases a 45 Mbps channel to Moscow from the Russian Satellite Communications Company (RSCC «Dubna»). JINR has access to the Russian networks and information resources (up to 45 Mbps computer communication link), as well as access to the international channel through shared RBNet in the common data stream 622 Mbps and in the granted 10 Mbps bandwidth. Figure 1 shows a present-day status of the external channels used by JINR.

Figure 2 shows the incoming and outgoing JINR traffic in 2003. Total incoming traffic was 19.89 TB (9.73 TB in 2002) and outgoing traffic was 24.43 TB (1.92 TB in 2002).

Table 1 represents traffic distribution among the JINR subdivisions (> 300 GB on incoming traffic).

Table 1

JINR's subdivision	Incoming traffic	Outgoing traffic	Incoming traffic, %	Outgoing traffic, %
LIT	3.52 TB	7.92 TB	17.7	32.4
DLNP	2.84 TB	4.33 TB	14.28	17.72
Proxy+servers	2.68 TB	1.82 TB	13.47	7.44
FLNR	2.29 TB	1.36 TB	11.5	5.58
LPP	2.04 TB	849.15 GB	10.25	3.39
BLTP	1.65 TB	1.13 TB	8.28	4.63
VBLHE	1.64 TB	2.79 TB	8.23	12.00
Uni-Dubna	1.1 TB	539.37 GB	5.53	2.16
FLNP	984.96 GB	2.27 TB	4.84	9.31
Administr.	399.51 GB	761.21 GB	1.96	3.04

