Scientific report on the completion of Theme 1119 on 2014-2016

Gheorghe Adam, LIT-JINR & IFIN-HH

1. **Title of the theme.** 05-6-1119-2014/2019, “Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data”
   Priority: 1
   Leaders: Gheorghe Adam, Petr V. Zrelov
   Theme beginning: 2014
   Participating JINR Laboratories: LIT, VBLHEP, BLTP, FLNR, FLNP, DLNP, LRB, UC
   Participating Countries, Institutes and International Organizations:
   Armenia, Australia, Azerbaijan, Belarus, Belgium, Brazil, Bulgaria, Canada, CERN, China, Czech Republic, France, Georgia, Germany, Greece, India, Italy, Japan, Kazakhstan, Moldova, Mongolia, Poland, Portugal, Romania, Russia, Slovakia, South Africa, Switzerland, Taiwan, Tajikistan, USA, Vietnam.

2. **Abstract**

The present report summarizes the most important achievements obtained within the JINR research theme 05-6-1119-2014/2016, “Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data”.
The organization of the presentation selects the most outstanding examples from the multitude of specific tasks solved within the theme 1119.

3. **Introduction.**
The theme 1119 is placed at the crossroad of the JINR research topics which need the computing as an indelible part of the accomplished research effort toward the solution of their specific scientific objectives.

The period covered by the present report corresponds to the last three years of the seven-year plan for the development of JINR 2010-2016. Within the broad research effort deployed in JINR, the expertise of the LIT scientists was needed for the solution of computing tasks asked by over 40 JINR scientific projects.

The possibility to gather a large spectrum of particular questions under the common umbrella of the theme 1119 comes from the existence of a *common mathematical background* of all these projects. The basic requests to the solutions provided by the LIT scientists are their *reliability*, *stability to perturbations*, *low computational complexity*, and *rapid convergence* of the numerical algorithms. There are, nevertheless, features of the real research world which strongly counteract the efforts to derive *perennial* solutions to the raised problems.

One feature comes from the very nature of the physical problem. For instance, the derivation of sound algorithms for *Monte Carlo data simulations* or *data processing and analysis* heavily depend on the details of the experimental setup. The addition of new features aimed at improving the existing experimental setup may simply invalidate a previously derived *optimal* solution. Radical changes of the algorithm design and of its implementation into a software code may be asked in order to provide a sound solution able to cope with the new reality of the setup. This feature illustrates the empirical observation that the implementation and maintenance of the software support to a given experiment are needed during the whole lifetime of the experiment itself.

Other instances regard the failure of the attempts to use brute force numerical methods for the solution of complex mathematical models of physical phenomena for which the perturbation theory does not work. Then the expectation that the straightforward discretization of the definition domain will hopefully converge to a meaningful solution under *discretization refinement* can fail badly. Problem adapted approaches can alleviate the difficulties and result in solutions with physically meaningful features.

The *rapidly evolving hardware-software environment* (HSE) is a source of (sometimes severe) *inefficiency* of the numerical algorithms and software which were previously optimized for other generation hardware. The substantial hardware changes ask for fundamentally different software implementations able to fully exploit the new possibility opened by the new hardware parallelism. This asks, first, for new mathematical methods and algorithms enabling efficient information flow inside the new hardware. Second, it asks for the grasp of alternative programming paradigms and programming languages.

The evolving HSE allows the solution of more sophisticated theoretical models, characterized by newly added features which make them more realistic. The reliable numerical or symbolic-numerical solution of such models asks, in its turn, for the development of new approaches to their solutions.

From the wealth of scientific results derived during 2014-2016 within the theme 1119 on the symbolic-numerical and numerical solution of a wide range of topics of interest to the JINR research, the present report will be selectively focused on cases of utmost difficulty.

4. The heterogeneous computing cluster HybriLIT, strategic development for high performance computing in JINR

The broad spectrum of the computing intensive tasks asking for symbolic-numerical or numerical solutions in JINR needs adequate computing facilities. The strategic mission of the heterogeneous computing cluster HybriLIT, under development in LIT-JINR as an indelible part of the Multifunctional Information Computing Complex (MICC) [1-3], is to provide the coverage the high performance computing (HPC) in JINR.

The basic motivation for the HybriLIT implementation in LIT-JINR followed from the *hardware revolution* which started about a decade ago and became since pervasive all over the world. In the context of the full replacement of the *single-processor chips* with a variety of *multi-core processor* dies, *manycore processor* dies, GPU *accelerators* in conjunction with multi-core processors, it became obvious that the *parallel computing* is the most necessary future development in JINR, which needs adequate infrastructure support in LIT.

After a necessary clarification process, which requested the corroboration of several key issues, the conception concerning the HybriLIT development has been formulated by the LIT management and steps for its practical implementation were taken, with the approval of the JINR Direction, during the second quarter of the 2014.

The HybriLIT cluster has had a short but rapid evolution driven by the supervision and the key decisions of the LIT management concerning its design and implementation: Modular development based on the most successful new hardware offers on the market. This decision mainly followed from the study of the trends in the buildup of the largest HPC facilities worldwide. Periodic scrutiny of the biannual TOP 500 lists [4].

A major component of the information-computing infrastructure is the *on-line information and organizational user support* through: the HybriLIT web-page [5], the HybriLIT devoted Indico system [6], the HybriLIT user support service [7] (for registered users), the HybriLIT GitLab service [8].

Bilingual support in Russian and English of all web resources meets the needs of scientist and specialist users from different countries.

The nowadays HybriLIT can be characterized as a scalable top level HPC facility which adequately covers the needs of a wide variety of users from the JINR and JINR Member States within a threefold way: (a) design of parallel algorithms and their implementation into software packages enabling running parallel jobs on modern HPC facilities; (b) use of program packages and specialized mathematical libraries adapted to the newest computing architectures; (c) carrying out massive-parallel and resource-intensive tasks.

This is not the end of the HybriLIT development but rather the beginning of a long process for its future extension. This process involves, among others, *correlated* HybriLIT developments with the other MICC components, deep investigation of the HybriLIT features enabling automatic control and enforcement of the *consistency* of its operation, *optimization* of the inner resource distribution and organization through a variety of techniques, etc.

►HybriLIT Enables Implementation of Efficient Numerical Methods for Hardly Solvable Problems

(1) The Asynchronous Differential Evolution Method (ADE) [9] allows efficient global numerical optimization for functions which are non-differentiable, non-continuous, and multi-modal. Its properties of asynchronicity, restart to get out from a fake minimum, and directionality of the search by taking into account pair correlations have been implemented in an efficient HybriLIT code able to solve complex different physical models: the ADE-SFF structural analysis of vesicular systems [10,11] (Fig.1) and the hybrid optical potential description of various nuclear processes like the elastic scattering and fragmentation processes [12, 13] and the computation of total interaction cross-sections of exotic nuclei [14].

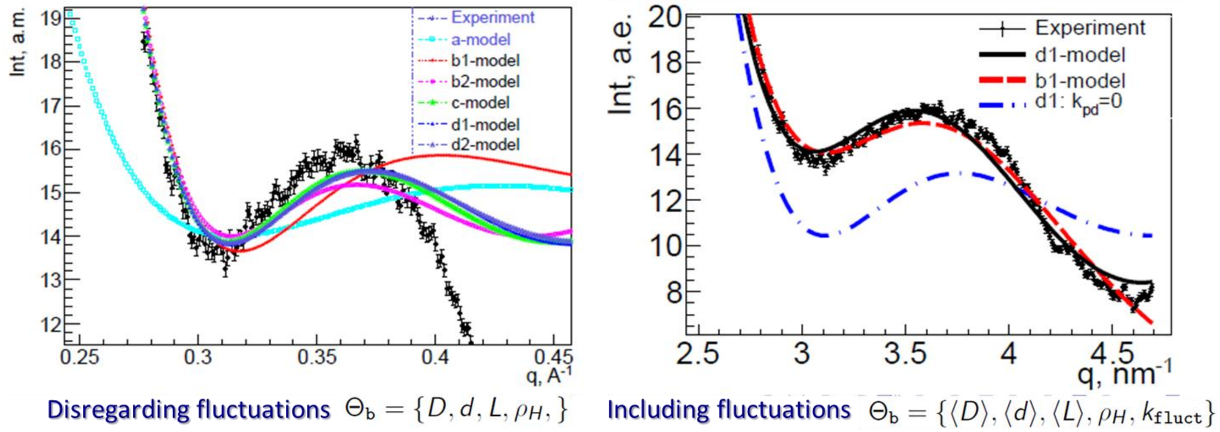


Fig. 1. Modeling the structure of poly-dispersed lipid DMPC (1,2-dimyristoyl-sn-glycero-3-phosphocholine) vesicles solvated in 40% sucrose solution. Analysis of small-angle scattering of synchrotron radiation data used the method of Separate Form Factors (SFF), modified in order to include the fluctuations of the lipid bilayers. The fitting of the parameters responsible of the vesicular structures was based on the ADE algorithm.

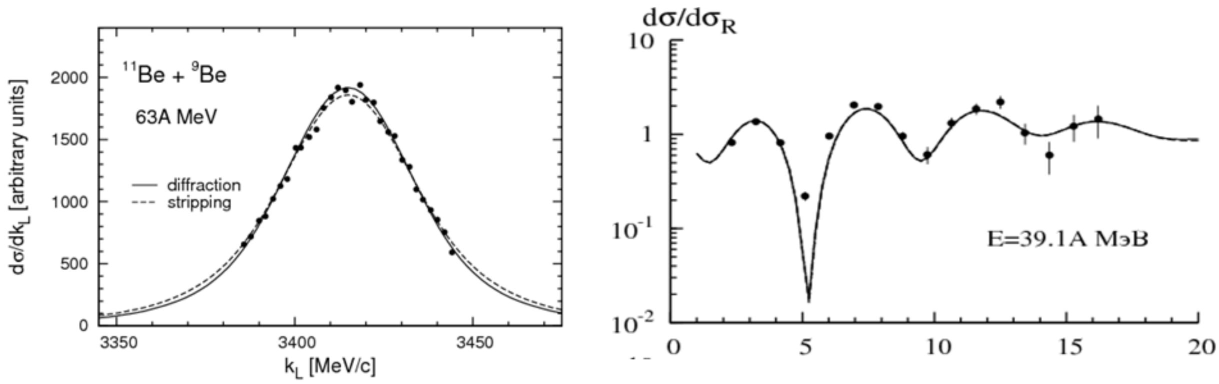


Fig. 2. Analysis of elastic scattering and fragmentation processes of ^{10}Be+^{12}C [PRC 91 (2015) 034606]

(2) In the framework of the ongoing collaboration between Many-Body Theory of Bosons group at the Center for Quantum Dynamics, Heidelberg University and the LIT, theoretical investigations of the highly-non-equilibrium quantum dynamics realized in trapped systems of ultra-cold atoms and molecules were performed. In particular, the development and optimization of the Multiconfigurational Time-Dependent Hartree for Bosons (MCTDHB) package designed to solve the many-body Schrödinger equation for bosons were done. The program modules designed for the MCTDHB package are intended to perform 1D, 2D and 3D computations on hybrid computing systems including multicore/many-core CPU and graphical accelerators. Parallel modules have been realized on the basis of present-day parallel programming technologies MPI+CUDA (MPI + PGI CUDA). The modules developed will be included into a new version of the package. A few instances of MCTDHB outputs are shown in Fig. 3. The development, implementation and preliminary computations were performed on the heterogeneous computing cluster HybriLIT (LIT JINR) and on the hybrid K100 cluster (Keldysh Institute of Applied Mathematics) [15]. A cross-platform package (working under operating systems Windows, Linux, and OS X), which is freely distributed and possesses a convenient graphic interface was developed

(http://QD-lab.org). On the basis of this package systematic studies of the dynamic properties of multiparticle quantum systems have been conducted [16].

