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LABORATORY OF INFORMATION TECHNOLOGIES

REPORT ON RESEARCH ACTIVITIES IN 2001

Report to the 91st Session
of the JINR Scientific Council
January 17–18, 2002

Dubna 2001

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In 2001 the Laboratory of Information Technologies (LIT) staff concentrates its activities on the maintenance of operation and the development of the computing and networking infrastructure of the JINR following the decision of the 88th session of the JINR Scientific Council.

The JINR computing and networking infrastructure as a basic facility includes:

- Telecommunication service, external computer communication channels, and distributed information systems;
- JINR Local Area Network (LAN) and High-Performance Computer Centre (HPCC);
- Support and development of standard software and modern tools of computational physics for users.

In 2001, the scientific programme of the LIT covered three first-priority topics of the "Topical Plan for JINR Research and International Cooperation in 2001". The Laboratory staff participated in 10 more topics of the Topical Plan in collaboration with other JINR Laboratories on the project level and in other 14 topics on the level of cooperation. The main aim of the Laboratory is the performance the works on the "Development and Maintenance of the Networking, Information and Computing Infrastructure at JINR" (topic 09-6-1019-96/2001, headed by I.V.Puzynin, R.Pose, and V.V.Korenkov) and the research in the field of the "Nonlinear Problems of Computing and Mathematical Physics: Algorithms, Investigation and Software" (topic 6-0996-93/2001, headed by I.V.Puzynin). Main results of the investigations performed within this topic have been published in the well-known journals, proceedings of the scientific conferences and preprints.

In the year 2001, 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 12 grants of the Russian Foundation for Basic Research. Six projects are devoted to the creation and development of informational, computing and telecommunication resources for performing fundamental research, and the other six are initiative scientific projects.

A confirmation of high level of these investigation and an interest of world scientific community is the regular organization of international conferences by Laboratory of Information Technologies.

In the year 2001, LIT participated in organizing four conferences:
on February 21-22, a workshop «Role of the Operating System Linux in the Computing Infrastructure of the Future» was organized in cooperation with the company "Hewlett Packard"; on June 28-30, an international workshop "Computer algebra and its applications to physics" (CAAP-2001) was held; on July 3-4, the first conference held in Russia on data storage systems "Solutions on Data Management in Scientific Research" was organized together with the company

"TechnoServ A/C"; on September 12-18, XVIII JINR International symposium on nuclear electronics and computing (NEC'2001) was held in Varna (Bulgaria).

First "Information bulletin of LIT" (JINR publication, 4-7998, Dubna, 2001) was published and contains information for users of JINR networking, computing and information resources.

External telecommunication systems

At present JINR leases 2 Mb/sec channel to Moscow from the Russian Satellite Communications Company (RSCC «Dubna»); thus JINR has access to the Russian networks and information resources (up to 2 Mb/sec) as well as access to the international channel through shared RBNet in the common data stream up to 1 Mb/sec (there is no granted bandwidth). The leasing of the channel to Moscow and payment for the Russian part of the traffic at the rate of 2500 US dollars per month is carried out from the interdepartmental programme «Creation of the national network of computer telecommunications for science and higher school» through the Russian Research Institute for development of public networks (ROSNIIROS) which bears responsibility for operation and development of the Russian BackBone RBNet (fig.1).

However, such a throughput of the channel is inadequate to satisfy the JINR's needs. Fig.2 shows the increasing peak load (grey colour) of the link to Moscow at daytime in November 2000 - November 2001.

Paid in 2001
RBNet - 35.8k$
CONTACT -8.43K$
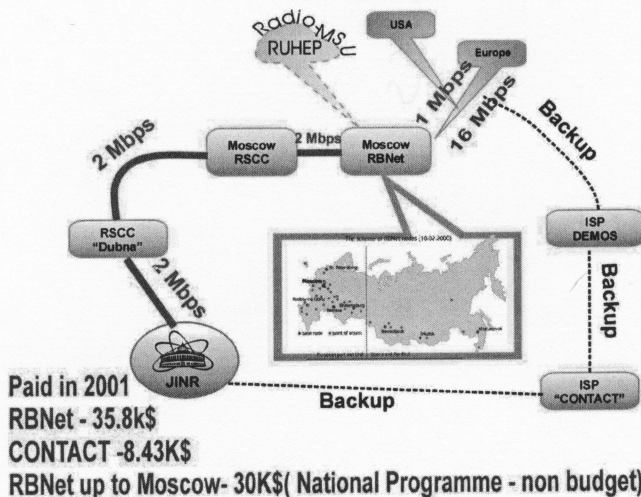RBNet up to Moscow- 30K$(National Programme - non budget)
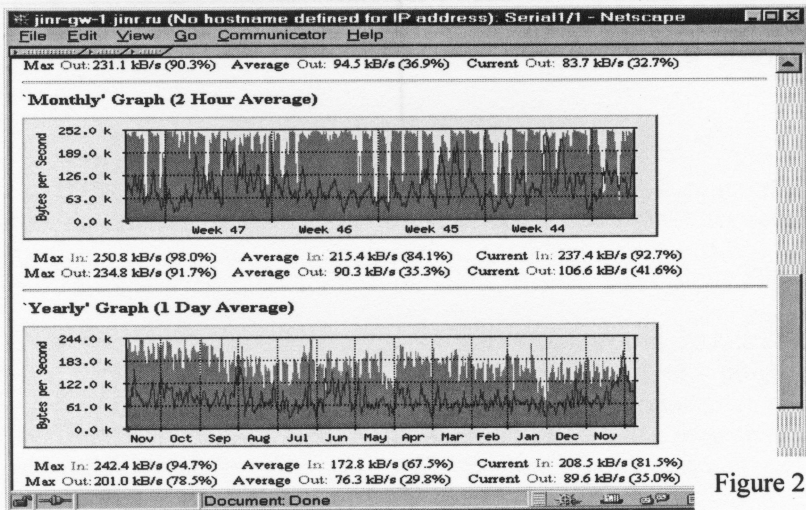
Figure 1.

Figure 2.

Tab.1 shows the incoming JINR traffic from 2001-01-01 to 2001-12-03 (total 3.7 TB) distribution among the JINR divisions. The University of Dubna (Uni-Dubna) and the modem pool (Tab.2.) take a noticeable share in the common traffic.

Table.1 JINR Incoming Traffic

JINR laboratories and subdivisions (>25MByte)	Traffic Mbytes
LIT+proxy+servers	1400
FLNR	669
DLNP	342
Uni-Dubna	271
Modem pool	223
LHE	214
BLTP	205
LPP	182
FLNP	110
Adm.	67
UC	26

Table.2 JINR Modem pool statistics

JINR laboratories and subdivisions	Hours from 01.2001 to 11.2001
FLNP	12930
DLNP	10778
Adm.	9236
FLNR	7930
LHE	7337
LIT	6552
LPP	3965
OTHERS	1096
BLTP	216

At the end of 2001, the JINR channel to Moscow will be increased up to 30 Mb/sec by leasing the bandwidth in the ATM155 channel from the RSCC "Dubna". The monthly cost of leasing the communication link Dubna - Moscow is 6000 US dollars per month. A partial payment of the channel lease can be carried out within the Russian program «Creation of the national network of computer telecommunications for science and higher school». Thus JINR will have access (up to 30 Mb/sec) to the Russian networks and information resources as well as access to the international channel through shared RBNet 155 Mb/sec channel in the common data stream. The guaranteed capacity for JINR in the international channel is supposed to be ranged from 2 Mb/sec up to 4 Mb/sec for the same level of payment.

