

78978

3m



JOINT INSTITUTE FOR NUCLEAR RESEARCH

2005-203

V. V. Ivanov, T. A. Strizh

**LABORATORY OF INFORMATION
TECHNOLOGIES**

**REPORT ON RESEARCH ACTIVITIES
IN 2005**

Report to the 99th Session
of the JINR Scientific Council
January 19–20, 2006

Dubna 2005

V. V. Ivanov, T. A. Strizh

**LABORATORY OF INFORMATION
TECHNOLOGIES**

**REPORT ON RESEARCH ACTIVITIES
IN 2005**

Report to the 99th Session
of the JINR Scientific Council
January 19–20, 2006

Dubna 2005

Объединенный институт
ядерных исследований
БИБЛИОТЕКА

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

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, V.V.Korenkov, and P.V.Zrelov) and in the field of the "Mathematical Support of Experimental and Theoretical Studies Conducted by JINR" (topic 09-6-1060-2005/2007, headed by V.V. Ivanov, Gh. Adam, and P.V. Zrelov). The Laboratory staff participated in research work done within 16 topics at the project level and within 16 topics at the cooperation level. Main results of the investigations performed within these topics have been published in well-known journals, proceedings of scientific conferences and preprints.

A number of scientific projects involving members of LIT staff have been financed by grants afforded by the Commission of the European Community in the frames of the EU-Russia collaboration and INTAS. Thirteen grants were afforded by the Russian Foundation for Basic Research. Among them, seven were directed to the creation and development of information, computing and telecommunication infrastructure, while six supported various projects of scientific interest.

During the year 2005, LIT was the main organizer of the 9-th Workshop on Computer Algebra "DUBNA 2005", Dubna, May 17-18, 2005, 3-rd International Workshop "Quantum Physics and Communication", Dubna, 26-30 June, 2005, Workshop on a current status of the "Dubna-Grid" project, Dubna, 21 July, 2005, and one of the organizers of the XX

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

Networking, computing, information support, and Grid technologies

The provision of JINR with high-speed telecommunication data links has had as the major target getting the 1 Gbps JINR-Moscow data link operational during the 2005 year. All the necessary equipment was already deployed such that, at the beginning of November, the test runs started. This achievement will secure significant increase of a total network traffic which reached 40 Tb both in the ingoing and outgoing directions during the first eleven months of 2005 under a 45 Mbps JINR-Moscow link.

Figure 1 shows the incoming and outgoing JINR traffic in 2004 and 2005. Total eleven month incoming traffic was 43.52 TB (32.69 TB in 2004) and outgoing traffic – 39.4 TB (40.22 TB in 2004).

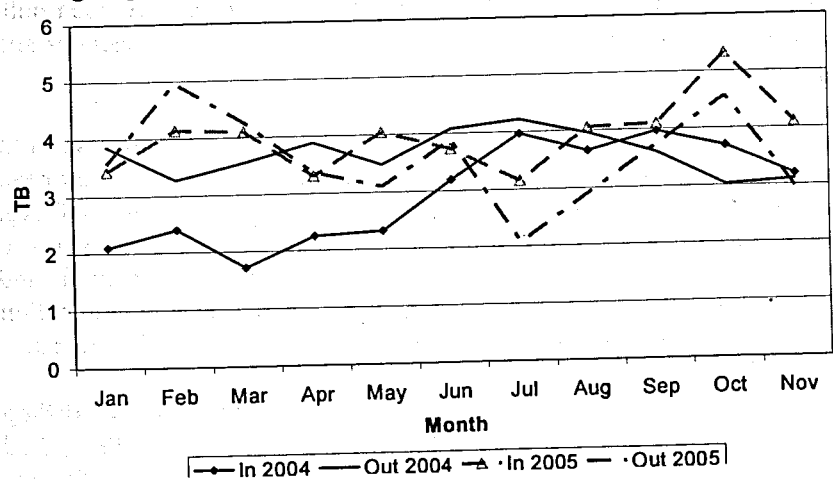


Fig. 1. Incoming and outgoing JINR traffic in 2004 (solid line) and 2005 (dashed line)

The table below shows an eleven month traffic distribution among the JINR divisions (>500 GB of incoming traffic).

JINR Laboratories	Incoming TB	Outgoing TB	Incoming %	Outgoing %
LPP	9.12	5.24	20.96	13.29
LIT	8.31	8.15	19.1	20.7
DLNP	7.88	6.95	18.11	17.65
FLNR	5.1	3.71	11.71	9.43
VBLHE	3.44	4.85	7.9	12.31
Uni-Dubna	2.62	2.32	6.03	5.89
BLTP	2.08	1.91	4.79	4.84
FLNP	1.94	4.58	4.46	11.64
Adm.	0.861	0.171	1.93	0.43
Servers	0.857	0.476	1.92	1.18

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

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

The JINR network structure is a complex of high diversity, which consist of specialized network software and versatile hardware. This structure is the basis of the distributed JINR information technologies (IT) services, in another words the virtual platform on which different and various network and computer services and applications function and develop. The creation of a high-speed, reliable and protected LAN has progressed significantly. The crucial problem of securing the LAN protection involved the development of network monitoring tools able to accomplish the look-ahead assessment of the entire network environment.

The gigabit networking structure of JINR (Fig.2) represents integration of hard- and software facilities that are the basis of the JINR network and information structure, the basis on which the mentioned infrastructure is built up and developed. The gigabit networking structure solves following tasks:

- integration of all JINR computer resources into a unified information environment;
- organization and provision of network access to informational – computational resources for various groups of users, provision of remote access to informational resources of Russian and foreign scientific centres for researchers of all JINR subdivisions;
- creation of a unified information space for all JINR staff, thus providing a way for data exchange between the Institute's subdivisions and between subdivisions and JINR Directorate;
- provision of services of remote access to JINR resources from home PCs of JINR staff members.