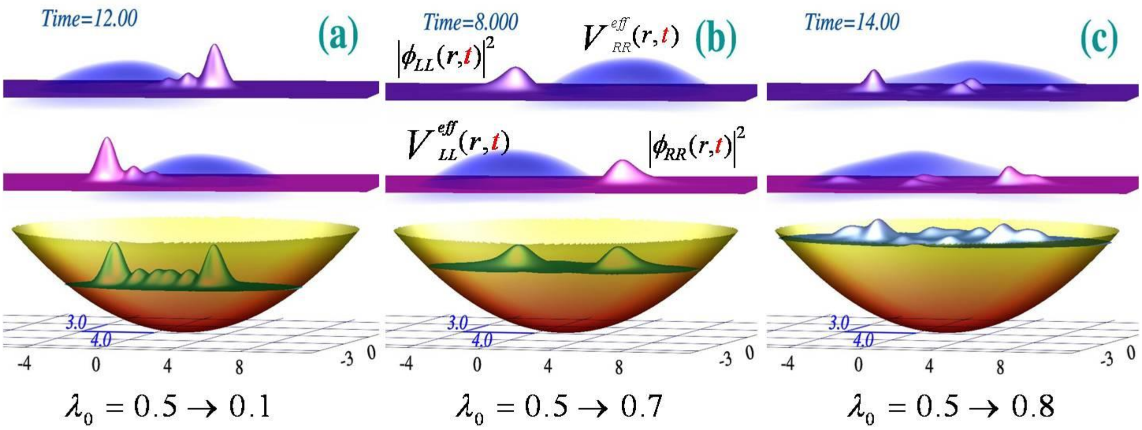


Fig. 3. Visualization of the interaction-induced time-dependent barriers in the two generic dynamical regimes of strongly-interacting trapped bosons (2D case) Evolutions of a two-fold fragmented initial state induced by a sudden displacement of the harmonic trap V(x, y) → V(x-1.5, y-0.5) with the simultaneous quench of the inter-particle repulsion: (a) strong decrease λ_0=0.5 → 0.1, snapshot at t=12; (b) moderate increase λ_0=0.5 → 0.7, snapshot at t = 8; (c) strong increase λ_0=0.5 → 0.8, snapshot at t=14.

(3) Dynamical model of the hydrated electron (polaron) [17, 18]. The boundary value problem of the polaron model was formulated and solved using our MPI/C++ code. The comparison of numerical outputs with experimental data (Fig. 4) shows that the developed model consistently describes the dynamics of the electron photoemission in water under the laser radiation in the ultra-violet range.

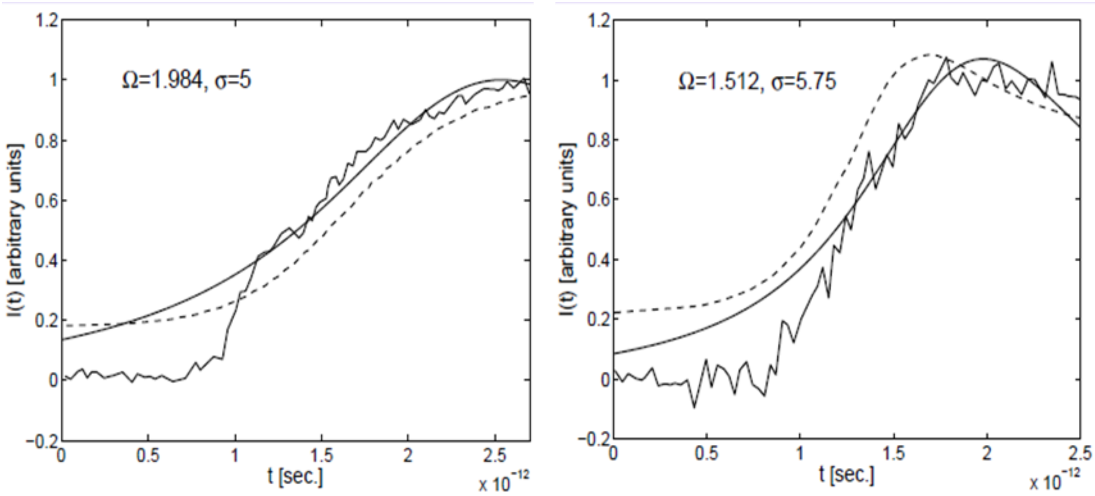
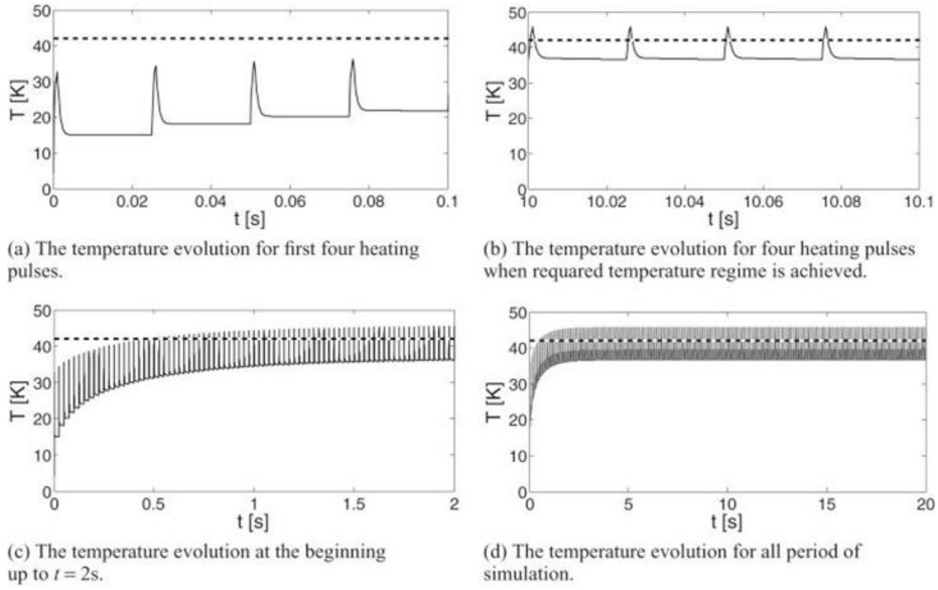


Fig. 4. Comparison of experimental data with theoretical predictions for electron photoemission in water under the laser radiation in the ultraviolet range

(4) Optimization of the design of an ion source cryogenic cell [19, 78] (Collaboration with VBLHEP). Simulation of the thermal behaviour of a multi-cylindrical device with a non-trivial design area and nonlinear thermodynamic properties of materials at cryogenic temperatures describes the model of a cryogenic cell designed for pulse feeding of working gases in the chamber of a source generating multiply charged ions. The mode of operation of the cryogenic cell asks for periodic valve opening and closing for injection of a gaseous substance in the millisecond range. The numerical simulation unveiled the existence of a transient regime at the beginning of the functioning cycle (Fig. 5).



(a) The temperature evolution for first four heating pulses.

(b) The temperature evolution for four heating pulses when requared temperature regime is achieved.

(c) The temperature evolution at the beginning up to $t = 2$s.

(d) The temperature evolution for all period of simulation.

Fig. 5. Regimes of the temperature evolution at the surface of the ion source cryogenic cell.

5. Support of Experimental Data Processing and Analysis

New mathematical methods and emerging software for reliable data acquisition are developed. Methods for dynamical image recognition under neutron diffraction on polycrystals enabling analysis of crystalline matter concerning crystallographic symmetry analysis, microstructural analysis, investigation of the kinetics of the matter processes at FLNP detectors; Methods for solving problems of the high "intellectuality" pattern recognition serving to the elaboration of new software for the automatic calibration of multi-detector systems in FLNR; Methods for solving ill-posed problems which emerge in the analysis of multidimensional distributions enabling elaboration of new software for the determination of times of decay by scintillators using an autocorrelation delayed coincidence time spectrometer in DLNP.

►Breakthrough advances in the analysis of spectroscopic data

The program VMRIA (Visual Multiphase Rietveld Analysis) (Fig. 6) denotes a continuously upgraded complex of program packages. It allows unique analysis of the widest possible classes of spectrometric data (including peaks of arbitrary shapes, 3D data) through pattern recognition of spectral components of arbitrary forms both by parametric and non-parametric methods [20, 21]. It enables reliable and unrivaled processing of Fourier diffractometer data. It is widely used in JINR (FLNP, DLNP), PNPI-Gatchina, MSU (Chemistry Faculty, INP-MSU), etc.

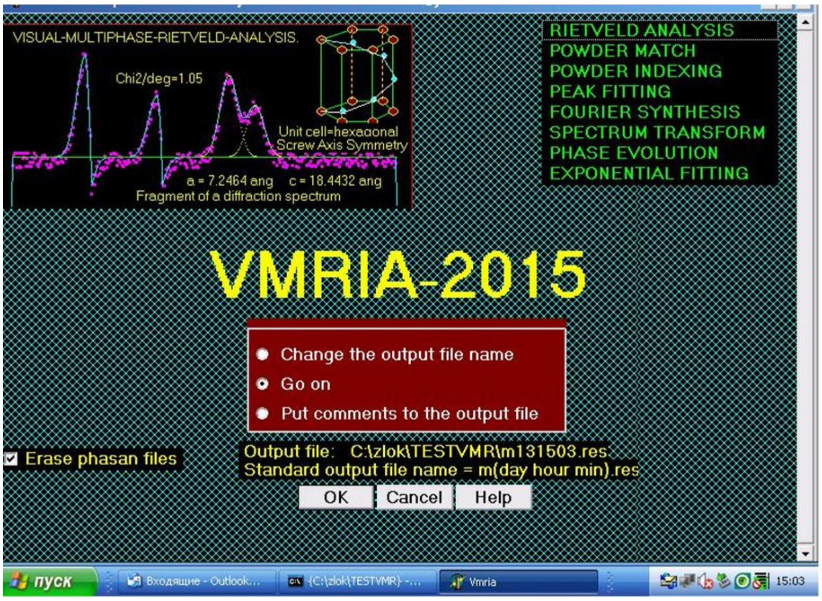


Fig. 6. Visual interface to a continuously evolving package for spectroscopic data analysis [V.B. Zlokazov, LIT]

►Automation of on-line data storage on modernized YUMO spectrometer at IBR2

An inspection of the JINRLIB software library, maintained both in English and Russian shows that a same LIT author (A.G. Soloviev) has contributed, among others, to the creation of the repeatedly upgraded programs SAS [22] and FITTER [23] which provide the online respectively offline information-computing environment for data processing and analysis of the most demanded IBR-2 detector, YUMO. The YUMO upgrade with position sensitive detectors will radically change the design and implementation of these packages in the near future.

