LABORATORY OF INFORMATION TECHNOLOGIES

The main tasks of the Laboratory of Information Technologies consist in the provision with modern telecommunication, network, and information resources, as well as with mathematical support of theoretical and experimental studies conducted by JINR, Member-State institutes at JINR, and other scientific centres. The development of the activity «Networks, Computing, and Computational Physics» is outlined here taking into account the ultimate importance of the progress in the information and computing infrastructure for the JINR activities, and the prospect of drastic changes in the information technologies.

The Laboratory does work on the «Information, Computer, and Network Support of the JINR's Activity» (topic 09-6-1048-2003/2007, headed by V. Ivanov, V. Korenkov, and P. Zrelov) and on the «Mathematical Support of Experimental and Theoretical Studies Conducted by JINR» (topic 09-6-1060-2005/2007, headed by V. Ivanov, Gh. Adam, and P. Zrelov).

The Laboratory staff participated in research work done within 16 topics at the project level and within 16 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 members of LIT staff have been financed by grants afforded by the Commission of the European Community in the framework of the EU–Russia collaboration and INTAS. Thirteen grants were afforded by the Russian Foundation for Basic Research. Among them, seven were directed to the creation and development of information, computing and telecommunication infrastructure, while six supported various projects of scientific interest.

During the year 2005, LIT was the main organizer of the 9th Workshop on Computer Algebra «DUBNA 2005» (Dubna, 17–18 May), the 3rd international workshop «Quantum Physics and Communication» (Dubna, 26–30 June), the workshop on the current status of the «Dubna-Grid» project (Dubna, 21 July), and one of the organizers of the XX International Symposium on Nuclear Electronics & Computing (NEC'2005) (Varna, Bulgaria, 15–20 September).

A third issue of the «Information Bulletin of LIT» (JINR, 4-8255, Dubna, 2005; http://lit.jinr.ru/Inf_Bul_3/) was published. The scientific report of the Laboratory for 2004–2005 was prepared and published.

NETWORKING, COMPUTING, INFORMATION SUPPORT, AND GRID TECHNOLOGIES

The provision of JINR with high-speed telecommunication data links has had as major target getting the 1 Gbps JINR–Moscow data link operational during the year 2005. All the necessary equipment was already deployed such that, at the beginning of November, the test runs started. This achievement will secure significant increase of the total network traffic during 2005 under a 45 Mbps JINR–Moscow link. Total year traffic was 45.88 TB (32.69 TB in 2004) and outgoing traffic was 41.53 TB (40.22 TB in 2004). Table 1 shows the traffic distribution among the JINR divisions ($>$ 500 GB of incoming traffic).

Table 1

JINR subdivision	Incoming traffic, TB	Outgoing traffic, TB	Incoming traffic, %	Outgoing traffic, %
LPP	9.35	5.64	20.37	13.58
LIT	8.79	8.61	19.16	20.73
DLNP	8.51	7.17	18.56	17.28
FLNR	5.33	3.75	11.62	9.03
VBLHE	3.66	5.09	7.98	12.25
Uni-Dubna	2.72	2.38	5.92	5.73
BLTP	2.19	1.99	4.77	4.79
FLNP	2.12	5.17	4.62	12.46
Adm.	0.943	0.191	2.01	0.45
Servers	0.888	0.495	1.89	1.16

Currently the database of IP addresses contains 5335 registered JINR Local Area Network (LAN) elements (4801 in the year 2004).

Systematic work on the LAN management was performed by the Network Operation Centre (http://noc.jinr.ru/): registered users — 3070, 1021 dialup- and VPN-users. 1070 JINR staff members use @jinr.ru for e-mailing. Investigated were approximately 15–20 incidents per month related to violation of the network security — viruses, scanning, breaks, etc. About 30 000 electronic messages are delivered every day, more than 200 000 messages were blocked as spam, 250–300 messages per day are infected by various types of viruses.

The JINR network is a complex structure of high diversity, which consists of specialized network software and versatile hardware. This structure is the basis of the distributed JINR information technologies (IT) services. The creation of a high-speed, reliable and protected LAN has progressed significantly. The crucial problem of securing the LAN protection involved the development of network monitoring tools able to accomplish the look-ahead assessment of the entire network environment. In 2005 the activities on the creation of the Gigabit Backbone were awarded the First Prize of JINR.

