JOINT INSTITUTE FOR NUCLEAR RESEARCH

97-378

R. Pose

# MAIN RESULTS OF THE LABORATORY OF COMPUTING TECHNIQUES AND AUTOMATION IN 1997

Report to the 83rd Session of the JINR Scientific Council
January 15–16, 1998

Dubna 1997

R. Pose

# MAIN RESULTS OF THE LABORATORY OF COMPUTING TECHNIQUES AND AUTOMATION IN 1997

Report to the 83rd Session of the JINR Scientific Council
January 15–16, 1998



Dubna 1997

The main efforts of the Laboratory of Computing Techniques and Automation have been directed towards provision of adequate networking, information, computing and software support of research under way at JINR. Limited financing is a retarding factor in carrying out the work.

In 1997, following the world tendency in the field of computing for science and higher schools and the progressive requirements of users, the Laboratory developed a conception of establishing a High Performance Computing Center (HPCC) at JINR. It should be read as a balanced development of four main components of HPCC, namely

- **Telecommunication systems:**
  - External communication channels (INTERNET);
  - High-speed JINR Backbone;
- **Systems for powerful computations and mass data processing:**
  - General High-performance server;
  - Clusters of workstations of JINR laboratories and experiments;
  - Computing farms (PC-farms);
- **Data storage system:**
  - File servers system based on AFS;
  - Mass storage system;
  - Information servers and database servers;
- **Software support systems:**
  - Systems for application creation and maintenance;
  - Visualization systems.

## Telecommunication systems

In 1997 was physically started an external communication for the 2Mbps fiberoptic link "JINR-RSCC"Dubna"-Shabolovka-Moscow Backbone-M9" comprising 6 tracks. Actually JINR obtained a new 2 Mbps computer communication link to Moscow (M9). The financing came from the Ministry of Science and Technology in the framework of the programme "Creation of the National Computer Telecommunications Network for Science and High Schools" on the project "Creation of the Rbnet Infrastructure (earth channels)". Thus, the problem of the computer communication link "JINR-Moscow (M9)" has been solved. The new channel is 16 times higher than the currently available one as regards to its throughput. Its operation is financed by the Russian Ministry of Science and Technology at the expense of funds allocated in a centralized form within the programme mentioned above. The question is under solution on routing and start up of the channel for a wide range of JINR users.

## JINR LAN

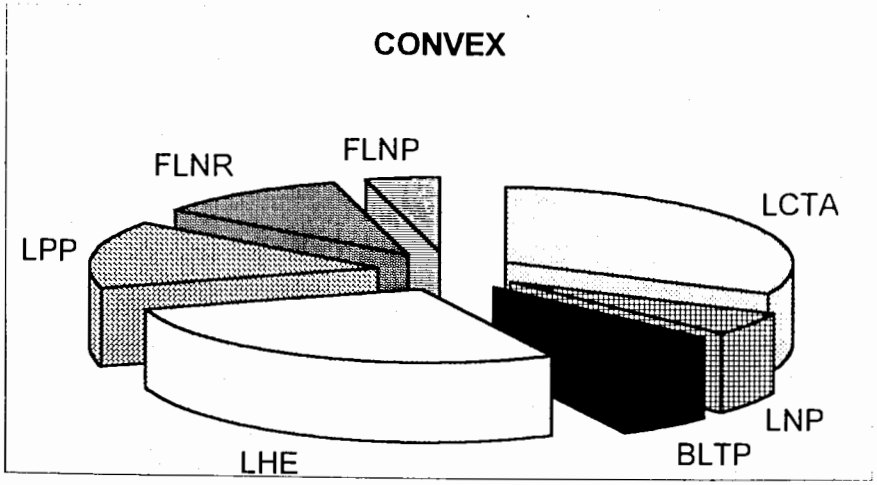
In June 1996 the regular meeting of the Committee for users of the JINR networking informational-computational infrastructure considered the question on a new version of the project on the upgrade of the JINR LAN. The meeting unanimously approved a programme changing the JINR LAN towards advanced communication technology, based on ATM technology. The committee also defined a sum of the top-priority financing required for realization of the programme, i.e. 200,000US$. The contract itself provided purchase and installation of network equipment for the segments of the JINR LAN incorporating all JINR Laboratories. However, in view of the difficult financial situation at JINR and after long discussions, the JINR Directorate decided to restrict itself by funding 116,000US$. This allows only purchase of the main part of the equipment and three segment complexes.