►Robust fitting for the estimation of hidden parameters in experimental distributions on the plane [24, 25]

The robust fitting is shown to be the only effective automatic approach to the derivation, with acceptable accuracy, of the scintillator decay time τ from a measured energy dependence E=g(t; τ) (Fig. 7).

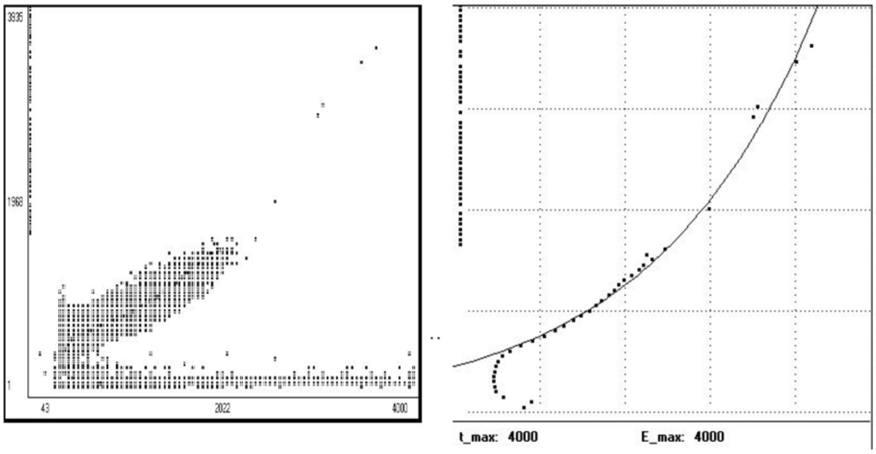


Fig. 7. Left: A raw 2-dimensional recorded distribution A(E; t). **Right**: The fitting function goes correctly through the points where it is adequate to the model, and ignores those where it is not (on the left side and at the bottom). The obtained result agrees with the known data (τ= 230ns)

► Reliable statistical inferences under low statistics and incomplete observation [26, 27]

This is a permanent problem asked for scrutiny by the low-statistics experiments. Instances: Confidence interval optimization for testing hypotheses under data with low statistics (Radioactivity: rare events); Robust fitting for the estimation of hidden parameters in experimental distributions on the plane.

New concept: *Optimal confidence interval*, based on the order statistics, enables both the parameter (mean) estimation and the statistical tests. On the one hand, this provides clear and natural data interpretation, and, on the other hand, means a good compromise between the criteria: ”the shortest interval length” – ”the largest size of the covering probability”.

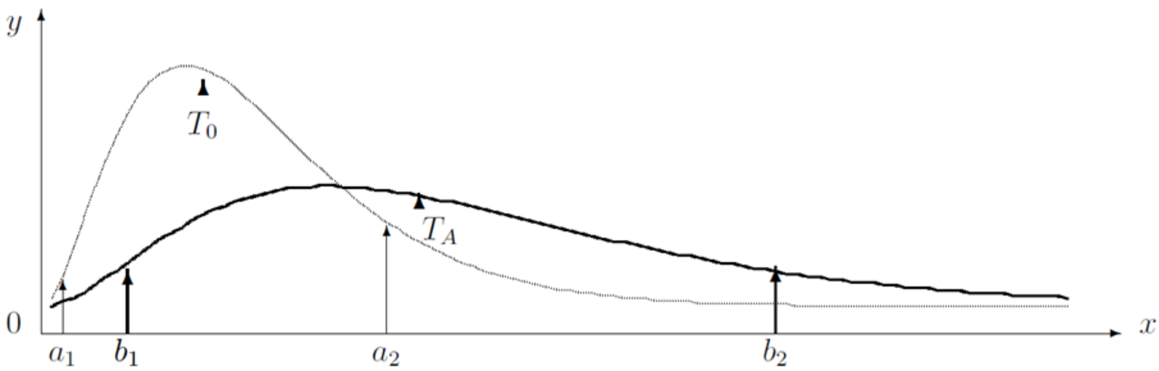


Fig. 8. Application of the concept of optimal confidence interval to the exponential distribution, which characterizes the radioactive decays and is very intolerant to the low statistics (m = 1-4 events): The gamma-distribution at m = 3. The confidence intervals [a1, a2] (thin line) and [b1, b2] (thick line) for the discrimination of the hypotheses T0 = 20 and TA = 40.

6. Development of Modern Investigation Tools in Large Scale International Collaborations

► Contribution to the upgrade of Geant4 package

Geant4 is a toolkit for the simulation of detector setup and response concerning the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, studies in medical and space science. The main Geant4 capability of simulating the hadronic interactions and electromagnetic showers is widely used by existing experiments at RHIC, LHC, as well as for simulations at the future accelerators FAIR and NICA.

Main yield of JINR scientists (V.V. Uzhinsky-LIT, A. Galoyan-VBLHEP): Development of the Fritiof (FTF) hadronic model, within the Quark-Gluon String Model (QGSM) originated by N.S. Amelin (LIT-JINR), for the simulation of interactions π, K, p, n, Λ, Nucleus+Nucleus, as well as Anti-proton, Anti-Nucleus+Nucleus. The series of proposed improvements have been included in successive Geant4 releases. Specific tasks solved: Improvement of string fragmentation; Improvements of processes cross sections; Inclusion of the Reggeon cascading for correct description of nucleus breakups; Improvement of parton momenta sampling.

Illustrations of the improvements of the FTF model are given in Figs. 9 and 10.

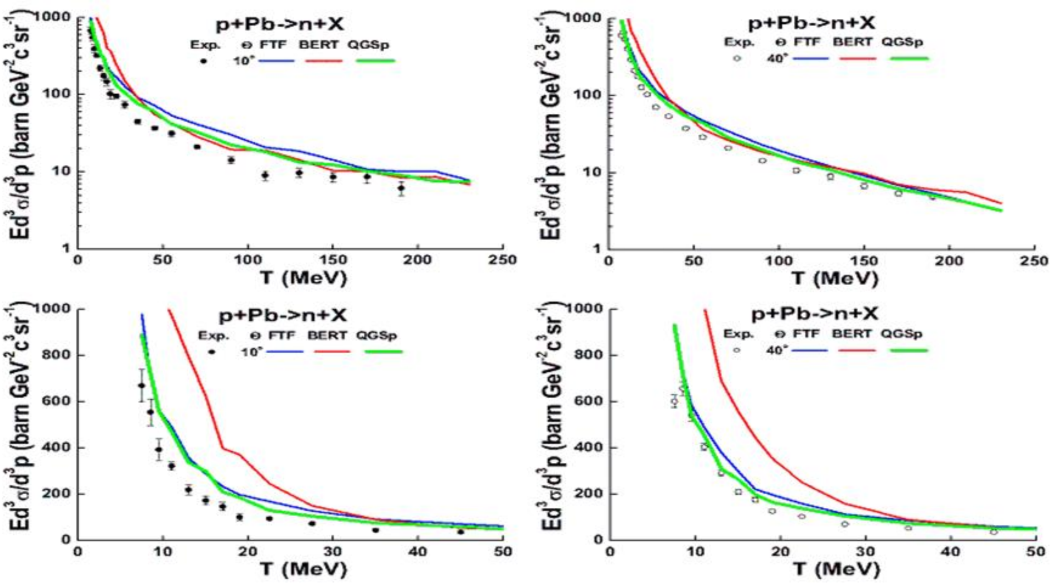


Fig. 9. Shower shape improvement of the slow neutron production (ITEP experimental data, 1983)

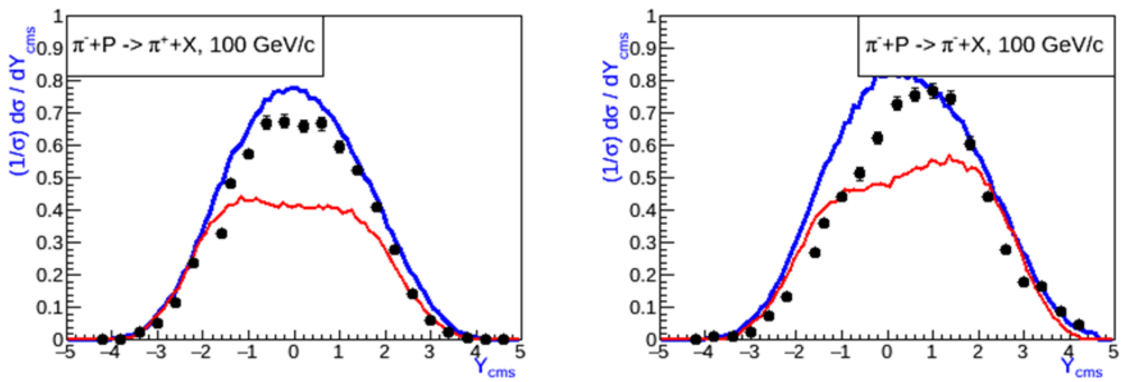


Fig. 10. πP interactions at 100 GeV/c. Red lines – old QGSp Blue lines – new QGSp

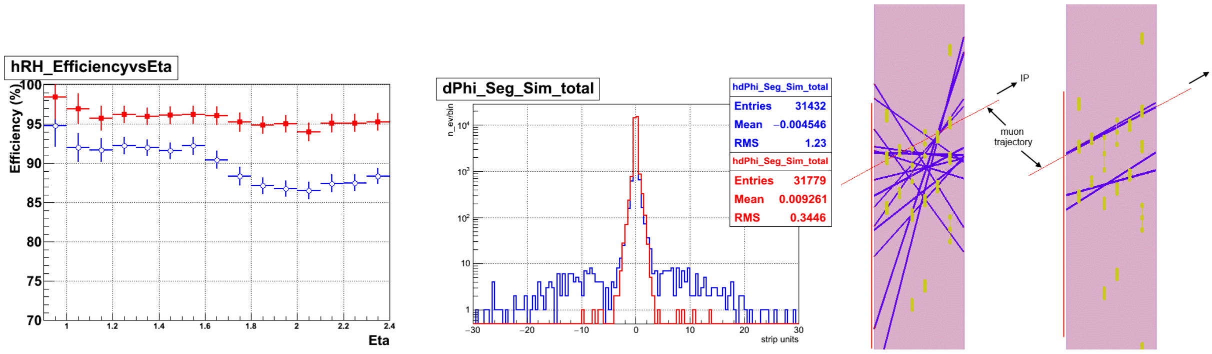
For the time being, the FTFP_BERT Physics List is a favorite Physics List of Geant4, QGSp being used by the ATLAS and CMS experiments. The present status of Geant4 [28] was defined with the important co-authorships of A. Galoyan (VBLHEP) and V.V. Uzhinsky (LIT).

