LABORATORY OF INFORMATION TECHNOLOGIES

The main task of the Laboratory of Information Technologies consists in provision with modern telecommunication, network and information resources together with providing the mathematical support of theoretical and experimental studies conducted by the JINR Member States institutes at JINR and other scientific centres.

In 2004, the LIT scientific programme covered mainly two first-priority topics of the Topical Plan for JINR Research and International Cooperation in 2004. The Laboratory staff participated in 13 more topics of the Topical Plan in collaboration with other JINR Laboratories at project level and in 17 topics at cooperation level. The main aim of the Laboratory is the performance of work on the «Information, Computer, and Network Support of JINR's Activity» (topic 09-6-1048-2003/2007, headed by V. Ivanov, V. Korenkov, and P. Zrelov) and in the field of the «Computer Physics for Theoretical and Experimental Research» (topic 09-6-1041-2002/2004, headed by I. Puzynin and A. Polanski). Main results of the investigations performed within these topics have been published in more than 140 articles in refereed journals, proceedings of scientific conferences and preprints.

In 2004, a number of scientific projects presented by LIT staff members received grants of the INTAS Foundation, the Commission of the European Community in the framework of the EU–Russia collaboration, and 13 grants of the Russian Foundation for Basic Research. Seven projects are devoted to the creation and development of information, computing and telecommunication resources for performing fundamental research, and the other six are initiative scientific projects.

During the year 2004, LIT participated in organizing two international conferences. On 25–31 January, the XI international conference «Mathematics. Computer. Education» was held. The purpose of such conferences is to integrate the efforts of Russian and foreign scientists, specialists and teachers directed towards developing science and higher education in Russia and other countries of CIS, as well as preserving the traditions of the Russian science and education and their integration in the international community.

On 29 June – 2 July, an international conference «Distributed Computing and Grid Technologies in Science and Education» was held. The conference was the first in Russia dedicated to the issues of implementation of advanced Grid technologies and distributed computing in all fields of human activities.

INFORMATION, COMPUTER AND NETWORK SUPPORT OF JINR'S ACTIVITY

External Telecommunication Channels

At present, JINR leases a 45 Mbps channel to Moscow from the Russian Satellite Communications Company (RSCC «Dubna»); thus, JINR has access to the Russian networks and information resources, as well as access to the international channel through shared RBNet + RUNNet in the common data stream 2.5 Gbps. The Dubna–Moscow channel bandwidth increasing up to 1 Gbps will be done in 2005. Figure 1 shows the immediate future of the JINR external channels.

Total 2004 incoming traffic was 36.1 TB (19.89 TB in 2003) and outgoing traffic was 43.64 TB (24.43 TB in 2003).

Table 1 shows year traffic distribution among the JINR subdivisions ($>$ 500 GB on incoming traffic).