The gigabit networking structure of JINR (Fig.1) integrates the hardware and software facilities providing the basis of the JINR network and information structure, upon which the mentioned infrastructure is built up and developed. The gigabit networking structure solves the following tasks:

• integration of all JINR computer resources into a unified information environment;

• organization and provision of remote network access to information-computational resources for various groups of JINR users, to information resources of Russian and foreign scientific centres;

• creation of a unified information space for the JINR staff for data exchange between the Institute's subdivisions and between subdivisions and JINR Directorate;

• provision of services of remote access to JINR resources from home PCs of JINR staff members.

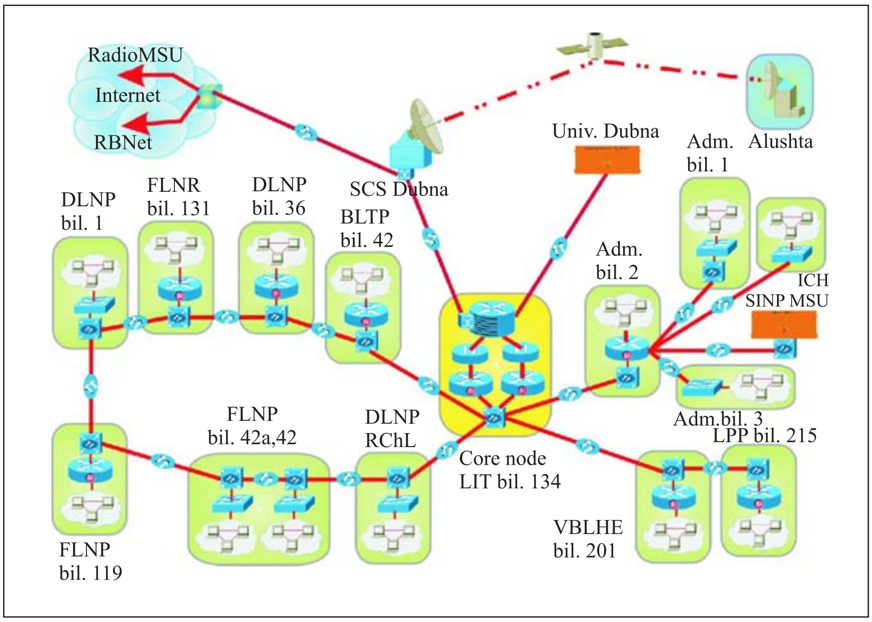

Fig. 1. JINR Local Area Network and telecommunication channels

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

More than 500 staff members of JINR and other research centres are using the JINR CICC. The JINR CICC is part of the Russian Grid segment used for LHC and other applications. 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, 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.), the LCG computing farm which is included in a worldwide computing infrastructure.

An approach to the implementation of a big mass storage in the CICC has been worked out. A structure of the 39 TB mass storage system CertonRAID 100 developed at the University of Heidelberg (Germany) has been purchased and is being tuned now. The system possesses high performance, flexibility, scalability, as well as additional tools of information protection. As soon as the system is put into operation, the total disk space will reach 50 TB for the CICC users.

Sixteen modern two-processor computing nodes have been put into operation (eight of them replace outdated general-purpose farm's nodes). Installed were a new data base server controlled by DBMS ORACLE 10G, a server for Grid-monitoring, several servers and workstations for a new software testing. Some computing nodes were modernized to perfect the cluster's performance. The process of transferring the CICC infrastructure to 1-GB Ethernet technology is coming to an end.

At present, the complex comprises more than 120 processors of total capacity of almost 100 kSI2K (1 kSI2K corresponds to the processor Intel Xeon 2.8 GHz) that are used as computing nodes, and several servers representing a common disk space, registration and authorization, mailing and other services. The main part of the computing resources is accessible for users through the batch processing system, while some part of the resources is connected to the global LCG infrastructure by Grid means. Preparation and edition of files, documents, jobs, programs, work with network services, applications, analysis and visualization of results is performed by the users during sessions on specialized interactive machines.

The transition has been realized from the OS Linux (CERN Red Hat 7.3) to the OS Scientific Linux CERN Release 3.0.5 (SLC3) with corresponding additional software: Gnu compilers (C, C++, F77) and Intel compilers (C, C++, F90), gdb and ddd debuggers, gnome and kde graphical shell, various users utilities (including ROOT), various libraries (including CERN library).