Passing all the above decisions took 9 months. Thus, currently JINR looks forward to receive the main part of the paid telephone-communication gadgets, which will provide a way for installation, tuning and putting into operation only the head part of the network equipment the high speed JINR Backbone, based on ATM.

By November, LCTA received software HP-Open View for network analysis and monitoring. It will be put into operation by the end of the year.

## Computing service

Below are given results of CONVEX computing server use by the Institute laboratories during the last 11 months.




It must be pointed out that LCTA uses computer time mainly for performing



computations in the field of computational physics. This work is performed in close collaboration with scientists from other JINR laboratories.

In 1997 the load of the main JINR servers has grown up. To make the users work better, a PROXY-server has been introduced into service.

A data-base for JINR IP addresses has been created and put into operation, based on the 'client-server' technology and visualization through WWW.

According to an agreement with Rossendorf/Germany, JINR has received a C3840 system comprising four 200Mflop scalar vector processors with 2Gb main memory, more than 40Gb disk storage. Work on its start up has been completed. In the nearest future it will be introduced into service for the users.

To provide normal operation of the network, one needs a set of powerful servers to maintain overall service.

Regarding the computing facilities, at JINR there is a whole diversity of computational problems in various fields of physics, which need powerful computing resources. They involve problems of theoretical and mathematical physics, solid state physics problems, experimental data processing problems, especially in HEP. To solve these issues, LCTA took part in the projects on creation of specialized centers by using extra budget funds for these purposes.

At the end of 1997 the JINR HPCC has the following equipment:

**Scalar-Vector system CONVEX C3840**

| | |
|---|---|
| OPERATING SYSTEM | CONVEXOS 11.5.0 |
| Number of Processors | 4 |
| Performance (peak) | 200 MFlops/1_CPU |
| Memory | 2 GB |
| Disks | 48 GB |

Ethernet, SCSI interface, DAT, 9-trk tape

**Scalar system Hewlett-Packard S class SPP2000**

| | |
|---|---|
| OPERATING SYSTEM | SPP-UX 10.20 |
| Number of Processors | 8 |
| Performance (peak) | 800 MFlops/1_CPU |
| Processor Type | PA8000 |
| Memory | 2 GB |
| Disks | 64 GB |

ATM, 100BaseT Ethernet

**Software:**

Batch processing, NQS, C, C++, Parallel Scientific Lib, Fortran, Message Passing Interface, Parallel Virtual Management, Parallel Application Development Tools

**Data Management System**
**D-class server + ATL 2640 Automated Tape Library**

**D-class server**

| OPERATING SYSTEM | HP-UX 10.20 |
|---|---|
| Number of Processors | 2 |
| Processor Type | PA8000 |
| Memory | 512 MB |
| Disks | 36 GB |

ATM, Ethernet, CD, SCSI
Software: HP-Open View Omni Back II, HP-Open View Omni Storage

**ATL 2640**

| NUMBER OF CARTRIGES | 264 |
|---|---|
| Capacity of the cartridge | 20 GB/40 GB |
| Total capacity | 5.28 TB/10.56 TB |
| Number of drives | 3 |

## Workstation clusters development

The SUN/SPARC cluster ultra.jinr.dubna.su at JINR is created as an OS SOLARIS environment server and is working under OS Solaris 2.5.1.

Site-licenses for JINR on Fortran F77-4.0 and C++-4.1 provide all JINR specialists complete conditions in the OS Solaris environment for their work, including use of current versions of CERNLIB. Site-licenses on F77-4.0 and C++-4.1 are available for any JINR hosts working under OS Solaris.

The latest versions of many FSF/GNU products widely used in JINR are installed at cluster in a proper way and can be used for installation at any other JINR hosts working under OS Solaris.

**CMS CLUSTER at JINR**

| HARDWARE | 3 SPARC-STATIONS ( 140 ULTRA SPARC STATION AND TWO SPARCSTATIONS-20) |
|---|---|
| Disk Space | 24 GB |
| Software | OS Solaris 2.5.1 |
| Compilers | C-4.0, C++-4.1, F77-4.0 |
| Number of users | 37 |



The computational environment is the same as at the CERN CMS cluster (cms.cern.ch). The CMS cluster at JINR supports both the tasks of simulation and data processing.