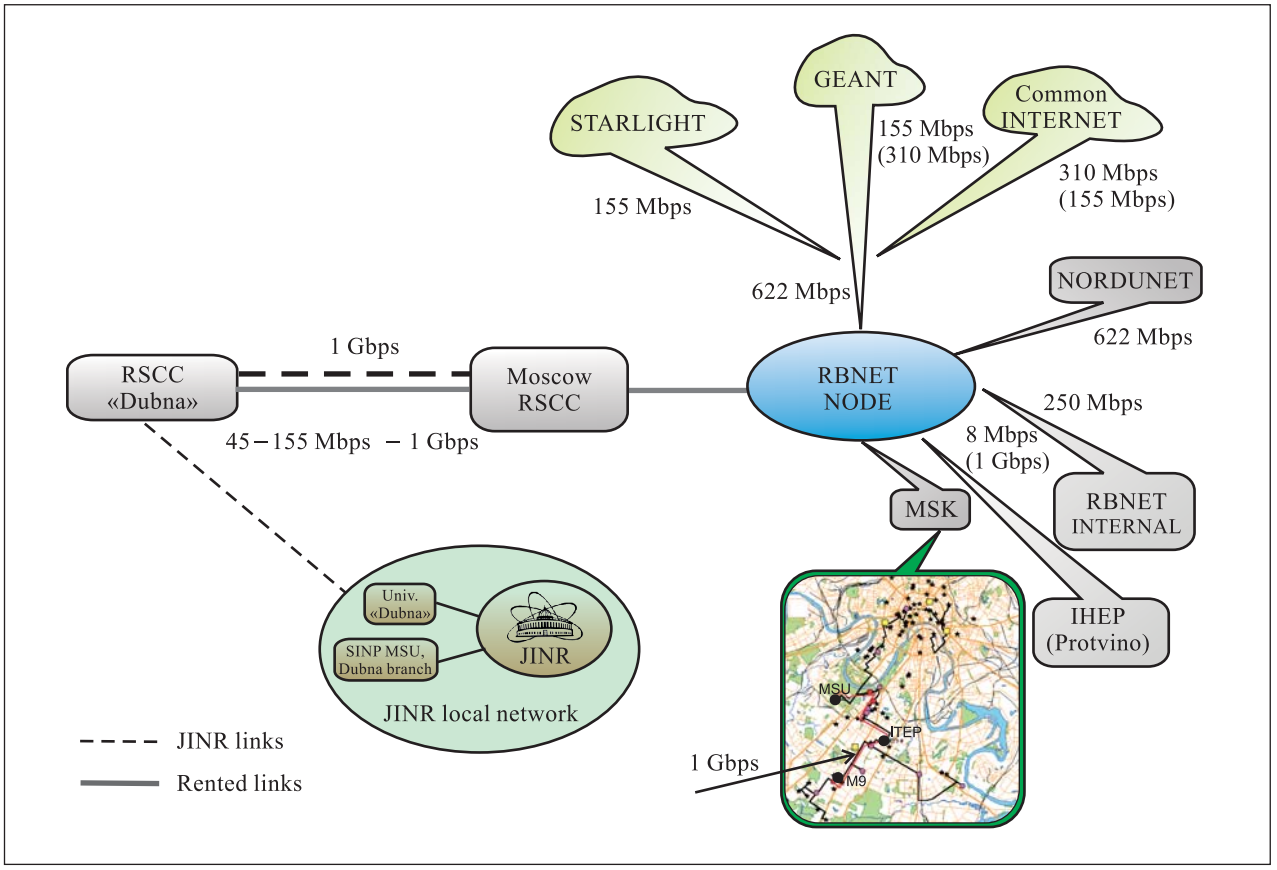

Fig. 1. Current state of external communications in Russia used by JINR

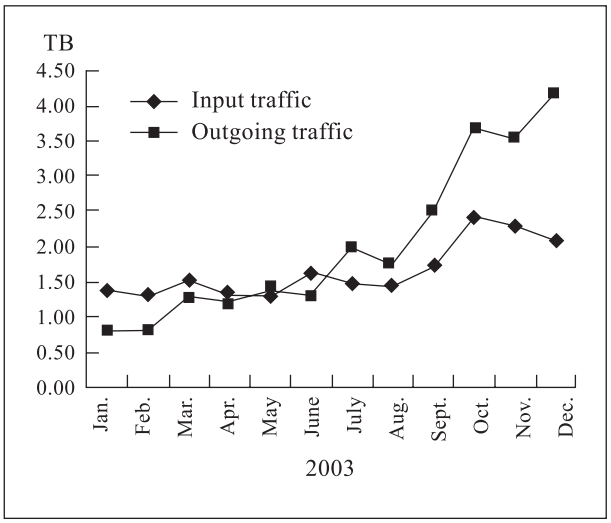

Fig. 2

Systematic work on the JINR local area network (LAN) management was performed by the Network Operation Centre (http://noc.jinr.ru/). Up-to-date JINR LAN statistics can be found at http://noc.jinr.ru/inform/inf_main_stat.shtml.

JINR LOCAL AREA NETWORK

At present, IP addresses database contains 4506 registered JINR LAN elements (4053 in the year 2002). As was outlined in the JINR Topical Plan for 2003, one of the main tasks to develop the information, computing and telecommunication structure at JINR was implementation of the first stage of a selected variant of the JINR Backbone on the basis of Gigabit Ethernet.

The core of the JINR LAN Gigabit Ethernet Backbone is Cisco Catalyst 6509 switch with 8-port Gigabit Interface Card. There are Cisco Catalyst 3550 switches installed at seven JINR Laboratories and in the building housing the JINR Administration. All these pieces of gigabit equipment are interconnected by 16-wired single-mode optical cables of 10 300 m (Fig. 3). To defend the perimeter of the JINR LAN, two Cisco firewall devices PIX-525 were installed (one is active, and the other is in a failover mode).

Work was in progress on research in the main features of the network traffic. The methods of nonlinear analysis and uniflow neural network were applied to reconstruction of a dynamic system describing the information traffic in a middle-size local area network.

The neural network trained on measuring the network traffic has played back a statistical distribution of the information flow, which is well featured by the logarithmically normal law. The analysis of key components of the traffic measurements has shown that already some leading components form a log-normal distribution, while the residual components play a role of casual noise. This result is confirmed by joint statistical, wavelet and Fourier analysis of traffic measurements. The log-normal distribution of the information flow and the multiplicative character of time series confirms applicability of the scheme developed by A. Kolmogorov to homogeneous fragmentation of grains, for the network traffic as well [1].