The further perspectives to improve the JINR computer telecommunications are related to the development in Russia of the system of international channels for science and education, to the development of the high-speed network infrastructure, especially for nuclear physics centres, and to the extension of cooperation with the Russian Satellite Communications Company and its branch in Dubna. Special commission of the Russian Ministry of Industry, Science and Technology will distribute the limits of capacity between scientific directions and institutes. The representative of JINR Dr.V.V.Korenkov will take part in the work of Commission as a member of HEP group. The construction of dedicated channels to CERN and DESY is an urgent task.

The commission of JINR network users for improvement of external computer communication links was organized by Director of JINR.

Systematic work on the LAN management was performed by the Network Operation Centre (http://noc.jinr.ru/). To make operation of the central mail server @jinr.ru more comfortable and reliable, a number of new services have been provided for its users: e-mail stream antivirus check-up, mail pseudonyms, protection from comical and undesired messages (SPAM). One can use the www-interface https://webmail.jinr.ru/ for fast access to mailboxes (fig.3). The interface is a multi-language one (Russian, English, etc.). The access
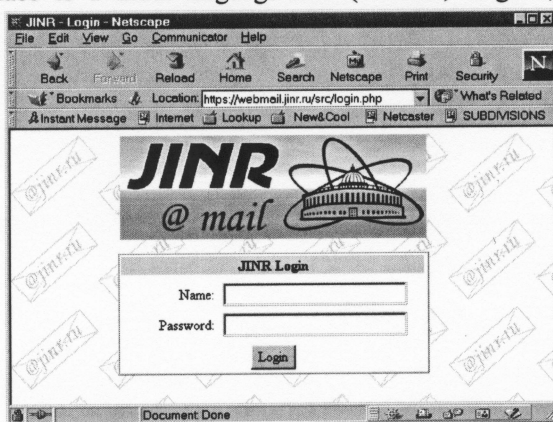

Figure 3.

through the webmail seems more preferable for the users outside the JINR network.

In 2001 JINR received the License A018377 n.19049 on data transfer services and now the Reglament and the Rules on user connection to JINR data transfer links are in preparation.

JINR Local Area Network (LAN).

At present IP addresses database contains 3451 registered JINR LAN elements (3105 in year 2000).

Currently the JINR network operates in non-standard configuration in a critical, temporary mode using Fast Ethernet technology as a result of ATM-backbone destruction.

A project on modernization of the network topology and choosing an adequate technology of its design is in development stage now, and LAN backbone construction will be the main task for future years. The basis for the work on the project is the recommendation of the 89-th sessions of the JINR Scientific Council on the further development of remote access to experimental installations, data processing and data transfer, participation in the collaborations under the projects Data Grid and Grid in Europe and America. The high-performance network will allow one to organize distributed computations, effectively using large computer complexes in the JINR laboratories. It is of particular importance for data processing for experiments LHC in CERN where JINR takes an active part.

There were a number of discussions of the future Local Area Network (LAN) backbone. It was reported on the several institute's forums that during the year of 2001 the JINR backbone used two technologies: the unreliable ATM and
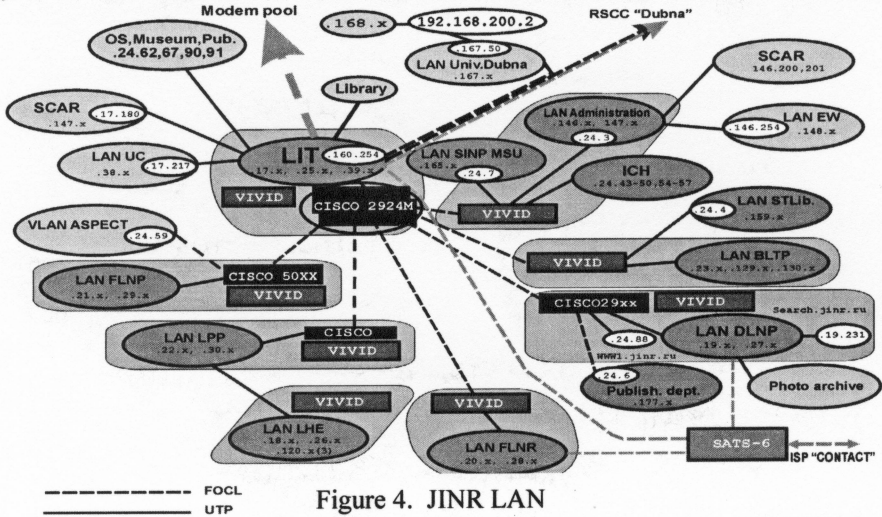

Figure 4. JINR LAN

30.X.2001г.

Fast Ethernet in three laboratories, and since October 30, 2001, the whole JINR backbone has been using Fast Ethernet (fig.4) due to central ATM-backbone equipment crash.

Two information technology dealers from Moscow (JetinfoSystems and TechnoServ A/C) and the telecommunication faculty of the Russian Institute for Friendship were invited to take part in the discussions.

All external experts, network specialists from the Institute's laboratories, and Directors of some JINR Laboratories have come to the conclusion that the Institute scientific programmes and participation in the international research programmes demand creation of a high speed reliable backbone, which can be realized through the transfer to Gigabit Ethernet technology. All information about the LIT projects on computing and networking are available at **http://noc.jinr.ru/projects.htm.**

The LIT Directorate together with SCAR organized training for fourteen network specialists with the help of lecturers invited from Moscow. Five of them have passed the examination with the excellent mark and received certificates.

The department of Information Technologies in the Moscow Technical University of Radio Engineering, Electronics, and Automation was organized on the LIT basis. The first enrolment of 10 students started in the year 2001.

Distributed informational systems, HPCC

More than one thousand staff members of JINR and other research centres are the HPCC users. JINR HPCC (fig.5) is one of the ten largest Russian

SPP2000
8 CPU x 720 Mflops;
1 GB memory;
~70 GB disk space

ATL
ATL

D370/1-server
ATL-2640 tape library 10.56 TB
(3 DLT 4000 drives);
HP OmniBack v.2.55 & OmniStorage v.3.11

PROJECT
PC-cluster
20 CPU 800MHz
MaryNet
for MD

ATM

SUN CMS Cluster
NIS+cluster: 3 Sun Sparc stations;
24 GB disk space; Solaris 2.5.1;
Iris Explorer license server, LHC++

APE100

8 batch-nodes dual PIII-500 MHz, 512 MB RAM, 9 GB HD;
2 interactive PC 333 MHz, 128 MB RAM, 8 GB HD;
Server: dual PIII-600 MHz, 512 MB RAM; 170 GB RAID-5;
DLT-4700 tape library;
Linux Red Hat 6.1; cernlib 2000; ROOT 2.25.03;
LHC++; PBS; total perf. of PC-farm: 400 SI 95

Upgrade by the end of
December, 2001
+32 CPU 800MHz (+1.5 K SI95)
File server with 1 TB disk space
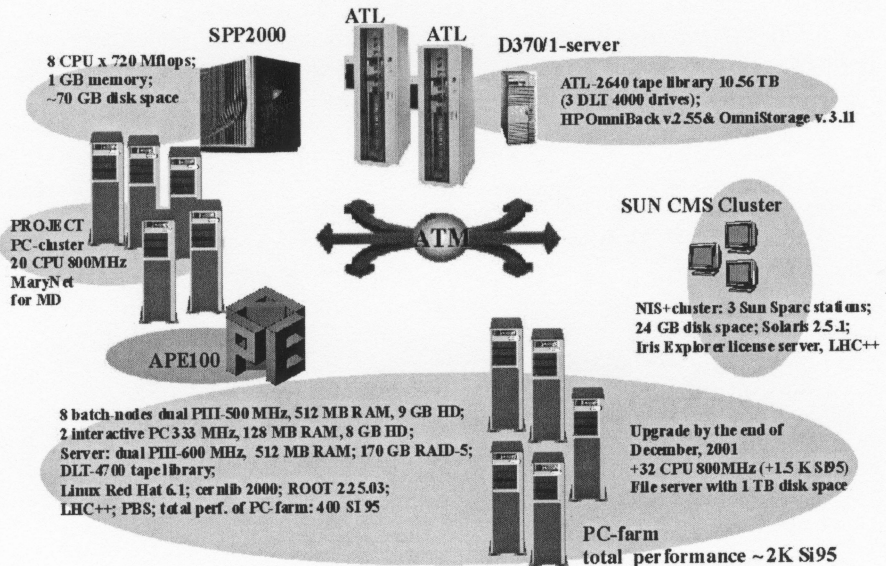
PC-farm
total performance ~2K Si95