Work has been in progress on maintenance of the LINUX environment at JINR.

## DATABASE SERVERS

In order to make work on world data bases and information systems more effective, software for the PROXY-server to buffer the information requested and obtained through external communications has been installed at a general LCTA server ( put into service according to the BAPHYS project).

Work has been in progress on realization of the BAPHYS project for creation at JINR of an information centre for institutions involved in fundamental and applied nuclear physics research (JINR, IHEP in Protvino, St.Petersburg Institute of Nuclear Physics, Novosibirsk Institute for Nuclear Physics, Institute for Nuclear Research (Troitsk), ITEP and Research Institute of Nuclear Physics MSU (Moscow)). A data base connected to the JINR Library Reference system is maintained on the basic server (http://dbserv.jinr.ru/library/) of this centre, fitted with a WWW-ORACLE system *[V.Korenkov et al., JINR Commun., P11-97-278, P11-97-277]*. The subsections "High Energy Physics (HEP)", "Low and Medium Energy Physics", "Physics Conferences, Workshops and Summer Schools" in the subsystem "Physics Information Servers and Data Bases" as well as "Publishing Offices" have been modified. Financial support for the BAPHYS work came from the Russian Foundation for Basic Research (in the frame of the interdepartmental programme). Besides, at the expense of JINR funds, an extra external memory has been purchased for the general server (disks and DLT-tapes).

Within the activities on creation of database (DB) applications, work performed together with the scientific department of Computer-Aided Management Systems/JINR to optimize the administrative activities should be noted. In particular, some variants of the program subsystems created by 1997 have been developed. That was caused by new requirements of various services in the JINR Board, expansion of higher-ups of the accounted information and introduction experience gained on the workplaces. It is mainly related to issues of creation of interfaces for number of systems.

Several versions have been realized on introducing the JINR topical plan for research and relevant data into the information retrieval systems, including WWW (http://www.jinr.ru/jinr/plan/planr.htm).

## WWW-SERVICE

Work has been in progress on development of information support for the multilevel set of WWW-servers at JINR, in particular, the general JINR and LCTA servers. Regarding the JINR general server, main modifications were re-

lated to the INFO and NEWS sections. The LCTA server has got its new content (home page), so the relevant subsections were respectively modernized.

The home page for the "Dubna" newspaper has been introduced and is maintained currently at the JINR WWW-server.

A procedure has been worked out from the methodical viewpoint for introducing full-text data bases from the JINR Publishing Department. It requires purchase of licensed software to provide proper access to the information needed.

The CMS informational system is heavily based on the world-wide web (WWW). The web-server http://sunct2.jinr.dubna.su was designed at LCTA and contains information on RDMS CMS collaboration activities. This web-server was adopted as an official web-server of the RDMS CMS collaboration by its in June 1997.

Now there are references on the RDMS CMS web-server http://sunct2.jinr.dubna.su from CERN CMS web-servers CMSDOC and CMSINFO. LCTA is responsible for further development and support of the RDMS CMS web-server

## SOFTWARE

At the same time, maintenance and development of the general-purpose program libraries have been progressing at LCTA. There are:

- free software (*http://jicom.jinr.ru/LCTA/freesoft.html*);
- licensed software (*http://jicom.jinr.ru/LCTA/Soft lic 1.html*);
- main purpose libraries - JINRLIB (*http://www.jinr.ru/~tsap/Koi/jinrlib/project.htm*), NAGLIB, CPC,CERNLIB (*http://www.jinr.ru/~tsap/Koi/sss.htm*). The version of CERNLIB for Windows NT/Windows95 98a was compiled with Microsoft Powerstation Fortran v.4.0 and Digital Visual Fortran v.5.0;
- FTP-archive (*http://jicom.jinr.ru/LCTA/FTP Soft.html* )

An original method for graphic digitizer has been developed and realized at a user interface level *[ A.P.Ierusalimov et al. - JINR Rapid Comm., N6,-1997]*

Software based on up-to-date technologies has been designed: Web-Oracle gateway Oralink (*http://oradb1.jinr.dubna.su/software/oralink/*), Russian Web Survey (*http://oradb1.jinr.dubna.su/rws/* ), Java applets etc.

Special client-server IDL facilities were used as 3D visualization for DEMON setup.