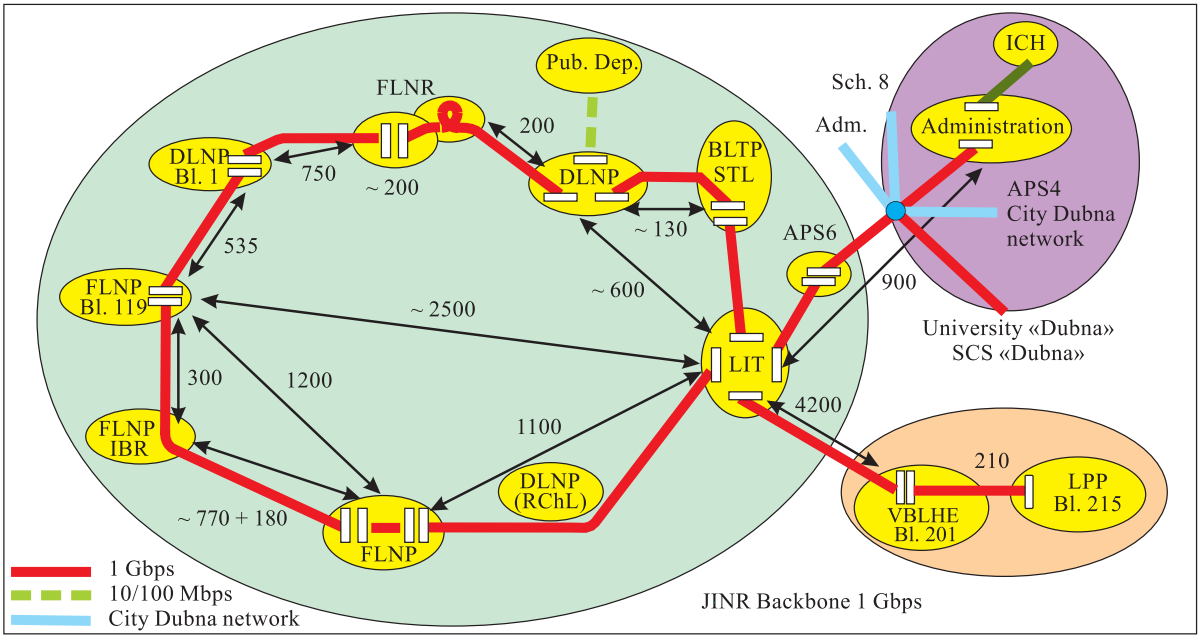

Fig. 3. JINR Gigabit Backbone

Distributed Information Systems, JINR Central Computing and Information Complex

The JINR Central Computing and Information Complex (JINR CCIC) is part of the Russian Information Computing Complex for processing information from the Large Hadron Collider. It comprises: an interactive cluster of common access; a computing farm for carrying out simulation and data processing for large experiments; a computing farm for the tasks of the LHC project; a computing farm for carrying out parallel calculations on the basis of modern network technologies (MYRINET, SCI, etc.); mass storage resources on disk RAID-arrays and tape robots.

CCIC PC-farms performance is: CPU 4.3 kSPI95, disk space 7.7 TB and ATL tapes 16.8 TB. Average total CPU loading was 25%. In October, 2003, the loading was 60.98%. JINR CCIC resources were used by the experiments E391A (KEK), KLOD, COMPASS, D0, DIRAC, HARP, CMS, ALICE for mass event modelling, data simulation and analysis. For the experiments ALICE, ATLAS and CMS, sessions of the mass modelling of physical events were conducted in the framework of JINR's participation in DC04 (Data Challenge 2004). More than 300 staff members of JINR and other research centres are using the JINR CCIC. Table 2 shows statistics of CPU time used by JINR's Laboratories on CCIC PC farms.

