LABORATORY OF INFORMATION TECHNOLOGIES

The main problems of the Laboratory of Information Technologies in 2002 were related to provision of the reliable operation and development of the JINR's network telecommunications and to the software and computer support of the scientific research which is under way at the Institute in the framework of the research field «Networks, Computing, Computational Physics».

In 2002, the LIT scientific programme was determined by three first-priority topics of the Topical Plan for JINR Research and International Cooperation. The employees of the Laboratory were also involved in research on 12 topics at a project level and in other 14 topics at a cooperation level.

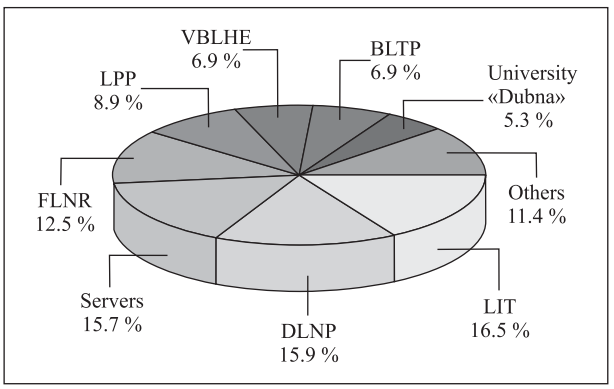
In 2002, LIT was an organizer of the Vth International Congress on Mathematical Modelling (V ICMM), the 4th All-Russia Conference on Digital Libraries (RCDL'2002), international workshop «Quantum Physics and Communication», the 9th international conference «Mathematics. Computer. Education».

In 2002, four scientists received a Doctor of Science degree and three received a Candidate of Science degree at LIT.

A series of work «Statistical Model of Information Traffic» was rewarded the JINR Second Prize for 2002.

EXTERNAL TELECOMMUNICATION CHANNELS

In 2002, the JINR external computer communication channel of 30 Mb/s for the Russian Internet segment and of 10 Mb/s for international computer networks demonstrated its reliable performance across the RBNet



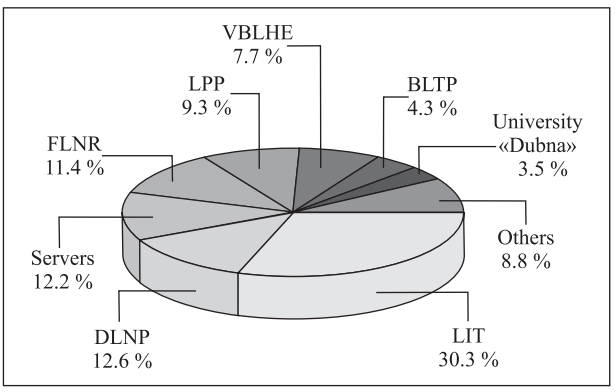


Fig. 1. Incoming traffic distribution over JINR divisions ($> 5\,\%$)

Fig. 2. Outgoing traffic distribution over JINR divisions ($> 3\,\%$)

network using the TELIA and STARTAP channels. For the year 2002, the incoming traffic reached 9.72 TB (4.14 TB in 2001) (Fig. 1), outgoing — 1.9 TB (Fig. 2).

The further development of the JINR's external communications is connected to implementation of the interdepartmental programme «Creation of a National Scientific Computer Network of the New Generation for 2002–2006» and the Russian GRID-segment. The first project has been implemented in the framework of creation of the JINR corporative computer network in cooperation with the RSCC «Dubna», a computer network for JINR's Crimean resort «Dubna» was mounted and adjusted in Alushta. Thus, a computer link and conditions for teleconferencing were provided for the participants of three international forums.

JINR LOCAL AREA NETWORK

In 2002, the reliable operation of the Fast-Ethernet-technology-based JINR Local Area Network (LAN) was provided (Fig. 3). There are 4053 network elements incorporated in the JINR LAN at present (there were 3451 in 2001), including 113 general-purpose and specialized servers. 821 home PCs are connected to the JINR modem pool.