► Contribution to the CMS experiment support

The new segment building algorithm [29] for the Cathode-Strip Chambers (CSC) from the CMS experiment was developed in order to improve the reconstruction for high hit rate and big backgrounds generated by "hard" muons. The efficiency with respect to pseudorapidity is shown in

Fig.11-a. The efficiency of the new algorithm is high and almost constant, while the efficiency of the standard algorithm decreases with the increase of the pseudorapidity [30]. The comparison of the difference in the azimuthal coordinate of the reconstructed and simulated segments (Fig.11-b) shows that the new algorithm reconstructs segments closer to the actual muon trajectory than the standard one.

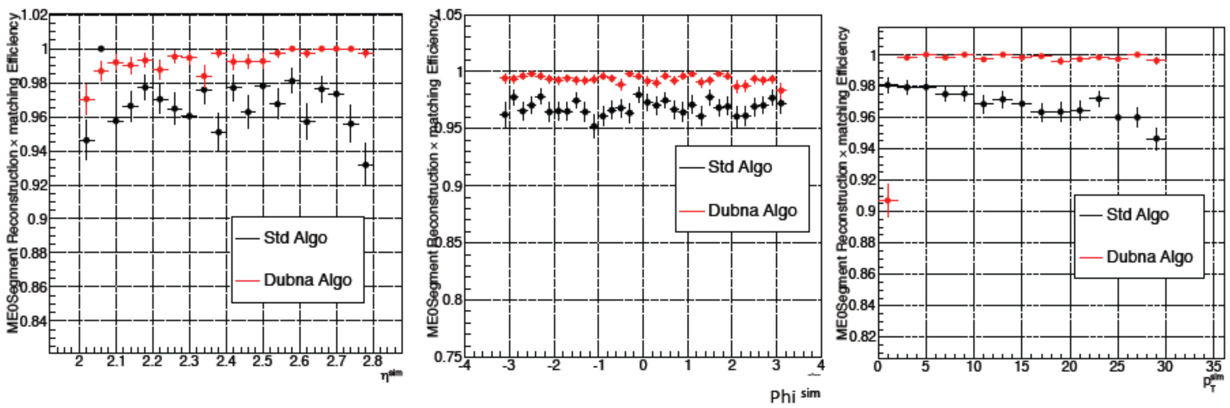
The developed algorithm takes into account the interaction point (IP) while reconstructing segments. As a consequence, the number of fake segments is considerably reduced in comparison with the standard algorithm. An example of a high hit multiplicity event is presented in Fig.11-c. The actual trajectory of the passing muon is drawn as a thin red line and almost coincides in direction with the IP. The reconstruction result of the standard algorithm is visualized on the left side of the picture. A lot of segments (blue lines) were reconstructed and all of them fail to reproduce the direction of the real particle. The new algorithm outputs for the same event are shown on the right part of the picture. Two segments are almost perfectly reproducing the trajectory of the muon and the overall number of segments is lowered to a reasonable amount.



a b c

Fig. 11. a – Reconstruction efficiency vs. pseudorapidity (standard algorithm – blue, new algorithm - red); b – the distance in strip units between the reconstructed and the simulated segment (standard algorithm – blue, new algorithm - red); c – example of a high hit multiplicity event (standard algorithm – left, new algorithm – right).

The new algorithm was implemented in the official CMS software package in July 2016. It proved to be effective, stable and robust. It was easily adopted as the reconstruction algorithm for the *new* GEM *detectors* that will be included in the experimental setup for the next major upgrade. The reconstruction efficiencies of the new (red) and the standard (black) algorithms with respect to different parameters are shown in Fig. 12. The new algorithm shows a high (~100%) and constant efficiency, regardless the parameter of interest. There is hope that new algorithm will become the default reconstruction algorithm both for the CSC and the GEM detectors of the CMS experiment.



a b c

Fig. 12. Reconstruction efficiency vs. different parameters of the simulated data. a – efficiency vs. pseudorapidity; b – efficiency vs. azimuthal coordinate; c – efficiency vs. transverse momentum of the muon.

► Contribution to the CBM experiment support

The planned CBM (Compressed Baryonic Matter) experiment at FAIR (Facility for Antiproton and Ion Research), GSI Darmstadt, Germany, has a rich program of investigations. The LIT-JINR team brings significant contributions to the solution of several tasks foreseen within the agreed activities defined in the frame of the CBM collaboration. Excerpts:

(1) The measurements of $J/\psi \rightarrow e^+e^-$ decays are among the basic tasks of the CBM experiment. The main results obtained during 2014-2016 may be summarized as follows (Fig. 13):

- An articulated methodology, including a chain of mathematical models and their algorithmic implementation was developed for the fast recognition and reconstruction of the rare decays J/ψ→e+e- registered by the CBM setup under the dominating hadronic background [31].

- Within the developed approach there have been defined the significant variables and boundaries enabling maximum background suppression and reliable signal identification [32].

- Comparative analysis of the efficiency of signal resolution has been done for two different approaches to the identification of the charged particles within the TRD detector based respectively on an artificial neural network (ANN) and a modification of the ωnk consistency criterion. Both have been found to show comparable effectiveness, nevertheless, the ωnk criterion has been found to show a number of advantages [31, 32].

- The ωnk based fast parallel algorithm allows a real time identification of the charged particles recorded by the TRD detector [33, 34].

O.Yu. Derenovskaya has successfully defended the PhD thesis “Methods and algorithms for recognition and reconstruction of the $J/\psi \rightarrow e+e^-$ decays in the CBM experiment”, on 24.04.2015.

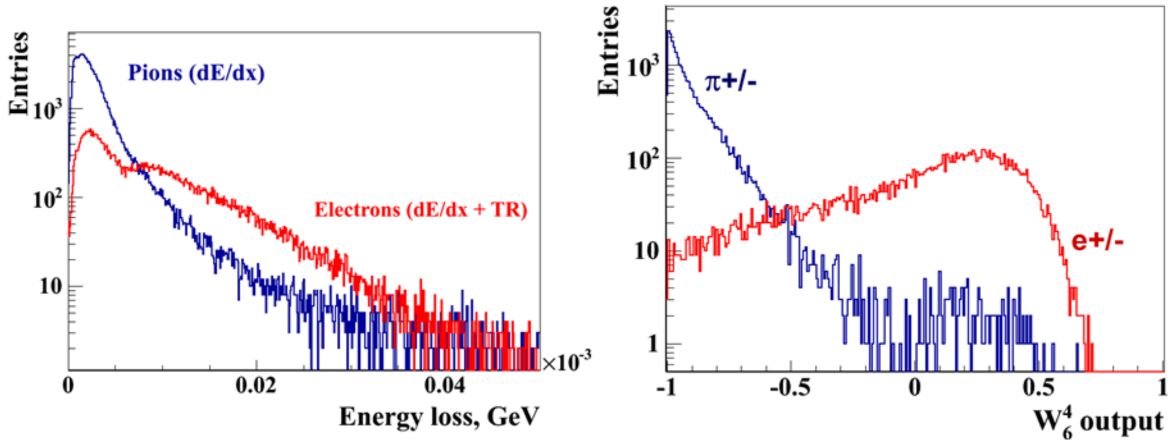


Fig. 13. Efficiency of the reconstruction of the $J/\psi \rightarrow e+e^-$ decays in the CBM experiment

(2) Investigation of event reconstruction in the muon MUCH station of the CBM setup. A fast ANN algorithm was developed for the identification and reconstruction of linear trajectories of the charged particles registered within the muon MUCH station. Based on these results, selection criteria for the $J/\psi \rightarrow \mu+ \mu-$ decays have been proposed which enabled the background suppression by a factor of 1000 [35].

► Software support for the microstrip GEM chambers of the BM@N experiment of the NICA project

(1) Track Reconstruction in Drift Chambers (DCH) and Momentum Estimation in BM@N experiment (excerpts) [36] (Figs. 14-16)

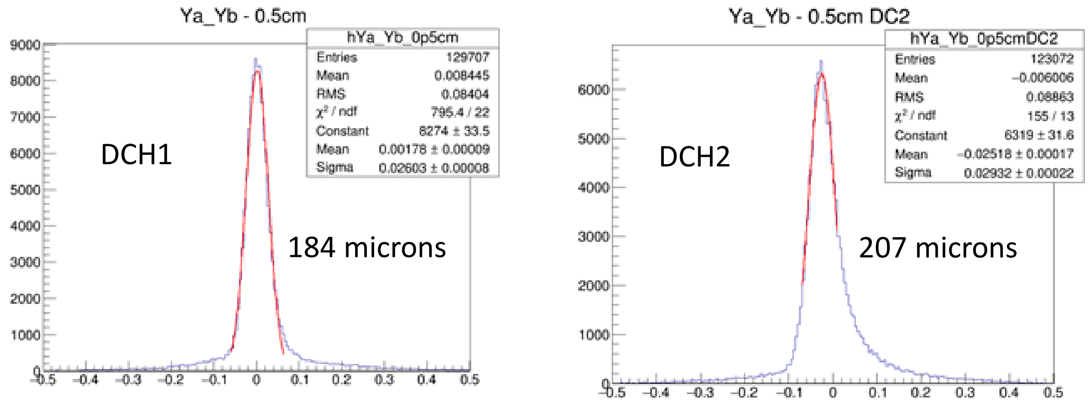


Fig. 14. BM@N First Test Runs with Nuclotron beams [February-March 2015]: Two DCHs have been used. The best resolution was obtained for the Y-coordinate