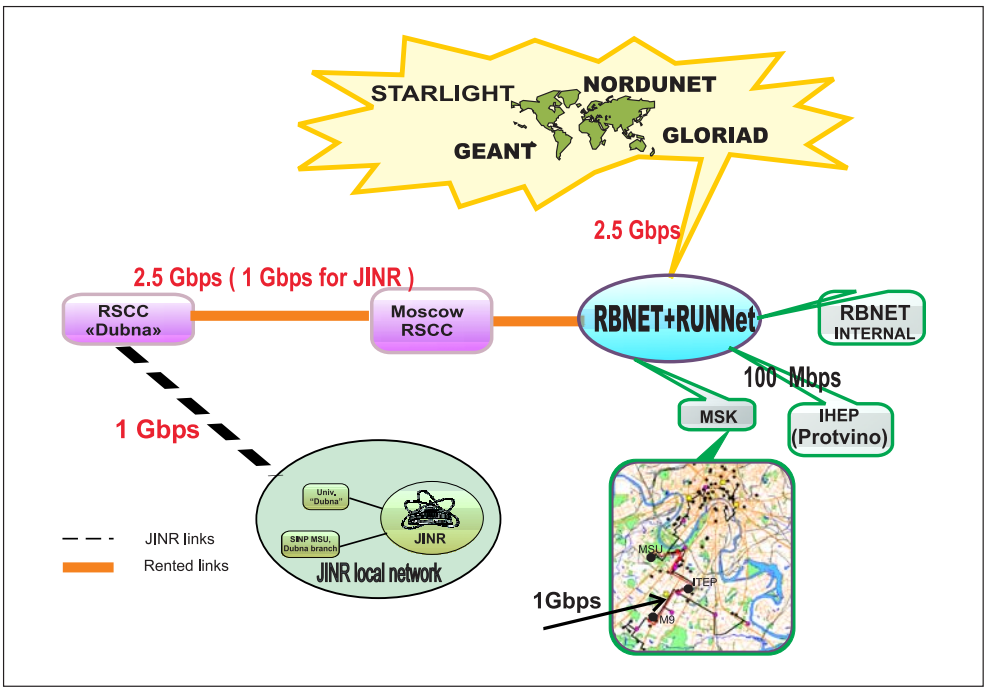

Fig. 1. Planned JINR external channels

Table 1

JINR subdivision	Incoming traffic, TB	Outgoing traffic, TB	Incoming traffic, %	Outgoing traffic, %
LIT	8.5	11.24	23.54	25.75
DLNP	5.34	6.24	14.8	14.29
FLNR	3.98	4.01	11.03	9.2
Servers	3.96	1.31	10.98	3.0
LPP	3.6	3.86	9.98	8.85
VBLHE	2.4	1.6	6.64	3.66
Uni-Dubna	2.26	2.09	6.26	4.78
BLTP	2.23	2.0	6.17	4.59
FLNP	1.73	8.42	4.78	19.3
Adm.	0.66	1.53	1.79	3.5

JINR Local Area Network (JINR LAN)

Currently the IP addresses database contains 4801 registered JINR LAN elements (4506 in 2003).

The spectrum of activities aimed at creation of a reliable, protected and high-speed JINR LAN includes:

— Development of a fault-tolerant architecture of the JINR LAN Backbone.

— Creation of a system to monitor and control the JINR LAN.

— Carrying out organizational and technical measures to provide the 1 Gbps data transfer rate across the JINR Laboratories.

— Creation of a network security system of the JINR LAN.

— Optimization of the information traffic across the JINR LAN.

All fiber optic cabling to have the transport media for the JINR Gigabit Ethernet LAN was made in 2003. The communication equipment to make this Gigabit Ethernet LAN was purchased in 2003 too.

During the 1st quarter of 2004 all the work to launch Gigabit Ethernet LAN was done: testing of the new single-mode fiber optic communication lines, creation of the switches configuration files and verifying the proper functioning of first component parts of the structure and then the entire JINR Gigabit Ethernet LAN.

The JINR Gigabit Ethernet LAN became available for users in March 2004. Cisco Catalyst 3550 family switches in 8 JINR main divisions, being connected by the fiber optic segments to the main Cisco Catalyst 6509 switch in LIT, formed the «star» topology of the JINR Gigabit Ethernet LAN backbone (Fig. 2).

The investigations on network traffic were continued. The Principal Component Analysis, especially the «Caterpillar»-SSA approach, was applied to the network traffic measurements. This approach is proved to be very efficient for understanding the main features of terms forming the network traffic. The statistical analysis of leading components has demonstrated that a few first components already form the main part of informa-