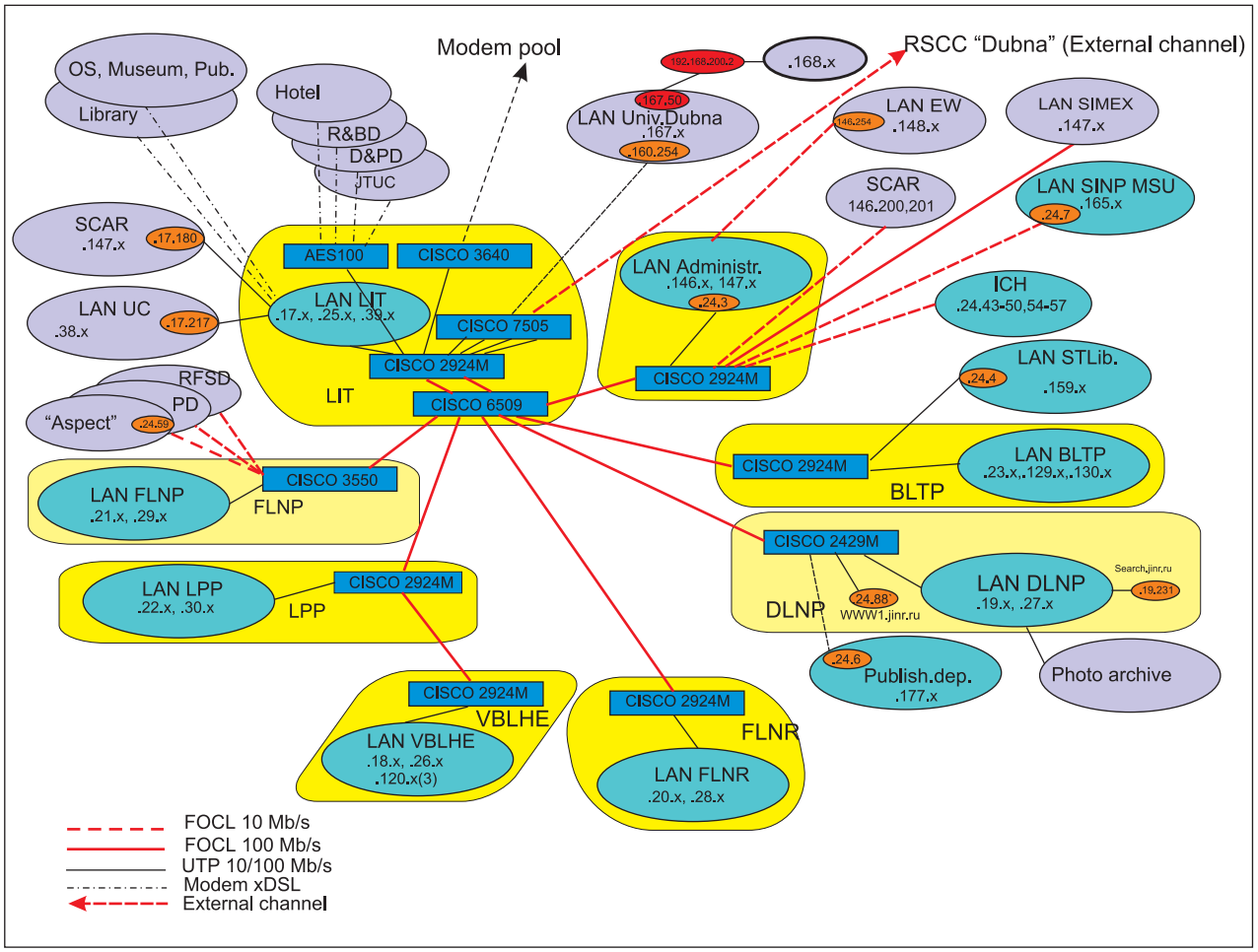


Fig. 3. JINR Local Area Network

Distributed Information Systems, JINR Central Computing Complex

The development of the JINR Central Computing Complex (CCC) was in progress on the basis of general-purpose and specialized clusters and computer farms. A distributed PC/Linux cluster has been installed at JINR CCC. The cluster comprises four separate interconnected components of various hardware nature and functional purposes. It includes an interactive farm of four dual-processor PCs Pentium III 1 GHz, 512 MB RAM, where the basic mathematical and special-purpose software, required for computations in the framework of several experiments, has been installed. The cluster also comprises specialized computing farms: a general-purpose farm, an LHC (Large Hadron Collider) farm, and a parallel computation farm. The computing general-purpose farm has eight dual-processor PCs Pentium III 500 MHz, 512 MB RAM. The LHC farm comprises 16 dual-processor PCs Pentium III 1 GHz, 512 MB RAM. The parallel computation farm includes eight dual-processor PCs Pentium III 1 GHz, 512 MB RAM connected by the communication network Myrinet 2000. Besides the general cluster, there are a number of specialized servers. The total general-purpose cluster's performance is almost 2500 SpecInt95.

The distributed file system AFS provides a transparent and protected access to the common disk space for information storage for the users of the JINR LAN and for all participants of international collaborations and projects of JINR. The total capacity of the JINR CCC disk space is 6 TB. The 15-TB automated tape library is used for the long-term storage of enormous information arrays and for the backup copying system (Fig. 4).

In 2002, work on creation of the JINR's GRID-segment and its incorporation in the global GRID structure was in progress. First steps towards creating a system of the global monitoring of the resources of the large-scale GRID–LHC virtual organization including the LAN segments of several institutes (MSU SINP, JINR, SSC RRC «Kurchatov Institute», RAS KIAM) in accordance with the GRID-architecture were initiated. The monitoring system operates in a test mode, its experimental use for simulation and analysis of simulated data for the experiments CMS, ALICE, and ATLAS was carried out. First results on practical application of the hierarchical mass-storage control system in the GRID–LHC virtual organizations with optimal use of the backup resources, fragmentation and replication of data were obtained.