According to Memorandum of Understanding of collaboration between the LCTA and the SPS/LEP Division of the CERN during 1997 following work has been done:

- TDM Monitoring System (*http://hpslz24.cern.ch:8080/cgi-bin/tdm_protect.vi*)



- MOPOS timing diagnostics system (*http://hpslz24.cern.ch:8080/examples/ex_mopos.html*)
- LabVIEW on the WEB (*http://hpslz24.cern.ch:8080/*)
- TCP/IP based Message Handler (LV_mhm) (*http://hpslz24.cern.ch:8080/others/rem_exec.html*)
- Synchronization of LabView application with an accelerator's cycle (*http://hpslz24.cern.ch:8080/sync/LV_sync.html*)
- An Object-Oriented technology in LabVIEW programming (*http://hpslz24.cern.ch:8080/others/LV_oop.html*).

According to CERN-JINR Cooperation Agreement on PC-based distributed computing - NICE (Novell Integration, Coordination and Evolution), in 1997 the following has been done:

- Extension of NICE environment to the Windows NT and Windows 95 operating systems.
- The work to prepare the replacement of NICE by NICE-95/NICE-NT at JINR. Now NICE-95/NICE-NT are under experimental operation at JINR.
- The beginning of the replacement of Novell Netware servers by Microsoft Windows NT servers.
- The joint CERN-JINR development of the different approaches in creating a scaleable management scheme for Windows NT.
- Development of the installation for Windows NT 4 desktops from network .
- Extension of Web-service under NICE95 (nicewww) to support the interactive applications.

# COMPUTATIONAL PHYSICS

In 1997 research in computational physics were in progress. More than 100 scientific works were published and reported at the international conferences.

Work has been progressed on modification of codes developed on the basis of the mathematical methods of cellular automata and artificial neural networks for the solving problems of track recognition, search and identification of secondary vertexes in experiments DISTO, ATLAS, CERES/NA-45, EXCHARM and STAR *[S.Baginyan et al., Comp.Phys.Commun., 1266, 1997; M.P.Bussa, V.V.Ivanov et al., NIM, A389, 1997, p.208; G.Agakishiev, E.Kolganova et al., NIM, A394,1997, pp.225-231]*. Within the DIRAC collaboration the modelling programs GEANT-DIRAC were developed and maintained, and research on designing a 3-level neural net trigger to measure dimesoatoms lifetime was in progress *[V.V.Ivanov, P.V.Zrelov, to be publish. in Int.J.Comput. and Math. with Applications]*. Research on parametric and nonparametric meth-

ods for the Gaussian form's peak separation was performed. *[G.Agakishiev,...,G.Ososkov et al., JINR Commun. E10-97-105, 1997].* The algorithms developed have been tested on model and real data. The problem were solved on the basis of a wavelet transformation of initial data.

Numerical methods have been developed for a description of a behavior of the complicated dynamic systems. Computational models for dipole magnet projects VULKAN-1 and VULKAN-2 of ALICE setup are elaborated. Calculations of 3D magnetic field and magnet characteristics are performed *[P.G.Akishin, et.al. JINR Rapid Comm, N1 (81), 1997, pp.81-941].* The work on development of EXCARM setup SP-40 magnet's computational model is carrying out by means of measured field data analysis and inverse problem solution. Measured magnetic field quality criterions are proposed and the field is analyzed.

Calculations were continued, algorithms and software were elaborated related to the development of wave theory of nature of elementary particles and the research of their structure and the resonance mass distribution *[F.A. Gareev, M. Yu. Barabanov and G.S. Kazacha, JINR P2-97-292, subm.to Izvest.RAN; JINR E4-97-183 subm. Yad.Fiz.].*

With the help of a mathematical model of inelastic collisions of high energy nuclei developed at LCTA when analyzing experimental data of the international collaboration EMU-01/12 on interaction of aurum ions and photoemulsion nuclei, an unknown feature of the high energy fission reaction - a spherically symmetric emission of a large number of nuclear fragments at once - has been discovered *[M.I.Adamovich,..,V.V.Uzhinskii et al., Zeit.fur Phys A, 1997,358,p.337].*

Computations have been performed for M1- and E1 strength distribution up to Giant resonances in deformed nuclei. It has been shown that the calculated fragmentation of the M1 force lower than 4 MeV in Er-166, Er-168, Yb-172, Yb-174 and Hf-178 was stronger than that in Dy and Gd. This was in agreement with experimental data *[V.G.Soloviev, A.V. Sushkov, N.Yu.Shirikova - RIKEN Symposium on Giant Resonances, 1997, Editors: N.Dinh Dang and S. Yamaji, pp 47-60; Yad.Fiz., 60 N10, 1997, pp.1754-1764].*