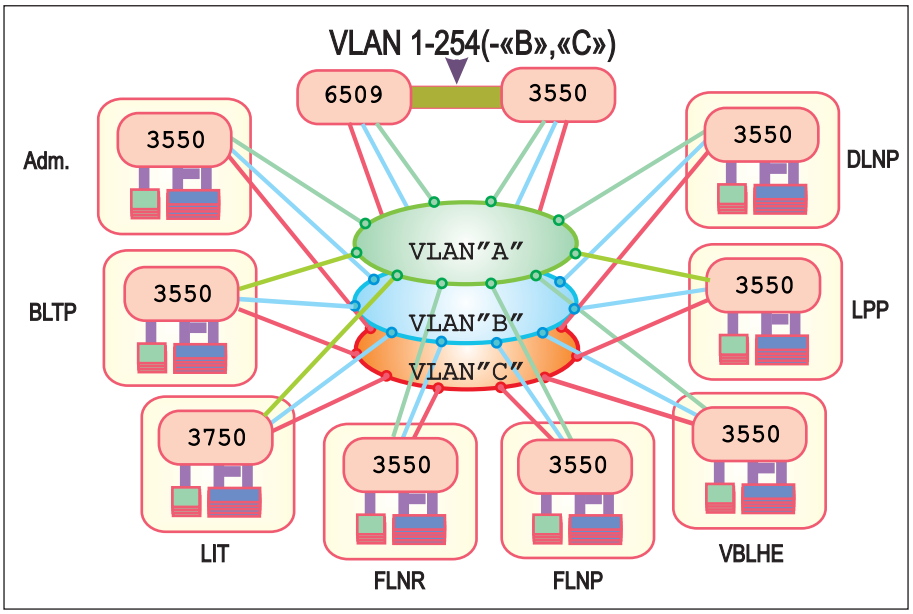

Fig. 2. Logical scheme of JINR LAN

tion traffic. The residual components play a role of small irregular variations which do not fit in the basic part of network traffic and can be interpreted as a stochastic noise. Based on the feature characteristics of residual components, a statistical method for the selection and elimination of residuals from the whole set of principal components was developed [1].

A modification of the Prigogine–Herman kinetic equation related to the network traffic was presented. A solution of this equation for homogeneous time-independent situations and for the log-normal desired speed distribution function clearly shows two modes corresponding to individual flow patterns (low concentration mode) and to collective flow patterns (traffic jam mode). For situations with low concentration there is almost a linear dependence of the information flow on the concentration and the higher the average speed, the lower the concentration at which the optimum flow takes place. When approaching the critical concentration, there are no essential differences in the flow for different average speeds, whereas for individual flow regions there are dramatic differences [2].

JINR Central Computing and Information Complex

About 450 staff members of JINR and other research centres are using the JINR Central Computing and Information Complex (JINR CCIC). The JINR CCIC users distributed over JINR divisions are shown in Table 2.

The JINR-CCIC is part of the Russian Grid Segment used for LHC and other applications.

Nowadays the JINR CCIC 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; a computing farm for the tasks of the LHC experiments; a computing farm for carrying out parallel calculations on the basis of the modern network technologies (Myrinet, SCI, etc.); LCG-2 computing farm included into a worldwide computing infrastructure; mass storage resources on disk RAID arrays.

The total CCIC performance is 8.0 kSPI95, disk space 14.0 TB. The average CCIC loading was 32%. The average loading of a common access farm is 50% during the year and 82.25% in April 2004.

JINR CCIC facilities were used by the experiments E391A (KEK), KLOD, COMPASS, D0, DIRAC, HARP, CMS, ALICE, ATLAS, HERAb, H1, NEMO, OPERA, HERMES, IREN for mass event production, data simulation and analysis.

Table 3 shows the percentage of CPU time used by JINR Laboratories on CCIC PC farms.

Table 2

LIT	DLNP	LPP	VBLHE	FLNR	BLTP	Other institutes	FLNP	Adm.
157	100	52	42	28	14	24	12	8

Table 3

Subdivision	LIT	FLNR	DLNP	LPP	FLNP	BLTP	VBLHE	Event production	Others
CPU time, %	7	1	14	15	3	14	8	36	2

Computing Service and Creation of a JINR Grid Segment

The Dubna-Grid Project was elaborated in 2004 in collaboration of LIT, University «Dubna», Directorate of the Programme for development of the science city of Dubna, University of Chicago (USA), and University of Lund (Sweden). The main aim of the project is creation of a Grid testbed on the basis of resources of Dubna scientific and educational establishments, in particular, JINR Laboratories, International University «Dubna», secondary schools and other organizations. This project will allow one to use more than 1000 CPU on the basis of Grid technologies.

In 2004, the Laboratory also continued the work on creation of computing services and Grid-technology deployment in data processing. Adaptation and support of new versions of ANAPHE (former LHC++) Library for Linux, Windows and Sun Solaris platforms were performed. Technical and programming assistance of the software development for LHC experiments was continued. Maintained were the existing software for LHC (ATLAS, ALICE, CMS, and LHCb) and non-LHC experiments.

Participation in Pre-Challenge production for ALICE, ATLAS, CMS, and LHCb and DC04 was continued in 2004. In the framework of JINR participation in the LCG (LHC Computing Grid) project, a number of works were performed. Tests on data transferring by the GridFTP protocol (GlobusToookit 3) were made. The server for monitoring of Russian LCG sites was installed and study of GridICE and MapCenter tools usage for monitoring of Russian sites was performed; the toolkit GoToGrid on the automatic installation and tuning of the LCG-2 package was developed; software for installation and control of MonaLisa clients on the basis of RMS (Remote Maintenance Shell) was designed.

