

#### JOINT INSTITUTE FOR NUCLEAR RESEARCH

2003-229

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# LABORATORY OF INFORMATION TECHNOLOGIES REPORT ON RESEARCH ACTIVITIES IN 2003

Report to the 95th Session of the JINR Scientific Council January 15–16, 2004

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# LABORATORY OF INFORMATION TECHNOLOGIES REPORT ON RESEARCH ACTIVITIES IN 2003

Report to the 95th Session of the JINR Scientific Council January 15–16, 2004 The main task of the Laboratory of Information Technologies consists in provision with modern telecommunication, network and information resources of theoretical and experimental studies conducted by the JINR Member State institutes at JINR and other scientific centers.

Information, computer and network support of the JINR's activity in year 2003 comprises:

- Provision of JINR and its Member States with high-speed telecommunication data links.
- Creation of a high-speed, reliable and protected local area network (LAN) of JINR.
- Creation and maintenance of the distributed high-performance computing infrastructure and mass storage resources.
- Provision of information, algorithmic and software support of the JINR research-and-production activity.
- Elaboration of the JINR Grid-segment and its inclusion in European and global Grid-structures.

In 2003, the scientific programme of the LIT covered three first-priority topics of the "Topical Plan for JINR Research and International Cooperation in 2003". The Laboratory staff participated in 13 more topics of the Topical Plan in collaboration with other JINR Laboratories on the project level and in 17 topics on the level of cooperation. The main aim of the Laboratory is the performance of work on the "Information, Computer, and Network Support of the JINR's Activity" (topic 09-6-1048-2003/2007, headed by V.V.Ivanov, and V.V.Korenkov) and in the field of the "Computer Physics for Theoretical and Experimental Research" (topic 09-6-1041-2002/2004, headed by I.V.Puzynin and A.Polanski). 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 2003, 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. Seven projects are devoted to the creation and development of informational, computing and telecommunication resources for performing fun-

damental research, and the other five are initiative scientific projects.

In the year 2003, LIT participated in organizing two conferences: on July 29 – August 2, Focus Symposium "Quantum Physics and Communication", and the XIX International Symposium on Nuclear Electronics & Computing "NEC' 2003", Varna, Bulgaria, September 15 – 20.

Second "Information bulletin of LIT" (JINR publication, 4-8160, Dubna, 2003, http://lit.jinr.ru/Inf\_Bul\_2/) was published and contains information for users of the JINR networking, computing and information resources.

#### External telecommunication systems

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

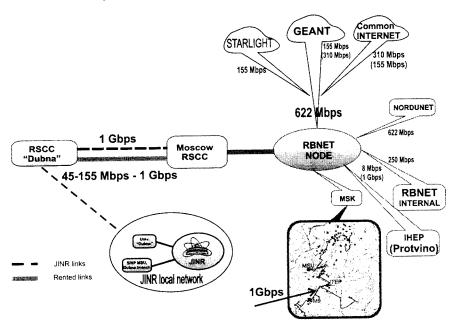


Figure 1: Current state of external communications in Russia used by JINR

Figure 2 shows the incoming and outgoing JINR traffic in 2003. Total eleven month incoming traffic was 18.55 TB (9.73 TB in 2002) and outgoing traffic was 21.8 TB (1.92 TB in 2002).

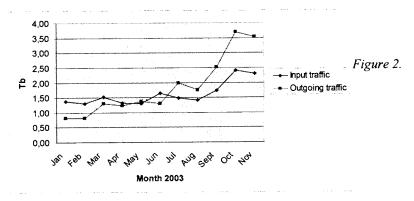


Table below shows an eleven month traffic distribution among

the JINR divisions (>300 GB on incoming traffic).

| JINR<br>laboratories | Incoming<br>(IN) | Outgoing<br>(OUT) | % (IN)  | % ( OUT) |  |
|----------------------|------------------|-------------------|---------|----------|--|
|                      | 3.31 TB          | 6.97 TB           | 17.85 % | 31.97 %  |  |
| LIT                  |                  |                   |         |          |  |
| DLNP                 | 2.62 TB          | 4.04 TB           | 14.12 % | 18.54 %  |  |
| Proxy+servers        | 2.54 TB          | 1.71 TB           | 13.67 % | 7.85 %   |  |
| FLNR                 | 2.13 TB          | 1.22 TB           | 11.48 % | 5.6 %    |  |
| LPP                  | 1.95 TB          | 770.53 GB         | 10.52 % | 3.45 %   |  |
| VBLHE                | 1.55 TB          | 2.69 TB           | 8.36 %  | 12.32 %  |  |
| BLTP                 | 1.56 TB          | 1.06 GB           | 8.4 %   | 4.88 %   |  |
| Uni-Dubna            | 998.2 GB         | 459.8 GB          | 5.25 %  | 2.06 %   |  |
| FLNP                 | 836.16 GB        | 1.59 TB           | 4.4 %   | 7.28 %   |  |
| Adm.                 | 368.14 GB        | 701.03 GB         | 1.94 %  | 3.14 %   |  |