Service User Interface has been implemented on one of the interactive machines of the JINR CICC (lxpub03.jinr.ru) for access of the users to the Grid global infrastructure. The following services have been provided on the LCG infrastructure of JINR: Storage Element (SE) based on the DPM system, Grid queue of jobs' batch processing (Computing Element, CE), Resource Broker (RB), information service (BDII), expanded service to provide permission to work in the Grid environment (MyProxy).

At the LCG farm, comprising 20 computing nodes, applied software for the LHC experiments has been installed: VO-alice-geant42ndProd_p01, VO-cms-CMKIN_4_4_0_dar, VO-cms-OSCAR_3_6_5_SLC3_dar, VO-cms-ORCA_8_7_1_SLC3_dar, VO-cms-ORCA_8_4_0, VO-lhcb-RTTC-v1, VO-lhcb-Gaudi-v15r5.

Instead of the old package processing system PBS, its new modified version Torque and intellectual dispatcher Maui have been installed.

In order to increase the performance of the CICC networking segments, the NFS protocol was replaced by the AFS protocol for software access, while for data access the intellectual tools DPM (Disk Pool Manager) and dCache were introduced.

The users involved in 17 physical experiments (ALICE, ATLAS, CMS, COMPASS, D0, DIRAC, H1, HARP, HERMES, KLOD, LHCb, NA48, NEMO, OPERA, STAR, etc.) are joined into specific subgroups (more than 130 users). To each subgroup, dedicated additional disk space has been allocated to perform simulation, storage and processing experimental and simulated data, a specialized software has been installed. 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	FLNR	Non-JINR Grid users	BLTP	FLNP	Adm.
171	104	53	44	34	28	14	12	9

Table 3

BLTP	LIT	DLNP	VBLHE	LPP	FLNP	LHC-production	FLNR
25%	23%	17%	15%	7%	5%	5%	3%

At the end of 2005 the electric power system was modernized. Symmetra power supply system is considered as the most appropriate solution. Modern modular technology of the distributed power supply system able to provide reliable protection and real uninterrupted power supply for the entire CCIC computer facility will be in use.

The elaboration of the JINR Grid segment and its inclusion in the European and global Grid structures has had as directions of activity the participation in LHC Computing Grid (LCG) project, the development of LCG/EGEE infrastructure, the participation in the development of the Russian Tier2 Cluster, Grid middleware evaluations, participation in the LHC experiments.

As part of the JINR participation in the LCG project, some work was performed. Production in the framework of DC's was accomplished at local JINR LHC and LCG farms. Tests on data transferring by the GridFTP protocol (GlobusToookit 3) were made. The server for monitoring Russian LCG sites was installed and the 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 package was developed; the software for installation and control of MonaLisa clients on the base of RMS (Remote Maintenance Shell) was designed (http://rocmon.jinr.ru:8080). The LIT team represents JINR in the RDIG (Russian Data Intensive Grid) consortium, a national federation in the EGEE (Enabling Grids for E-science) project. JINR's role and work in EGEE involves the following directions: EGEE-RDIG monitoring and accounting, middleware deployment and resource induction, participation in the OMII and GT4 evaluation and in the gLite testing, LCG SC activity coordination in Russia.

Among the other activities performed, worthy of notice are the development of the CASTOR2 system that includes the realization of a subservient module serving as a garbage collector, the development of the MCDB system (http://mcdb.cern.ch), the development of the data base structure and hierarchy for the CMS experiment.

Last but not least, the development of the Dubna-Grid project. The project is aimed at the creation of a distributed meta-computing environment on the basis of vacant computing resources of «office» computers in the Dubna University, secondary schools and other organizations of higher education in Dubna. This foresees the creation of a common pool of accessible nodes of more than 1500 units. The project is based on an Agreement between the Administration of Dubna, Joint Institute for Nuclear Research and University «Dubna» for creation of a city-wide multipurpose new-generation information infrastructure based on the Grid technologies and is partially financed by grants from the town of Dubna and the Russian Foundation for Basic Research.