Development of the LCG web-portal was in progress: a new system on collecting, keeping and visualization of monitoring data on CPU and Storage Resources usage at the Russian LCG sites and a new informational block on the CPU and Storage Resources which are available at the Russian LCG sites were included.

Events database and repository of generators were created. Dynamical home-page http://hepweb.jinr.ru has been created for testing Monte Carlo Generators of physical processes. The page also allows one to estimate the main properties of hadron–nucleus and nucleus–nucleus interactions (includes FRITIOF model, HIJING model, and tools for Glauber and Reggeon theories calculation).

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 (20 new programs have been included and tested).

Database and WWW Service

A systematic supplement and maintenance of the earlier created 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/).
- Information system «JINR Topical Plan for Research" (http://www.jinr.ru/plan/ptp-2004/title.htm).
- Electronic catalog at JINR Library (http://lib.jinr.ru/dmitry/uni/rus/simple.html).
- System for online sending lists on preprints, JINR communications, etc., at the JINR Library (http://lib.jinr.ru/maillist/newslistru.html).

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

The LIT employees fulfilled necessary work for the JINR's STD AMS on the software and centralized support of administrative databases, including modernization of the interface and contents of the database «JINR Staff», software support of the JINR Accounting Department and accounting departments of the Institute's subdivisions, processing of information on pension benefits at JINR for the Pension Foundation, etc.

COMPUTER PHYSICS FOR THEORETICAL AND EXPERIMENTAL RESEARCH

Development of Methods for Modeling and Processing Experimental Data

A new algorithm Jetfinder based on a wavelet analysis has been developed in the framework of the VBLHE–LIT collaboration that realizes a jet reconstruction under conditions of intensive background. The algorithm works in the space of pseudorapidity η versus φ, using as weights transverse momenta for STAR TPC or ECAL energy. The main advantages of the Jetfinder algorithm, as compared to the standard procedure LUCELL (UA1) which uses tree parameters, are in using the only control parameter λ and remarkable robustness of this algorithm. Besides, the Jetfinder analyzes all scales automatically by one pass of the algorithm [3].

Simulation of the processes of multifragmentation and spallation in reactions of separated Sn isotopes with proton and deuteron beams at the energies 0.6, 3.5 and

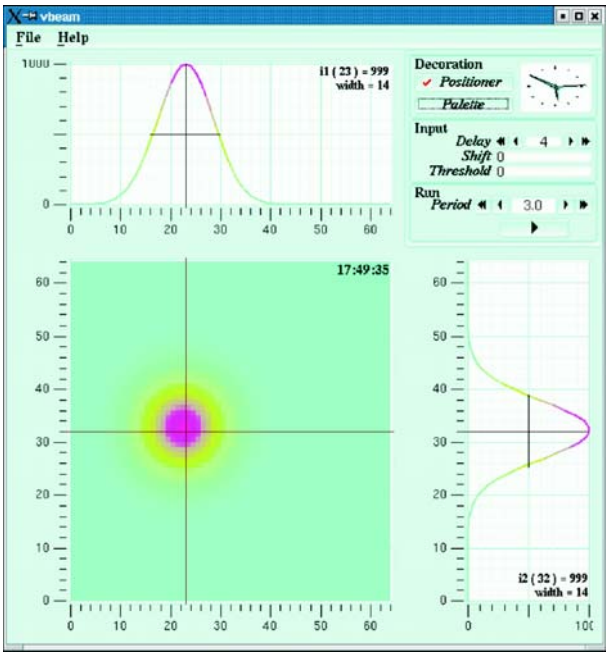

Fig. 3. Visualization of the beam profile

8.1 GeV/nucleon has been performed. Results of the simulation are compared with experimental data obtained at VBLHE synchrophasotron [4].

A visualization package for observation of the profile of a primary beam and its location on the target for effective operation of the fragment-separator COMBAS was developed. The package allows one to visualize data both in on-line and off-line modes. When starting the package, a window containing a central field of survey of the beam profile and two auxiliary fields for its projections onto axes X and Y appear (Fig. 3) By small modifications the package can be used for a broad spectrum of set-ups which use accelerator beams [5].