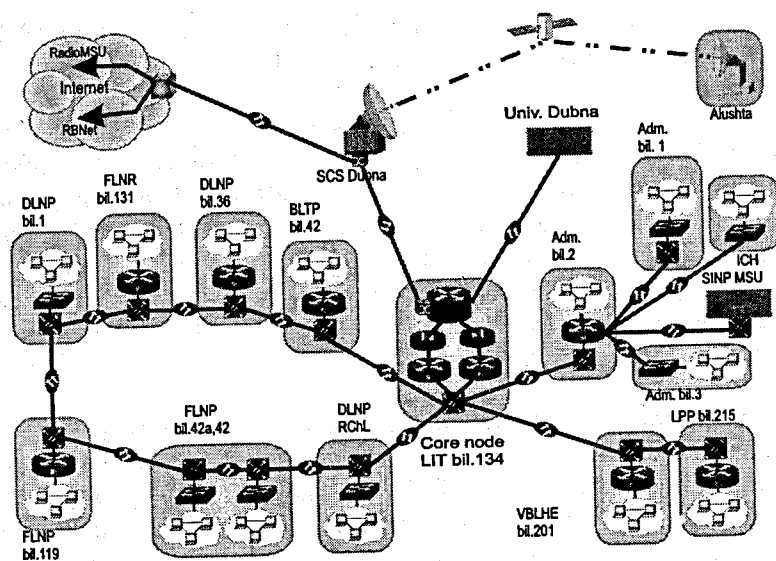


Fig.2. JINR Local Area Network and telecommunication channels

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

More than 500 staff members of JINR and other research centres are using the JINR-CICC. The JINR-CICC is part of the Russian Grid segment used for LHC and other applications. Nowadays the JINR-CICC comprises: an interactive cluster of common access, a common access computing farm for carrying out simulation and data processing for a number of physics experiments in which the JINR participates, a computing farm for the tasks of the LHC experiments, a computing farm for carrying out parallel calculations on the basis of the modern network technologies (Myrinet, SCI, etc.), LCG computing farm is included into a worldwide computing infrastructure.

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

Sixteen modern two-processor computing nodes have been put into operation (8 of them replace outdated general-purpose farm's nodes). Installed were a new data base server controlled by DBMS ORACLE 10G, a server for Grid-monitoring, several servers and workstations for new software testing. Some computing nodes were modernized to perfect the cluster's performance. The process of transferring the CICC infrastructure to 1 GB Ethernet technology is coming to the end.

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

The transition has been realized from the OS LINUX (CERN Red Hat 7.3) to the OS Scientific Linux CERN Release 3.0.5 (SLC3) with corresponding additional software:

- compilers Gnu C, C++, F77;
- compilers Intel C, C++, F90;
- debuggers gdb, ddd;
- graphical shell gnome, kde;
- various users utilities, including ROOT;
- various libraries, including CERN library.

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

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

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

Software MPI to support the paralleling of user's tasks has been installed on a cluster for parallel computations where the nodes are connected by the high-speed network Myrinet.

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

The users involved in the physical experiments ALICE, ATLAS, CMS, COMPASS, D0, DIRAC, H1, HARP, HERA-B, HERMES, IREN, KLOD, LHCb, NA48, NEMO, OPERA, STAR (more than 130 users) are

joined into specific sub-groups. For each subgroup some additional disk space has been allocated to perform simulation, storing and processing of experimental and simulated data and specialized software has been installed. The JINR CICC users distributed over JINR divisions are tabulated as follows:

LIT	DLNP	LPP	VBLHE	FLNR	Non JINR Grid users	BLTP	FLNP	Adm.
171	104	53	44	34	28	14	12	9

The table below shows the percentage of CPU time using by JINR Laboratories at CICC:

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

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

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

The work on creation of computing services and Grid-technology deployment in data processing was in progress. Adaptation and support of new versions of ANAPHE (former LHC++) Library for Linux, Windows and other platforms were performed. Technical and programming assistance of the software development for LHC experiments was continued.

In accordance with CERN-JINR participation plans, the researches are

aimed to develop, configure, and start-up the TDAQ ATLAS system. The experiment schedule assumes that, starting in 2007 and continuing during the following 10 to 15 years of cooperation, the ATLAS experiment will collect, process, and analyze experimental data. LIT researchers take part in the development of the control Supervision HLT system, and on-line TDAQ ATLAS monitoring system. In LIT, a mini test-bed HLT TDAQ was developed to provide the means for debugging and software tests in the environment similar to in real use in CERN.

In the framework of the JINR participation in the LCG (LHC Computing Grid) project, some work was performed. Production in frames of DCs was accomplished at local JINR LHC and LCG farms. Tests on data transferring by the GridFTP protocol (GlobusToolKit 3) were made. The server for monitoring Russian LCG sites was installed and study of GridICE and MapCenter tools usage for monitoring of Russian sites was performed; the toolkit GoToGrid on the automatic installation and tuning of the LCG package was developed; software for installation and control of MonaLisa clients on the base of RMS (Remote Maintenance Shell) was designed (<http://rocmon.jinr.ru:8080>).

Work to develop the CASTOR2 system was in progress. Among other activities were: development of the control process of the garbage collection module, communication to the Oracle Databases, participation in the work to create the TESTBED of a new gLite Middleware, development of the MCDB system, test of a new OMII software, test of the GT4, development of tests for gLite, data base structure and hierarchy designing and development for the CMS experiment.

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

Last but not least, the development of "Dubna-Grid" project. The project is aimed at the creation of a distributed meta-computing environment on the basis of vacant computing resources of "office" computers in the "Dubna" University, secondary schools and other high educational organizations in Dubna. The project foresees creation of a common pool

of accessible nodes of more than 1500 units. The project is based on an Agreement between Administration of Dubna, Joint Institute for Nuclear Research and University "Dubna" for creation of a city-wide multi-purpose new generation informational infrastructure based on the Grid technologies and is partially financed by grants from the town of Dubna and the Russian Foundation for Basic Research.