Various approaches to the installation of the computational infrastructure at such a scale were discussed at LIT and available technologies were studied. Since the Microsoft Windows OS that is used everywhere for office computers does not support complicated and resource-consuming computing tasks in the distributed environment, it has been decided to apply the Linux-based technology for construction of the meta-cluster. In order to reach the goals, several technologies and all the potential resources have to be integrated into the computing infrastructure of the Dubna-Grid meta-cluster, controlled by a unified centre from LIT, JINR.

The logical structure of the meta-cluster is shown in Fig. 2.

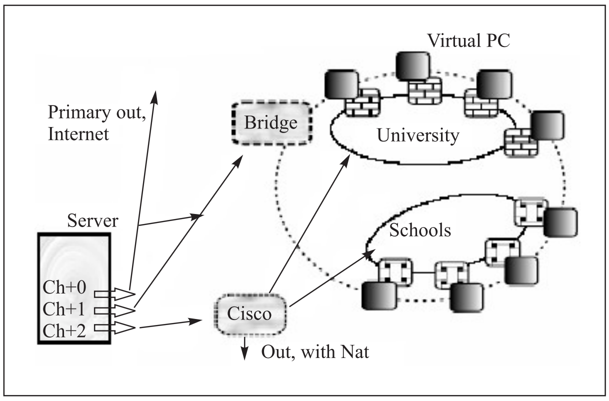

Fig. 2. Logical scheme of the Dubna-Grid meta-cluster

At LIT a Grid laboratory, GridLab, is created. The aim of the GridLab is to develop an educational programme of Grid technologies for scientists from JINR and the Member States, students, PhD students and teaching staff of Dubna schools. Technically the GridLab is a specialized segment of the Dubna-Grid project consisting of a module of seven working nodes and one server. The nearest term plans involve the deployment of lectures and sets of specialized practical works in the field of Grid technologies.

Traditional provision of information, algorithmic and software support of the JINR research-and-production activity included a wide spectrum of activities both at LIT and at 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.

The Backward Proportional Chamber (BPC) of the H1 setup at DESY is under responsibility of the Dubna group. The BPC alignment has been performed to both nearest detectors: Central Jet Chamber (CJC) and backward Spaghetti Calorimeter (SpaCal) on 2004–2005 experimental data. Also the BPC alignment has been done for the Backward Silicon Tracker (BST), which is the closest to the interaction point. After the BPC alignment ΔR, Δx, Δy, residuals between detectors, became less than 0.1 cm (while being 1–2 cm before alignment). An additional track filtering in the BPC was done for concurrent tracks in a region of radius of 3 cm by selecting the best track with the usage of the goodness-of-fit χ^2-criterion. The codes created have been implemented into the official release of the H1 software [1].

Significant progress has been achieved in efficiency and transverse momentum P_T reconstruction for hard single muons in CMS software: up to $P_T = 1$ TeV the efficiency of reconstruction was increased above 96%, with a P_T-resolution less than 8%. The most significant result has been obtained for Drell–Yan dimuon reconstruction efficiency, which has been increased by 12–20% (see Fig. 3). These improvements have been achieved by modifications implemented in the CMS software for track-segment building in CSCs and for muon trajectory seed generator [2].

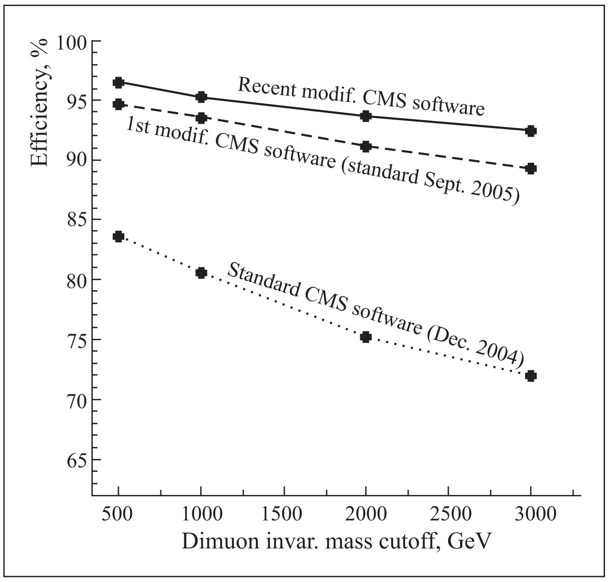

Fig. 3. Drell–Yan dimuon reconstruction efficiency in standard and modified CMS software for samples with mass cutoffs 0.5, 1, 2, and 3 TeV