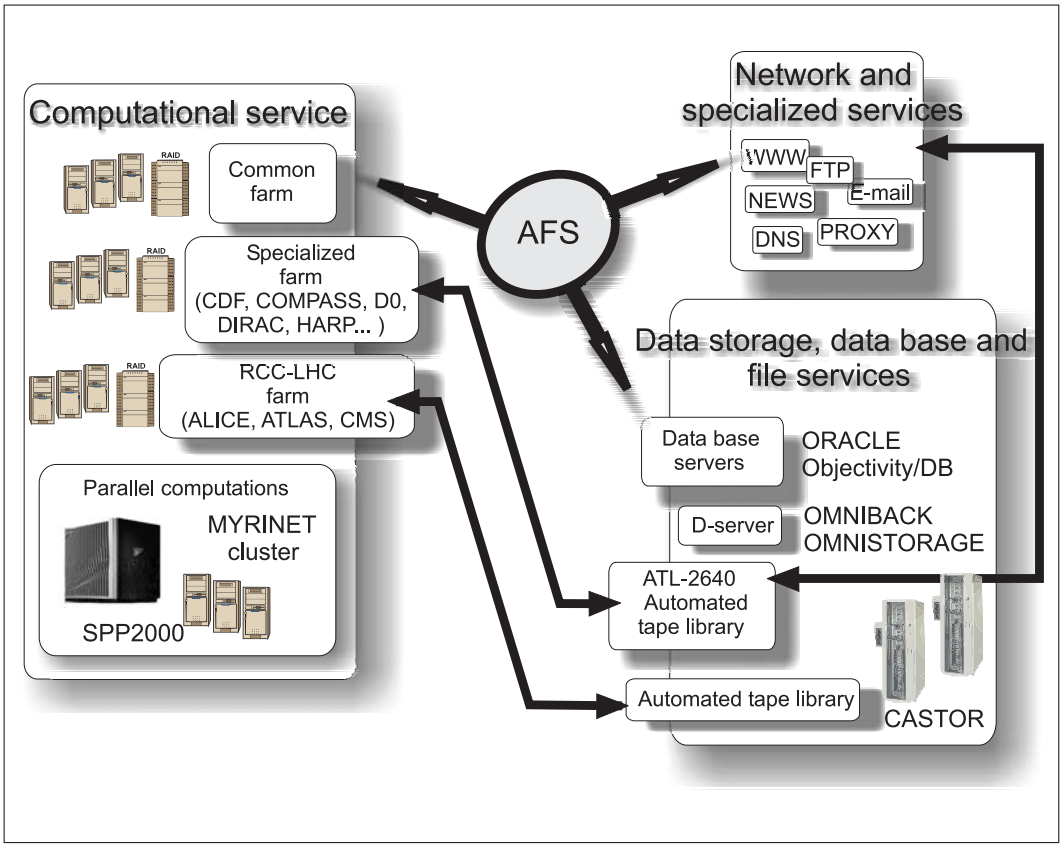


Fig. 4. Services at the JINR computing centre

Mass event production runs for the CMS experiment were prolonged in 2002. More than 110 000 physical events with a possible production of electrons, photon and hadron jets were generated at the specialized farm of the JINR CCC. The size of the generated data reached 25 % of the total number of events generated by the Russian participants of mass event production runs (MSU SRINP, ITEP, IHEP, MSU Research Computer Centre). The participants of the autumn session of the mass event production for CMS were also CERN, Italian and French physics centres, the CMS distributed GRID-Centre in the USA.

A series of works within the projects LHCb, DIRAC, and DUBTO has been performed, including:

• for the LHCb project, java-units and programs of the simulation system for the first-level trigger of the LHCb installation were designed;

• for the DIRAC project, a new version of the program for simulation GEANT–DIRAC V2.61 was put into operation;

• for the DUBTO project, based on the GEANT package a program was designed to simulate various channels of π^{+4}He interaction in the experimental setup.

The maintenance and support of the information WWW-servers of JINR and LIT (http://www.jinr.ru, http://lit.jinr.ru) was continued. Necessary work on software support and centralized support of databases of a scientific and administrative type was fulfilled. The general-purpose and specialized libraries were maintained on the JINR's computer platforms. The filling and possibilities were extended on using the JINRLIB library based on programs created or adapted by JINR employees. The library was tested on the platforms SPP, Convex, Windows 9x/NT/2000/, versions for computer platforms Linux and FSF (GNU) were prepared, what is important in view of change-over to the use of the tools of Linux-clusters at the LIT general-purpose computer centre. In 2002, the content of the library was enlarged by 20 new programs mirroring a wide spectrum of the JINR's scientific tasks. A Web-page was prapared for the JINRLIB, providing electronic access to the descriptions of programs and rules of their usage in case of compilers calls. The modern state of the JINR program libraries is shown on the web-page: http://www.jinr.ru/∼tsap/Koi/sss.htm.

COMPUTATIONAL PHYSICS

In 2002, computer simulation methods and software for data processing were developed on the basis of new methods of information filtering, compression and visualization, and image recognition [1].

An effective algorithm for selection of useful events based on a multilayer feed-forward neural network was proposed and applied to simulated and real data analysis for the DUBTO experiment [2].

A series of works on the development of a statistical model of information traffic has been completed on the basis of a detailed study of its main features. The detailed nonlinear analysis of measurements of the information traffic was performed for the first time. It shows that the aggregation of these measurements (Fig. 5) forms a statistical distribution, which is approximated with a high accuracy by the log-normal distribution (Fig. 6). The log-normal distribution of the traffic measurements and their multiplicative character (Fig. 7) confirm that the scheme developed by A. Kolmogorov for the homogeneous fragmentation of grains can also be applied to the network traffic. The developed model provides a basis for creating new ef-