In the framework of the Glauber–Sitenko microscopic optical-limit model, calculations are made of the nucleus–nucleus total reaction cros sections. Satisfactory agreement with existing experimental data at energies higher than 50 MeV/nucleon is obtained without introducing any free parameters. On the basis of the model, calculations of the $^{6,8}\mathrm{He} + {}^{28}\mathrm{Si}$ total reaction cross sections at intermediate energies have been performed. The results of the calculations are compared with the existing experimental data (Fig. 4). The effects of the density tails of the projectile nuclei, as well as the role of shell admixtures and short-range correlations, are analyzed [6].

A phenomenological and semimicroscopic analysis of data acquired in experiments on elastic and inelastic scattering of 50-MeV alpha particles resulted from their collisions with $^{112,114,120,124}\mathrm{Sn}$ nuclei has been carried out within the optical potential approach and techniques of distorted waves and coupled channels [7].

Anomalous decays π^0, $\eta \to \gamma\gamma$ in the framework of the three-flavour Nambu–Jona-Lasinio (NJL) model, in the vacuum and in quark matter in β equilibrium are studied. It is found that the behaviour of the relevant observables essentially reflects a 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 [8].

Phase transitions in hot and dense matter and the in-medium behaviour of pseudoscalar mesons are investigated, in the framework of the three flavour Nambu–Jona-Lasinio model, including the 't Hooft interaction, which breaks the $U_A(1)$ symmetry. It is found that the appearance of strange quarks, above certain densities, leads to meaningful changes in different observables, especially in matter within β equilibrium. The behaviour of mesons in the T–ρ plane is analyzed in connection with possible signatures of restoration of symmetries [9].

The photon–proton scattering reactions $\gamma p \to \gamma'\pi'$, $\gamma p \to \pi^0 p'$ and $\gamma p \to \gamma'\pi^0 p'$ are investigated via the field-theoretical one-particle $\pi\omega\rho$-meson, nucleon and Δ-isobar exchange model [10].

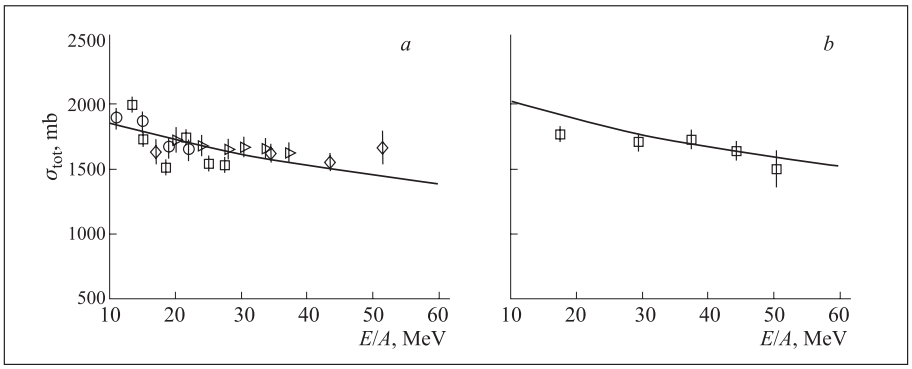

Fig. 4. Total cross section for reaction $^{6}\mathrm{He} + {}^{28}\mathrm{Si}$ (*a*) and $^{8}\mathrm{He} + {}^{28}\mathrm{Si}$ (*b*) calculated in the framework of the high-energy approximation

Creation of Numerical Methods and Software for Mathematical Simulation of Complex Physics Systems

The solutions of Klein–Gordon equation in the gravitational field of a massive point source in GR were considered for the first time. The basic bounded quantum state and the next few states in the discrete spectrum for different values of the orbital momentum were examined numerically. A novel feature of the solutions under consideration is the essential dependence of their physical properties upon the gravitational mass defect of the point source. It yields a repulsion or an attraction of the quantum levels and to their quasi-crossing [11].