The LIT team of the CBM collaboration contributed to the development of methods and algorithms for event reconstruction in the CBM experiment. The track reconstruction problem can be split into track finding and track fitting. Different competitive approaches to both track finding and reconstruction of the initial track parameters were applied by the LIT specialists. For the track finding, 3D track following and cellular automaton methods have been used. The Kalman filter and global fitting methods like the polynomial approximation are applied to the problem of the momentum reconstruction. The Kalman filter was also used for the determination of primary and secondary vertices. The efficiency of track reconstruction for particles detected in at least four stations is presented in Fig. 4. Tracks of high-momentum particles are reconstructed very well with efficiencies of 99.45%, while multiple scattering in detector material leads to lower reconstruction efficiency of 89.46% for slow particles.

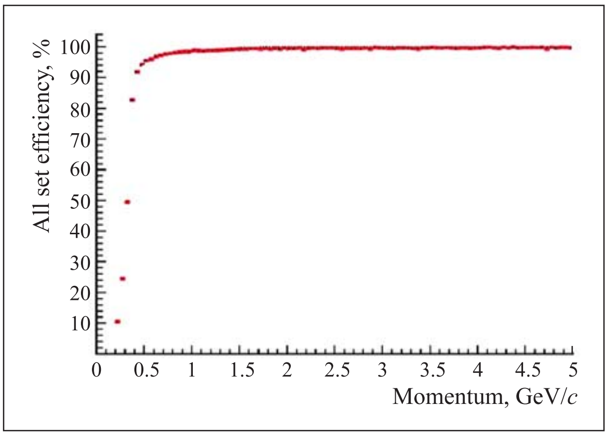

Fig. 4. Track reconstruction efficiency as a function of momentum

The reconstruction efficiency for fast primary tracks with momentum higher than 1 GeV/c is almost 100%, while the efficiency of all fast tracks is slightly lower because of the presence of secondary tracks, originating far downstream from the target region. Total efficiency for all tracks with a large fraction of soft secondary tracks is 96.98% [3].

Elastic Net for standalone RICH ring finding was worked out. Standalone finding of rings in this detector is based on the elastic neural net. The method does not require any prior track information and can be used for triggering. Application of the method to the RICH detector of the CBM experiment shows an efficiency of 94.3% and high speed (5.4 ms per event with about 1400 hits in the RICH detector). In view of its computational simplicity and high speed, the hardware implementation of the algorithm, which can increase the speed by some another orders of magnitude, is foreseen [4].

Generalized numerical solutions were obtained for solving the 3D nonlinear magnetostatic problems by the finite element method (FEM). In the general FEM theory the calculations of errors are based on the estimation of nearness between approximated solution and the unknown exact solution. The formulas connecting the computational error of finite element problems with easily calculated local characteristics are presented. An example of using the characteristics under computation of a dipole magnet model for the PANDA experiment is considered (Figs. 5 and 6) [5].

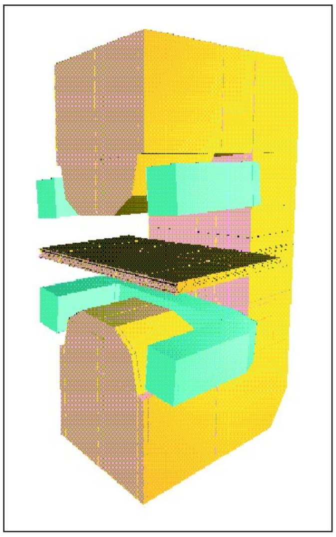

Fig. 5. Computer dipole model for PANDA forward spectrometer (1/2 symmetrical part)

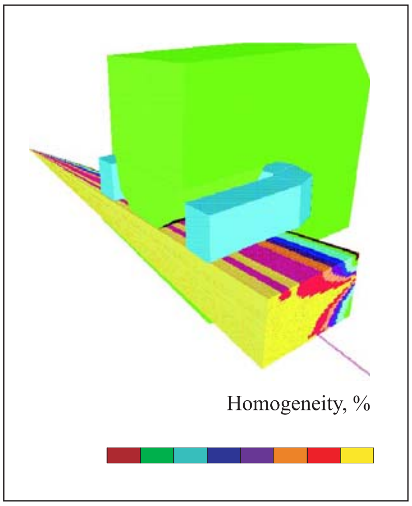

Fig. 6. Distribution of bending power homogeneity in the working region (1/4 symmetrical part)