Implementation of the project will allow one:

- to create a consolidated computing environment (meta-cluster) of the Dubna city on the basis of resources of scientific, research and educational institutions, in particular, JINR subdivisions, University "Dubna", secondary schools and other organizations concerned;
- to create a segment of the international Grid infrastructure operating in frames of various Grid systems (LGG/EGEE, NorduGrid and OSG);
- to perform the research in the areas of control, security and stability within the Grid environment;
- to provide the execution of large-scale computing tasks of the JINR and other enterprises of the Dubna scientific-industrial complex and other organizations concerned;
- to share the experience in creation of a city segment of the Grid infrastructure in order to create similar systems in other Russian cities.

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

The logical structure of the meta-cluster is shown in Fig.3.

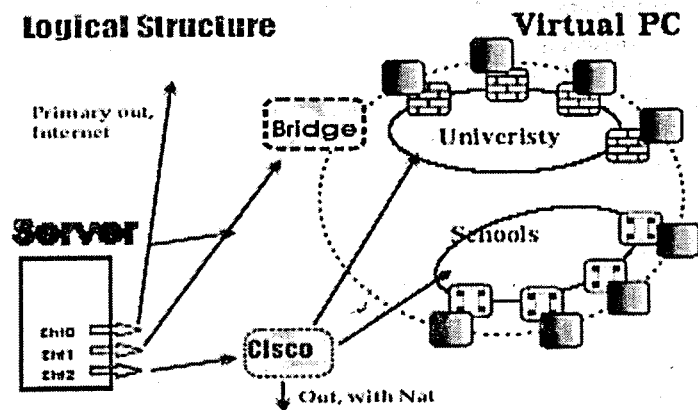


Fig.3. Logical scheme of the "Dubna-Grid" meta-cluster

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

The LIT team represents JINR in the RDIG (Russian Data Intensive Grid) consortium - a national federation in the EGEE (Enabling Grids for E-science) project. JINR role and work in EGEE involves following directions:

- SA1 - *European Grid Operations, Support and Management* - EGEE-RDIG monitoring and accounting. Middleware deployment and resource induction. Participation in the OMII and GT4 evaluation and in the gLite testing. LCG SC activity coordination in Russia.
- NA2 - *Dissemination and Outreach* - coordination of this activity in Russia, organization of EGEE RDIG Conference, creation and run the RDIG Web site (<http://www.egee-rdig.ru>), dissemination in JINR Member states.
- NA3 - *User Training and Induction* - organization of grid tutorials, induction courses and training courses for administrators.

- NA4 - *Application Identification and Support* - coordination of this activity in Russia, organization of HEP applications in Russia through the EGEE infrastructure.

Traditional provision of information, algorithmic and software support of the JINR research-and-production activity included a large spectrum of activities both at LIT and JINR levels. Hard work was undertaken towards systematic development and maintenance of databases and information systems taking into account the user needs. The work was also in noticeable progress on the development of the WWW tools at the JINR and LIT main information servers: www.jinr.ru and lit.jinr.ru. Members of the LIT staff provided necessary work for the JINR's STD AMS on the software and centralized support of the administrative databases.

Software and computer complexes for experimental data processing

The Backward Proportional Chamber (BPC) of the H1 setup at DESY is under responsibility of the Dubna group. The BPC alignment to both nearest detectors has been performed: Central Jet Chamber (CJC) and backward Spaghetti Calorimeter (SpaCal) on 2004-2005 experimental data. Also the BPC alignment has been done for the Backward Silicon Tracker (BST) which is most close to the interaction point. After the BPC alignment DR, Dx, Dy - residuals between detectors became less than 0.1 cm (and were 1-2 cm before alignment). An additional track filtering in the BPC was done for concurrent tracks in the region of radius of 3 cm by selecting the best track with the usage of the goodness of fit χ^2 -criterion. The codes created have been implemented into the official release of the H1 software. [V.Palichik, M.Kapishin, BPC alignment to CJC and SpaCal, H1 Tracking Group Meeting, DESY, Hamburg, August 17, 2005, <https://www-h1.desy.de/idet/itracker/TrackingGroup/AgnMin/Meet050817>; A.Aktas, ..., V.Palichik et al. (H1 Collaboration), *Elastic J/Psi Production at HERA, DESY 05-161, 2005; hep-ex/0510016, submitted to Eur.Phys.J.*]

A significant progress has been achieved in efficiency and transverse momentum P_t reconstruction for hard single muons in CMS software: up to $P_t = 1\text{TeV}$ the efficiency of reconstruction remains not less than 96% and P_t -resolution stays less than 8%. The most significant result has been

obtained for Drell-Yan dimuon reconstruction efficiency which has been increased by 12-20% (see Fig.4). These improvements have been achieved by the modifications implemented in the CMS software for track-segment building in CSCs and for muon trajectory seed generator. [I.A.Golutvin, V.V.Palichik, M.V.Savina, S.V.Shmatov. Search for Neutral Gauge Bosons at Large Hadron Collider. JINR Preprint P2-2005-78, submitted to "Nuclear Physics".]