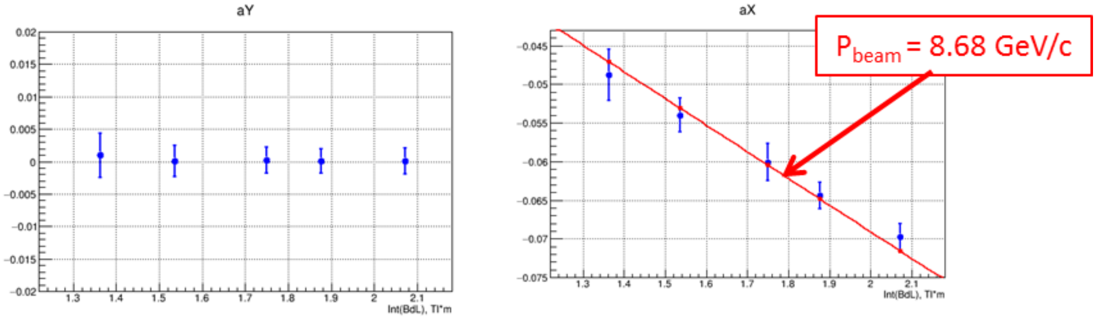


Fig. 15. The DCHs have been aligned to the beam (track reconstruction with the both DCHs): Y-slope is close to zero; X-slope [extrapolated to magnetic field B=0] is close to zero

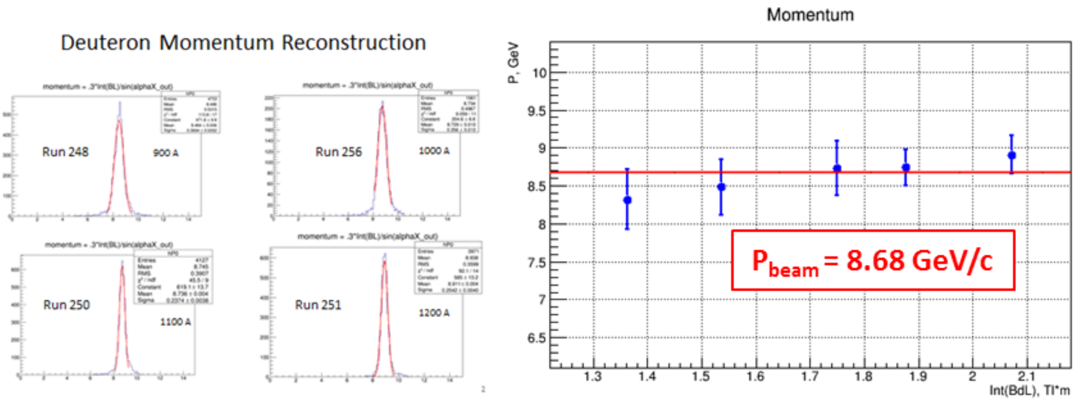


Fig. 16. Estimation of deuteron beam momentum at different magnetic fields using X-slope

(2) Software for BM@N GEM (Gas Electron Multiplier) tracker [37] involves two tasks.

- *Realistic Simulation of the GEM detector* needs development of data generation algorithms which take into account features controlling the actual data in the GEM chamber: the signal deviation under external magnetic fields and the influence of the angular deviation of the flying particle from the beam axes to the shape and the size of the strip cluster (signal). Fig. 17 – left provides Garfield++ simulation of the process of formation of avalanches of electrons (signal) inside the GEM chamber.

- The coordinate reconstruction of the track spatial points registered by the detectors (hit reconstruction algorithms) assumes the development of algorithms able to restore the coordinates of the particle trajectories across the detector planes (hits). The hits serve as inputs to track finding methods.

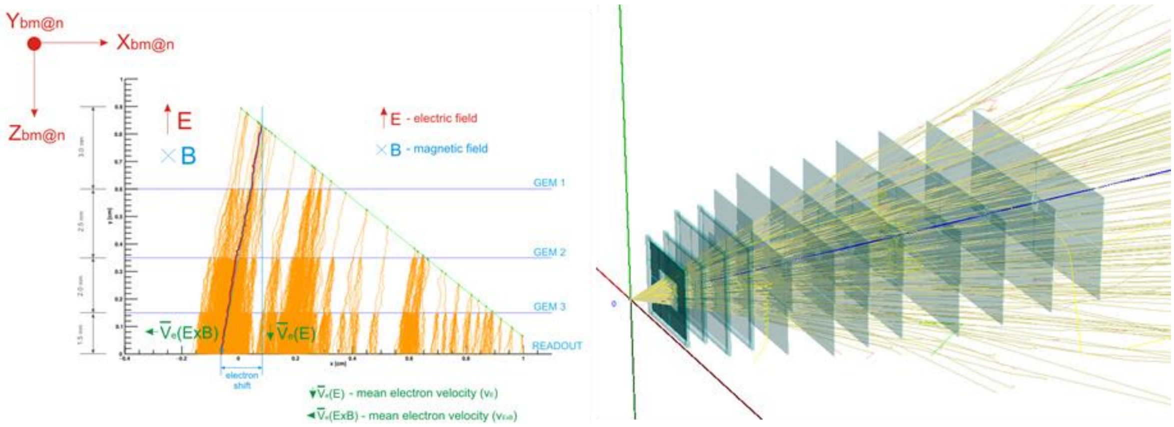


Fig. 17. Left: Garfield++ modeling the process of formation of avalanches of electrons (signal) inside the GEM chamber. The green line denotes the track of the particle traversing the GEM chamber. The orange color marks electron trajectories provoking avalanches. The avalanche signal is registered by the readout plane. **Right**: A realistic version of the complete configurations of the GEM detector of the BM@N experiment.

► **Modeling magnetic components of large scale facilities** [115-119]

The buildup of 3D computing models of the dipolar and quadrupole superconducting magnets entering the NICA (JINR) and SIS100 (GSI) facilities, the computation of the distributions of the magnetic fields within the working regions of the magnets are intrinsic parts of the certification process of the newly constructed magnet modules in VBLHEP.

Two cases worked out by P.G. Akishin are shown in Figs. 18 and 19.

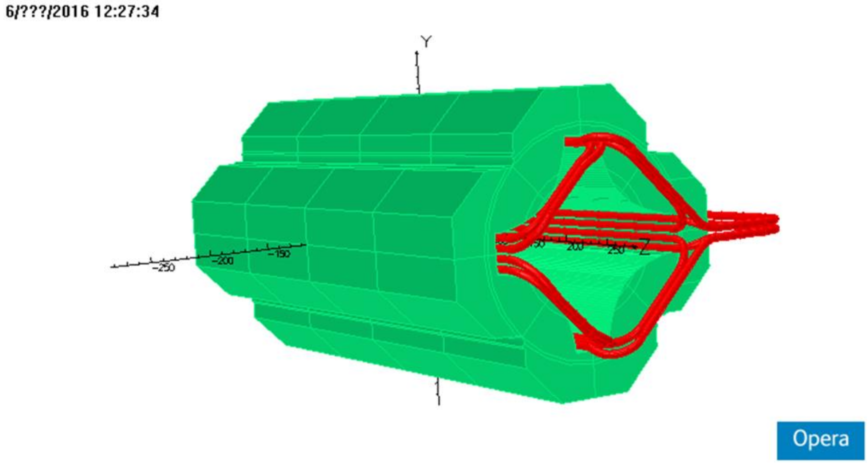


Fig. 18. Analysis of the distribution of the magnetic field inside the booster quadrupole magnet (NICA)

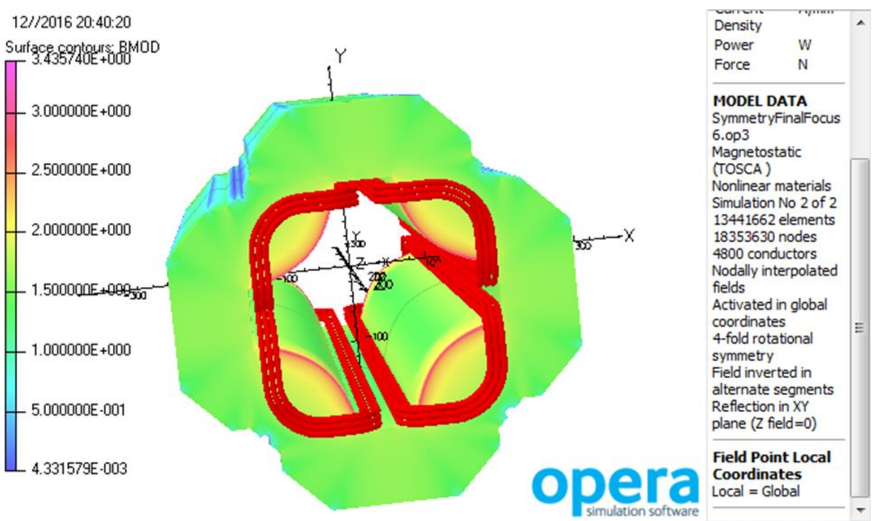


Fig. 19. Analysis of the magnetic field distribution inside the final focus lense (NICA)

7. Solution of difficult mathematical problems with guaranteed output under controlled accuracy

► New Ways of Reducing Extreme Inner Problem Complexity

- ***Embedding the original problem in a different approximation space*** enables considerable extension of the grasp of particular solutions. A striking example is the derivation of unified symbolic-numerical solution of boundary-value, resonance, and scattering problems by means of finite element method based on interpolatory Hermite polynomials [38-50].

Successive developments combining together the Kantorovich method, the finite element method, and asymptotic methods resulted in a complex algorithm implemented in a series of symbolic-numerical and numerical packages for the investigation and simulation of few-body quantum systems with application to nuclear and atomic physics. The designed algorithms and created programs allow solving, with high accuracy, the boundary-valued problems for the multidimensional Schrödinger equation and for certain systems of second-order ordinary differential equations, to compute the related eigenvalues and eigenfunctions, to compute metastable and resonance states, to solve scattering problems and problems of tunneling through repulsive barriers. These program packages, which are quite useful for a wide range of users, were published in the CPC Program Library and in JINRLIB. Four LIT authors (O. Chuluunbaatar, A. Gusev, V. Gerdt, and V. Rostovtsev from a total of ten) have been rewarded with the JINR Second prize (2015) for this problem-oriented complex of programs.

Two illustrations (Fig. 20 and Fig.21) show the power of the developed package.