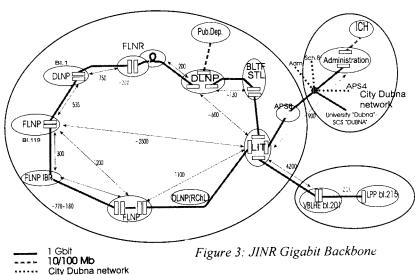
Systematic work on the LAN management was performed by the Network Operation Centre ( http://noc.jinr.ru/). Up-to-date statistics can be found at http://noc.jinr.ru/inform/inf\_main\_stat.shtml.

#### JINR Local Area Network (LAN)

At present IP addresses database contains 4506 registered JINR LAN elements (4053 in year 2002).

As it was outlined in the JINR Topical Plan for the year of 2003, one of the main tasks to develop the information, computing and telecommunication structure in JINR was "Implementation of the first stage of a selected variant of the JINR Backbone on the basis of Gigabit Ethernet".

The core of the JINR LAN Gigabit Ethernet backbone is Cisco Catalyst 6509 switch with newly installed Gigabit Interface Card (8 ports). There are Cisco Catalyst 3550 switches to be installed in 7 JINR Laboratories and the Administrative division. All these pieces of gigabit equipment are interconnected by a new cable structure (10 300 meters), based on 16-wired single-mode optical cables (Fig. 3). To defend the perimeter of the JINR LAN, two Cisco firewall devices PIX-525 (one is in active, and another is in a failover mode) were installed.



Thus, in 2003 created was the network transport environment of the new generation: the Gigabit Ethernet backbone with the presented by Cisco Catalyst high technology 6509 switch, as the main switch in LIT and Cisco Catalyst 3550 switches in the JINR Laboratories and the Administrative division. The network switching and routing will be done in the same programming environment by means of the Cisco IOS 12.3 operating system.

A nonlinear analysis has been applied to the traffic measurements obtained at the input of a medium size local area network. The reliable

values of the time lag and embedding dimension provided the application of a layered neural network for identification and reconstruction of the underlying dynamical system. The trained neural network reproduced the statistical distribution of real data, which well fits the log-normal form. The detailed analysis of traffic measurements has shown that the reason of this distribution may be a simple aggregation of real data. The Principal Components Analysis of traffic series demonstrated that a few first components already form the fundamental part of network traffic, while the residual components play a role of small irregular variations that can be interpreted as a stochastic noise. This result has been confirmed by application of the wavelet filtering and Fourier analysis to both the original traffic measurements and individual principal components of original and filtered data. The log-normal distribution of traffic measurements and a multiplicative character of traffic series confirmed the applicability of the scheme, developed by A.Kolmogorov for the homogeneous fragmentation of grains, also to the network traffic.

P.Akritas, P.G.Akishin, I.Antoniou, A.Yu.Bonushkina, I.Drossinos, V.V.Ivanov, Yu.L.Kalinovsky, V.V.Korenkov and P.V.Zrelov. Chaos, Solitons & Fractals, 17 (2003) 305-309. I.Antoniou, V.V.Ivanov, Valery V.Ivanov and P.V.Zrelov. In: Proc. Int. Conf. Mathematics and Informatics for Industry, MII 2003, 14-16 April 2003, Thessaloniki, Greece, pp.170-181. I.Antoniou, V.V.Ivanov, Valery V.Ivanov and P.V.Zrelov. Nucl. Instr.& Meth. in Phys. Res. A 502 (2003) 768-771. I.Antoniou, V.V.Ivanov, Valery V.Ivanov and P.V.Zrelov. Physica A 324 (2003) 733-753.