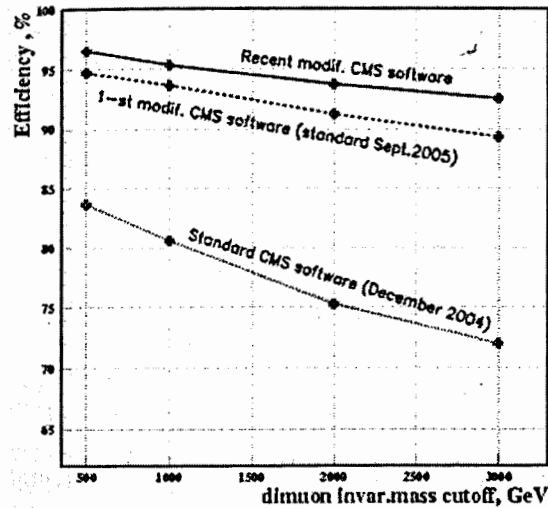


Fig.4. Drell-Yan dimuon reconstruction efficiency in standard and modified CMS software for samples with mass cutoffs 0.5, 1, 2, and 3 TeV

The LIT team of the CBM collaboration contributed into the development of methods and algorithms for event reconstruction in the CBM experiment. The track reconstruction problem can be split into track finding and track fitting. Different competitive approaches to both track finding and the reconstruction of the initial track parameters were applied by the LIT specialists. For the track finding 3D track following and cellular automaton methods have been used. The Kalman filter and global fitting methods like the polynomial approximation are applied to the problem of the momentum reconstruction. The Kalman filter was also used for the determination of primary and secondary vertices. The efficiency of track reconstruction for particles detected in at least four stations is presented in Fig.5. Tracks of high momentum particles are reconstructed very well with efficiencies of 99.45%, while multiple scattering in detector material leads to lower reconstruction efficiency of 89.46% for slow particles.

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

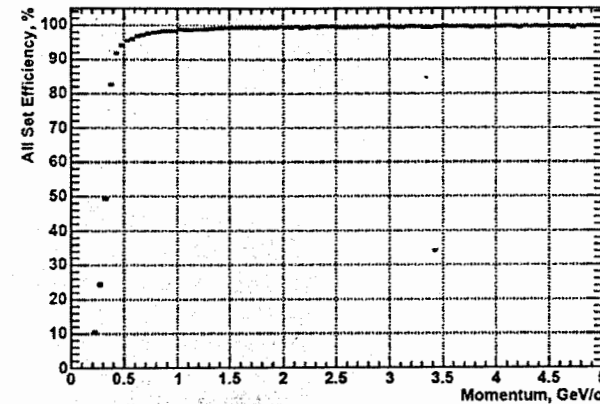


Fig.5. Track reconstruction efficiency as a function of momentum

Tracking in the CBM experiment, Workshop on Tracking in High Multiplicity Environments (TIME05), 03-07 October, 2005, Zurich, Switzerland (to appear in Nucl. Instr. and Meth. A); S. Gorbunov and I. Kisel, Analytic formula for track extrapolation in non-homogeneous magnetic field, X International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT 2005), May 22-27, 2005, DESY, Zeuthen, Germany (to appear in Nucl. Instr. and Meth. A)]

Elastic Net for standalone RICH ring finding was worked out. Standalone finding of rings in this detector is based on the elastic neural net. The method does not require any prior track information and can be used for triggering. Application of the method to the RICH detector of the CBM experiment shows an efficiency of 94.3% and high speed (5.4 ms per event with about 1400 hits in the RICH detector). In view of its computational simplicity and high speed, the algorithm is considered to be further implemented in hardware which can increase the speed by another few orders of magnitude. [S. Gorbunov and I. Kisel, Elastic net for standalone RICH ring finding, X International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT 2005), May 22-27, 2005, DESY, Zeuthen, Germany (to appear in Nucl. Instr. and Meth. A)]

Methods and numerical algorithms for modeling magnetic systems

The generalized numerical solutions was obtained for solving the 3D nonlinear magnetostatic problems by the finite element method (FEM). In the FEM general theory the calculations of error are based on the estimation of nearness between approximated solution and the unknown exact solution. The formulas connecting the computational error of finite element problems with easily calculated local characteristics are presented. The characteristics are residuals for equations of the problem in classical

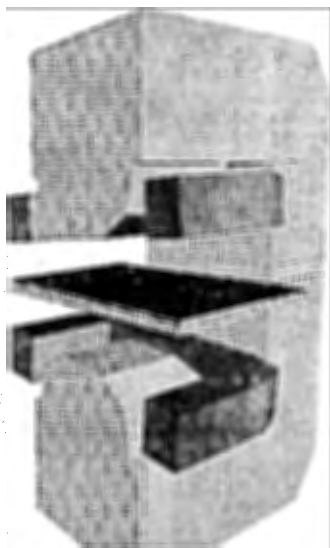


Fig. 6. Computer dipole model for the PANDA (1/2 symmetrical part)

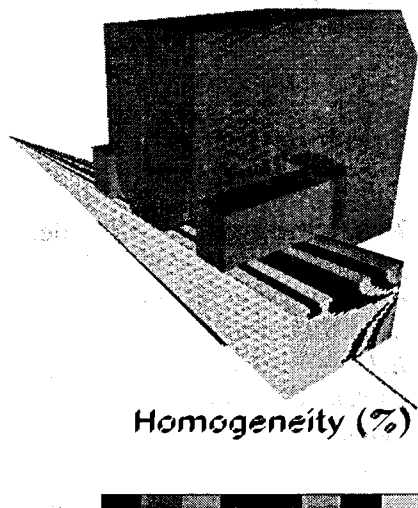


Fig. 7. Distribution of bending power homogeneity in the working region (1/4 symmetrical part)

sense. An example of using the characteristics under computation of a dipole magnet model for the PANDA experiment is considered (Fig.6-7). [J.Ritman, O.I.Yuldashev, M.B.Yuldasheva. An algorithm for construction of dipole magnets computer models with quality control and its application for the PANDA Forward Spectrometer. JINR, E11-2005-49, Dubna, 2005; [http://www1.jinr.ru/Preprints/2005/049\(E11-2005-49\).pdf](http://www1.jinr.ru/Preprints/2005/049(E11-2005-49).pdf); E.P.Zhidkov, O.I.Yuldashev, M.B.Yuldasheva. About accuracy control of computations under the 3D magnetic fields simulations. Bulletin of Peo-