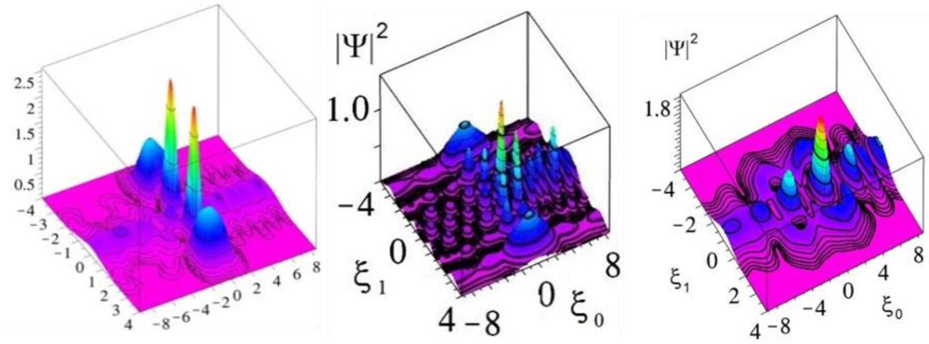
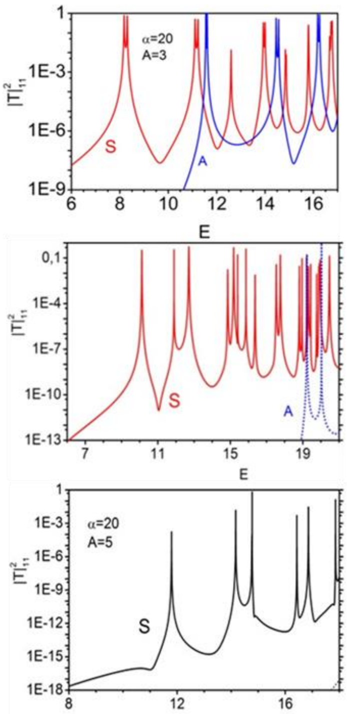


Fig. 20. Probability densities of sub-barrier resonance transmission, over-barrier and over-well resonance reflection of two-particle cluster



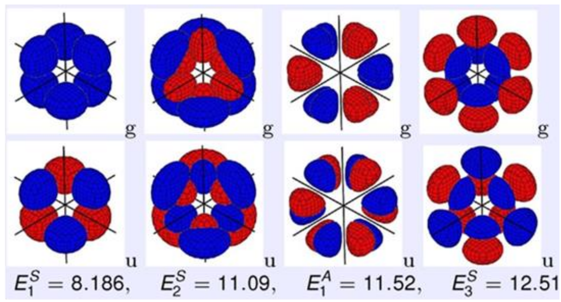


Fig. 21. Left: The isosurfaces of first g-u doublets of symmetric (S) and antisymmetric (A) metastable states corresponding to the first four peaks of the transmission coefficient for a resonance transmission of composite system of three identical particles A=3 through the repulsive Gaussian barrier.
Fig. 21. Up-right: The total transmission probabilities vs the energy E from the ground symmetric (S) or antisymmetric (A) state of clusters of 3, 4 and 5 identical, particles coupled by the oscillator potential, through the Gaussian potential barriers.

- ***The general frame enables numerical solutions in agreement with the experiment*** for a great many few-particle problems [51-57]. Fig. 22 compares a high-resolution experiment on electron emissions in fast proton helium collisions with theoretical expectations from standard scattering theory with a deep node between the binary and recoil peak in all directions [53].

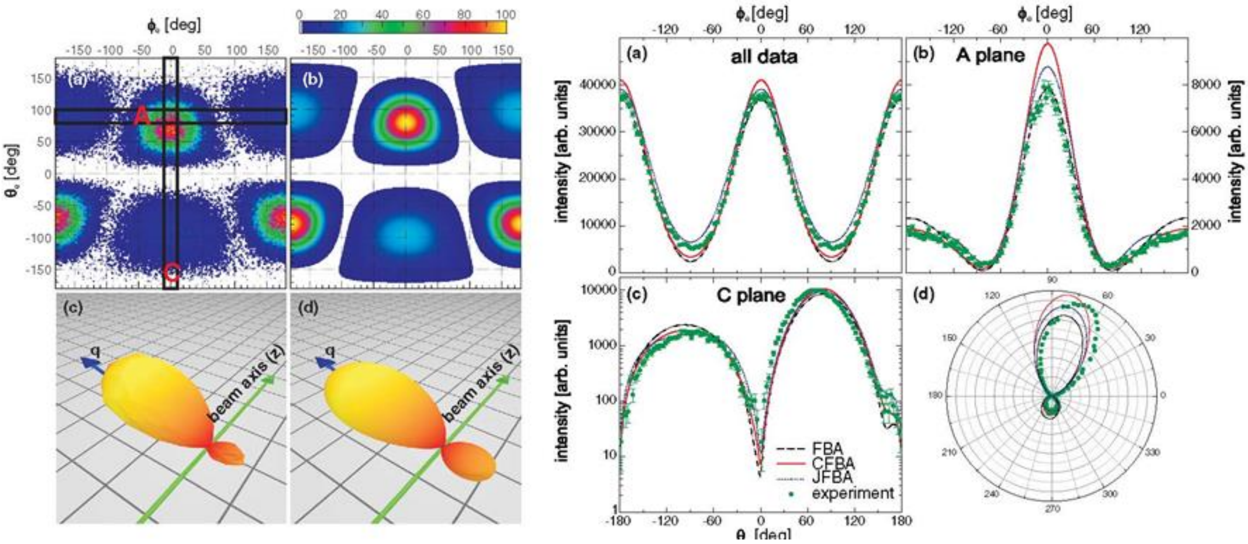


Fig. 22. Left: Electron angular distributions for a fixed energy of E= 6.5± 3.5 eV and momentum transfer of q=0.75±0.25 a.u: (a) Experimental result and (b) theoretical distribution based on the First Born Approximation (FBA) calculations. The areas marked as A and C correspond to the azimuthal plane and the coplanar geometry, respectively. (c) and (d) depict 3D representations of the contour plots (a) and (b). The blue arrow indicates the direction of q and the green arrow the initial beam axis (z). The experimental data shown in (c) are mirrored at ϕ=0 to reduce statistical fluctuations. **Right**: Experimental (green dots) and calculated (FBA, black line; J-matrix FBA, blue line; Correlated wave function FBA, red line) electron angular distributions for E=6.5 eV, q=0.75 a.u: in the plane as indicated in Fig.22 left-(a). Right: (a) All data; (b) azimuthal plane (θ=90° ±10°); (c),(d) coplanar geometry (ϕ = 0°± 10°).

- ***Increasing the number of pivotal points for function expansions***. In contradistinction to the existing floating point computing dogma, the three-point basic element method (BEM) [59-60] allows reliable use of high order polynomial expansions: to reliably solve difficult data smoothing problems; to get efficient recognition and parametrization of high-dimensional patterns (Fig.23-24).

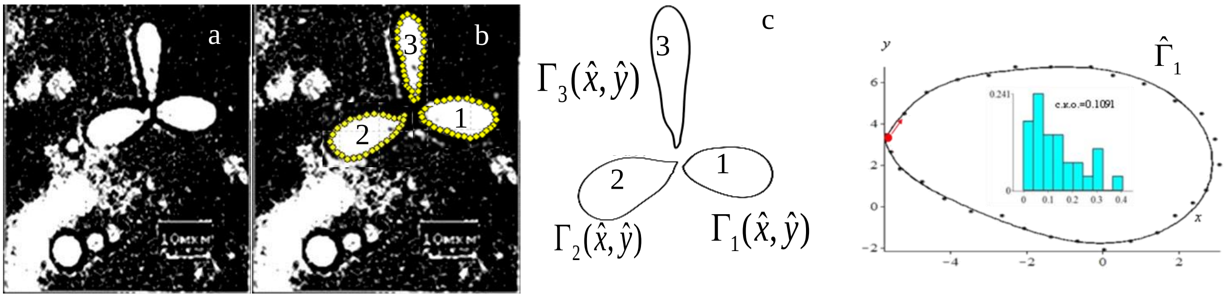


Fig. 23. Contour smoothing of the α-particle tracks on a microphotograph containing residuals of the interaction of fast neutrons with nuclei of polymers (a) [Г.Н. Зорин и др. “Изучение возможности регистрации термоядерных нейтронов в условиях высокого фона атомного реактора”, Атомная энергия, 1996, Т.80, №6, с. 473-474] is shown on the parametric approximation with 11-th degree BEM polynomials. The 30 point measurements along each track (b) are smoothed with the help of a 11-th degree BEM polynomial resulting in the curves (c).

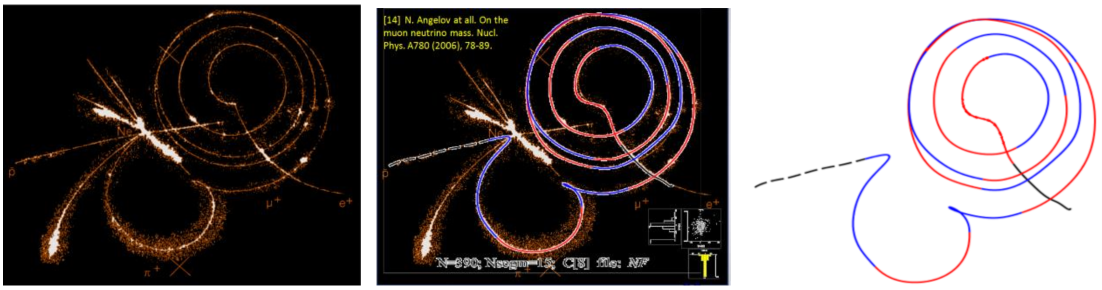


Fig. 24. Smoothing and segmentation of a track with complex topology got on a streamer chamber [N. Angelov at al., “On the muon neutrino mass”, Nucl. Phys. A780 (2006), 78-89]. The coordinates of 390 points are shown. The piecewise analytic description of the 15 track segments is done by means of 30 polynomials of 11-th degree.

- ***Developing problem adapted multi-scaling algorithms*** [60-62]

The discovery that the algebraic degree of precision of a quadrature sum is not its universal characteristic over the range of the floating point machine numbers [63] has fundamentally changed the approach to the definition of the control decisions in the Bayesian automatic adaptive quadrature. The multi-scaling is needed in order to cover consistently all the integration domains of interest. Moreover, the binary tree structure of the Chebyshev coefficients enabled the definition of new effective inference criteria concerning Bayesian diagnostic of convergence (Fig. 25).

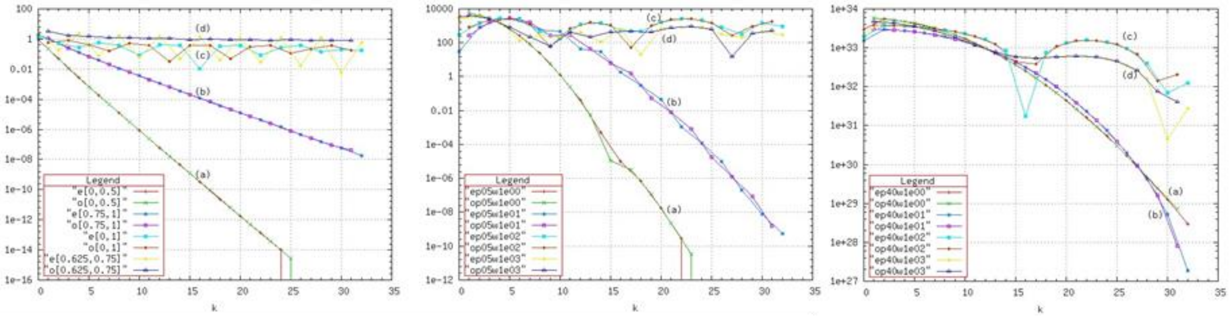


Fig. 25. Typical patterns of variation of the absolute magnitudes of the Chebyshev expansion coefficients within the even and odd rank subsets versus the coefficient labels for different families of integrals

► NICA driven numeric-theoretical studies

The search for a phase transition from high density hadronic matter to quark-gluon plasma asks for numerical-based theoretical investigations devoted to the exploration of this terra incognita. Here there are a few instances of studies aimed at understanding the underlying phenomena.