## <u>Distributed informational systems, JINR Central Computing and Informational Center</u>

More than 300 staff members of JINR and other research centres are using the JINR Central Computing and Informational Center (JINR-CCIC). The JINR CCIC users distributed by JINR divisions are tabulated:

| LIT | DLNP | LPP | VBLHE | FLNR | BLTP | Other<br>Institutes | FLNP | Adm. |
|-----|------|-----|-------|------|------|---------------------|------|------|
| 136 | 88   | 45  | 38    | 24   | 13   | 13                  | 12   | 4    |

The JINR-CCIC is part of the Russian Information Computing Complex for processing information from the Large Hadron Collider. It comprises:

- An interactive cluster of common access;
- A computing farm for carrying out simulation and data processing for large experiments;
- A computing farm for the tasks of the LHC project;
- A computing farm for carrying out parallel calculations on the basis of modern network technologies (MYRINET, SCI, etc.);
- Mass storage resources on disk RAID-arrays and tape robots.

Total CCIC PC-farms performance is: CPU 4.3 kSPI95, disk space 7.7 TB and ATL tapes 16.8 TB. The eleven month (of year 2003) total CPU time used was 4 605 688.37 hours, average loading was 37.14%. In October 2003 the loading was 60.98%.

JINR CCIC facilities were used by experiments E391A (KEK), KLOD, COMPASS, DO, DIRAC, HARP, CMS, ALICE for mass event modelling, data simulation and analysis.

For experiments ALICE, ATLAS and CMS, sessions of the mass modelling of physical events have been conducted this year in frames of the JINR's participation in DC04 (Data Challenge 2004).

The table below shows the percentage of CPU time using by JINR Laboratories on CICC PC farms.

| LIT  | FLNR | DLNP  | LPP  | FLNP | BLTP  | VBLHE | Prod.run | Others |
|------|------|-------|------|------|-------|-------|----------|--------|
| 5.72 | 1.94 | 14.71 | 8.83 | 8.18 | 23.48 | 3.49  | 29.56    | 4.09   |

### Computing service and creation of a Grid-segment of JINR

In 2003, LIT actively worked on using the Grid technologies for experimental data processing. At present, the scientific community begins intensive use of the Grid concept that guesses creation of an infrastructure providing the global integration of information and computing resources. JINR has a possibility of a full-scale involvement in this process. The progress reached in the field of organizing distributed computing, as well as the experience gained in the participation in the international Grid projects, in particular, in high-energy physics, will allow successful development of this direction. The LHC project that is unique on scales of obtained data and from the viewpoint of computer technologies, provides

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

V.Ilyin, V.Korenkov, A. Soldatov. Open Systems, No.1, 2003, pp.56-66.

In the autumn of 2003, a first variant of the global infrastructure was working for actual tasks of a full-scale simulation of experiments. Work was under way to create a system of the global monitoring of the resources of the large scale Russian virtual organization, including LAN segments of several institutes (SINP MSU, JINR, ITEP, IHEP, IAM RAS) in accordance with Grid architecture.

The main activities were:

- Adaptation and support of new versions of ANAPHE (former LHC++) Library for Linux, Windows and Sun Solaris platforms.
- Support of the existing software for LHC (ATLAS, ALICE and CMS) and non-LHC experiments.
- Participation in Pre-Challenge data production for ALICE, ATLAS, CMS and LHCb.
- Measurements of Globus Toolkit 3 (GT3) performance under heavy load and concurrency.
- Development of the software for the organization stress testing of Data Management.
- AliEn server installation for distributed data processing of ALICE in Russia.
- Elaboration of LCG portal at JINR for Russia (http://lcg.jinr.ru).
- Installation and a testing of Castor at JINR CCIC.

During the year 2003 JINR has participated in the CMS Pre-Challenge production (PCP03). 250K events have been already simulated in frames of the CMSIM v.133 package. A volume of data produced was 320 GB. The further processing with the usage of ORCA (vers.7\_5\_0) will result in creation of a data base with a size about 600 GB. A new Grid tool, Storage Resource Broker (SRB), was used for the CMS production. SRB client installed at JINR provides a direct access to CMS common data bases at SRB server at Great Britain (Bristol) and gives new opportunities for storage and exchange of data inside the CMS collaboration.

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

V.Pose, B.Panzer-Steindel. NIM A502 (2003) 478-480.

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

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

The protocol between CERN, Russia and JINR on participation in the LCG Project was approved in 2003. The tasks in the LCG are:

- •Testing Grid middleware (component test, Grid functionality testing);
- •Common solutions for event generators (events database, repository of generators);
- •Grid technology evaluation (Globus toolkit-3.0, other industrial Grid software).

The Russian memorandum on creation of a Grid type computing infrastructure on distributed processing of huge data volumes in Russia was signed in September, 2003 by the Directors of the eight institutes: IHEP - Institute of High Energy Physics (Protvino),

IMPB RAS - Institute of Mathematical Problems in Biology (Pushchino).