METHODS AND TOOLS FOR MODELING PHYSICAL PROCESSES AND EXPERIMENTAL DATA ANALYSIS

The development of methods for mathematical description of nonlinear self-organizing structural changes in UO_2 during its burn-up in nuclear reactors on the basis of cellular automata (CA) has been in progress. This provides a way for effective extraction, by CA methods, of every possible quantitative characteristics of the structures represented in those micrographs, for their subsequent use in theoretical models of the process.

Besides, what is even more important, under these circumstances, one can formulate mathematical models of the process directly in terms of the entities imprinted in the micrographs. In particular, the micrographs corresponding to a smaller burn-up can be accepted as initial data for a program of calculation (with the help of some local rules of interaction given in elementary image elements — pixels) of the visual image of fuel state at advanced terms of exploitation. In order to check up the agreement between the theoretical model and experiment, the obtained thus theoretical image was compared, using the CA programs of image analysis, with a micrograph of real fuel at the same burn-up. Some strict mathematical results of the theory of cellular automata (related to Ising models, voting, etc.) were useed for the interpretation of some features of fuel behaviour observed in the experiment. Various methods of calculating the fractal dimension of spatial structures formed in UO_2 during operation of a nuclear reactor were applied for the first time to the description of a burn-up degree. The fractal dimension of microstructures was found to be a natural and important characteristic feature describing the degree of radiation destruction and hence it can show the level of emergency danger when using fuel at this burn-up stage [6].

A model based on the thermal spike concept for an explanation of latent track formation in $YBa_2Cu_3O_{7-x}$ single crystal has been studied by LIT and VBLHE scientists. The model demonstrates some interesting peculiarities such as electronic quenching and existence of bifurcation points. Arguments why the energy spent on damage creation in the track should be equal to melting heat and why the so-called «epitaxial regrowth» is impossible are given [7].

The analysis of the relation between variables is one of the main tasks of technical and scientific research. A major problem in data/signal denoising, compression and forecasting is to find an optimal or good representation. A new approach to the analysis of complex dependence with relatively small noise using the four-point methodology was suggested. The suggested algorithm LOCUSD divides the interval/curve into subintervals/segments of various lengths, provides for every segment local cubic estimations and gives a technique for obtaining integral cubic approximants. Finding the breakpoints in an autotracking mode and the iterative computation schemes are the two main features of the proposed method that use a special approximation model. An automatic knot detection and a piecewise-cubic approximation method are proposed. In this method the continuity of the first derivatives of the approximants for functions presented by data without errors are acceptable; smaller δ results in more segments with more precise approximants; for noisy data it is advisable to choose greater sampling step and δ; the goal is to find such δ that yields desirable approximation quality and an acceptable count of segments [8].

In recent years, progress in experimental techniques of the Electron Momentum Spectroscopy (EMS) (where at least two electrons emerge at the final stage of reaction and are studied in coincidence), in particular, the development of cold-target recoil-ion momentum spectroscopy (COLTRIMS) has made it possible to perform precise, kinematically complete studies of complex atomic collisions. The double processes of He in electron-impact ionization, single ionization with simultaneous excitation and double ionization, have been studied at large momentum transfer using an energy- and momentum-dispersive binary $(e, 2e)$ spectrometer. The experiment has been performed at an impact energy of 2080 eV in the symmetric noncoplanar geometry. In this way, it has been achieved a large momentum transfer of 9 a.u., a value that has never been realized so far for the study of double ionization. The measured $(e, 2e)$ and $(e, 3{-}1e)$ cross sections for transitions to the $n = 2$ excited state of He^+ and to doubly ionized He^{2+} are presented as normalized intensities relative to that to the $n = 1$ ground state of He^+. The results are compared with first-order plane-wave impulse approximation (PWIA) calculations using various He ground-state wave functions (to study models of dynamics of the processes and quantum correlation structure of two-electronic states). It is shown that the shapes of the momentum-dependent $(e, 2e)$ and $(e, 3{-}1e)$ cross sections are well reproduced by the PWIA calculations only when highly correlated wave functions are employed [9].