Figure 5. The main JINR computing centre facilities.

centres. It actively cooperates with other leading centres - Intergovernmental Supercomputer Centre, Institute of high-performance computations and data bases (St.Petersburg). In collaboration with the leading nuclear physics centres of Russia, HPCC JINR participates in creating the Russian Regional Center for LHC Data Handling.

In 2001, the creation of the GRID segment in Russia was in progress. Ten more institutes of the Russian Federation take part in the project. The main LIT activity consists in the installation of GLOBUS toolkit, creation of GRIS (Grid Resource Information Service) and GIIS (Grid Index Information Service), certification, testing of metadispatcher, development of monitoring tools, data management, physical event mass generation and creation of a distributed database at the LIT PC-farm and HPCC servers.

In 2001, the available software suitable for solving the tasks of increasing the availability and effective use of the network services and resources of the JINR's central servers, central computing farms and clusters as well as mass data storages, was analysed and the best one for JINR HPCC has put in operation. An new web-interface for its usage was developed.

In the year 2001, SPP200 was used by 81 of 142 registered users. The CPU usage was 96% and the total CPU time was 58500 hours. Table below shows the percentage of CPU time using by JINR laboratories.

LIT	FLNR	DLNP	LPP	FLNP	BLTP	LHE
22%	13%	9%	8%	15%	22%	11%

The CONVEX 220 was used as the computing, e-mail, and http-server by 1215 users. Active e-mail users are 1031. Table below shows the registered users distribution over JINR laboratories

FLNR	DLNP	LPP	FLNP	BLTP	LHE	LIT	Adm.
165	166	124	57	109	129	372	93

There is a plan to replace the old Convex computers with a cluster of Intel-based servers. Convex 220 has a 25 Mhz processor frequency, and Convex 3840 – 60 Mhz, while Intel produce PCs with processor frequency more than 1Ghz. Then Convex 220 has 10 GB of disks, and modern desktop PC has twice as much. These old machines consume enormous electric power.

Computing service

Information and computer support of the JINR participation in the experiments at CERN, DESY and BNL was in progress in 2001. The installation of Globus toolkit at two computers at LIT was performed. One of them is used as an informational grid-server for the whole JINR and as a server for a specialized LIT Linux PC-farm. So way, the farm is included into a EU Data Grid and into a prototype of the Russian Regional Informational Computing Center for LHC accordingly. The other computer is used for testing new versions of software in

the framework of the EU Data Grid Project. The further adaptation and support of current versions of LHC++ Library for Linux and Windows NT platforms was performed. Software for monitoring the resources and services of the JINR high performance computing centre has been installed and is in operation.

In 2001, new run of mass event production was performed at a PC-farm, LIT JINR (16 processor units of 500 MHz) for the CMS high level trigger. The volumes of simulated data up to 75 GB are generated at the LIT PCfarm. The data production is performed with the use of the Pythia program and CMSIM, a program for simulation and reconstruction of events for the CMS experiment.

An investigation of the specialized computing system APE-100 based on the SIMD architecture has been in progress. A system of starting a task in a background that allows one to release the workstation terminal for execution of other operations has been designed. An Web-page has been prepared. It is devoted to the APE project and informs on the current status of the project. It also contains documentation on hard- and software as well as references to the main web-sites of Italy and Germany (http://www.jinr.ru/~tsap/Koi/ape/ape.htm).

New documents have been prepared and introduced in WWW. They include realization at JINR of electronic access to the texts of the program library CPCLIB (Belfast, Northern Ireland) and the Elsevier Publishing House (Amsterdam) for the readers of the CPC (Computer Physics Communications) journal; maintenance of the NAG Library; maintenance of CERNLIB on the JINR computer platforms; filling the JINRLIB with the new codes was in progress (http://www.jinr.ru/~tsap/Koi/sss.htm).

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:

- Information system IPDB - a web-interface of the JINR IP addresses database(http://iss.jinr.ru/ipdb/).
- Accelerator Data Bases (http://iss.jinr.ru/acc/).
- System for accounting and statistics of operating the JINR basic facilities (http://iis.jinr.ru/basic-fac/) was performed using ASP technology.
- A system for monitoring activities on preparing elements of the ATLAS detector in Dubna has been put into operation and is maintained (http://wnlse50.jinr.ru/wf/new/wf.html). It was designed at St-Petersburg Institute of Nuclear Physics. In frames of the project, application OAS to PL/SQL has been provided for mapping the DB status in the global network. The database has been transferred from WinNT server to the Linux Redhat server. A Perl module has been written for the weekly DB archiving in a semiautomatic mode.
- Digitizing of graphics at users' requests, preparation of bibliographic data on HEP for the PPDS database(http://www.jinr.dubna.su/~diginfo/). Almost

150 scientific papers have been prepared for the PPDS database. More than 50 papers were coded and included into the database. The other 50 are being prepared now. The work was carried out in cooperation with IHEP, BNL and other physics centres. 148 graphics have been digitized at the requests of JINR and foreign physicists.

- Information system «JINR Topical Plan for Research» (http://dbserv.jinr.ru/~deadhead/tp/). Software has been added for automated file translation from LaTeX into DB Oracle.
- Information System "System of accounting between JINR and Experimental Production Plant (Access, VBA)" for the JINR Accounting Department.

One of the most important activities was the development of the system of WWW/FTP servers of the Institute's subdivisions and the maintenance of the main WWW/FTP Server of JINR. In order to maintain and develop a specialized WWW/FTP server FAXE (http://faxe.jinr.ru and ftp://faxe.jinr.ru) with program products for the JINR users, have been modernized.

Among the activities related to the main JINR and LIT servers (http://www.jinr.ru, http://lit.jinr.ru), the following work should be noted: actualization of the divisions in accord with the main scientific results and the programs of JINR activities; information on conferences, schools and workshops held at JINR; News; updating the presentation about JINR and Dubna.

The development and maintenance of the www-JavaStation was in progress (http://dbserv.jinr.ru/js/).

Computational Physics

The main problems of the Computational Physics include the algorithmic and software support of experimental and theoretical research under way at the Institute as well as the provision of the effective use of its computing facilities.

About 80 scientific publications, reports on conferences and JINR preprints were published and presented.

1. Mathematical modeling and information support of experimental investigations.
1.1. Data processing support in particle physics

The main works were related to the development of basis resources (both the tool and target computing) of experiments in high energy physics. The main gains were directed to the development and installation of the system for processing experimental and simulated (Monte-Carlo) data of the experiment EXCHARM on the new powerful server of the Linux-cluster RISK. It should be noted that in scales, entirety, comprehensive approach and the level of the scope

of the problems, this direction connected with the creation and application of the Data Processing System is very useful.

The experience and methodical results obtained in experiment EX-CHARM are applied in other experiments including the experiments with JINR participation at CERN, etc. [1-2].