ITEP - Institute of Theoretical and Experimental Physics (Moscow),

JINR - Joint Institute for Nuclear Physics,

KIAM RAS - Keldysh Institute of Applied Mathematics,

PNPI - Petersburg Nuclear Physics Institute (Gatchina),

RRC KI - Russian Research Center "Kurchatov Institute",

SINP-MSU - Skobeltsyn Institute of Nuclear Physics (MSU).

This consortium RDIG (Russian Data Intensive Grid) was made up as a national federation to participate in the EGEE (Enabling Grids for E-science in Europe) project which will start in year 2004.

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

#### DATABASE and WWW SERVICE

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

- System for accounting and statistics of operating the JINR basic facilities (<a href="http://iis.jinr.ru/basic-fac/">http://iis.jinr.ru/basic-fac/</a>).
- Digitizing of graphics at users' requests, preparation of bibliographic data on HEP for the PPDS database (http://www.jinr.dubna.su/~diginfo/). More than 40 papers were coded and included into the PPDS database. The work was carried out in cooperation with IHEP, BNL and other physics centers. 235 graphics have been digitized at the requests of JINR and foreign physicists.
- Information system «JINR Topical Plan for Research» (<a href="http://iis.jinr.ru/tp/">http://iis.jinr.ru/tp/</a>).
- <a href="http://lcg.jinr.ru">http://lcg.jinr.ru</a> Webportal for the project «LHC Computing Grid Project at Russia».
- <a href="http://Grid.jinr.ru">http://Grid.jinr.ru</a> Informational web site about Grid activites in JINR.
- http://Lcg.jinr.ru/egee RDIG-EGEE web portal prototype.
- (<u>http://lib.jinr.ru/dmitry/uni/rus/simple.html</u>) electronic catalog from the year 2000<sup>th</sup> at JINR Library.
- <a href="http://lib.jinr.ru/maillist/newslistru.html">http://lib.jinr.ru/maillist/newslistru.html</a> online sending lists on preprints, JINR communications, etc. at JINR Library.

Work was in progress at LIT on the development of WWW-tools on the main information servers as part of the JINR Central Computing and Information Complex (CCIC): <a href="www.jinr.ru">www.jinr.ru</a> and <a href="lit.jinr.ru">lit.jinr.ru</a>. The following main results of the work should be noted:

- Allocation and support in the "Web-hosting" mode of information sites of a number of JINR's subdivisions and external organizations.
- Introduction and support jointly with the service of JINR's Chief Engineer of the information system on the Basic Facilities of JINR (Nuclotron, U-400, U-400M, IBR-2, Phasotron, Project IREN) with the description of the general performances of each facility and the dynamic mapping of the state of their service capability in accordance with the scheduled plan of their operation.
- Mapping a current state of both technical and software support of JINR's CCIC and its communication facilities (together with the main services of the Complex and JINR's NOC).

Steady support of one of the main general-purpose FTP-servers was provided: <u>faxe.jinr.ru</u>. This server also was utilized for support and load on call of anti-virus programs into JINR's PCs.

The employees of the LIT fulfilled necessary work for the JINR's STD AMS on the software and centralized maintenance of administrative databases, including:

- modernization of the interface and contents of the database "JINR Staff",
- creation and modifications of the software complex on registration of currency bank in the environment of the common 1C system for the JINR's Accounting Department,
- creation of the journal for accounts' registration in the 1C environment and document "Rendering services for Chief Power Engineer Department".

Work was in progress on the development and maintenance (Section <a href="http://dbserv.jinr.ru/js/">http://dbserv.jinr.ru/js/</a> of the <a href="http://dbserv.jinr.ru/js/">dbserv.jinr.ru</a> server) of the archive of documentation and software related to the advanced technologies of "interlayer" (middleware). Computer programs were designed in the Java

language for automation of unrolling the client and server applications on the mentioned technology.

#### Computational Physics

The main tasks of the Computational Physics are:

- Development of methods for modeling physical processes and experimental data analysis.
- Creation of methods and numerical algorithms for modeling magnetic systems and transportation of charged particle beams.
- Elaboration of software and computer complexes for experimental data processing; their application in JINR experiments.
- Elaboration of numerical schemes and software for complex physical systems simulation.
- Development of methods, algorithms and software of computer algebra.

In 2003, more than 60 scientific publications, reports at conferences and JINR preprints were published and presented.

## Development of methods for modeling physical processes and experimental data analysis

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

A.Soloviev, E.Litvinenko, G.Ososkov, A.Islamov and A.Kuklin. NIM A 502(2003) 500-502.