The analyses and numerical study of the structure and properties of the polydispersed DMPC vesicles population in three phases: gel, ripple, and liquid, were performed. Dependence of the DMPC membrane thickness on temperature was restored from the SANS experiment on the basis the SFF-HH model. It was demonstrated that DMPC membrane thickness in liquid phase ($T = 30\,^{\circ}$C) depends on the membrane curvature [10].

The properties of a model of the moisture evaporation in a porous building material of a rectangular form have been investigated. Algorithms of solving a nonlinear diffusion equation with initial and boundary conditions simulating the dynamic distribution of moisture concentration, calculation of coefficients of a polynomial describing transport of moisture, with usage of experimental measure of moisture concentration in a sample were developed. Research of the properties of the model was carried out depending on the polynomial degree and the set of its coefficients and the quantity of the used experimental data [11].

NUMERICAL ALGORITHMS AND SOFTWARE FOR SIMULATION OF COMPLEX PHYSICAL SYSTEMS

The advection of a passive scalar quantity by incompressible helical turbulent flow has been investigated in the framework of an extended Kraichnan model. Statistical fluctuations of the velocity field are assumed to have the Gaussian distribution with zero mean and defined noise with finite time correlation. Actual calculations have been done up to two-loop approximation within the field-theoretic renormalization group approach. It turned out that the space parity violation (helicity) of a stochastic environment does not affect anomalous scaling which is the peculiar attribute of corresponding model without helicity. However, the stability of asymptotic regimes, where anomalous scaling takes place, and the effective diffusivity strongly depend on the amount of helicity [12].

Methods of numerical description of open quantum systems by the deterministic methods of approximate differential integration were developed. A representation of a propagator for open quantum systems in the form of a double functional integral with respect to conditional Wiener measure was proposed. It allows one to apply the approximate formulas exact for functional polynomials of a certain power to calculation of such integrals. Within this deterministic approach the problem is reduced to the evaluation of usual (Riemann) integrals of low multiplicity. The formulas are in fact the basis of a numerical method of studying the time evolution of the systems. The features of the method are discussed and some examples of calculations are given [13].

In cooperation with the University of Cape Town, the particle-like excitations of nonlinear dispersion matter have been studied within models of condensed matter theory and nonlinear optics based on the nonlinear Schrödinger (NLS) equation. It has been shown that unlike the bright solitons, the parametrically driven kinks of the NLS equation are immune to instabilities for all damping and forcing amplitudes; they can also form stable bound states. In the undamped case, the two types of kinks and their complexes can stably travel with nonzero velocities. The bistability of the Bloch and Néel walls within the NLS contrasts the properties of these solutions within the Ginzburg–Landau equation, where they cannot stably coexist [14].

The parametrically driven damped NLS equation serves as an amplitude equation for a variety of resonantly forced oscillatory systems on the plane. Its nodal soliton solutions are considered. It is shown that although the nodal solitons are stable against radially symmetric perturbations for sufficiently large damping coefficients, they are always unstable to azimuthal perturbations. The corresponding break-up scenarios are studied using direct numerical simulations. Typically, the nodal solutions break into symmetric «necklaces» of stable nodeless solitons [15].

The study of a late time acceleration of the universe, together with the initial singularity and isotropization process, remains among the attractive problems of modern cosmology. The problem of singularity has been thoroughly addressed by us in a number of papers for the last few years for both plane symmetric and Bianchi-type universes. The interacting spinor and scalar fields in a plane symmetric space-time are considered and the possibility of the formation of soliton-like configurations is investigated. The investigation is performed on the role of nonlinear spinor field in elimination of space-time singularity for Bianchi universes when a self-consistent system of scalar, spinor, electromagnetic and gravitational fields given by a Bianchi-type I model is involved [16].

Stationary solutions to the Gross–Pitaevskii equation define the topological coherent modes, representing nonground-state Bose–Einstein condensates. These modes can be generated by means of alternating fields whose frequencies are in resonance with the transition frequencies between two collective energy levels corresponding to two different topological modes. The theory of resonant generation of these modes was generalized in several aspects: multiple-mode formation was described; a shape-conservation criterion was derived, imposing restrictions on the admissible spatial dependence of resonant fields; evolution equations for the case of three coherent modes were investigated; the complete stability analysis was accomplished; the effects of harmonic generation and parametric conversion for the topological coherent modes were predicted. It was demonstrated that the dynamical transition between the mode-locked and mode-unlocked regimes was accompanied by noticeable changes in the evolutional entanglement production [17].