On the basis of the separated form-factor model, parameters of the polydispersed unilamellar DMPC vesicle population are analyzed. The neutron scattering length density across the membrane is simulated on the basis of a fluctuated model of a lipid bilayer. The hydration of vesicle is described by sigmoid distribution function of water molecules. The results of fitting (Fig. 5) the experimental data obtained at the small-angle spectrometer SANS-I, PSI (Switzerland) are as follows: average vesicle radius (272 ± 0.4) Å, radius polydispersity 27%, membrane thickness (50.6 ± 0.8) Å, thickness of hydrocarbon chain region (21.4 ± 2.8) Å, number of water molecules per one DMPC molecule 13 ± 1, area per one DMPC (59 ± 2) Å^2. The calculated water distribution function across the bilayer directly explains why the lipid membrane is easily penetrated by water molecules [12].

Algorithms and codes have been developed for constructing stationary regular solutions to the Yang–Mills-dilaton system and obtaining unstable eigenmodes of those solutions. Corresponding problems (boundary value problem and Sturm–Liouville matrix problem) were solved on the basis of the continuous analogue of Newton's method. An effective algorithm has been

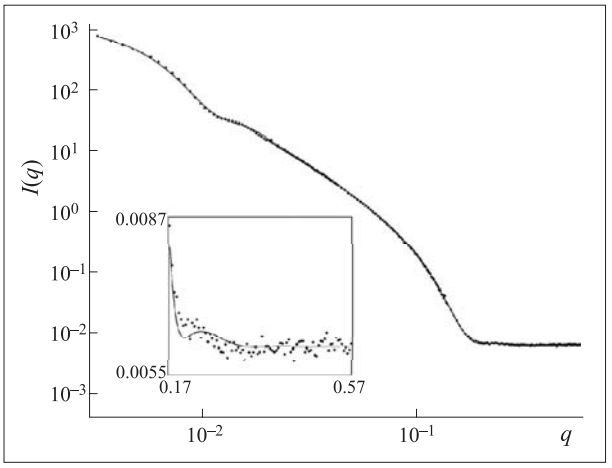

Fig. 5. The results of fitting the experimental data obtained at the small-angle spectrometer SANS-I, PSI (Switzerland)