Methods and tools for modeling physical processes and experimental data analysis

The development of methods for a mathematical description of nonlinear self-organizing structural changes in UO_2 during its burn-up in nuclear reactors on the basis of cellular automata (CA) has been progressing. The advisability of such an approach follows from the fact that the scanned micrographs of fuel, after preliminary processing with the help of the visual images editor and subsequent digitizing, can be presented in the form of the CA checkerboard. It provides a way for effective extraction, by CA methods, of every possible quantitative characteristics of the structures represented in those micrographs, for their subsequent use in theoretical models of the process. Besides, what is even more important, under these circumstances, one can formulate mathematical models of the process directly in terms of the entities imprinted in the micrographs. In particular, the micrographs corresponding to a smaller burn-up, can be accepted as initial data for a program of calculation (with the help of some local rules of interaction given in elementary image elements - pixels) of the visual image of fuel state at enormous terms of exploitation. In order to check-up agreement between the theoretical model and experiment, the obtained thus theoretical image was compared, using the CA-programs of image analysis, with a micrograph of real fuel at the same burn-up. Some strict mathematical results of the theory of cellular automata (related to Ising models, voting, etc.) were applied to interpretation of some features of fuel behaviour observed in experiment. Various methods of calculating the fractal dimension of spatial structures formed in UO_2 during operation of a nuclear reactor were applied for the first time to the description of a burn-up degree. The fractal dimension of microstructures was found to be a natural and important characteristic feature describing the degree of radiation destruction and hence it can show the level of emergency danger when using fuel at this burn-up stage. [Akishina E.P., Ivanov V.V., Kostenko B.F. - Particles and Nuclei. 2005. V.2, No.1(124). P. 59-72.]

A model based on the thermal spike concept for an explanation of latent track formation in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ single crystal has been studied by LIT and VBLHE scientists. In order to explain the track formation processes

in the monocrystal $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$, a description based on a thermal peak model, is suggested. The model demonstrates some interesting peculiarities such as electronic quenching and existence of bifurcation points. Arguments why the energy spent on damage creation in the track should be equal to melting heat and why the so-called "epitaxial regrowth" is impossible are given. [Kostenko B.F., Pribis J., Goncharov I.N. – JINR Preprint E17-2005-61, Dubna, 2005, Submitted to "Particles and Nuclei, Letters"]

The analysis of dependence between variables is one of the main tasks of technical and scientific research. Methods of approximations are used every day in data analysis and information gain process, and the associated problems are of wide interest in theoretical and experimental sciences. One of the main problems in data/signal denoising, compression and forecasting is to find an optimal or good representation. Once it is achieved many things can be done about drawing information from data. A new approach to the analysis of complex dependence with relatively small noise using the four point methodology was suggested. The suggested algorithm LOCUSD divides the interval/curve into subintervals/segments of various lengths, provides for every segment local cubic estimations and gives a technique for obtaining integral cubic approximants. Finding the breakpoints in an auto-tracking mode and the iterative computation schemes are two main features of the proposed method that uses a special approximation model. An automatic knot detection and a piecewise - cubic approximation method are proposed. In this method the continuity of first derivatives of the approximants for functions presented by data without errors are acceptable; smaller δ results in more segments with more precise approximants; for noisy data it is advisable to choose a greater sampling step and δ ; the goal is to find such δ that yields desirable approximation quality and an acceptable count of segments. [Dikoussar N.D., Torok Cs. Automatic Knot Detection in the Piecewise-Cubic Approximation (Algorithm and MS.NET Components), Proceedings of the Conference PRASTAN 2005, Banska Bystrica, June 11-17, 2005. Slovak Statistical and Demographical Society, Bratislava, December 2005, pp.160-165.]

In recent years, progress in experimental techniques, particularly the development of cold-target recoil-ion momentum spectroscopy (COLTRIMS), has made it possible to perform precise, kinematically

complete studies of complex atomic collisions. The double processes of He in electron-impact ionization, single ionization with simultaneous excitation and double ionization, have been studied at large momentum transfer using an energy- and momentum-dispersive binary (e,2e) spectrometer. The experiment has been performed at an impact energy of 2080 eV in the symmetric noncoplanar geometry. In this way has been achieved a large momentum transfer of 9 a.u., a value that has never been realized so far for the study on double ionization. The measured (e,2e) and (e, 3-1e) cross sections for transitions to the $n=2$ excited state of He^+ and to doubly ionized He^{2+} are presented as normalized intensities relative to that to the $n=1$ ground state of He^+ . The results are compared with first-order plane-wave impulse approximation PWIA calculations using various He ground-state wave functions. It is shown that shapes of the momentum-dependent (e,2e) and (e, 3-1e) cross sections are well reproduced by the PWIA calculations only when highly correlated wave functions are employed. [N. Watanabe, Y. Khajuria, M. Takahashi, Y. Udagawa, P.S. Vinitzky, Yu.V. Popov, O. Chuluunbaatar and K.A. Kouzakov, (e,2e) and (e, 3-1e) studies on double processes of He at large momentum transfer, Phys. Rev. A 72, pp. 032705-1-11 (2005); P.S. Vinitzky, Yu.V. Popov and O. Chuluunbaatar, Fast proton-hydrogen charge exchange reaction at small scattering angles, Phys. Rev. A 71, pp. 012706-1-9 (2005)]