Within the collaboration of LCTA and FLNR, St.Peterburg Institute of Physical Research and the Russian Research Centre "Kurchatov Institute", computations have been in progress on quasielastic scattering and total cross-section for some systems using densities created in nuclear-structural models and the full M3Y effective nucleon-nucleon forces *[O.M.Knyazkov,I.N.Kuchtina,S.A.Fayans, Particles&Nuclei, 28, N4, 1997].*

An elasto-dymanical model of macroscopic dynamics of symmetric nuclear fission has been formulated. Modelling has been performed and, for example, obtained was a macroscopic barrier of symmetric nucleus fission of a superheavy element $^{114}298$, the fusion of which has been planned at experiments under



way at FLNR/JINR *[S.I.Bastrukov et al., Int.J,Mod.Phys., E6:(Nucl.Phys.),N1, 1997,p89-110; J.Phys., G23 (nucl.Phys.), 1997,L322].*

In order to describe direct interaction processes of heavy ions with nuclei, a method of high-energy approximation has been developed, allowing one, in fact, to get the amplitudes of elastic, inelastic scattering and nucleon transfer reaction in explicit form *[A.I. Embulaev et al., JINR P7-97-185,subm. to Izv. RAN].*

Numerical solution of nonlinear heat equation is performed to simulate the evolution of thermal field induced by high current ion beam treatment of the metallic target. The dependence of the heating rate and the melting depth are obtained as a function of ion beam intensity *[E.A.Airyan et al.- JINR Rapid Comm, N6 , 1997].*

The development of effective methods and algorithms for numerical investigation of Cauchy problems for the classical Hamiltonian systems is in progress at LCTA in 1997. This problem resulted from modelling the process of nuclei fragmentation at FOBOS experiment. The efficiency of the approach is shown in dynamic computations for few-body systems with some pair potentials *[P.G.Akishin, I.V.Puzynin, S.I.Vinitsky, Int.J.of Modern Phys., 12,N1,1997,119-124; Comp. Math.Applic. v.34.N2-4, pp.45-73, N5-6, pp.613-625, 1997].*

The fractal properties of some objects (irradiated thin films, pictures taken in cosmic space, chaotic signals) were investigated. On the basis of a computer analysis of the objects some conclusions have been made on nature of the respective processes. In addition, research has been carried out on fractal properties of the signals from a function analysis viewpoint *[M.V.Altaiski, et al., JINR Rapid Commun.,2[82]-97,pp.37-46].*

A two Fortran 77 codes are developed. The first one (ASYMPT) calculates asymptotics of potential curves and adiabatic potentials with an accuracy of $O(\rho^{-2})$ in the framework of the hyperspherical adiabatic (HSA) approach. It is also shown that matrix elements of the equivalent operator corresponding to the perturbation $\rho^{-2}$ have a simple form in the basis of the Coulomb parabolic functions in the body-fixed frame and can be easily computed for high values of total orbital momentum and threshold number. The asymptotic potentials obtained can be used in the second code (HSEIGV) developed for the calculation of the energy levels and radial wave functions of two-electron systems in the adiabatic and coupled-channel approximations of the HSA approach. In this approach, the solution of the six-dimensional Shrödinger equation describing the dynamics of a two-electron atomic system is reduced to the solution of a system of coupled second-order ordinary differential equations in scattering (radial) coordinate $\rho$. The program is applied to the calculation of the energy values of the ground state and several double excited states of $H^-$ below the $n=2$ threshold. *[A.G.Abrashkevich, I.V.Puzynin et al., Preprint JINR, E11-97-326, E11-97-335, 1997].*

Approaches to construction of asymptotically optimal interface solvers are elaborated for the solution of nonlinear elliptic problems with anisotropic coefficients varied sharply within the domain *[B.N.Khoromskij, G.Wittum.to apper in Numer. Math.]*. The approaches are based on an efficient sparse approximation to the related Schur complement matrices and on the construction of efficient multilevel iterative methods for solving arising interface equations.