1.2. Development of new methods for data processing

One of perspective methods of the analysis of experimental data is a wavelet analysis based on a wavelet transformation.

The WASP (Wavelet Analysis of Secondary Particles angular distributions) package was developed. It is a C++ program aimed to analyse secondary particles angular distributions in high energy nucleus-nucleus interactions. (WASP was designed for data analysis of the STAR and ALICE experiments). WASP provides a user-friendly Graphical User Interface (GUI) implemented by using ROOT GUI-classes.

The first version of WASP was successfully applied to data analysis. Angular distributions of secondary particles produced in the interactions of sulphur and oxygen nuclei with photoemulsion nuclei at the energies of 200 and 60 GeV/nucleon were analyzed. With the help of the wavelet analysis it was observed that the pseudorapidity distributions of the particles summered on all the events had three sub-structures. The distributions in separate events have more than one sub-structure in 40% of the cases. The wavelet analysis allows one to separate events with different sub-structures (fig. 6)[3].
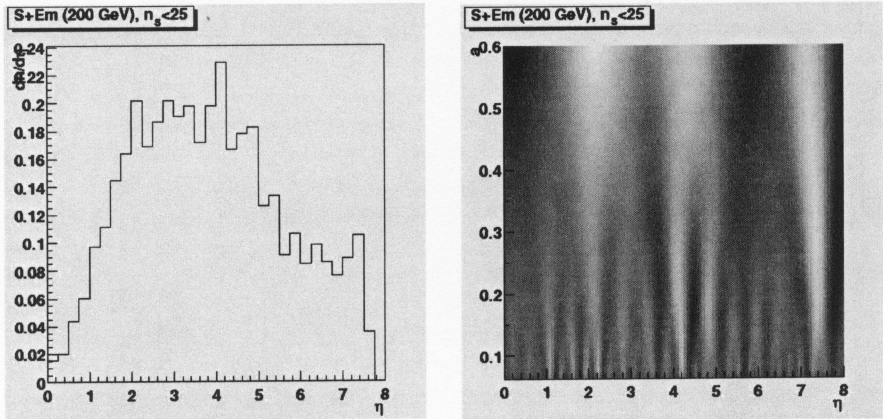

Fig. 6 Shower particles pseudorapidity distribution in events with $n_S < 25$ (left) and its wavelet spectrum (right). Tree sub-structures arise at scale 0.4.

New WASP version allows one to perform both one- and two-dimensional wavelet analysis. Thus it can be used for ring-like structures detecting. [4-8].

A study of software efficiency improvements for the pattern recognition chambers (PC) of the HERA-B outer tracker (OTR) has been accomplished in frames of the planned LPP work in the HERA-B collaboration. A new version of the PC calibration program was developed on the basis of the consistent applying of the robust approach to both: track-finding algorithms and calibration function calculation. In addition to the improvement of the calibration accuracy, it allowed one to accelerate the calibration procedure by the order of magnitude in comparison to the conventional calibration program. The most effective was the robust fit of cubic splines directly to raw data which are the many thousands of the drift time measurements. The fit results are shown in fig.7.
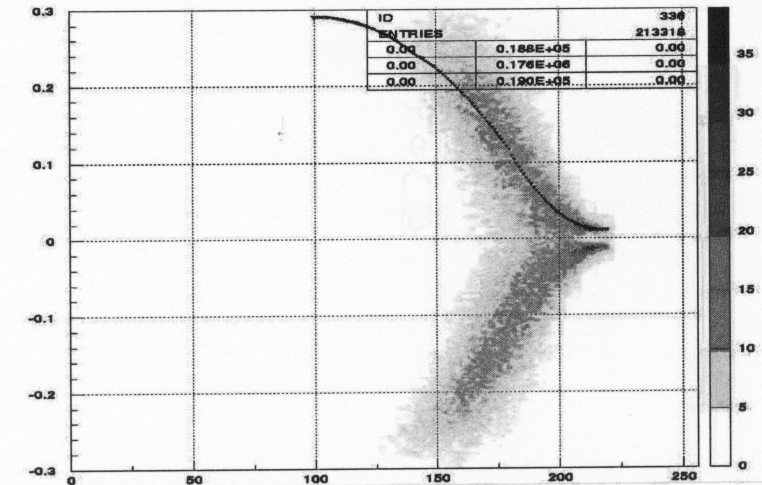

Fig.7 Result of the cubic spline fit to 5mm PC drift data

Two versions of the Radon-Hough transform for the track reconstruction in OTR PC were developed. The first, most substantial version takes into account the drift chamber specifics including their left-right ambiguity. The method and program descriptions and testing results are submitted to Particle & Nuclei Lett. The second, very fast version was developed on the basis of the variable slope histogramming method. It was applied as a seeding algorithm for the Ranger program and also tested on real PC data. Although it shows a satisfactory performance, its further development is needed in order to improve its speed characteristics. The C++ program for OTR PC alignment with simultaneous fitting of all shifting and rotation parameters on the basis of the MIL-

LEPEDE program was developed and tested on real PC data. Its possible robustification is studied [9].

Cathode strip chambers (CSC), i.e. six-layer multiwire proportional chambers with a strip cathode readout, are used as muon detectors in the forward region of CMS. About 10-20% of the muon hits in CSC will be contaminated by heavy physical background. As a result, the traditional least squares method (LSQ) looses its optimal properties. Therefore, it has been developed an iterative robust track fitting procedure with a sub-optimal polynomial weight function. The results obtained demonstrate the advantages of the proposed robust approach, which gives the parameter estimation very close to the optimal one. Track parameters obtained by the robust method have a value of RMS in 2 - 2.4 times better than the parameters obtained by the LSQ method [10].

The research of collective streams is actual now especially after the discovery of the great quantity of an elliptic stream at the RHIC energies. Plans have been made of the study of streams at the JINR synchrophasotron. With the purpose of theoretical data analysis it is necessary to develop and utilize the models taking into account potential interactions of particles. One of such models is the model of relativistic quantum molecular dynamics (RQMD). In order to test the model, a description of basic characteristics of nucleus - nucleus interactions at the energy of 3,3 GeV/nucleon was considered. The model RQMD has appeared to unsatisfactory play the spectra of protons in NN- and AA- interactions. Therefore, the further use of RQMD at the indicated energies seems inexpedient. For the analysis, data of LHE and calculations over the modified model FRITIOF were used [11].

Research on exotic states of hadron structures has been in progress. Experimental observations of the anomalous-narrow resonant hadronic structures K(1630), N(3520), Σ (3170) are discussed. These supposed exotic states are produced in the processes with large 4-momentum transfers. The special feature of the decay points out a space clusterization of colorless decay products of K(1630) and N(3520), their angular separation in two parts [19].

1.3. Application of the Method of Volume and Boundary Integral Equations in Models of Magnet Systems with Superconducting Shields

The modeling of magnet systems with superconducting shields is considered. Nonlinear volume and boundary integral equations are derived that govern the magnetization distribution over a non-linear medium and the current distribution over the superconductor boundary. Methods for discretization of the continuous equations and for iterative solving of the nonlinear systems thus obtained are suggested. The results of a simulation of the magnet system employed in the ALICE experiment (CERN, Geneva) are presented [12].

1.4. Application of the Mathematical Modeling in Low and Intermediate Energy Physics.

Using the model of a temperature peak as well as the measured radii of tracks in a high-temperature superconductor YBCO and its thermal characteristics, an effective electron - phonon relaxation time has been calculated for this material. It was in a good agreement with experimentally measured (by methods of laser technique) values of this magnitude. Thus, for the first time, a self-consistent description of the process of track formation in the high-temperature superconductor, not containing any matching parameters, has been constructed [13].