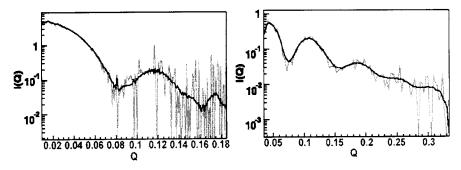


Figure 4: Smoothing window results (black) over "raw" data (gray) for "new" (left) and "old" (right) ring detectors of YuMO

Formation of high burn-up structures in UO<sub>2</sub> nuclear fuel materials, known as *rim effect*, attracts attention mainly due to its possible catastrophic influence on the operation conditions of modern nuclear power stations. This process, resulting in the gross structural damage, grain subdivision, is of particular scientific interest as well, because physical mechanisms and relevant parameters of it are still poorly understood. A new, based on the cellular automata (CA), approach for processing and modelling the structure dynamics of nuclear fuel at different burn-ups was proposed. Some evidences for existence of self-organization processes in the fuel at high burn-ups were established. It has been found that the fractal dimension of the surface structures strongly depends on the radiation damage of the material.

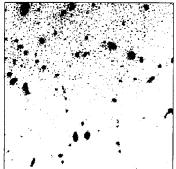
A micrograph of original pattern transformed into CA checkerboard is shown in Figure 5. Black points are pores filled with fission gas products, white background is ceramic UO<sub>2</sub>.

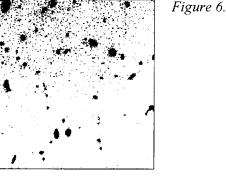


Figure 5.

Black points are pores filled with fission gas products, white background is ceramic UO<sub>2</sub>. Results of Ising CA simulation of pattern evolution under temperature changes are shown in Figures 6 and 7. The processes of pores coalescence and dissolution are seen at different temperature modes.

I.Antoniou, V.V.Ivanov, B.F.Kostenko, J.Spino and A.D.Stalios. Chaos, Solitons & Fractals, 19 (2004) 731-737. E.P.Akishina, I.Antoniou, V.V.Ivanov, B.F.Kostenko and A.D.Stalios. Chaos. Solitons & Fractals, 18 (2003) 1111-1128.





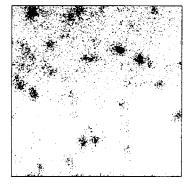


Figure 7.

I.Antonoiu, E.P.Akishina, V.V.Ivanov and B.F.Kostenko. The WSEAS Transactions on Computers, Issue 4, Vol.2, October 2003, 1061-1066.

Since its discovery in 1993, quantum teleportation (OT) has been a subject of intense theoretical and experimental studies. Experimental demonstration of QT has so far been limited to teleportation of light. A new experimental scheme for QT of heavy matter was proposed. It was shown that the standard experimental technique of nuclear physics experiment could be successfully applied to teleportation of spin states of atomic nuclei. It was claimed that there are no theoretical prohibitions upon a possibility of a complete Bell measurement, therefore, the implementation of all four quantum communication channels is at least theoretically possible. A general expression for scattering amplitude of two 1/2-spin particles was given in the Bell operator basis, and peculiarities of Bell states registration were briefly discussed.

V.V.Ivanov, B.F.Kostenko, V.D.Kuznetsov, M.B.Miller and A.V.Sermyagin. Particles and Nuclei, Letters, 2003, No.1[116] 96-107.

The Dubna Cascade Model in its version DCM-CEM was employed to calculate the neutron spectrum at different positions of target system. Three well-defined geometrical positions were chosen for this calculation. The dependence of the neutron spectra on the length l, being in the upstream position of the first blanket, was calculated for three values of the parameter l. In this set-up an exceedingly hard neutron spectrum as practically no low-Z moderating materials has been included.

M.I.Krivopustov,.., A.N Sosnin,..., A.Polanski et al., Kerntechnik, 68 (2003) 1-2, 48-55.

Expressions approximating the integral cross-sections for elastic and inelastic interactions of light and heavy nuclei at the energies up to several GeV/nucleon were elaborated. The calculated cross-sections are inside the range of experimental errors or very close to it. A FORTRAN code and a corresponding numerical example of the cross-section approximation were described in details.

Barashenkov V.S., Kumawat H. – Submitted to Kerntechnik.