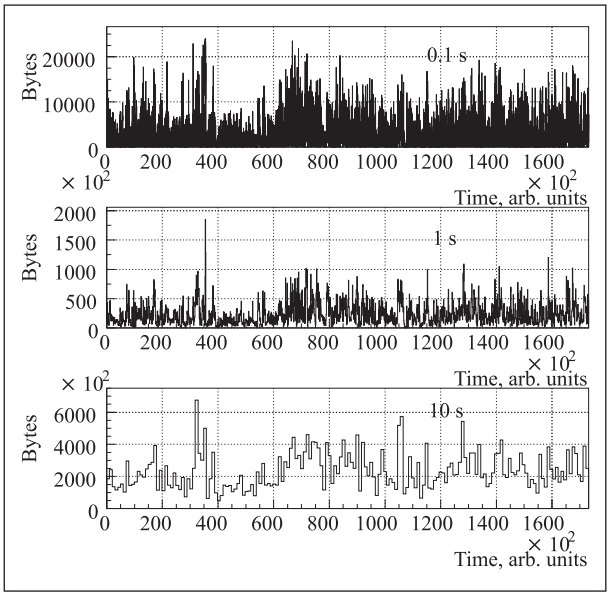


Fig. 5. Traffic measurements aggregated with different sizes: 0.1, 1 and 10 s

fective tools for optimal control over the traffic in computer networks, increasing data flows and decreasing information loss. It also provides new possibilities for implementation of traffic monitoring and for computer networks protection against unauthorized intrusions [3].

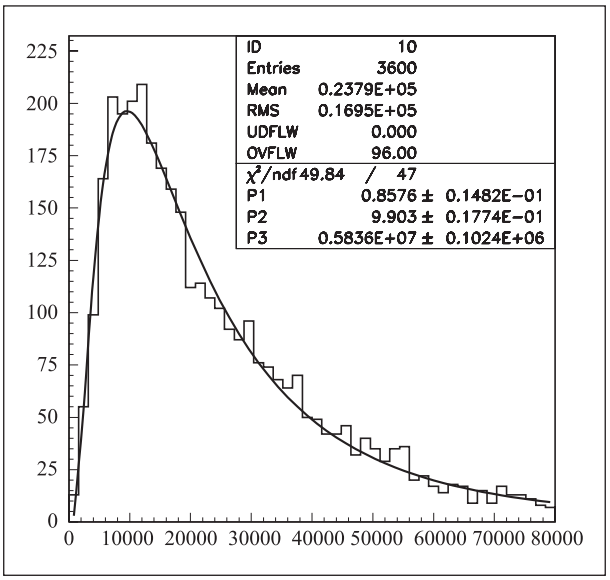


Fig. 6. Packet size distribution for daily traffic measurements aggregated with 1 s window: fitting curve corresponds to the log-normal function

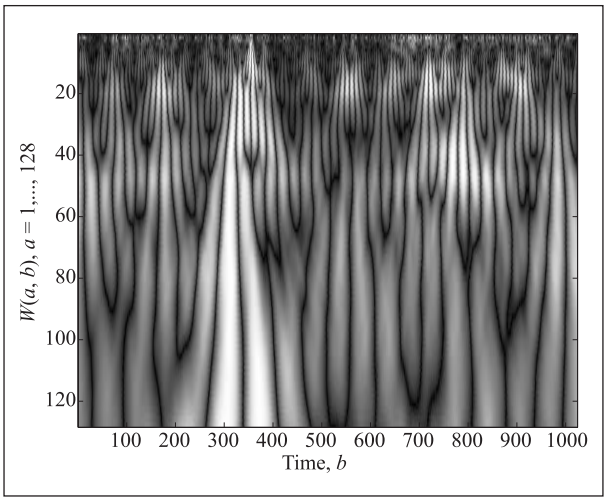


Fig. 7. Shade plot of the continuous wavelet transformation coefficients for traffic measurements aggregated with 1 s window

Algorithms and software have been developed for the analysis of angular distributions of secondary particles with the help of wavelet transformations (WASP), for data filtering with the use of a lifting scheme (WALF), for experimental data fitting (FITTER) [4].

One of the results obtained in 2002 is related to creation of a distributed CHARM system for data processing and data storage in the field of particle physics. The hard- and software complex, based on the local Linux-cluster RISK-2002, the LPP computer farm, and the robotized central mass memory, is used for processing of simulated information and experimental data obtained from the EXCHARM set-up [5].