With the purpose of solving some modern problems of quantum computing and quantum data links, the opportunity of quantum teleportation of states of heavy substance was investigated using the JINR experimental installations. A new scheme and a protocol of quantum teleportation of heavy substance have been proposed [14].

The development of Monte-Carlo models and algorithms for description of interactions of hadrons with nuclei at intermediate and high energies has been in progress. A model of the hadronization processes based on analogy between the processes of transition of·quark – anti-quark pairs into observed mesons and generation of electromagnetic radiation in gas lasers has been constructed. The model allows one to take into account the effects of stimulating effects of the meson field on the sources generating it [15].

The curve smoothing is a fundamental problem of mathematics, statistics, and data analysis. A goal of the present-day computing technologies is the development of effective methods and algorithms of smoothing. A new approach to the local curve approximation and the smoothing is proposed. The relation between curve points is defined using a special cross-ratio weight function. The coordinates of three curve points are used as parameters for both the weight functions and the three-point cubic model (TPS). A very simple in computing and stable to random errors cubic smoother in an adaptation mode (LOCUS) is constructed. The free parameter of TPS is estimated independently of the fixed parameters by recursion with the effective error suppression and can be controlled by the cross-ratio parameters. The efficiency and the noise stability of the algorithm are confirmed by examples and by comparison with other known non-parametric smoothers [24].

Parameters of a subcritical cascade reactor driven by a proton accelerator and based on a primary lead-bismuth target, main reactor constructed analogously to the molten salt breeder (MSBR) reactor core and a booster-reactor analogous to the core of the BN-350 liquid metal cooled fast breeder reactor (LMFBR) have been estimated. It is shown by means of Monte-Carlo modeling that the reactor under study provides safe operation modes $(k_{eff} =0.94\text{-}0.98)$, is capable to transmute effectively radioactive nuclear waste and reduces by an order of magnitude the requirements on the accelerator beam current. Calcula-

tions show that the maximal neutron flux in the thermal zone is 10^{14} cm^2 s^{-1}, in the fast booster zone is $5.12*10^{15}$ cm^{2}s^{-1} at k_{eff} =0.98 and proton beam current I=2.1 mA [25].

2. Algorithmic and software support of theoretical investigations.
2.1. Open quantum systems and numerical functional integration method.

The problem of description of time evolution of open quantum systems (OQS), i.e. systems interacting with their environment, is interesting from both methodological and practical points of view. Such an approach is a natural framework for description of nonequilibrium irreversible processes accompanied by a dissipation of energy that finds use in various areas of quantum physics and chemistry. This approach is suitable for studying the evolution of the dinuclear system in the framework of the new model proposed in the Flerov Laboratory of Nuclear Reactions. The path integral approach appears to be a convenient tool for studying the open quantum systems. In the framework of this approach the representation of propagator for open quantum systems in the form of a double functional integral with respect to conditional Wiener measure is obtained. Numerical method which allows reducing the calculation of multiple Wiener integrals to calculation of usual (Riemann) integrals of low multiplicity can now be applied to studying the time evolution of open quantum systems. An iterative formula improving the results of numerical calculations for enlarged time intervals is derived. In collaboration with FLNR and BLTP the applicability of the obtained formula for propagator as well as efficiency of the approximation formula for its evaluation is examined on a problem of calculation of the density matrix of OQS in the dinuclear system model [17-18].

2.2. Computational molecular dynamics methods and software.

An optimized version of the DL_POLY molecular dynamics simulation code has been used to study the cluster–surface impact processes for metallic phases. The characteristics of the cluster–surface collisions were studied in a wide range of the cluster impact energies (Einc = 0.035–3.5 eV/atom). Modification of the surface, exposed to the cluster-beams, was studied by monitoring the molecular dynamics configurations of the system in real time. The density and temperature distributions in the system under the energetic irradiation has been investigated in detail. The three major channels of the impact yield (viz., soft landing, droplet spreading and implantation) were distinguished and estimated. Based on the density and temperature distributions data the low energy cluster–surface impact has been analyzed and a novel interpretation of droplet spreading process is given [20-23]. Fig.8 shows the top (left), side (middle) and cut (right) views of MD configurations at t = 1.3 ps (top), t = 2.1 ps (middle), and t = 5.0 ps (bottom) for the cluster incident energy Einc = 0.56 eV/atom.
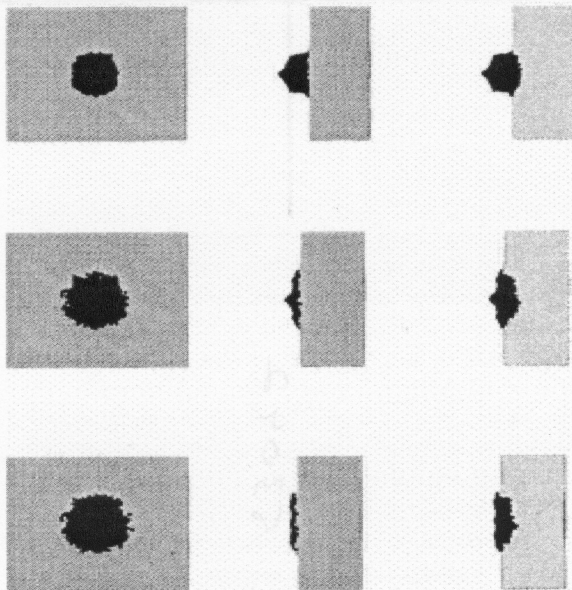
Figure 8.

2.3. Thermoelastic computational approach to beam-surface interaction modeling.

A method of numerical analysis of Stefan's problem for a metal sample exposed to a high-current pulse ion beam has been developed [16]. In supposition that the lateral areas of the sample are thermo-isolated, the dynamics of moving the interphase $\zeta=\zeta(t)$ separating the melted and firm parts of the sample was investigated. It has been found that the form of the source influences the form of the interphase $\zeta=\zeta(t)$. Therefore, choosing the characteristics of the source, one can control the evolution of the interphase $\zeta(t)$.

Fig.9 gives the graphs of time dependence of temperature of the metal surface $T(0, t)$ for three cases:
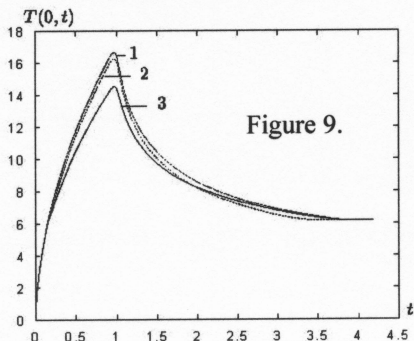

Figure 9.

1. $c_1 = c_2 = 456$ J/kgK (without taking into account the phase moves);

2. $c_1 = c_2 = 456$ J/kgK (taking into account the phase moves without changing heat capacity);

3. $c_1 > c_2$, $c_2 = 456$ J/kgK, $c_1 = 700$ J/kgK (phase moves with changing heat capacity).
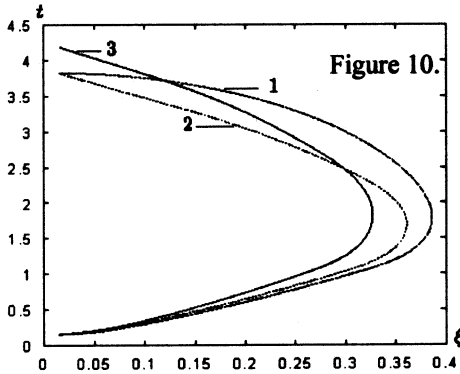
Figure 10.