Table 2

Subdivision	LHC prod. run	DLNP	BLTP	LPP	FLNP	LIT	Others	VBLHE	FLNR
CPU time, %	33.32	20.77	18.71	6.70	5.78	5.23	4.47	2.57	2.44

Computing Service and Creation of a Grid Segment of JINR

In 2003, LIT actively worked on using the Grid technologies for experimental data processing. At present, the scientific community begins intensive use of the Grid concept, which guesses creation of an infrastructure providing the global integration of information and computing resources. JINR has a possibility of a full-scale involvement in this process. The LHC project, which is unique in scale of obtained data and from the viewpoint of computer technologies, provides

processing and analysis of experimental data using the Grid. The analytical review in the journal «Open Systems» prepared in cooperation with SINP MSU and SSC RRC «Kurchatov Institute» is devoted to the analysis of work performed in this area at JINR and the Russian centres [2].

Work was under way to create a system of the global monitoring of the resources of the large-scale Russian virtual organization, including LAN segments of several institutes (SINP MSU, JINR, ITEP, IHEP, IAM RAS) in accordance with Grid architecture. The adaptation and support of new versions of ANAPHE (former LHC++) Library for Linux, Windows and Sun Solaris platforms were performed. The existing software for LHC experiments (ATLAS, ALICE and CMS) and non-LHC experiments was supported. Measurements of Globus Toolkit 3 (GT3) performance under heavy load and concurrency were done. AliEn server was installed for distributed data processing of ALICE in Russia. The Castor system was installed and tested at the JINR CCIC.

During the year 2003 JINR participated in the CMS Pre-Challenge production (PCP03). 250K events were simulated with the help of the CMSIM v.133 package. A volume of data produced was 320 GB. A new Grid tool, Storage Resource Broker (SRB), was used for the CMS production. The SRB client program installed at JINR provides a direct access to CMS common databases at SRB server in UK (Bristol) and gives new opportunities for storage and exchange of data inside the CMS collaboration.

The LIT staff members take part in the development of monitoring facilities for computing clusters with a large number of nodes (10 000 and more) which are used in the EU Data Grid infrastructure. In the framework of a task of Monitoring and Fault Tolerance they participate in creation of a Correlation Engine system. This system serves for an operative discovering of abnormal states at cluster nodes and taking precautions to prevent them. A Correlation Engine Prototype was installed at CERN and JINR for accounting abnormal states of nodes [3].

Some tests were performed on data transfer from Protvino (sirius-b.ihep.su; OS Digital UNIX Alpha Systems 4.0) to ATL-2640 mass storage system in Dubna (dtmain.jinr.ru; OS HP-UX 11.0) to estimate a transmission capacity and a stability of a system including communication channels and a mass storage (OmniBack disk agent in Protvino and OmniBack tape agent in Dubna). No abnormal terminations have been fixed. The average transmission speed was 480 Kbps. The maximal speed was 623 Kbps, while the minimal one was 301 Kbps. (The distance between Dubna and Protvino is about 250 km; the capacity of communication channel Protvino–Moscow is 8 Mbps.)

The storage of data obtained during CMS Monte-Carlo Mass Production runs was provided by using Omnistorage: the volumes of data from SINP MSU ($\sim$ 1 TB) have been transferred to Dubna to ATL-2640.

Maintenance of the JINR Program Library was in progress. New documents have been prepared and introduced in WWW. They include realization at JINR of electronic access to the CPCLIB, CERNLIB (http://www.jinr.ru/programs/), adaptation programs on the JINR computer platforms, and filling the JINRLIB (about 80 programs have been included and tested).