- ***Lattice studies of* QCD *Landau gauge gluon and ghost propagators*** [64, 65]

The study of the propagators within lattice Quantum Chromodynamics (QCD) has to face the problem of Gribov ambiguity when fixing the gauge (e.g., Landau, Coulomb etc.). This can lead to large differences of the observables found for different Gribov copies generated for the same Monte-Carlo (MC) configuration (in other words, to large "Gribov noise"). Fig. 26 illustrates the solution proposed for the suppression of the Gribov noise associated to gluon propagators. For this cycle of works, I.L. Bogolubsky (LIT) and five other authors have been awarded the JINR Second Prize (2015).

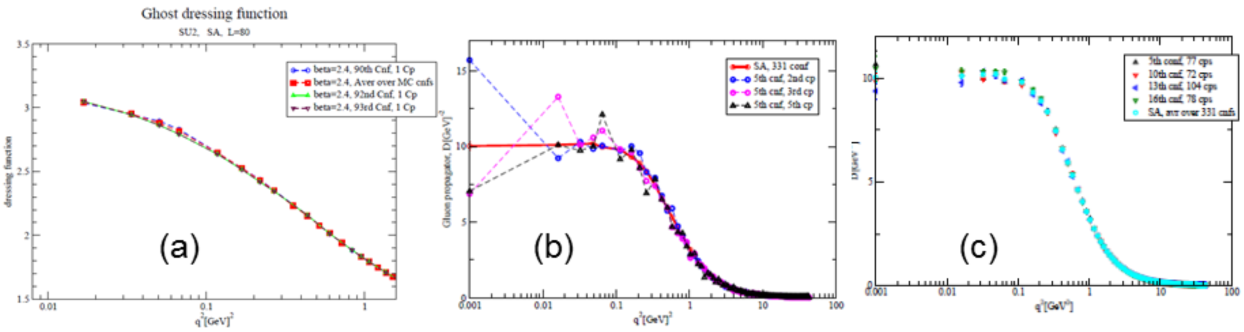


Fig. 26. (a) Ghost dressing function $J(q^2)$ [at β=2.4, L=80] as compared to $J(q^2)$ averaged over three MC configurations; (b) Gluon propagator $D(q^2)$ [at same β and L] and three Gribov copies at a single MC configuration as compared to standard $D(q^2)$ average over 331 MC configurations; (c) Same as (b), but average taken over many Gribov SA copies for a single MC configuration.

- ***Study of the meson properties and of the thermodynamics of the system in the Nambu–Jona–Lasinio* (NJL) *model with different regularizations*** [66-72]

The effect of the regularization scheme and parameter sets on the phase diagram of matter is studied. It is noted that the first-order phase transition in the system may *vanish* if a certain parameter set is used in the NJL model with the Pauli-Villars regularization. Effects of the vector interaction in the NJL model with Polyakov loop are studied in combination with the entanglement interaction between the quark and pure gauge sectors.

The investigation of the QCD phase diagram showed that the first order chiral phase transition at finite baryon chemical potentials and its critical endpoint disappear for sufficiently large values of the vector interaction constant G_V. The presence of an entanglement interaction between quark and pure gauge sectors leads to an increase of the value G_V at which the first order transition disappears. Figs. 27 and 28 illustrate model predictions.

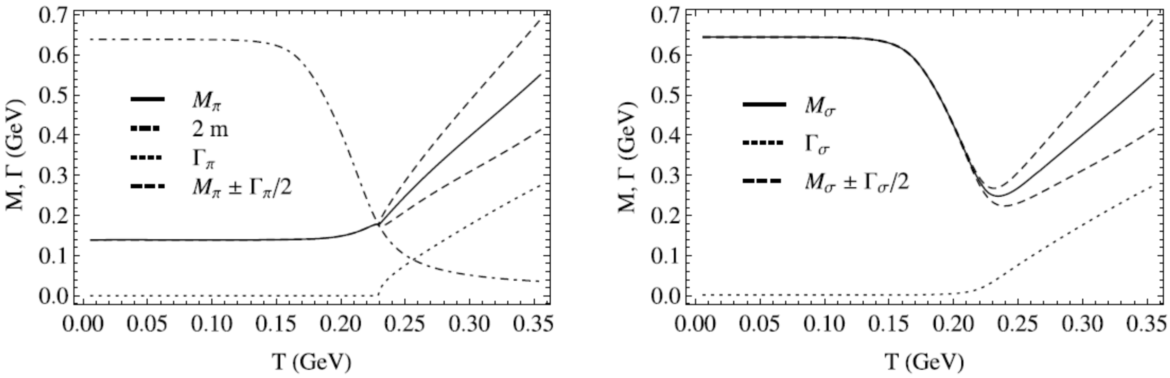


Fig. 27. Modeling and prediction of hadron properties at finite temperature and density (two-flavor Polyakov-loop-extended NJL model: Meson masses $M_{\pi/\sigma} \pm \Gamma_{\pi/\sigma} / 2$, the double quark mass and the meson width $\Gamma_{\pi/\sigma}$).

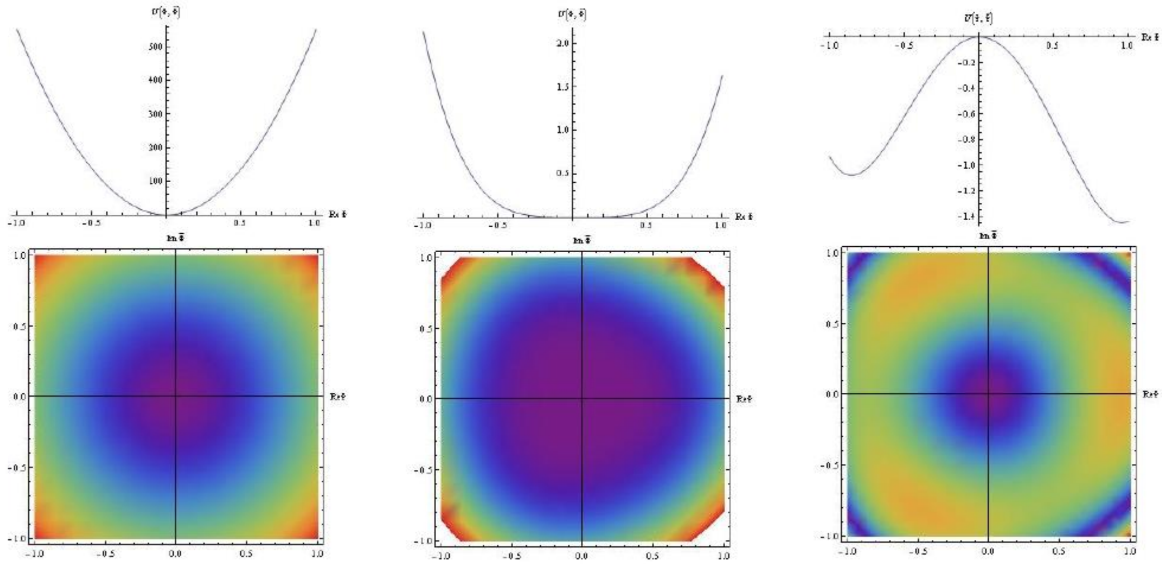


Fig. 28. Deconfinement transition description using the Polyakov loop

- ***Studies of* NJL*-type models of equations of state of the super-dense matter*** [73-77]

For the cycles of papers under the last two directions, Yu. Kalinovsky and O. Grigorian (LIT) [plus other seven authors] have received two 2014 awards for outstanding results in the investigation of the QCD-phase diagram and means of diagnosing the onset of the deconfinement from hadron structure and their reactions: *Small Prize of the International Academic Publishing Company Nauka/Interperiodika* and *Best Publication in PEPAN Letters*.

► **Numerical Studies of Physical Processes in Exotic Materials** [79-95]

The study of physical processes based on numerical solutions of theoretic models concerns several classes of modern materials of interest in biology, the physics of materials, nanotechnology, quantum computing, etc. Below an excerpt is given of four remarkable results.

- ***Generalization of Bogolubov theory of weakly interacting Bose gases*** [83]. The ground state of homogeneous Bose gas of hard spheres has been computed for Bose systems characterized by arbitrarily strong interactions. Numerically calculated characteristics such as condensate fraction and ground state energy are in very good agreement with Monte Carlo simulations (Fig. 29).

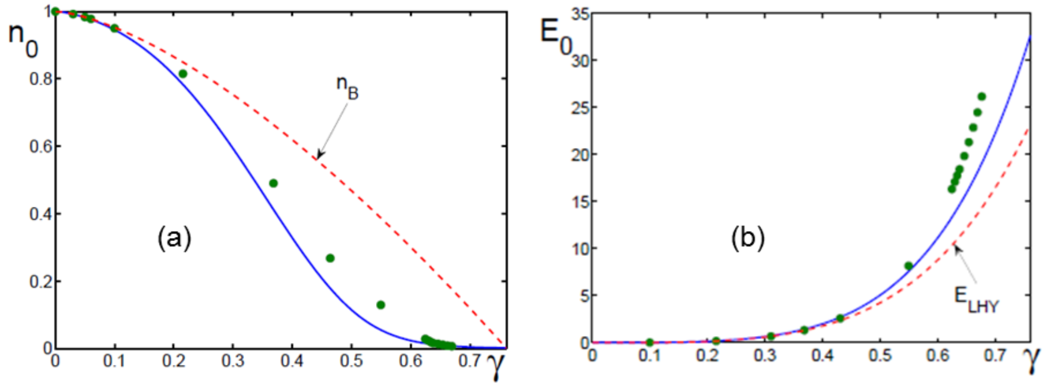
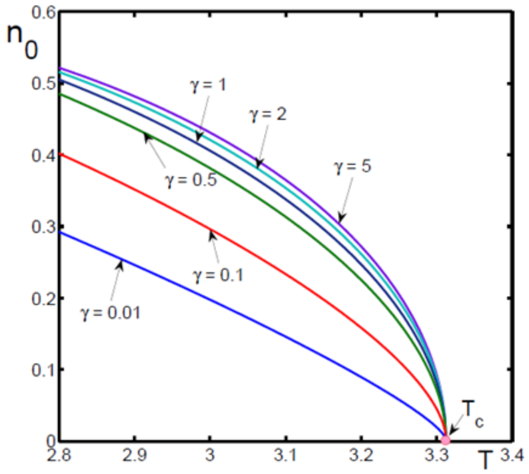


Fig. 29. (a) Condensate fraction n_0 (solid line) as a function of the gas parameter γ, compared with the Monte Carlo results, shown by dots, and with the Bogolubov approximation n_B (dashed line); (b) Dimensionless ground-state energy E_0 (solid line) as a function of the gas parameter γ, compared with the Monte Carlo results, shown by dots, and with the Lee-Huang-Yang expression E_{LHY} (dashed line).