Fig.10 gives the graphs of moving the phase boundary $\zeta=\zeta(t)$ (depth of penetration of the temperature equal to the melting point into the sample as a time function). Taking into account the change of the heat capacity leads to a diminution of the maximal value of temperature on the surface, and also to a diminution of the value of the melting depth of metal.

2.4. High level accuracy computational schemes for quantum systems investigations.

With the project Few-Body Physics the ^{4}He trimer system at ultra-low energies was investigated using a hard-core version of the Faddeev differential equations and realistic ^{4}He -^{4}He interactions. The binding energies of the Helium trimer and scattering observables were calculated. The mechanism of formation of the Efimov states of the ^{4}He trimer was also studied. It was shown that the Efimov levels arisen from virtual levels which were in turn formed (quasi)resonances settled on the real energy axis. The resonances including virtual levels are calculated [26-28].

An uncoupled correlated variational method for the calculation of helium isoelectronic bound states is proposed. New projective coordinates s = r1 + r2 ,v = r12/(r1 +r2),w = (r1 -r2)/r12 are introduced instead of the conventional ones s = r1 + r2 ,t = r1 - r2, u = r12. All matrix elements of the total Hamiltonian and the weight function are expressed as simple products of three one-dimensional integrals. The variational basis is formed by a set of Laguerre polynomials with a single nonlinear parameter and two sets of Jacobi polynomials for the projective coordinates s, v,w, respectively. It provides a reasonable rate of convergence of the energy, E = E(N), with respect to a number N of the basis components of the eigenvector. The proposed method yields the best available energies for the isoelectronic ground states of the helium atom. New estimations of the isotope helium ground states are also presented [29].

A Newtonian iteration scheme has been constructed in frames of research on computational physics for solving a scattering problem using the Schwinger variational functional. The scattering problem is formulated as an eigenvalue problem with respect to a pair of unknowns: a phase shift and a wave function. The efficiency of the proposed iteration scheme and its accuracy are

demonstrated on exact solvable problems of the elastic scattering problem with Morze and spherical potentials [30].

2.5. Numerical Calculations for Nuclear Models.

Numerical methods and software for applications in the nuclear theory were developed.

The problem of production and survival of the very long-lived isomeric state of ^{180}Ta nuclide is a real challenge for a theory of nucleosynthesis. Numerical calculations are performed within the Quasiparticle-Phonon Nuclear Model (QPNM) using the formalism developed in works of V.G.Soloviev. The calculations performed show that a decisive role is played by the collective (i.e. strong) E2 transitions from the intermediate states $|IS\rangle \otimes |E1_i\rangle$ to some states of the $|g.s.\rangle \otimes |vib\rangle$ type in the range from 2.7 to 4.0 MeV. These high-intensive K-allowed two-step γ-transitions are responsible for the strong de-excitation of ^{180}Ta^m in the (γ, γ') reaction [31].

The quasiparticle-phonon nuclear model (QPNM) was adopted to compute the M1 strength distribution in the energy range $4 \div 10$ MeV in the deformed ^{154}Sm, where two distinct wide peaks are visible at ~ 6 MeV and ~ 8 MeV respectively. This peculiar structure has captured the interest of theorists, as testified by many calculations which followed the experimental discovery. It was shown that the coupling with two-phonon configurations enhances considerably the fragmentation of the M1 strength with respect to the random-phase approximation (RPA). The resulting QPNM spectrum has a two-hump profile with much broader humps with respect to RPA and in close agreement with the experimental data. The results obtained contribute also to shed light on the controversial properties of the M1 spectrum in this energy range [32].

The spiral magneto-electron waves in the gas-dust interstellar medium (ISM) were investigated. The electrons, both relativistic and thermal, are ones of the most abundant and mobile charged components of ISM, and their small mass provides the most strong coupling with intercloud magnetic fields. Therefore it is natural to expect that the collective behavior of electrons may essentially affect the interstellar gasdynamics. An idealized model is considered of the gaseous magnetically supported cloud whose gasdynamics is dominated by thermal electrons in the regime of strong coupling between the densities of the electron current and the magnetic flux threading the cloud; the mobility of ions and neutral molecules is regarded to be heavily suppressed. It is shown that the cyclotron waves are heavily damped in the interstellar medium and, therefore, cannot affect the gasdynamics of star-forming molecular clouds. Based on the equation of electromagnetic induction for the magnetic flux density driven by Hall and Ohmic components of electric field generated by flows of thermal electrons an analytic model of helicoidal magneto-electron waves is developed. It was found that the helicons can propagate in the interstellar medium without noticeable attenuation. The presented numerical estimates for the group velocity of inter-

cloud helicons suggest that this kind of spiral circularly polarized magneto-electron waves can be responsible for the broadening of molecular lines detected from dark interstellar clouds [57-58].

2.6. Computer Algebra

To solve systems of nonlinear algebraic equations in many variables, these systems should to be transformed into a canonical form. One of such canonical forms is an involutive basis which is a Groebner basis of some special structure. Janet bases together with Pommaret bases are currently most important types of involutive bases. While Pommaret bases are more convenient for many theoretical questions faces the problem of δ-regularity of differential systems, i.e. in certain coordinate systems no finite Pommaret basis exists. It has been shown that Pommaret whenever it is finite is also a minimal Janet basis. As checking whether a Janet basis is also a Pommaret basis requires only some trivial computations, this allows for an efficient construction of Pommaret bases without bothering about termination issues.

The original highly efficient algorithms for computation of Janet bases were designed and implemented in Reduce, C and C++.

These algorithms exploit a very useful data structure called Janet tree for representing the multiplicative variables with respect to the Janet division of a given monomial set. Based on this data structure the completion to involution of both monomial and polynomial sets can be performed extremely fast. The search for an involutive divisor becomes now even faster than with the classical binary search in a sorted array. The new algorithms admit the further optimization. Extensive benchmarking was performed in comparison with the special purpose computer algebra system SINGULAR. This is a system dedicated to polynomial computations and is considered as very fast for Groebner basis computations. In most examples, the implementations of the new algorithms turned out to be faster.

Moreover, the new algorithms unlike classical Buchberger algorithm for computation Groebner bases admit effective parallelization what was explicitly demonstrated on a two-processor Pentium based computer. Modelling multi-processor computations on this machine reveals a behaviour of the computing time which is close to inversely proportional with respect to the number of processors.

General involutive algorithms for polynomial as well as linear systems of partial differential equations were also implemented in Mathematica [33-38].

Numerical integration of the complicated dynamical systems is suffered by drifting of the integral of motion and possible constraints from their initial values. This problem has been attacked by many authors. However, up to now a general solution of it has not been found. An approach based on the optimal control theory is proposed. A point of the phase space of the dynamical system (derived by numerical simulation) is piloted by an additional control gradient

term in the equations. In result this point has a component of the velocity towards the surface fixed by initial values of the integral of motion and possible constraints. Numerous numerical experiments show advantages of the stabilization properties of the control method in compare with the well known Dirac's Hamiltonian dynamics for the constrained systems [39].

In the 90s, very fundamental experimental results were derived in cosmology: a spectrum of the cosmic background radiation was measured and acceleration of the Universe expansion was established. There are many theoretical questions following from new experimental facts and they need sophisticated computer simulations. A version of the cosmological quantum-field model in the case of conformably flat space-time is formulated. The main goal is to explain the expansion of the Universe as quantum gravitational effect like a phase transition. In the future it is planned to do numerical simulations of the derived model using the stabilization method developed at the previous stage [40-41].