DATABASE AND WWW SERVICE

A systematic supplement and maintenance of the earlier constructed databases and information systems continued taking into account the users' needs. Among these are:

- System for accounting and statistics of operating the JINR basic facilities (http://iis.jinr.ru/basic-fac/).
- Preparation of bibliographic data on HEP for the PPDS database (http://www.jinr.dubna.su/~diginfo/) and digitizing of graphics at users' requests. More than 40 papers were included into the PPDS database. The work was carried out in cooperation with IHEP, BNL and other physics centres. 235 graphics have been digitized at the requests of JINR and foreign physicists.
- Information system «JINR Topical Plan for Research» (http://iis.jinr.ru/tp/).
- Webportal for the project «LHC Computing Grid Project at Russia» (http://lcg.jinr.ru).
- Information web site about Grid activites at JINR (http://Grid.jinr.ru).
- RDIG-EGEE web portal prototype (http://www.egee-rdig.ru).
- Electronic catalog starting in 2000 in the JINR Science and Technology Library (STL) (http://lib.jinr.ru/dmitry/uni/rus/simple.html).
- Online sending lists on preprints, JINR communications, etc. in the JINR STL (http://lib.jinr.ru/maillist/newslistru.html).

Work was in progress at LIT on the development of WWW-tools on the main information servers www.jinr.ru and lit.jinr.ru. The following main results of the work should be noted:

- Allocation and support in the «Web-hosting» mode of information sites of a number of JINR's subdivisions and external organizations.
- Introduction and support jointly with the service of JINR's Chief Engineer of the information sys-

tem on the Basic Facilities of JINR (Nuclotron, U400, U400M, IBR-2, Phasotron, IREN project).
- Mapping a current state of both technical and software support of JINR's CCIC and communication facilities.

Steady support of one of the main general-purpose FTP-servers was provided: faxe.jinr.ru. This server was also utilized for support and load on call of antivirus programs.

The employees of LIT fulfilled work for JINR's STD AMS on the software and centralized maintenance of administrative databases, including:
- modernization of the interface and contents of the database «JINR Staff»;
- creation and modifications of the software complex on registration of currency bank in the environment of the common 1C system for JINR's Accounting Department;
- creation of the journal for accounts' registration in the 1C environment and document «Rendering Services for Chief Power Engineer Department».

Work was in progress on the development and maintenance (Section http://dbserv.jinr.ru/js/ of the dbserv.jinr.ru server) of the archive of documentation and software related to the advanced technologies of «interlayer» (middleware). Computer programs were designed in the Java language for automation of unrolling the client and server applications on the mentioned technology.

COMPUTATIONAL PHYSICS

In 2003, more than 150 scientific publications, reports at conferences and JINR preprints were published and presented.

Work was done on an improvement of the resulting scattering spectra quality due to the use of the spectrometer resolution during both wavelet filtering and traditional smoothing of the small-angle neutron scattering data. This result leads to a better fitting of the form-factor curve at the next step of data analysis (Fig. 4). Besides, the wavelet analysis permits one to extract and analyze a background (noisy) component and, what is more, to carry out instrumental hardware corrections [4].