### Algorithmic and software support of theoretical investigations

The process of nuclear multifragmentation has been implemented, together with evaporation and fission channels of the disintegration of excited remnants in nucleus-nucleus collisions using percolation theory and the intranuclear cascade model. Colliding nuclei were treated as face centered cubic lattices with nucleons occupying the nodes of the lattice. The site – bond percolation model was used. An algorithm of calculation of the number of percolation clusters inside nuclei was developed. The code can be applied to calculation of the fragmentation of nuclei in spallation and multifragmentation reactions.

G. Musulmanbekov, A. al-Heydari, Phys. Atom. Nucl. Vol. 66, No. 9, 2003, pp. 1671 – 1679.

Multiparticle production in high energy proton – proton collisions has been analysed in the framework of the Strongly Correlated Quark Model (SCQM) of hadron structure. It was shown that inelasticity decreases at high energies and the violation of KNO – scaling was a con-

sequence of total cross section growth and increasing with collision energy masses of intermediate clusters.

G. Musulmanbekov, Yad. Fizika Vol. 67, No. 1, 2004 (in press).

Calculation of the cross sections for single ionization of the ground 1 S and excited 2 P helium states by relativistic impact of a bare uranium ion of charge  $Z_p$ =92 with energy 1~GeV/u was performed. The heavy particle collision is treated within the semi-relativistic first Born approximation. The non-relativistic initial and final two-electron correlated atomic states are obtained by numerical procedures from variational principles. The continuum final states are considered below the n=2 threshold of the He<sup>+</sup> ion. The differential ionization cross section d $\sigma$ /dE s obtained for electron energies E < 37 eV. This energy range includes a wide non-resonant region as well as the resonance structures due to the autoionizing states  $(2s^2)^1$ S,  $(2s^2p)^1$ P and  $(2p^2)^1$ D.

A. V. Selin, A. M. Ermolaev and C. J. Joachain. Phys. Rev. A 67 (2003) 012709.

A semi-relativistic symmetric eikonal distorted wave method for treating collisions of fast projectiles with light atomic targets was proposed. The projectile interaction with target electrons was described by the Li'enard-Wiechert potential, within the impact parameter approach. This model allows one to estimate two-centre effects in fast heavy-particle collisions. It is found that in the dipole approximation the first-order eikonal cross sections differ from the corresponding Born cross sections by a simple factor that accounts for the forward-backward asymmetry of the ejected electron with respect to the direction of the projectile motion. In order to illustrate the method, calculations of single ionization for collisions of fast U<sup>92+</sup> ions (1 GeV/u) with helium targets have been carried out.

A. V. Selin, A. M. Ermolaev and C. J. Joachain, J. Phys. B: At. Mol. Opt. Phys. 36 (2003) L303-L309.

A global analysis of experimental data on the elastic and inelastic scattering of alpha particles by  $^{90,94}$ Zr nuclei and on the total cross sections for their interaction with these nuclei was performed. The deformation length and the neutron-to proton multipole matrix-element atios for the  $2_1^+$  and  $3_1^-$  states of the  $^{90,92,94,96}$ Zr nuclei were obtained for various projective species, and a comparative analysis of these quantities was

performed. With the aim of revealing the origin of the phase shifts found in that study, experimental data on the inelastic scattering of 35.4, 40.0, 50.1, and 65.0 MeV alpha particles on <sup>90,94</sup>Zr nuclei were analyzed on the basis of a unified approach.

A.D.Duysebaev, K.A.Kuterbekov, I.N.Kuhtina, B.M.Sadykov, L.I.Slusarenko, V.V.Tokarevsky, S.A.Fayans. Yadernaya Fizika, 2003, V.66, N4, p.1-13.

A heavy fermion model was used to describe the jet production in the interaction of the gluon with the proton implying further averaging over its mass. As usual in one-spin correlations, the imaginary part of the double gluon exchange amplitude plays the relevant role. The asymmetry in the inclusive set-up with the pion tagged in the fragmentation region of the polarized proton does not depend on the centre of mass energy in the limits of its large values. The lowest order radiative corrections to the polarized and unpolarized contributions to the differential cross sections are calculated in the leading logarithmic approximation. In general, a coefficient of logarithm of the ratio of cms energy to the pion mass depends on the transversal momentum of the pion. This ratio of the lowest order contribution to the asymmetry may be interpreted as a partial contribution to the odderon intercept. The ratio of the relevant contributions in the unpolarized case can be associated with the partial contribution to the pomeron intercept. The numerical results given for the model describe the iet as heavy fermion decay fragments.

A.Ahmedov, E.Antonov, E.Bartos, E.A.Kuraev, E.V.Zemlyanaya. J.Phys. G 29: Nucl.Part.Phys. No.3 (2003) 521-529.