Computation of Cohomologies for Lie Algebras and Superalgebras Explicit computation of Lie (super)algebra cohomologies is of great importance for studying modern models of theoretical and mathematical physics. A new algorithm has been designed. The new algorithm splits cochain complexes containing spaces of very high dimension into a smaller one. In many applications this strategy leads to significantly faster computations. The algorithm has been implemented in C and applied to some concrete examples of physical interest. This approach can also be applied to explicitly determine the Spencer cohomology of Z-graded Lie (super)algebras [42-43].

International cooperation

In accordance with the Agreement between JINR and the Research Centre Rossendorf, Germany, about a cooperation in the field of application and development of computing systems, LIT specialists took part in the realization of the project "Zentrale Nutzerdatenbank" for administration of the computer complex FZR with the use of WWW technology. Work on creation of the automated system of administrating the computer complex with application of WWW technology was carried out. A number of the Java-programs is developed. An opportunity was investigated of using software on base of LDAP (Lightweight Directory Access Protocol) for automated remote administrating of personal computers with different operational systems (W2000 and LINUX) .

In cooperation with DESY (Zeuthen), joint work on the development and creation of applied and system software for high-performance multiprocessor computing complex APEMille and development and creation of apeNEXT was performed. Debugging and testing of both software and hardware for APEmille were performed. A simulation on the preliminary VHDL model of apeNEXT was done. A prototype version of a C compiler, including a first interface to the TAO front-end was developed. Testing with the functional simulator of the apeNEXT architecture running on Linux PCs was performed.

Joint work is carried out in cooperation with CERN IT Division in frames of the CERN-Intas project on the creation of a system "Correlation Engine". The purpose of the system is a timely detection of anomalous states on PC-farm's nodes and failure prevention. A first prototype of the correlation system has been designed in the language Perl and statistics is being accumulated. In parallel, the possibilities of the prototype are being extended.

In cooperation with CERN and Brookhaven National Laboratory the following work has been carried out [46-48]:

1. Development in cooperation with CERN of the object-oriented program environment (framework ROOT) for solving a wide class of scientific problems using workstations and PC (http://root.cern.ch)

2. Elaboration, development and realization of an informational model of processors for acquisition, reconstruction and physical analysis of data for large experiments.

3. Introductions of modern object-oriented technologies for experiment STAR.

4. Development of an object-oriented input/output system for ATLAS experiment

Due to these works, the possibilities of the system of C++ classes for a description of complex hierarchically organized OO models of reconstruction and analysis of complex events for HEP have been essentially extended (http://www-root.fnal.gov/root2001/). The possibilities of the subsystem of 3D graphics of the ROOT package have been extended, too. The results were presented at the international workshop (http://www.atsweb.neu.edu/hepvis01/) and at the international conference (http://www.ihep.ac.cn/~chep01/ and http://www.ihep.ac.cn/~chep01/paper/3-034.pdf

The investigation on common DFG/GSI/JINR project "Non equilibrium strongly dense matter in nucleus-nucleus collisions" was in progress. The aim of the project is to further develop transport schemes including off-shell effects, in particular, such as finite particle widths, and possible phase transitions in dense matter and implement these schemes into various dynamical models, i.e., to study evolution of resonance matter and dynamics of phase transitions.

Charmonium dissociation in a hot meson gas was investigated in collaboration with Rostock University (Rostock, Germany). The results are applied to heavy-ion collisions within a modified Glauber model scenario and the phenomenon of anomalous J/ψ suppression is addressed [44-45]. Results are applied to the case of Pb-Pb collisions at CERN.

Active collaboration was continued with Germany in the field of computer Algebra. With Tech. Univ. (RWTH), Aachen, two *Maple* packages called Involutive and Janet implementing original algorithms designed in LIT for transformation (completion) of systems of nonlinear algebraic equations and linear systems of PDEs, respectively, into the canonical involutive form have been developed.

With Univ. Greifswald, a *Mathematica* tool Invo for completion of nonlinear algebraic and linear differential systems to involution was created. This software tool allows a user to experiment with various involutive divisions generating different algorithmic procedures for the completion [38].

The development of a *Mathematica* facilities for finding closed form solutions of differential equations was carried out in cooperation with Univ. Appl. Sci. (FH) Ravensburg-Weingarten.

The effective cooperation with the International Salvay Institute of Physics and Chemistry (Brussels, Belgium) progressed in 2001 on the basis of developed computational tools and methods based on artificial neural networks, cellular automata. A nonlinear time series analysis was applied to the traffic measurements, obtained at the input of a medium size local area network. In order to reconstruct the underlying dynamical system, the correlation length τ and the embedding dimension d_E of the traffic time series were estimated. In order to extract the regular part from traffic data, the high-frequency, "noisy" part was filtered out. The reliable values of τ and d_E permitted to apply a layered neural network for the identification and reconstruction of the underlying dynamical system [53].

Applied research.

A graphic version of the program Progress++ for calculation and optimization of city electric supply lines has been put into operation. The program works at IBM PC under Windows environment. At present, it is exploited at all 35 electric power supply enterprises of Moscow region as well as at some plants of other regions of Russia. The program is an effective tool for power loss analysis. Following the directions of the program allows one to minimize energy loss from 8-10% down to 5-8%. The program can create and screen schemes of various complexity. It also can determine the network graph connectivity index and detect cycles in the scheme. The solving of the system of N Kirchhoff equations is performed during the time of the order N of operations. A certificate has been received from the Ministry of Energy, registration No.001.

A number of investigations in cooperation with the International Salvay Institute of Physics and Chemistry (Brussels, Belgium) in the field of applied research were performed in 2001:

- The review devoted to the computational methods and tools for modeling and analysis of various complex processes in physics, medicine, social dynamics and nature. There are considered: 1) the multivariate data analysis based on Ω_n^k-criteria and artificial neural networks (ANN), 2) the applications of neural networks for the function approximation and for the reconstruction and prediction of chaotic time series, and 3) the use of cellular automata (CA) in pattern recognition and in modeling of complex dynamical systems [49].
- The ability of artificial neural networks to reconstruct discrete chaotic

maps with singular points was investigated. As a simple test model, the Cusp map was used. The traditional Multilayer Perceptron, the Chebyshev Neural Network, and the Wavelet Neural Network were compared. The numerical scheme for the accurate determination of a singular points is also developed. It has been shown that combining a neural network with the numerical algorithm for the determination of the singular points one can accurately approximate the discrete chaotic maps with singularities [50].

- A new approach to the problem of efficient resources distribution in different types of economic systems was proposed. The usage of the entropy as an indicator of the efficiency of resources distribution was also proposed. This approach is based on the methods of statistical physics in which the states of economic systems are described in terms of the density functions $p(g,\alpha)$ of the variable g parameterized by α. The parameter α plays a role of the integral characteristic of the state of the economic system. Having the density function $p(g,\alpha)$, one can use the corresponding entropy to evaluate the efficiency of the resources distribution. The theoretical study has been tested on real related to the portfolio investment [51].

- The using of the elastic neural nets (ENN) to find the initial estimation in automated procedures of locating seismic events was proposed. The advantages of ENN are the simplicity of the algorithm, the fast convergence and the high efficiency. The results were shown on simulated seismic events [52].

Collaboration with Belarus

Some investigations in LIT are conducted in collaboration with researchers from the Republic of Belarus, particularly, from the Institute of Mathematics (IM) of the National Academy of Sciences of Belarus in Minsk. This collaboration is realized in the form of common research, exchange of results and new ideas, and mutual visits of scientists in the framework of the topical plans for research at LIT and IM.

The main direction of the joint research is the development of theory, creation of numerical methods for integration in the topological and metric spaces and its applications in the problems of theoretical physics. There is a strong background in these areas both in LIT and in IM which forms a basis for collaboration. The investigations in the field of measure theory are traditionally performed in IM, the development of numerical methods and algorithms is usually done in both institutes and the creation of computer codes and practical application of the methods is carried out at LIT.