An extensive study of the 0^+ states in ^{158}Gd was carried out recently, within the quasiparticle-phonon model (QPM). The QPM study has been extended to ^{168}Er and some Th and U isotopes. An intention have been made to test if the QPM can account for the huge number of 0^+ levels observed in ^{168}Er and is able to offer a consistent picture of the properties of the 0^+ states in deformed nuclei of different regions. The study performed shows that it is necessary to go beyond the mean field approximation (RPA) in order to account for a large number of 0^+ levels observed in ^{168}Er . RPA, in fact, generates only 15 0^+ states below 4 MeV. Moreover, according to QPM calculation performed, several levels, specially above 3 MeV, correspond to states with appreciable, often dominant, two-phonon components. The QPM results suggest that the octupole correlation is not a common feature of the 0^+ states in all nuclei, but is to be associated to the peculiar shell structure of some nuclei, in this case ^{158}Gd . The QPM analysis of the E2 and E0 transitions leads to a conclusion that the quadrupole collectivity is lacking in all 0^+ states of ^{168}Er and is more

appreciable, but still not strong, in the actinides. On the whole, the present QPM calculation provides a fairly satisfactory description of the existing properties of the 0^+ states in deformed nuclei. In order to assess its complete reliability, however, it is desirable to complete the characterization of those states by systematic measurements of their E2 and E0 decay strengths. [N.Lo. Iudice, A.V. Sushkov, and N. Yu. Shirikova, *Phys. Rev. C* in press (2005)]

Theoretical and numerical investigation of the magnon Bose-Einstein condensation (BEC) in quantum antiferromagnets is started. This phenomenon predicted earlier theoretically was observed this year for the first time in low-temperature experiment on antiferromagnet Cs_2CuCl_4 at Max Planck Institute for Chemical Physics of Solids (MPI CPfS), Dresden. Magnon BEC is a magnetic phase transition induced by an applied strong magnetic field near the saturation field B_c . Calculation of the phase transition temperature $T_c(B)$ as a function of a magnetic field B is based on a realistic Hamiltonian with parameters derived from inelastic neutron scattering experiments. On the first stage, the analytical derivation and numerical analysis of the magnon energy spectrum and density of states in Cs_2CuCl_4 are carried out. Results are used to calculate the phase boundary $T_c(B)R(B_c - B)^\alpha$. It is found that in the vicinity of B_c the critical exponent tends to the value $\alpha_{\text{BEC}}=2/3$ characteristic of the universality class of BEC transitions. Obtained theoretically the phase boundary $T_c(B)$ in Cs_2CuCl_4 is in a good agreement with the experimental data. [D.L. Kovrizhin D.L., Yushankhai V., Siurakshina L. - Submitted to *Phys. Rev. B*.]

The analyses and numerical study of the structure and properties of the polydispersed DMPC vesicles population in three phases: gel, ripple, and liquid was performed. Dependence of the DMPC membrane thickness on temperature was restored from the SANS experiment on the basis the SFF-HH model. It was demonstrated that DMPC membrane thickness in liquid phase ($T=30^\circ\text{C}$) depends on the membrane curvature. [M.A.Kiselev, E.V.Zemlyanaya, V.K.Aswal, R.H.H.Neubert. *JINR Preprint E14-2005-93, Dubna, 2005; ArXiv: physics/0507140; submitted to the European Biophysics Journal*]

The properties of a model of the moisture evaporation in a porous building material of a rectangular form are investigated. Algorithms of solving

a nonlinear diffusion equation with initial and boundary conditions simulating the dynamic distribution of moisture concentration, calculation of coefficients of a polynomial describing transport of moisture, with usage of experimental measure of moisture concentration in a sample are developed and investigated. Research on the properties of the model is carried out depending on the polynomial degree and a set of its coefficients and the quantity of the used experimental data. [I.V.Amirkhanov, E.Pavlushova, M.Pavlush, T.P.Puzynina, I.V.Puzynin, I.Sarkhadov. *Numerical Investigation of a Moisture Evaporation Model in Building Materials, Bulletin of Peoples' Friendship University of Russia. Series Applied and computer mathematics, v.4, N 1, 2005, pp. 96-106.*]

Numerical algorithms and software for simulation of complex physical systems

The advection of a passive scalar quantity by incompressible helical turbulent flow has been investigated in the frame of an extended Kraichnan model. Statistical fluctuations of the velocity field are assumed to have the Gaussian distribution with zero mean and defined noise with finite time-correlation. Actual calculations have been done up to two-loop approximation in the frame of the field-theoretic renormalization group approach. It turned out that the space parity violation (helicity) of a stochastic environment does not affect anomalous scaling which is the peculiar attribute of corresponding model without helicity. However, the stability of asymptotic regimes, where anomalous scaling takes place, and the effective diffusivity strongly depend on the amount of helicity. [O.G. Chkhetiani, M. Hnatich, E. Jurcisinova, M.Jurcisin, A.Mazzino, M. Repasan, *Scaling regimes in model of passive scalar advected by the turbulent velocity field with finite correlation time. Influence of helicity in two-loop approximation, Communication of JINR (2005) E17-2005-135; O.G. Chkhetiani, M. Hnatich, E. Jurcisinova, M.Jurcisin, A.Mazzino, M. Repasan, Influence of helicity on scaling regimes in extended Kraichnan model*}, Will be published in proceedings of RG2005, 30 August - 3 September 2005, Helsinki, Finland.]

The temperature dependence of the heavy-quarkonium interaction based on the Bhanot-Peskin leading order perturbative QCD analysis was explored. The Wilson coefficients are computed solving the Schroedinger equation in a screened Coulomb heavy-quark potential. The inverse Mel-

lin transform of the Wilson coefficients then allows for the computation of the 1S and 2S heavy-quarkonium gluon and pion total cross section at finite screening/temperature. As a phenomenological illustration, the temperature dependence of the 1S charmonium thermal width is determined and compared to recent lattice QCD results. [F. Arleo, J. Cugnon, Yu. Kalinovsky, *Phys. Lett. B* 614, 44-52, 2005.]