A mathematical procedure was developed to calculate the probability of generating a compound nucleus at nuclei interaction in reactions with heavy ions within the model of the double nuclear system, created at FLNR and developed at BLTP [6].

Analytical and numerical methods have been developed to model the electromagnetic activity of a paramagnetic neutron star. The periods of nonradial torsional pulsations have been studied analytically and numerically [7]. The model is currently used in interpreting observational data on pulsars and magnetars.

In the framework of the development and application of algorithms and software for numerical research in the heavy ion relativistic collisions, a combination of the quantum molecular dynamics model and the evaporation model of de-exciting nuclei describes well the spectra of secondary protons and neutrons up to the energies of striking particles $\sim$ 300 MeV [8]. Investigation on colour transparency, exotic nuclei properties, fragmentation and multifragmentation processes in hadron and nucleus–nucleus collisions was performed [9].

A high-accuracy approximation method for linear evolutionary operators in Hilbert space has been created and theoretically proved. The method is based on discretization of the time variable of the original equation with the help of Magnus expansion for evolution operator and subsequent approximation of this expansion by rational functions of stability [10].

New variation-iteration algorithms were constructed and implemented in the FORTRAN language for solving with a predetermined accuracy the bound state problems and three quantum particle scattering problems with point or Coulomb pair interactions in the adiabatic representation. A numerical analysis and testing of the designed algorithms on the models of three quantum particles with point interactions and for the study of the transfer ionization reactions at supersmall scattering angles have been performed [11].

An analysis of relativistic field-theoretical equations was presented for photon–proton scattering reactions [12]. The numerical solutions of these equations were compared to new experimental data for reactions with $\gamma\Delta \to \pi p\gamma$ final states. A generalization for the inverse scattering problem was considered.

The interlacing operator technique is applied to discrete equations. It allows one to generate new families of precisely solved Jacobi matrices. It shows that the obtained thus Jacobi matrices lead to new precisely solved nonlocal potentials of the Schrödinger equation [13]. Discrete algebraic Darboux transformations and a factorization procedure have been obtained for a system

of coupled Schrödinger equations, permitting generation of series of potential matrices with predetermined spectral characteristics for which the system of discrete Schrödinger equations has precise solutions [14].

A program [15] has been worked out for a numerical solution of the system of partial differential equations, describing the energy relaxation in the vicinity of an ion trajectory moving in a substance and in the field of a pulsed energy release stipulated by slowing down the ion beams in the substance. A mathematical model of radiation damages appearing in a number of radiation-stable insulators has been constructed.

A new method [16] for computing the coil potential in modelling the 3D nonlinear magnetic fields, which does not result in accumulation of errors, was suggested. The method has been developed on the basis of field measurements of data for the EXCHARM experiment.

Some topics on applicability of the involutive bases technique to optimization problems of integer programming were considered. Restrictions have been revealed with the help of computer experiments, and some ways of modifying the involutive approach directed at overcoming these restrictions have been planned [17].

The designed original algorithms and software were applied to investigate the mechanical model for $SU(2)$ gauge theory. It was found out that, in contrast to the instant form of this mechanical model, its light-cone version possesses not only the first-class constraints but also the second-class ones [18].

A new much more effective algorithm of calculating cohomologies has been proposed which is based on splitting large cochain complexes into minimally possible subcomplexes [19].

Some procedures of semiclassical quantization of normal forms based on the algebraic perturbation theory were implemented in Reduce and included in the QUANTGIT computer program. This program is a core of the software complex oriented to simulation of dynamic and atomic systems in external fields [20].

The electronuclear systems consisting of two «cascade» subcritical assemblies, a liquid metal reactor on fast neutrons used as a booster, and a thermal reactor, where main heat production takes place, were simulated by the Monte-Carlo method. Reactors of VVER-1000, MSBR-1000, and CANDU-6 types are considered. The research results show that the two-reactor systems with an enriched uranium booster and a liquid cadmium valve are the most effective ones from the viewpoint of high output characteristics and safe functioning [21].