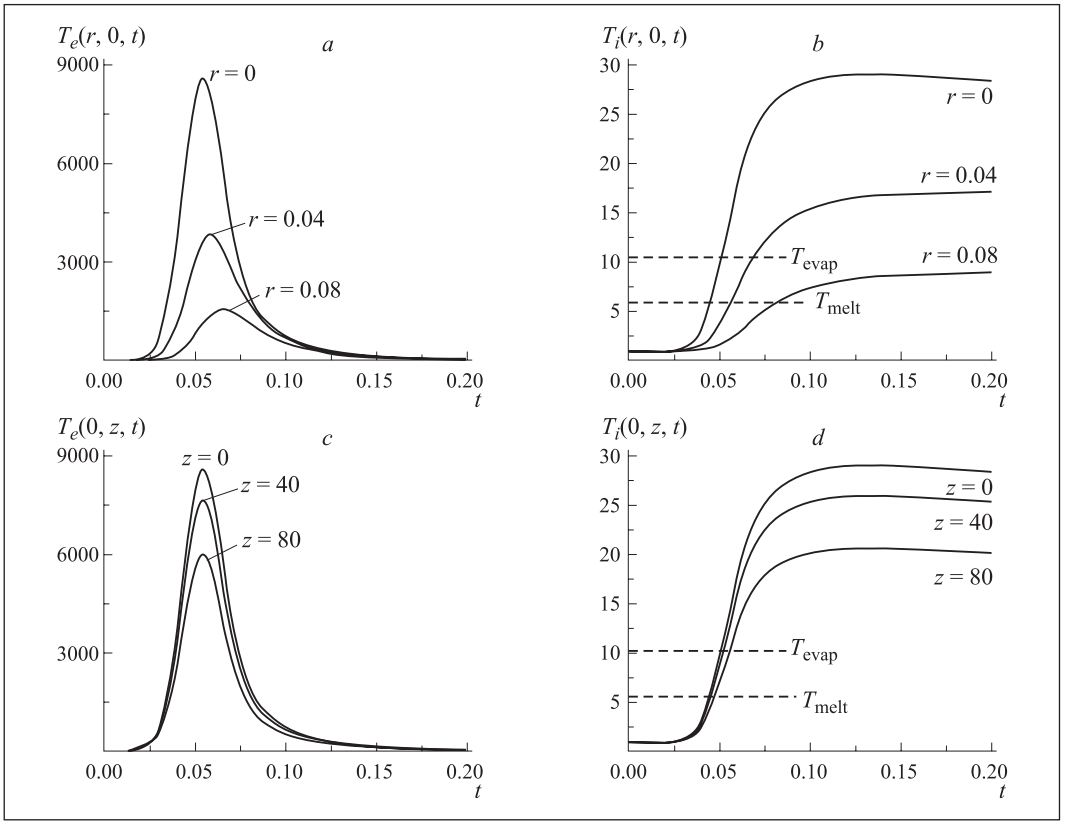

Fig. 6. Time dependence of the temperature of electron gas (*a*) and lattice (*b*) on the surface ($z = 0$) of nickel irradiated with uranium ions for various distances from the track axis. Time dependences of temperatures of electron gas (*c*) and lattices (*d*) in the place of passing a uranium ion through a surface ($r = 0$) for different depths z in the target. The shaded straight lines on panels *b* and *d* show the temperatures of melting $T_{\rm melt}$ and evaporation $T_{\rm evap}$

developed and a program complex has been designed for solving a system of nonlinear wave equations [13].

Based on the principles of classical hydrodynamics and Newtonian gravity, the theory of hydrogravity formulated in the manner of hydromagnetic theory has been developed to provide constructive account of the gravitational effect of global pulsations of a neutron star on the motions of ambient gas-dust interstellar medium. Particular attention was given to gas-dynamical oscillations generated by a pulsating neutron star in an unbounded spherical shell of gas and dust promoted by circumstellar gravitational stresses and damped by viscosity of the interstellar matter. Computed in the long wavelength approximation, the periods of these gravity-driven shear modes, referred to as quasistatic modes of hydrogravity, are found to be proportional to periods of the gravity modes in the neutron star bulk [14].

A 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 is solved numerically in the cylindrical 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 (Fig. 6). The maximal sizes of radius and depth in target where the melting and evaporation processes can take place have been estimated [15].

Coherent modes of trapped Bose gases were investigated. The conditions of appearing resonance excitations of the modes have been figured out [16].

Development of Methods, Algorithms and Software of Computer Algebra

A traditional two-day Workshop on Computer Algebra was held in Dubna on 25–26 May 2004. The workshop was dedicated to the memory of the outstanding Russian physicist and organizer of science M. Mescheryakov.

An efficient parallelization of algorithms for computing involutive polynomial bases of Janet type and with integer coefficients of unbound length was demonstrated. Apart from Janet bases, the parallel version of the algorithm can also be applied for computing reduced Gröbner bases. In so doing, there are no needs in extra reductions, since reduced Gröbner bases form internally fixed subsets of involutive bases [17].

It was argued that the most general and universal algorithmic approach to reduction of multiloop Feynman integrals to basic integrals was based on computation of Gröbner bases for recurrence relations derived from the integration by parts method. In this connection, one considers generic recurrence relations when propagators have arbitrary integer powers treated as symbolic variables (indices) for the relations [18].

A number of discrete algorithms for symbolic computation of topological phases in optical interference microscopy were designed and analyzed. These algorithms have been implemented as Maple and Mathematica packages [19].

The problem of solving the Schrödinger equation for bound states in space of dimension D was investigated for the central potentials of a polynomial type and the coefficients dependent on $2q$ of arbitrary constants. By a numerical-analytical solving of the algebraic system of equations that is equivalent to the Schrödinger equation (the Magjari system), some interesting laws in distribution and behaviour of the roots of that system were found out depending on value D. In particular, at great enough values of D, the energy spectrum gets equidistant [20].

With the help of the program implementing an original algorithm, cohomologies of the limited Lie algebras of Hamiltonian vector fields were investigated. Such algebras (or Lie p algebras) of vector fields are finite-dimensional analogs, determined over fields of positive characteristic p, of corresponding classical algebras. Their finite dimensionality removes a number of difficulties, arising at calculation of cohomologies of classical Lie algebras of vector fields [21].