The development of methods, algorithms and program tools of computer algebra is in progress. Main attention was done to development of algorithmic and computer algebra aspects of Feynman diagrams computation, program for constructing finitely presented Lie algebras and superalgebras *[Gerdt V.P., Kornyak V.V. Nucl. Instr. and Meth. in Phys. Res. A 389, 1997, 370-373; V.P.Gerdt, V.V.Kornyak, Russian Journal "Programming and Computer Software", 3, 1997, 58-71]*.

## Maintenance of the UC computational-informational structure

The UC/JINR computing complex has been upgraded jointly with the UC staff.

- A UNIX-server has been put into operation (computer ALPHA-400 under the UNIX Digital operating system); a Samba system, providing network access to home-directories (disk assembly) from PCs; a system for WWW-pages and an e-mail system for UC staff and students, including the POP3 system have been installed.
- A multi-media server MMS to provide graphic, video and audio information processing has been installed.
- One more computer classroom has been equipped.
- The network architecture of the complex has been reorganized, all computers are operating in a "twisted pair" network environment.
- A network server (Novell server and network router) was modernized.

## PARTICIPATION IN RUSSIAN INTERDEPARTMENTAL PROGRAMMES

In 1997 LCTA took an active part in realization of several interdepartmental programmes:

**1. "Creation of a National Network of Telecommunications for Science and Higher Schools"**

- development of the network RBNet and earth channels (section of the Programme 3.3.2. jointly with RosNIIROS);



- development of the network RUHEP - "Dubna-Moscow" link creation (jointly with the Research Institute for Nuclear Physics MSU);
- head organization within the project BAPHYS - creation of a data base network for nuclear physics.

**2.** Working out an interdepartmental programme **"Creation of high-performance computer centres in Russia"** ( funds have been allocated for organization of HPCC at JINR).

**3.** A project "A computing farm for solving the problems of modeling and mass processing of homogeneous physics information" has been worked out for participation in the programme **"Advanced Information Technologies".**

## PLAN FOR THE YEAR 1998

- To finish the ATM-project on creation of the ATM-based backbones in all JINR laboratories.
- To provide a reliable operation of the external communication links by means of a tender selection of the service-provider.
- The most reasonable strategy for development of external computer communications for JINR, in view of the limited funds, involves aid in solving the question on creation of a node for a high-speed Europe Backbone (project TEN34) in Moscow, as well as a high-speed communication link to the USA in frames of projects on the development of the national network of computer telecommunications for science and higher schools.
- To start up the HPCC at JINR at its first stage -SPP2000+DLT robot+mass memory system.
- To realize a first step in creation of the computing farm.
- To work out a project on organizing an electronic complex for message exchange within JINR by using a unified data base of all registered JINR users.
- To install an electronic libraries server, based on HPC servers (full-text data bases, photoarchive data bases, physics data bases etc.)
- To design a centralized Backup system for general JINR servers by using the HPC facilities.
- To pursue a policy of software standardization and licensing for creation of workplaces for users of the JINR networking informational-computational infrastructure(NICE95/NT).
- Further development of algorithms and methods for researches under way at JINR:
  1. Development of new cascade models for simulation of complicated multifactor problems of nuclear and particle physics. Modelling the

nucleus-nucleus collisions taking into account pomeron interactions for experiments planned at CMS.

2. Maintenance of a data base and an electronic reference book of particle-particle and nucleus-nucleus interaction cross-sections.
3. Creating modern computational tools for data processing and data analysis on the basis of new statistical methods, artificial neural networks and cellular automata. Software design for experiments in low, intermediate and high energy physics: FOBOS, CORSET, DIRAC, NEMO, STAR, EXCHARM, ATLAS, etc.
4. Development of multilevel adaptive algorithms and software for modeling magnetic fields and beam transport problems and application to modern experimental set-ups (ALICE, EXCHARM, U400M-U400).
5. Creation of new algorithms and software for solving nonlinear multidimensional equations that simulate the behavior of complicated physics systems. Algorithmic and software support of theoretical and experimental investigations of nuclei structure.
6. Construction of high-accuracy computational schemes for numerical study of the dynamics of physics systems, taking into account randomness, fractal and stochastic factors of interaction.
7. Development of computer algebra methods to study non-linear algebraic equations, differential equations in partial derivatives; to describe the behavior of dynamic systems phase trajectories; for analytical computation of many-loop Feynmann diagrams in gauge theory with massive particles.