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

V.K.Lukyanov, E.V.Zemlyanaya, B.Slowinski, K.M.Hanna. Izv. RAN ser .fiz. V.67, N1, 2003,pp.55-61.

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

V.K. Lukyanov, E.V. Zemlyanaya, D.N. Kadrev, A.N. Antonov, K.Spasova, G.S. Anagnostatos. Izv. RAN ser .fiz. V.67, N5, 2003, pp.717-721.

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

A. A. Suzko. Phys. Lett. A 308, (2003) p.267 –279.

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

L.M. Nieto, B. F. Samsonov and A. A. Suzko. J.Phys., A: Mathematical and General, v.36, (2003) p. 12293-12301.

A passage of fast dimesoatoms through a matter was considered from a quantum-mechanical viewpoint. A set of quantum-kinetic equa-

tions for the density matrix elements describing their intrinsic state evolution was derived. It was shown that probabilistic description of internal dynamics of hydrogen-like atoms was impossible even at sufficiently low energies because of the "accidental" degeneracy of their energy levels.

O. Voskresenskaya. J Phys. B At. Mod. Opt. Phys. 36 (2003) 3293-3302.

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

D. Blaschke, G. Burau, Yu. L. Kalinovsky, V. L. Yudichev. Prog. Theor. Phys. Suppl. 149, 182-189, 2003;

P. Costa, M. C. Ruivo, Yu. L. Kalinovsky. Phys. Lett. B 577 (2003) 129-136.

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

P. Costa, M. C. Ruivo, Yu. L. Kalinovsky. Phys. Lett. B560, 171-177, 2003.

A coupled system of spherically symmetric SU(2) Yang-Mills-dilaton equations in 3+1 Minkowski space-time was studied both analytically and numerically. It has been found that the system admits a hidden scale invariance which becomes transparent if a special ansatz for the dilaton field is used. This choice corresponds to a transition to a frame rotated in the *ln r-t* plane at a definite angle. An infinite countable family of self-similar solutions which can be parametrized by the N - the number

of zeros of the relevant Yang-Mills (YM) function was founded. According to the performed linear perturbation analysis, the lowest solution with N=0 only occurred to be stable. The Cauchy problem has been solved numerically for a wide range of smooth finite-energy initial data. It has been found that if the initial data exceed some threshold, the resulting solutions in a compact region shrinking to the origin attain the lowest N=0 stable self-similar profile, which can pretend to be a global stable attractor in the Cauchy problem. The solutions reside a finite time in a self-similar regime and then the unbounded growth of the second derivative of the YM function at the origin indicates a singularity formation, which is in agreement with the general expectations for the supercritical systems.

E.E. Donets, O.I.Streltsova, T.L. Boyadjiev. Phys. Rev. D. 58. 2003 (in press).

A new method for regularization of the stochastic perturbation expansion has been developed. This method, based on wavelet decomposition of dependent variables in spatial argument being applied to Langevin equation gives a finite theory. The crux of the method is the generalization of second order random processes to that with correlation function defined in wavelet space. The one-loop contribution to the surface tension in Kardar-Parisi-Zhang equation has been calculated.

M.V. Altaisky. Dok. Akademii Nauk 392(2), 2003, pp.180-182.

A macroscopic model of the dissipative magneto-elastic dynamics of viscous spin polarized nuclear matter was discussed in the context of seismic activity of a paramagnetic neutron star. The source of the magnetic field of such a star was attributed to Pauli paramagnetism of baryon matter promoted by a seed magnetic field frozen into the star in the process of gravitational collapse of a massive progenitor. Particular attention was given to the effect of shear viscosity of incompressible stellarmaterial on the timing of non-radial torsionalmagnetoelastic pulsations of the star triggered by starquakes. By accentuating the fact that this kind of vibration is unique to the seismology of a paramagnetic neutron star it was shown that the high-frequency modes decay faster than the low-frequency modes. The obtained analytic expressions for the period and relaxation time of this mode, in which the magnetic susceptibility and viscosity enter as input parameters, were then quantified by numerical estimates for these parameters taken from early and current works on

transport coefficients of dense matter. It was found that the effect of viscosity was crucial for the lifetime of magnetotorsion vibrations but it did not appreciably affect the periods of this seismic mode which fall in the realm of periods of pulsed emission of soft gamma-ray repeaters and anomalous x-ray pulsarsyoung super-magnetized neutron stars, radiating, according to the magnetar model, at the expense of the magnetic energy release. Finally, arguments are presented that the long periodic pulsed emission of these stars in a quiescent regime of radiation can be interpreted as a manifestation of weakly damped seismicmagnetotorsion vibrations exhibiting the field induced spin polarization of baryon matter.