INTERNATIONAL COOPERATION

Together with seven institutes of Russia (IHEP, IMPB RAS, ITEP, KIAM RAS, PNPI RAS, RRC KI, and SINP-MSU), JINR participates in the EGEE (Enabling Grids for E-sciencE) project (led by CERN) which was started on 1 April 2004. In the framework of this work the first prototype for resource centre at JINR was installed and is working now. The farm consists of 20 CPUs; the LCG-2 software was installed. The site JINR LCG-2 is included in the GOC Grid monitoring (http://goc.grid.sinica.edu.tw/gstat/lcgce01.jinr.ru/). The JINR LCG-2 site was actively used by some LHC experiments for testing and data production.

In cooperation with the Technical University of Cosice (Slovak Republic) and the Laboratory of Computing and Statistic Physics (Academia Sinica, Taiwan), research was in progress on mathematical simulation of formation of 3D protein structures. In order to study the thermodynamic properties and 3D structures of macromolecules of a protein type, an effective algorithm is required for computing the solvent accessible surface

area and the volume of macromolecules deposited in solvent. A method of constructing a special closed surface area made of triangles that allows one to determine if the given point is inside the molecule or else outside of it has been developed. A new analytic method earlier proposed for finding the macromolecules' square and volume was adapted for calculation with accounting a possible existence of intramolecular cavities [22].

In the framework of an agreement concluded between JINR and the University of Cape Town, the particle-like excitations of nonlinear damped systems in various models of condensed matter and nonlinear optics have been studied. Theoretical and numerical investigation of traveling solutions in the damped driven nonlinear Schrödinger equation has been performed. This equation has a number of applications in the fluid dynamics models, nonlinear optics, ferromagnet theory, etc. New classes of soliton solutions of NLS equation have been analyzed for the cases of parametric and external driving [23].

In cooperation with the International Solvay Institute for Physics and Chemistry (Brussels, Belgium) the Department of Mathematics of Aristoteles University (Thessaloniki, Greece), and Moscow Engineering and Physical Institute (Moscow, Russia), the approach for efficient resources distribution in economics based on entropy has been investigated. The scheme developed in previous work on the efficient resources distribution in economic systems with a small number of elements based on entropy was generalized. In order to take into account the asymmetric resources distribution, a new set of two-parameter interpolating functions was introduced. It is demonstrated that the maximal value of entropy is reached only in case of asymmetric distribution of resources. First results on application of the generalized approach to the analysis of incomes distribution for Sweden and Russia populations have shown that the new scheme allows efficient estimation of the state of the analyzed system and control over the resources distribution process [24].

APPLIED RESEARCH

The problem of a classification of the *E.coli* promoters with respect to their electrostatic potentials was studied at LIT in cooperation with the Institute of Theoretical and Experimental Biophysics and the Institute of Cell Research of RAS (Pushchino). The classification of promoters and other functionally important genome fragments according to their nucleotide sequences and physical-chemical properties is a key factor for understanding gene transcription, replication, recombination and their regulation. This work presents the approach that allows computation of electrostatic potentials of long nucleotide sequences of DNA for both procaryotic and eucaryotic species. The electrostatic potentials of *E.coli* promoters and periodic sequences were calculated. The electrostatic characteristics of the genome promoters, together with the primary structure, are expected to provide their reliable classification [25].

The results of recent studies on the development of new statistical models of stock market data were presented. On the basis of the analysis of a large number of stocks of various companies, it is shown that for some stock market data the statistical distribution of closing prices normalized by corresponding traded volumes (the index called by the authors as «Price/Volume ratio») fits well a log-normal law. For most stocks such a correspondence is reached with no additional detrending procedure. For other stocks, the distribution has a more complicated character and in most cases is described by a weighed sum of some functions of the log-normal distribution. However, after application of a detrending procedure all considered data can be described by a single log-normal distribution [26].

The problem of robust extraction of trend and chaotic components from stock market time series was considered. The proposed methods also allow one to extract a part of the chaotic component, the so-called anomalous term, which is caused by the transient short-time surges with high amplitudes. This provides more accurate determination of the trend component. The methods are based on the M-evaluation with decision functions of Huber and Tukey type. The iterative numerical schemes for determination of trend and chaotic components are briefly presented, which is resulting in a desired solution within a finite number of iterations. The optimal level for extraction of the chaotic component is determined by a new numerical scheme based on the fractal dimension of the chaotic component of the analyzed series. The forecasting scheme that uses the realized part of the analyzed series and a priori expert information was discussed [27].

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