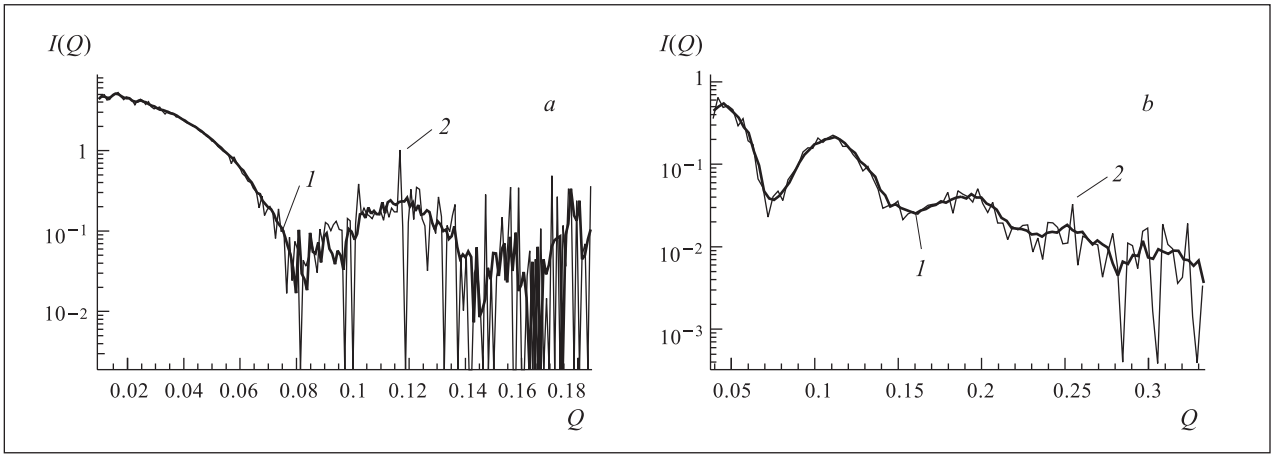

Fig. 4. Smoothing window results (*1*) over «raw» data (*2*) for «new» (*a*) and «old» (*b*) ring detector of YuMO

A new experimental scheme for quantum teleportation of heavy matter was proposed. It was shown that the standard experimental technique of nuclear physics experiment could be successfully applied to teleportation of spin states of atomic nuclei. It was claimed that there are no theoretical prohibitions upon a possibility of a complete Bell measurement, therefore, the implementation of all the four quantum communication channels is at least theoretically possible [5].

Calculations of the cross sections for single ionization of the ground and first excited helium states by relativistic impact of a bare uranium ion of charge $Zp = +92$ with energy 1 GeV/amu were performed. The uranium ion interaction with the target electrons was described by the Lienard–Wiechert potential, within the impact parameter approach. The differential ionization cross sections were obtained for electron energies $E < 37$ eV below $n = 2$ threshold of the He^+ ion. In these calculations the nonrelativistic initial and final two-electron correlated atomic states are obtained by numerical procedures from variational principles [6]. A semirelativistic symmetric eikonal distorted wave model treating the collisions beyond first Born approximation

was proposed. This model allows one to estimate two-centre effects in the fast heavy-particle collisions [7].

A global analysis of experimental data on the elastic and inelastic scattering of alpha particles by ^{90,94}Zr nuclei and on the total cross sections for their interaction with these nuclei was performed. The deformation length and the neutron to proton multipole matrix-element ratios for the 2_1^+ and 3_1^+ states of the ^{90,92,94,96}Zr nuclei were obtained for various projective species, and a comparative analysis of these quantities was performed. With the aim of revealing the origin of the phase shifts found in that study, experimental data on the inelastic scattering of 35.4, 40.0, 50.1, and 65.0 MeV alpha particles on ^{90,94}Zr nuclei were analyzed on the basis of a unified approach [8].

A heavy fermion model is used to describe the jet production in the interaction of the gluon with the polarized proton. Single-spin asymmetry appears due to the interference of single- and double-gluon exchanges between protons. The lowest and relevant contributions to the single-spin asymmetry may be associated with the partial contribution to the odderon and pomeron intercept, respectively. This information can be obtained in numerical analyses [9].

The nucleus–nucleus eikonal phases were calculated in the Glauber approach using realistic Fermi-type nuclear densities taken from electron scattering data. A special method of solving the inversion problem was suggested for restoring the Woods–Saxon-type optical potential. Comparisons were carried out between both of the restored potentials, the ones fitted to the experimental data, and the respective elastic differential and total reaction cross sections [10].

The elastic form factor of ^{12}C was calculated in the plane-wave Born approximation (BA) and also by accounting for distortions of electron waves in the nuclear Coulomb field both within the High-Energy Approximation (HEA) and by numerically solving the Dirac equation (SDE). The nuclear wave function includes peculiarities associated with the alpha-clusterization and short-range correlations of nucleons. It was shown that these correlations affect form factors at comparably large transfer momenta, where a considerable difference takes place between different schemes of calculations, namely, BA, HEA, and SDE methods. It was concluded that the SDE method was preferable when studying effects on form factors of the short- and middle-range nucleon correlations in nuclei [11].