S.I. Bastrukov, J. Yang, D.V. Podgainy and F. Weber, J. Phys. G: Nucl. Part. Phys. 29 (2003) p.683.

## Creation of methods and numerical algorithms for modeling magnetic systems and transportation of charged particle beams

A magnetic field distribution in a vicinity of a ferromagnetic corner domain for a magnetostatic problem was investigated. The magnetostatic problem arises when searching the distribution of the magnetic field generated by magnet systems encountered in many physical devices such as accelerators. The domain, in which a boundary value problem is solved, has often a piece-wise-smooth boundary. In such cases, numerical calculations of the problem require consideration of the solution behavior in the corner domain. An upper estimate of maximum possible growth of the magnetic field in the corner domain was given. In terms of this estimate, a method was proposed for condensing the differential grid in the vicinity of the corner domain.

E.P. Zhidkov, T.T. Perepelkin. Preprint JINR P11-2003-40, Dubna, 2003. Mathematical Modelling (in press).

New projection field vectors formulations for solving linear and nonlinear problems with divergence, curl operators have been suggested. Such a type linear problems arise in modern physics experiments with spectrometer magnets. The nonlinear problems arise in full general magnetic system modelling, when computations are required for the stored energy, for the forces, torques, acting on the coils, the ferromagnetic parts, and for another characteristics. In contrast to the known methods, based on numerical solving the second order 3D differential equations, the suggested approach not requires a numerical differentiation to com-

pute magnetic field, it permits to control the computational results and to compare the computed and measurement data more precisely.

E.P. Zhidkov, O.I. Yuldashev, M.B. Yuldasheva. Bulletin of RPFU, Series Applied and Computer Mathematics (in press).

## Elaboration of numerical schemes and software for complex physical systems simulation

In the calculation of thermodynamic properties and three dimensional structures of macromolecules, such as proteins, it is important to have a good algorithm for computing solvent accessible surface area and volume of macromolecules. A new analytical method have been proposed for this purpose. In the algorithm, the transformation was considered which maps the spherical circles of intersection of atomic surfaces in three-dimensional space onto the circles on a two-dimensional plane and the problem of computing solvent accessible surface area and volume was transformed into the problem of computing corresponding curve integrals on the plane. This allows one to consider only integrals over the circular trajectories on the plane. The algorithm is suitable for parallelization. Testing on several small proteins has shown a high accuracy of the algorithm and a good performance.

- S. Hayryan, Chin-Kun Hu, E. Hayryan et al. Journal of Computational Chemistry 2003 (in press).
- J. Busa, J. Dzurina, E. Hayryan, Sh. Hayryan, Chin-Kun Hu, et al. Com. Phys. Com. 2003 (in press).

A FORTRAN code PBSOLVE was created for a numerical solution of a linear Poisson-Boltzman equation. Finite different discretization and successive overrelaxation iterations on the sequence of grids were used to obtain the approximate electrostatic potential on the grid. Error control was provided by comparison of solutions on nested grids. A parallel version of the PBSOLVE which exploits the message passing interface has also been constructed. The performance of the program and the efficiency of parallelization have been tested on the small peptide Met-Enkephalin.

S. Hayryan, Chin-Kun Hu, E. Hayryan, I.Pokorny. Lecture Notes in Computer Science Publisher: Springer-Verlag Heidelberg, Vol. 2657, January 2003, pp. 54 - 62.

## Development of methods, algorithms and software of computer algebra

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

V.P.Gerdt, D.A.Yanovich, Programming and Computer Software, Vol. 29. No. 2, 2003, 72-74.

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

M.Znojil, D.Yanovich, V.Gerdt. Journal of Physics A: Mathematical and General 36, 2003, 6531-6545.

V.Gerdt, D.Znojil, D.Yanovich. In: "Computer Algebra in Scientific Computing / CASC 2003", Garching, 2003, pp. 143-162.

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

V.V.Kornyak. Programming and Computer Software, Vol.29, No.2, 2003, 94-99.

V.V.Kornyak. In: "Computer Algebra in Scientific Computing / CASC 2003", Garching, 2003, pp. 227-240.

#### Макет Т. Е. Попеко

Получено 15.12.2003. Подписано в печать 17.12.2003. Формат 60  $\times$  90/16. Бумага офсетная. Печать офсетная. Усл. печ. л. 1,68. Уч.-изд. л. 1,91. Тираж 185 экз. Заказ № 54223.

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