The results obtained within the collaboration include creation of numerical methods and approximations for functional integrals with respect to a

measure of the Gaussian type in complete separable metric spaces and their application to the Feynman path integrals of quantum physics.

The functional integral method is applied to the study of Markovian open systems for research in the evolution of the dinuclear system in the framework of the new model proposed in the Flerov Laboratory of Nuclear Reactions, JINR. The considered model takes into account the competition between complete fusion and quasi-fission processes in the nuclei collisions and enables one to calculate the probability of the compound nucleus formation after the capture stage. It is important for planning and carrying out experiments on super heavy element synthesis at JINR as well as at GSI (Germany) and GANIL (France).

The mutual activity of LIT and Republic Belarus in computer algebra over the last 5 years has covered both common research and conferences organization. The number of conferences in Belarus were organized with the help of the computer algebra team of LIT: the first in the Belarus history International conference "Computer Algebra in Fundamental and Applied Research and Education" (CAS-97), December 8-11, 1997 in Minsk; the second CAS conference "CAS-99" was also held in Minsk, September 23-25, 1999; on September 19-22, 2000, another international conference on computer algebra "Differential Equations and Computer Algebra Systems" was organized in the city of Brest. This year the docent of Brest State Technical University, A.N.Prokopenya, took active part in the 5th International workshop on computer algebra in physical research. Together with the head of computer algebra team of LIT they agreed to coorganize a special session at ACA'02, the "8th International conference on application of computer algebra" which is to be held in Volos, Greece, June 25-28, 2002. The title of their joint session that have been included in the ACA'02 schedule is "Mathematical physics and control theory" and a number of prominent scientist working in this research area expressed their wish to give talks at this session coorganized by specialist from LIT JINR and Belarus.

The cooperation of LIT with the Institute of Radiation Physics and Chemistry Problems (IRP&CP), National Academy of Sciences of Belarus in Minsk was active, too.

A method is elaborated of constructing a time-dependent periodic Hamiltonian for which a system of Schroedinger equations admits analytic solutions. Time-independent soluble problems are transformed into time-dependent ones by a set of unitary time-dependent transformations and a proper choice of initial states. As an application of the method, the expectation value of Hamiltonian, total, dynamical, and geometric phases are derived in terms of the obtained solutions [54].

Darboux transformations and a factorization procedure for a system of coupled finite-difference Schroedinger equations are presented. The conformity between Darboux transformations and the factorization method is established. Factorization chains and consequences of Darboux transformations are obtained for a system of coupled discrete Schroedinger equations. The approach suggested

permits construction of new series of potential matrices with the known spectral characteristics for which the coupled channel discrete Schroedinger equations have exact solutions [55].

During the last few years, interesting and fruitful collaboration with IRP&CP has lain in the field of investigations on computer simulation and calculations concerning the Project on sub-critical assembly with MOX fuel for research on nuclear waste transmutation. One of the last common published paper [56] deals with theoretical investigation of transmutation rates for a number of long-lived fission products and minor actinides as well as with neutron spectra formed in the sub-critical assembly driven with the following monodirectional beams: (i) 660 meV protons; (ii) 14 MeV neutrons. The main objective is the comparison of neutron spectrum in the MOX assembly for different external driving sources.

In the next year, 2002, the 5th International Congress on Mathematical Modeling, will be held at the Laboratory of Information. The main co-organizer of the Congress is the Council on Mathematical Modeling of the Russian Academy of Sciences.

The goal of the Congress is to discuss modern problems of computer simulation so important in the 21st century. The Congress is one of the traditional conferences covering a wide range of mathematical modeling topics. The scientific program of the Congress includes the following topics:

- Mathematical modeling with high-performance computing systems.
- Mathematical models and software support in computational physics.
- Mathematical models of transfer and evolution in nonlinear and information-active systems.
- Mathematical modeling of processes in micro- and nanoelectronics.
- Mathematical models of computer optics.
- Mathematical modeling of composite materials properties.
- Mathematical simulation of processes in the mechanics of deformed matter.
- Mathematical simulation of turbulent processes.
- Mathematical modeling of processes in transitional and boundary layers.
- Mathematical models of nonlinear dynamics and synergetics.
- Mathematical and computer models of intellectual systems.
- Mathematical models in economics and sociology.
- Mathematical models of chemical and ecological systems.
- Mathematical modeling of bio- and macromolecular systems.

Plans for the next years

Futher external telecommunication links development consists of
- Step-by-step increasing of JINR-Moscow telecommunication link throughput up to 155 Mbps on the basis of agreement between JINR, RSCC and RbNet during year 2002-2003 and up to 1Gbps in future using the JINR, RSCC and RbNet Memorandum on cooperation;
- Step-by-step increasing of the external telecommunication link capacity and throughput for JINR within the programme "Creation of the National Computer Telecommunications Network for Science and High School" and the FastNet project;
- Creation of dedicated specialized data links to various scientific organizations (CERN, FNAL, BNL and etc.)
- Development of a prioritization scheme to manage the external traffic using the priorities of experiments
- Participation in the creation of corporative networks for Russian institutions for nuclear physics with a high speed channel to CERN for the Russian regional centre for LHC computing

JINR Local Area Network Backbone Modernization
- Adopt a Project on creation a new JINR Backbone in 2002 from proposed by dealers the basis of discussions performed and provide its financing and realization.
- Provide in 2002 an additional optical cable link between LIT and SCC2; make T-type connection to reach LHE-site to install a hot reserve line JINR-SCC2.
- Perform the necessary measures to increase the level of security for the JINR network. Firewall cluster of 3-5 Intel PC with special "firewall" software will make check all of the traffic.
- Creation of the mail cluster to check up all incoming and outgoing mail traffic for the presence of the "bad" content or attachments.
- Develop Web hosting - the project assumes to make a centralized WWW resource in JINR.

Development of computing infrastructure
- Create a cluster of 5 Intel PCs under Linux operating system as a replacement for a cluster of old Convex computers.
- Creating specialized clusters using advanced technologies to solve complex computational problems (for example, molecular dynamics).
- Creation of a centre for data storage and data processing on the basis of mass storage memory, PC farms, and clusters.

- Development of the architecture for the new specialized high performance computer apeNEXT, its basic software for the systems of parallel computations in cooperation with INFN (Italy) and DEZY (Germany).
- Adaptation and maintenance of the appropriate programming and informational software to provide the functioning of the GRID segment at JINR in frames of participation in EU DATAGrid project and creation of the Russian Grid segment. Development of the special Grid Software for Grid -monitoring and data management.
- Information, algorithmic and software support of JINR and its Member States research programmes; maintenance and development of libraries (CERNLIB, NAG, CPC, DUBNA) and special programs GEANT4, ROOT, LHC++ for all computing platforms.

Computer physics for experimental and theoretical research
- Creation of a program library of fast monitoring of signals on the basis of the wavelets of the second generation.
- Creation of systems for experimental data processing in particle physics.
- Creation of methods and numerical algorithms for magnetic fields calculation and particle beams transport.
- Creation of numerical methods and software for mathematical simulation of complex physics systems.
- Mathematical simulation of thermal and diffusion processes of interacting accelerated ions with materials. Adaptation for simulation of the complex U400M + DECRIS-14 and U-400 + ECR4M.
- Simulation by the methods of molecular dynamics of thermoelastic processes arising in metals exposed to high-energy ions.
- Development of methods, algorithms and software of computer algebra. Introduction and maintenance of modern systems of analytical calculations for physics problems.

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