Methods of numerical description of open quantum systems by the deterministic methods of approximate differential integration are developed. A representation of a propagator for open quantum systems in the form of a double functional integral with respect to conditional Wiener measure is proposed. It allows one to apply the approximate formulas exact for functional polynomials of a certain power to calculation of such integrals. Within this deterministic approach the problem is reduced to the evaluation of usual (Riemann) integrals of low multiplicity. The formulas are in fact the basis of a numerical method of studying the time evolution of the systems. The features of the method are discussed and some examples of calculations are given. [Rushai V.D. and Lobanov Yu.Yu. - *Phys. Rev. E* 71, 066708 (2005)]

In cooperation with the University of Cape Town, the particle-like excitations of nonlinear dispersion matter have been studying in frames of the models of condensed matter theory and nonlinear optics based on the nonlinear Schroedinger equation (NLS). It has been shown that unlike the bright solitons, the parametrically driven kinks of the NLS equation are immune from instabilities for all damping and forcing amplitudes; they can also form stable bound states. In the undamped case, the two types of kinks and their complexes can stably travel with nonzero velocities. The bistability of the Bloch and Néel walls within the NLS contrasts the properties of these solutions within the Ginzburg-Landau equation, where they cannot stably coexist. [Zemlyanaya E.V., Barashenkov I.V., and Woodford S.R. - *Parametrically Driven Dark Solitons: a Numerical Study. Lecture Notes in Computer Science. 2005. V. 3401, Springer-Verlag, P. 590.*]

The parametrically driven damped NLS equation serves as an amplitude equation for a variety of resonantly forced oscillatory systems on the plane. Its nodal soliton solutions are considered. It is shown that although the nodal solitons are stable against radially-symmetric perturbations for

sufficiently large damping coefficients, they are always unstable to azimuthal perturbations. The corresponding break-up scenarios are studied using direct numerical simulations. Typically, the nodal solutions break into symmetric "necklaces" of stable nodeless solitons. [Alexeeva N.V. and Zemlyanaya E.V. - *Nodal two-dimensional solitons in nonlinear parametric resonance. Lecture Notes in Computer Science. 2005. V. 3401, Springer-Verlag, P. 91.*]

The study of a late time acceleration of the universe together with the initial singularity and isotropization process remains among the attractive problems of modern cosmology. The problem of singularity has been thoroughly addressed by us in a number of papers for the last few years both plane symmetric and Bianchi type universes. The interacting spinor and scalar fields in a plane symmetric space-time are considered and the possibility of the formation of soliton-like configurations is investigated. The investigation of a role of nonlinear spinor field in elimination of space-time singularity for Bianchi universes, whereas a self-consistent system of scalar, spinor, electro-magnetic and gravitational field given by a Bianchi type I model is performed. [Saha, Bijan and Shikin, G.N.: *Static plane-symmetric nonlinear spinor and scalar fields in GR (to be published in Intern. J. Theor. Phys.)*, (2005); Saha, Bijan and Shikin, G.N.: *Exact self-consistent plane-symmetric solutions to the spinor and scalar field equations, (to be published in Bulgarian J.Phys.)*; Saha, Bijan and Shikin, G.N.: *Nonlinear Spinor and Scalar Fields in General Relativity (to be published in Vestnik PFU)* (arXiv:gr-qc/0104089); Saha, Bijan and Todor Boyadjiev: *Interacting spinor and scalar fields in a Bianchi type-I Universe: Oscillatory solutions in the "Gravity, Astrophysics and Strings @ the Black Sea"* (Eds. P.P. Fiziev and M.D. Todorov) *St. Kliment Ohridski University Press, Sofia*, 226-233, (2005) [arXiv:gr-qc/0308061]; Saha, Bijan: *Interacting scalar and spinor fields in Bianchi type I universe filled with magneto-fluid* *J. Astrophys. Space Sci.* 299 (1), 149-158, (2005) (arXiv:gr-qc/0309062)]

Stationary solutions to the Gross-Pitaevskii equation define the topological coherent modes, representing nonground-state Bose-Einstein condensates. These modes can be generated by means of alternating fields whose frequencies are in resonance with the transition frequencies between two collective energy levels corresponding to two different topological modes. The theory of resonant generation of these modes was generalized

in several aspects: multiple-mode formation was described; a shape-conservation criterion was derived, imposing restrictions on the admissible spatial dependence of resonant fields; evolution equations for the case of three coherent modes were investigated; the complete stability analysis was accomplished; the effects of harmonic generation and parametric conversion for the topological coherent modes were predicted. It was demonstrated that the dynamical transition between the mode-locked and mode-unlocked regimes was accompanied by noticeable changes in the evolutionary entanglement production. [V.I. Yukalov, K.P. Marzlin, E.P. Yukalova, and V.S. Bagnato, *Topological coherent modes in trapped Bose gas*, *Am. Inst. Phys. Conf. Proc.* 770, 218-227 (2005); V.I. Yukalov and E.P. Yukalova, *J. Low Temp. Phys.* 138, 657-662 (2005)]

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

static Patterns and Recognition by Synthetases and Elongation Factor EF-TU". Accepted by *Biochemistry* (bi0516733), 2005; R.V. Polozov, V.S. Sivozhelezov, V.V. Ivanov and Yu.B. Melnikov. *On a Classification of E.coli Promoters According Their Electrostatic Potentials, Particles & Nuclei, Letters*, 2005, Vol. 2, No. 4(127), pp. 82-90.]