A method of constructing a time-dependent periodic Hamiltonian was elaborated for which a system of Schrödinger equations admits analytic solutions. Time-independent soluble problems were transformed into time-dependent ones by a set of unitary time-dependent transformations and a proper choice of initial states. A new class of 2×2 periodic time-dependent Hamiltonians with cyclic solutions was constructed in a closed analytic form. In particular, the periodic time-dependent Hamiltonians were generated whose expectation values for cyclic solutions and spin-expectation values do not depend on time. As a consequence, this approach can be used for modelling quantum dynamic wells and wires with the effect of the particle localization [12].

The intertwining operator technique was applied to difference Schrödinger equations with operator-valued coefficients. It was shown that these equations appear naturally when a discrete basis was used for solving a multichannel Schrödinger equation. New families of exactly solvable multichannel Hamiltonians have been found [13].

A passage of fast dimesoatoms through a matter was considered from a quantum-mechanical viewpoint. A set of quantum-kinetic equations for the density matrix elements describing their intrinsic state evolution was derived. It was shown that probabilistic description of internal dynamics of hydrogen-like atoms was impossible even at sufficiently low energies because of the «accidental» degeneracy of their energy levels [14].

The anomalous decays $\pi^0\eta \to \gamma\gamma$ in the framework of the three-flavor Nambu–Jona-Lasinio model, in the vacuum and in quark matter in β-equilibrium was studied. It was found that the behavior of the relevant observables essentially reflect manifestation of the partial restoration of chiral symmetry, in non-strange and strange sectors. The probability of such decays decreases with density, showing that anomalous mesonic interactions are significantly affected by the medium [15].

The behavior of neutral pseudoscalar mesons π^0, η and η' in hot and dense matter was investigated in the framework of the three-flavor Nambu–Jona-Lasinio model. Three different scenarios were considered: zero density and finite temperature, zero temperature and finite density in a flavor asymmetric medium with and without strange valence quarks, and finite temperature and density. The behavior of mesons was analyzed in connection with possible signatures of restoration of symmetries. In the high density region and at zero temperature it has been found that the mass of the η' increased, the deviation from the mass of the η being more pronounced in matter without strange valence quarks [16].

A macroscopic model of the dissipative magnetoelastic dynamics of viscous spin polarized nuclear matter is discussed in the context of seismic activity of a paramagnetic neutron star. The source of the magnetic field of such a star is attributed to Pauli paramagnetism of baryon matter promoted by a seed magnetic field frozen into the star in the process of gravitational collapse of a massive progenitor. Particular attention is given to the effect of shear viscosity of incompressible stellar material on the timing of nonradial torsional magnetoelastic pulsations of the star triggered by starquakes. By accentuating the fact that this kind of vibration is unique to the seismology of a paramagnetic neutron star we show that the high-frequency modes decay faster than the low-frequency modes. The obtained analytic

expressions for the period and relaxation time of this mode, in which the magnetic susceptibility and viscosity enter as input parameters, are then quantified by numerical estimates for these parameters taken from early and current works on transport coefficients of dense matter. It is found that the effect of viscosity is crucial for the lifetime of magnetotorsion vibrations but it does not appreciably affect the periods of this seismic mode which fall in the realm of periods of pulsed emission of soft γ-ray repeaters and anomalous X-ray pulsars — young supermagnetized neutron stars, radiating, according to the magnetar model, at the expense of the magnetic energy release. Finally, we present arguments that the long periodic pulsed emission of these stars in a quiescent regime of radiation can be interpreted as a manifestation of weakly damped seismic magnetotorsion vibrations exhibiting the field-induced spin polarization of baryon matter [17].

A portable universal program complex in C language has been created for symbolic-numeric solving of multivariate polynomial systems with finitely many roots. The complex is based on the original algorithms designed in the sector for converting of the initial system into equivalent another system called involutive and more appropriate for the root finding [18].

Based on the original and highly efficient algorithms a fast C program was developed for computing cohomologies of Lie algebras and Lie superalgebras of vector fields. Such computations are important in analyzing general mathematical features of modern supersymmetric models of particle physics and quantum field theory [19].