An urgent problem of nuclear waste transmutation and discussion of various approaches and methods of transmutation of the isotopes, which, in view of their high radioactivity and migrations in the biosphere, require obligatory transmutation, were considered in review [22].

The modern state of research in the area of computer simulation of physical and biological systems by molecular dynamics methods (MD) is given in review [23]. Special features of computer simulation of molecular and atomic systems based on parallel and vector calculations were analyzed. On the basis of application of methods of the MD simulation, calculations have been done allowing a dynamics analysis of condensed systems (clusters, liquids, etc.) and nuclei phenomena at a molecular level.

INTERNATIONAL COOPERATION

According to the Cooperation Agreement between JINR and the research centre FZR (Rossendorf, Germany), a series of investigations has been conducted, the main direction of which was the choice, analysis and testing of new technologies to create information distributed systems, in particular, for organization of access to relational databases [24].

In cooperation with CERN, monitoring tools were developed for computing clusters with a large number of nodes (10 000 and more) used in the EU DataGrid infrastructure. In the framework of the task on Monitoring and Fault Tolerance, an event correlation system (Correlation Engine) is being created. The task of the system is a timely detection of anomalous states on cluster's nodes and taking precautions to prevent failures. With the help of the created Correlation Engine Prototype, statistics is being accumulated on anomalous states of nodes based on the CERN computing clusters. The prototype has been installed for statistics accumulation at the computing clusters at CERN and JINR.

In cooperation with CERN and the Brookhaven National Laboratory, work was in progress on:

— development of the object-oriented software environment (framework ROOT) for the solving of a wide range of scientific problems using workstations and personal computers (http://root.cern.ch) [25];

— elaboration, development and implementation of an information model of processes of acquisition, reconstruction and physical analysis of data for large experiments;

— introduction (together with the BLHE) of modern object-oriented technologies for the STAR experiment.

Within the joint DFG–GSI–JINR project «Nonequilibrium Strongly Dense Matter in Nucleus–Nucleus Collisions», work was continued on creating the software for numerical research on heavy ions collisions in the framework of a hydrodynamic model for various type equations of nuclear matter state. With the help of the designed software, in cooperation with physicists of JINR BLTP and the Kurchatov Institute, possible manifestations of the quantum chromodynamics (QCD) deconfinement phase transition in heavy ion collisions [26] were investigated.

In the framework of the Cooperation Agreement between JINR and Cape Town University, a nonlinear Schrödinger equation with defocusing nonlinearity, the localized solutions among of which are «dark» solitons (domain walls), was under study [27].

In 2002, the cooperation with the International Solvay Institute for Physics and Chemistry (Brussels, Belgium) was in progress. A series of investigations was devoted to research in the information traffic [3].

APPLIED RESEARCH

In 2002, the cooperation with the International Solvay Institute for Physics and Chemistry (Brussels, Belgium) was continued in the field of applied research, which included:

• Investigations on the econophysics problems were performed. A new approach to the effective resources distribution has been developed, and a modification of the Cox–Ross–Rubenstein discrete model has been suggested which takes into account changing options prices depending upon percent rates [28].

• On the basis of elastic neural nets, new algorithms of solving the travelling salesman problem for a set of cities with known optimal tours [29] were developed.

• A simple and effective method has been suggested to find an initial approximation of an earthquake epicentrum based on the elastic neural net application [30].

• Generalization of the optical coherence tomography (OCT) images filtration algorithm has been obtained. It was developed to filter the OCT group images measured on the same skin area [31].

In cooperation with scientists from the Technical University of Kosice (the Slovak Republic) and the Laboratory of Computational and Statistical Physics of Academia Sinica (Taiwan), research on the mathematical modelling of proteins folding was continued [32]:

• An effective analytical algorithm has been developed for calculating the solvent excluded volume and the solvent accessible surface area of a protein molecule.

• Effective multigrid algorithms for the numerical solving of a boundary-value problem for the nonlinear Boltzmann–Poisson equation, which describes the electrostatic potential of the protein molecule in the solvent.

A FORTRAN code implementing the mentioned algorithms has been created and tested on the Linux clusters. The parallel version of the code was also created using the MPI package.

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