As part of joint research work on bioinformatics conducted by LIT in collaboration with the Institute of Theoretical and Experimental Biophysics (Pushchino) and the Institute of Cell Biophysics (Pushchino), calculations have been performed on research of transport tRNAs. The distribution of the electrostatic potential around several tRNAs was calculated with the help of the nonlinear Poisson–Boltzmann equation, for both free tRNAs and those linked to the proteins involved in translation: an aminoacyl-tRNA synthetase (ARS) and an EF-TU elongation factor. A comparison of various tRNAs has allowed the identification of several regions of the strong negative potential related to the tRNA typical structural patterns and invariant with respect to the tRNAs. These patterns were found to be conserved upon binding the tRNAs to proteins, but both the electrostatic potentials in the invariant patches and the areas occupied by these patches depend upon a particular tRNA-binding protein. The comparison of the calculated pK shifts of fluorescently labeled tRNAs with experimentally observed pK shifts shows that the tRNA total charge is at least $-40q$ (q — charge of proton) and even most likely close to $-70q$. This large charge leads to the high absolute values of the electrostatic potential around tRNAs and allows one to propose a mechanism of the electrostatic charge switching on a corresponding synthetase. In view of its strong negative charge, tRNA increases the proton concentration in its nearest neighborhood, thus inducing positive charges on histidine residues of the synthetase at the early stage of the protein-tRNA recognition. This study has shown that the electrostatic field of tRNAs is the key factor of tRNA recognition [18].

METHODS, ALGORITHMS, AND SOFTWARE OF COMPUTER ALGEBRA

The cohomologies of restricted Lie algebras of Hamiltonian vector fields have been studied in the framework of the research on computer algebra conducted at the Laboratory of Information Technologies. Restricted Lie algebras (or Lie p-algebras) of vector fields are finite-dimensional analogs of corresponding classical algebras defined over the fields of positive characteristic p. The computer-based calculations performed with the Lie p-algebras of vector fields preserving a symplectic structure (i.e., Hamiltonian and Poisson algebras) have revealed important and interesting peculiarities in the structure of their cohomologies. Statements explaining these peculiarities have been proved [19].

A new universal mathematical frame for constructing models in mathematical physics called «a system of discrete relations on an abstract simplicial complex» was proposed. This construction can be interpreted as a natural generalization of the notion of cellular automaton and as a set-theoretic analog of a system of polynomial equations. The algorithms in C for compatibility analysis of a system of discrete relations and for constructing canonical decompositions of discrete relations have been developed and implemented. A regular way to impose topology on an arbitrary discrete relation via its canonical decomposition was proposed. This allows one to evolve standard tools of the algebraic topology (homology group, cohomology ring, etc.) for relations. Applying the above technique to cellular automata — a special case of system of discrete relations — some new results were obtained. Most interesting of them is the observation that the presence of nontrivial proper consequences may determine global behavior of an automaton. If the number of states q is a power of a prime, i.e., $q = p^n$, one can express any discrete relation in terms of polynomials over the Galois field F_q and then use the standard Groebner basis method for the compatibility analysis. The Groebner basis computation for the cellular automaton «Life» with the help of Maple 9 takes 1 h 22 min. The proposed approach gives an analogous result about 5000 times faster — for less than 1 s [20].

An asymptotic heat kernel expansion for elliptic differential operators acting on compact closed curved manifolds has been studied by means of the computer algebra. The coefficients in this expansion are quantities of fundamental importance in the quantum field theory, quantum gravity, spectral geometry and topology of manifolds. Deriving explicit expressions for these quantities is quite a laborious task, especially in the problems of modern physics that deals with complicated operators (high-order and nonminimal ones) in a complicated geometric environment (with torsion and gauge fields in addition to the Riemann curvature tensor). In fact, the calculations cannot be performed without computer algebra tools. A covariant algorithm for computing the heat kernel coefficients and its implementation as two C programs CoincidenceLimits and DWSGCoefficient are described. Some results obtained with the help of these programs are presented for the first time. The most considerable results are related to nonminimal operators and manifolds with torsion [21].

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