- *Bose-Einstein condensation in self-consistent mean-field theory* [82]



Numerical investigations show that the phase transition of Bose-Einstein condensate is of *second order* for Bose systems with arbitrarily strong interactions. This is proved in the frame of self-consistent mean-field theory developed in [82]. All other variants of mean-field approach give incorrect first-order transition.

Fig. 30. Condensate fraction n_0 as a function of dimensionless temperature T in the critical region.

- *Optical lattice with heterogeneous atomic density* [87]

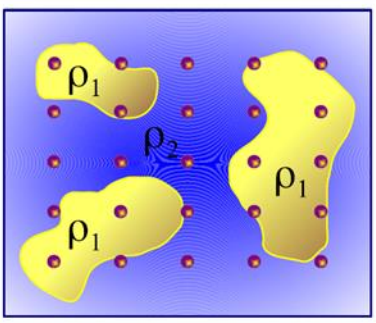


Fig. 31 (up**).** Snapshot of a heterophase two-density lattice system. Regions of higher density ρ_1 are randomly immersed into the matrix of lower density ρ_2, with $\rho_1 > \rho_2$.

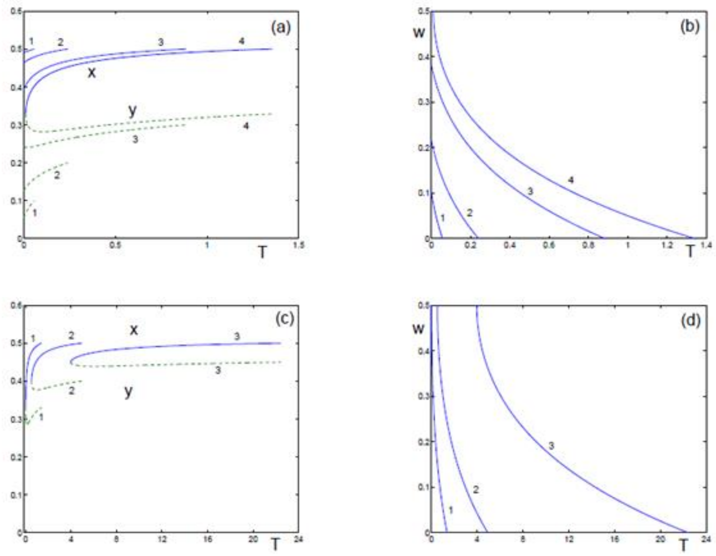


Fig. 31. (right) Solutions as functions of the dimensionless temperature T for different filling factors: (a) order parameters x (solid line) and y (dashed line) for ν=0.1 (line 1), ν=0.2 (line 2), ν=0.3 (line 3), and ν=0.328 (line 4); (b) dense-phase probability w for the same filling factors and enumeration as above; (c) order parameters x (solid line) and y (dashed line) for ν=0.33 (line 1), ν=0.4 (line 2), and ν=0.45 (line 3); (d) dense-phase probability w for the same filling factors and enumeration as in (c).

The formation of heterogeneous states in optical lattices characterized by a spontaneous mesoscopic separation into spatial regions with different atomic densities is investigated. The numerical results show that such states can arise if there are repulsive interactions between atoms in different lattice sites and the filling factor ν is less than one-half.

- Vortex rings and vortex ring solitons in shaken Bose-Einstein condensate [89]. In a shaking Bose-Einstein condensate confined in a vibrating trap, there can appear different nonlinear coherent modes such as vortex ring solitons and vortex rings. The energy required for creating vortex ring solitons is larger than that needed for forming vortex rings. The generation of vortex rings is illustrated by numerical simulations for trapped rubidium ^{87}Rb atoms.

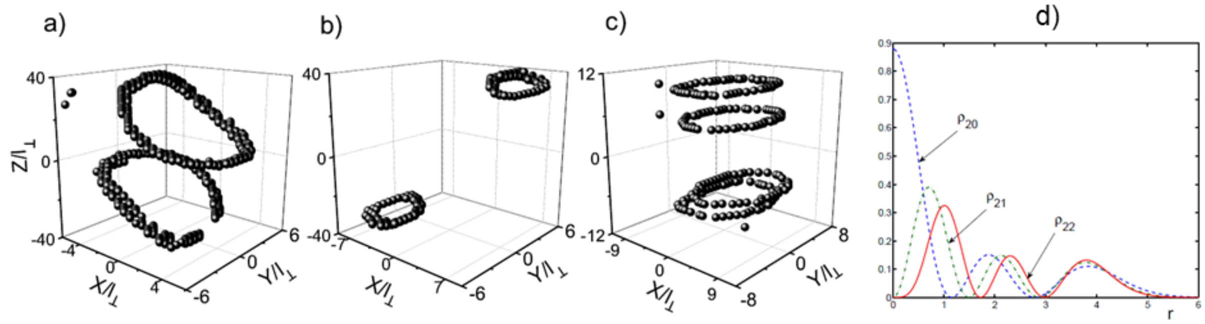


Fig. 32. Spatial location of vortex rings after different shaking time: a) t =10.5 ms; b) t=11ms; c) t=14.4 ms; d) Radial density of the double ring state (dashed line), composite vortex state + double ring states (dashed dotted line) and vortex state with the winding number m=2 (solid line)

8. Developments in Computer Algebra and Quantum Computing [96-105]

► **Development of symbolic algorithms controlling the extension of Kantorovich method to the solution of few-body problems** [96-97]

The above mentioned Kantorovich based extension of numerical methods [38-50] heavily relied on a number of underlying symbolic algorithms [96-97].

► **Investigation of the interplay between methods of computational group theory and Monte Carlo methods** [98-102]

In the study of finite quantum systems, combinatorial quantum models were investigated. The related computations revealed a high efficiency and accuracy of the Monte Carlo approach which in a number of cases can replace rather cumbersome exact computations with finite groups. In addition, the Lagrange equations for continuous approximations of combinatorial models have been studied.

►**General analysis of the Cosserat family of partial differential equations** (**PDE**) [103-105]

By using Lie symmetry methods implemented as the program packages DESOLV and SADE, written in Maple and included into the library of journal Computer Physics Communications, the general analytical solutions to the kinematic part of the nonlinear Cosserat PDE system describing dynamics of flexible slender structures (e.g. cables, cords, ropes, etc.) was found. This considerably simplifies their numerical simulation and makes it faster by two orders of magnitude.

►**Building up discretization schemes which inherit the basic algebraic properties of the original PDEs** [106-107] was possible by means of computer-algebra methods which reduce the difference equations into the canonical form of a Gröbner (standard) basis. A newly proposed approach (Fig. 33) is expected to shed new light on this topic.

►**Computing algorithmically the full set of algebraically independent constraints for singular mechanical and field-theoretical models with polynomial Lagrangians** [108] serves as a tool for the investigation of models of modern gauge field theories and elementary particle physics. If the model under consideration is not singular as a whole but has domains of dynamical (field) variables where its Lagrangian becomes singular, then such domains are detected and the relevant constraints are computed.

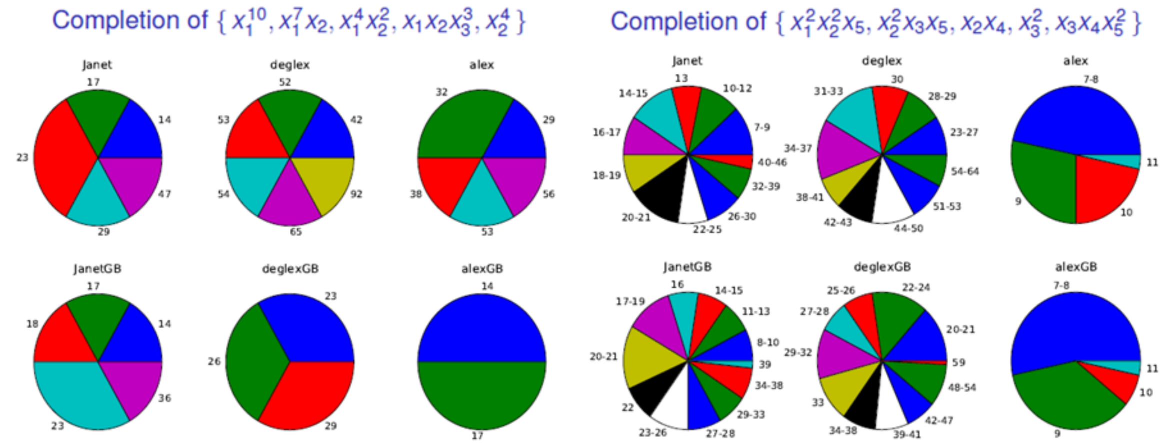


Fig. 33. New down-up approach to the derivation of involutive Groebner bases results in compact bases (third columns in each set) allowing the derivation of easily parallelizable algorithms.

►**Investigations in quantum computation and quantum information** [109-114]

Several rigorous solutions have been derived. The description of the mixed quantum states of d-dimensional quantum states (qudits) as the orbit space of the global unitary transformation group was given [109].

For the model example of 3-level quantum system (qutrit) with the local unitary group SU(2) x U(1), its entanglement space is described as the orbit space of this group [110]. Besides, the estimation of probability for mixed stated to be entangled were obtained [111, 112].

The dynamics of qubits, as particles of spin 1/2 under the action of strong laser field was modelled in [113,114].

9. Miscellanea

Besides the above mentioned aspects of the output of theme 1119, there are two more ones deserving consideration.

The first concerns the new JINRLIB program library developments [120-122]. The JINRLIB contains a total of 69 packages of software of general interest, the overwhelming contribution to which comes from LIT. Taking into account the modern trends in the development of the computing, in JINRLIB there has been created a section devoted to parallel programs. In this section there are parallelized versions of well-known and widely used programs like MINUIT and FUMILI. With the vigorous development of the new hybrid cluster HybriLIT, it is expected that this kind of contribution to JINRLIB will become prevailing.

The second aspect concerns the organization of periodic international conferences. The International MMCP Conferences (Mathematical Modeling and Computational Physics), organized once every two years, have got a solid international reputation, with the publication of the MMCP Conference Proceedings under a severe refereeing process (Editors Gh. Adam, J. Buša, M. Hnatič), MMCP 2011 – at Springer (vol. LNCS 7125) in 2012 (a real bestseller according to the Springer marketing reports) and MMCP 2015 – at EPJ Web of Conferences (vol. 108, 2016).

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