Effective algorithms for calculating the solvent accessible surface area and the volume of macromolecules deposited in solvent have been developed at LIT in cooperation with the Technical University of Cošice (Slovakia) and the Institute of Physics of the Academia Sinica Nankai.g (Taiwan). When calculating the solvation energy of proteins, the hydration effects, drug binding, molecular docking, etc., it is important to have an efficient and exact algorithms for computing the solvent accessible surface area and the excluded volume of macromolecules. A Fortran package is presented which is based on the new exact analytical methods for computing volume and surface area of overlapping spheres. In the considered procedure the surface area and the volume are expressed as surface integrals of the second kind over the closed region. Using the stereographic projection the surface integrals are transformed to a sum of double integrals which are reduced to the curve integrals. MPI Fortran version is described as well. The package is also used for computing the percolation probability of continuum percolation models. When calculating thermodynamic properties and a three-dimensional structure of macromolecules (for example, proteins), it is important to have an efficient algorithm for computing the solvent-accessible surface area of macromolecules. Here, we propose a new analytical method for this purpose. In the proposed algorithm, a transformation is considered that maps the spherical circles formed by intersection of the atomic surfaces in three-dimensional space onto the circles on a two-dimensional plane, and the problem of computing the solvent-accessible surface area is reduced to the problem of computing the corresponding curve integrals on the plane. This allows one to consider only the integrals along the circular trajectories on the plane. The algorithm is suitable for parallelization. Tests on many proteins as well as the comparison to other analogous algorithms have shown the efficiency of the method. [Ayryan E. et al. - *Comput. Physics Communications*. 2005. No. 165, P. 59-96. ; Ayryan E. et al. - *J. Comput. Chem.* 2005. No. 26, P. 334-343.]

Methods, algorithms, and software of computer algebra

The cohomologies of restricted Lie algebras of Hamiltonian vector fields have been studied in frames of the research on computer algebra conducted at LIT. Restricted Lie algebras (or Lie p -algebras) of vector fields are finite-dimensional analogs of corresponding classical algebras defined over the fields of positive characteristic p . The computer-based calculations performed with the Lie p -algebras of vector fields preserving a symplectic structure (i.e. Hamiltonian and Poisson algebras) have revealed important and interesting peculiarities in the structure of their cohomologies. The statements explaining these peculiarities have been proved. [Kornjak V.V. – *Programming and Computer Software, Vol.31, No.2, pp. 87-90. 2005*]

A new universal mathematical frame for constructing models in mathematical physics called “a system of discrete relations on an abstract simplicial complex” is proposed. This construction can be interpreted as a natural generalization of the notion of cellular automaton and as a set-theoretic analog of a system of polynomial equations. The algorithms in C for compatibility analysis of a system of discrete relations and for constructing canonical decompositions of discrete relations have been developed and implemented. A regular way to impose topology on an arbitrary discrete relation via its canonical decomposition was proposed. This allows one to evolve standard tools of the algebraic topology (homology group, cohomology ring, etc) for relations. Applying the above technique to cellular automata - a special case of system of discrete relations - some new results were obtained. Most interesting of them is the observation that the presence of non-trivial proper consequences may determine global behavior of an automaton. If the number of states q is a power of a prime, i.e., $q=p^n$, one can express any discrete relation in terms of polynomials over the Galois field F_q and then use the standard Groebner basis method for the compatibility analysis. The Groebner basis computation for the cellular automaton “Life” with the help of Maple 9 takes 1 h 22 min. Proposed approach gives an analogous result about 5000 times faster - for less than 1 sec. [Kornjak V.V. *On Compatibility of Discrete Relations. Lecture Notes in Comp. Sci. 3718, Springer-Verlag, 2005, 272–284, <http://arXiv.org/abs/math-ph/0504048>*]

An asymptotic heat kernel expansion for elliptic differential operators

acting on compact closed curved manifolds has been studied by means of the computer algebra. The coefficients in this expansion are quantities of fundamental importance in the quantum field theory, quantum gravity, spectral geometry and topology of manifolds. Deriving explicit expressions for these quantities is quite a laborious task, especially in the problems of modern physics that deals with complicated operators (high order and non-minimal ones) in a complicated geometric environment (with torsion and gauge fields in addition to the Riemann curvature tensor). In fact, the calculations cannot be performed without computer algebra tools. A covariant algorithm for computing the heat kernel coefficients and its implementation as two C programs CoincidenceLimits and DWSGCoefficient are described. Some results obtained with the help of these programs are presented for the first time. The most considerable results are related to non-minimal operators and manifolds with torsion. [Kornjak V.V. – *Focus on Numerical Analysis, Editors: J.P. Liu, Nova Science Publishers, NY, 2005, pp. 1-25*]

The modern laser physics and nanotechnologies have stimulated computer simulations for the dynamics of atomic systems in external fields and for control problems of finite dimensional quantum systems. For such subjects the symbolic-numerical algorithms based on procedures of normalization and quantization of polynomial Hamiltonians, and numerical methods for solving the time-dependent Schroedinger equation (TSDE) were developed. [Belyaeva I.N., Chekanov N.A., Gusev A.A., Rostovtsev V.A, Ukolov Yu.A., Uwano Y. and Vinitzky S.I. *A MAPLE Symbolic-Numeric Program for Solving the 2D-Eigenvalue Problem by a Self-consistent Basis Method. Proc. of the 8th International Workshop on Computer Algebra in Scientific Computing (September 12-16, 2005 Kalamata, Greece) Eds. V.G.Ganzha, E.W.Mayr, E.V.Vorozhtsov, Springer-Verlag Berlin Heidelberg 2005 pp.32–39; Gusev A., Gerdt V., Kaschiev M., Rostovtsev V., Samoylov V., Tupikova T., Uwano Y., and Vinitzky S., *Symbolic-Numerical Algorithm for Solving the Time-Dependent Schroedinger Equation by Split-Operator Method. Proc. of the 8th International Workshop on Computer Algebra in Scientific Computing (September 12-16, 2005 Kalamata, Greece) Eds. V.G. Ganzha, E.W.Mayr, E.V. Vorozhtsov, Springer-Verlag Berlin Heidelberg 2005 pp.244-258.*]*