APPLIED RESEARCH

Formation of high burn-up structures in UO_2 nuclear fuel materials, known as rim effect, attracts attention mainly due to its possible catastrophic influence on the operation conditions of modern nuclear power stations. This process is of particular scientific interest as well, because physical mechanisms and relevant parameters are still poorly understood. A new, based on the cellular automata (CA), approach for processing and modelling the structure dynamics of nuclear fuel at different burn-ups was proposed. Some evidences for existence of self-organization processes in the fuel at high burn-ups were established. It has been found that the fractal dimension of the surface structures strongly depends on the radiation damage of the material [20].

A micrograph of original pattern transformed into CA checkerboard is shown in Fig. 5. Black points are pores filled with fission gas products, white background is ceramic UO_2.

Results of Ising CA simulation of pattern evolution under temperature changes are shown in Figs. 6 and 7. One can see processes of joining the pores during their subdivision depending on temperature.

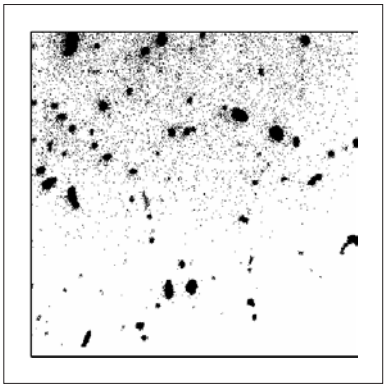

Fig. 5.

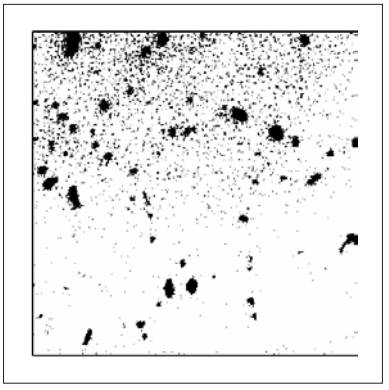

Fig. 6.

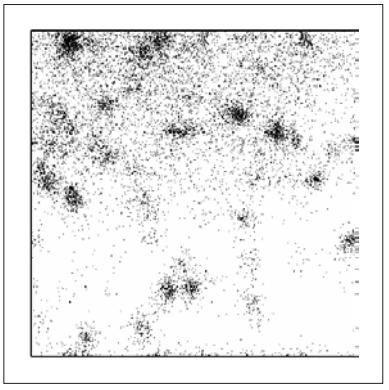

Fig. 7.

INTERNATIONAL COOPERATION

In cooperation with the scientists from the Technical University of Kosice, the Slovak Republic, and the Laboratory of Computational and Statistical Physics of Academia Sinica, Taiwan, research in the mathematical modelling of proteins folding was continued:

- In the calculation of thermodynamic properties and three-dimensional structures of macromolecules, such as proteins, it is important to have a

good algorithm for computing solvent-accessible surface area and volume of macromolecules. A new analytical method has been proposed for this purpose. This allows one to consider only integrals over the circular trajectories on the plane. The algorithm is suitable for parallelization. Testing on several small proteins has shown a high accuracy of the algorithm and a good performance [21].

- A FORTRAN code PBSOLVE was created for a numerical solution of a linear Poisson–Boltzman equation. Finite different discretization and successive over relaxation iterations on the sequence of grids were used to obtain the approximate electrostatic potential on the grid. A parallel version of the PBSOLVE has also been constructed. The performance of the program and the efficiency of parallelization have been tested on the small peptide Met-Enkephalin [22].

In cooperation with the Technical University of Aachen, Germany, the original involutive algorithms designed at LIT for constructing involutive bases were implemented in the form of Maple packages «Involutive» and «Janet» [23]. These packages are destined for computing Janet bases for polynomial systems and for systems of partial differential equations, respectively.

By using the above-mentioned program complex [18] and in cooperation with the Nuclear Physics Institute, the Czech Republic, a new type of exact solvability of the Schrödinger equation in a large spatial dimension and for central polynomial potential was found. This is because the solvability of Schrödinger equation under the conditions indicated is reduced to solvability of the overdetermined system of nonlinear algebraic equations (Magyari equations) [24].

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