Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data (05-6-1119-2014/2023)

(Written Report)

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Participating JINR Laboratories: LIT, VBLHEP, BLTP, FLNR, FLNP, DLNP, LRB

Participating Countries and International Organizations:
Armenia, Australia, Azerbaijan, Belarus, Belgium, Brazil, Bulgaria, Canada, CERN, China, Czech Republic, France, Georgia, Germany, Italy, Japan, Kazakhstan, Moldova, Mongolia, Poland, Portugal, Romania, Russia, Slovakia, South Africa, Switzerland, Tajikistan, USA, Vietnam.

April, 2023

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Main Achievements in the MLIT Topic 1119 during 2020−2023

Extended Abstract

Within the present Report, the "Topic 1119" stands for an abridged denomination of the JINR research topic 05-6-1119-2014/2023, "*Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data"*,

The research done within the Topic 1119 during 2020–2023 involves four activities, which agglutinate the different subject matters solved:

1. Mathematical and computation methods for simulation of complex physical systems;
2. Software complexes and mathematical methods for processing and analysis of experimental data;
3. Numerical methods, algorithms and software for multicore and hybrid architectures and Big Data analytics;
4. Methods, algorithms and software of computer algebra and quantum computing.

The written progress Report on the Topic 1119 status, made at the 52-nd Session of the JINR Programme Advisory Committee for Condensed Matter Physics (PAC-CMP) (02.07.2020) [1], evidenced two types of distinctive features, which differentiate this Topic in the JINR research.

The first type concerns prerequisites (input features) of the work done within this topic:

− *Work done in close cooperation* with research groups from all JINR Laboratories and with JINR Member State Institutions. This involves the use of the existent expertise of the LIT staff for the solution of challenging problems, in over 40 JINR projects, which ask for advanced research in computational mathematics and physics, directed to the creation of new mathematical methods and algorithms for the numerical or symbolic-numerical solution of topics arising in experimental and theoretical physics studies, their implementation into software packages. This subject area includes a wide spectrum of investigations approved for completion in JINR within the seven year period 2017–2023 in high energy physics, nuclear physics, physics of condensed matter and of nanostructures, biophysics, information technologies, the solution of which is inseparable from the use of computing. Such subject matters of the outmost importance in JINR are the NICA based projects, the neutrino program, the superheavy and exotic nuclei physics, the IBR-2 neutron based investigations*. Out of the 272 references quoted at the end of this Report, 135 (i.e. 50%) are done within international collaborations. The overwhelming part of the remaining titles are done in collaborations with other JINR Laboratories.*

− The promotion and support of a scientific environment in MLIT, which encourages and rewards a *deep and extensive professional expertise* along four critical directions: thinking as computer scientist with several computing paradigms; expert knowledge of the mathematical problems backing the topic of the collaboration; in depth grasp of the numerical analysis topics enabling the achievement of reduced complexity, robustness and reliability of the developed algorithms; deep knowledge of the physics side of the problem at hand as a precondition of significant mathematical modeling undertakings. The leadership of the Topic 1119 has put great efforts to back the agreed cooperation in the large scale projects by working groups the complementarity of the knowledge of the members of which secure the coverage of all the four mentioned critical directions. Inside the JINR ecosystem, we heavily rely on the decisions of the JINR Directorate and the Program Advisory Committees.

− Unfortunately, not everything went smooth during 2020–2023. The Covid-19 pandemic forced us to change substantially, for a while, the form (place and style) of the scientific work. While over 90 percent of the MLIT staff involved in the solution of the Topic 1119 tasks were passed at work at the distance, the pace of the scientific effort remained at a high level. New forms of communication, like the scientific webinars, came to the first plan and we have been forced to postpone for better times the face-to-face meetings at our traditional Conferences, Workshops and Schools. However, we paid the highest price in human lives. Particularly heavy was felt the loss of Prof. Vladimir P. Gerdt [2], uncontested long time promoter and leader of the computer algebra and quantum computing research.

The second type of features singles out *the Topic* 1119 *output* within the JINR research. The Resolution of the 52-nd Session of the PAC-CMP (see [3], p.5 and [4], p.6) fully endorsed the five kinds of achievements reported at this session and recommended their further continuation, namely:

(i) *Contributions to the large-scale advancement of the JINR research;*

(ii) *Advances to solutions of specific cooperation tasks within JINR conducted research projects;*

(iii) *Software packages implemented in general-purpose computing libraries;*

(iv) *Contributions to the JINR excellence in the worldwide research landscape;*

(v) *Grow up of the scientific competence in using the JINR computer tools.*

These five figures of merit enable in-depth characterization of the many facetted work done within the Topic 1119. They evidence the timeliness and the importance of the various achievements. The scrutiny of the progress made within the Topic 1119 during 2020–2023 unveils the following bird’s–eye view along these lines:

(i) The design, development, implementation, and maintenance of a user friendly environment on the MLIT heterogeneous computing platform, which involves the HybriLIT cluster and the “Govorun” supercomputer, is our main contribution to the success of the MICC (Multifunctional Information and Computing Complex) project and, throught it, to the vitally needed large scale computing in the JINR;

(ii) Instances of the valorization of the Topic 1119 MLIT staff expertize in computing and data handling are the highly needed and appreciated contributions to the three-dimensional simulations asked by the magnet validation for the future NICA facility, solutions of specific tasks within the BM@N and MPD projects at NICA, substantial contributions to software development, within the JINR contribution, for the CMS and ATLAS Phase 3 projects at CERN, development of data processing system software for the Baikal-GVD project, etc.;

(iii) The development and implementation of software packages dedicated to large projects (BM@NRoot, MPDRoot, CMSROOT, Geant4), or in general purpose computing libraries (9 packages in JINRLIB, 3 packages in CPC Library) are proofs of our lasting prestigious output, simultaneously based on in-depth grasp of right computing paradigms and the formulation of breakthrough ideas;

(iv) For the period covered by the present analysis, the staff of the Topic 1119 co-authored a number of 384 scientific papers in prestigious international journals (266 in foreign journals, 118 in Russian journals), together with 19 monographs or contributions to monographs. Co-authorship to 217 CMS Project research papers, 38 Baikal-GVD Project research papers complete the list of the scientific papers. The presentation of 40 plenary or invited lectures at international conferences completes the statistics of the contribution to the JINR excellence trough publications;

(v) A specific, particularly important facet of the activity of an important fraction of the staff of the Topic 1119 was the alleviation of the abrupt learning curve associated to the use of the large scale computing. In this respect, besides personal face-to-face help through conversations, the organization of dedicated events and/or the participation to them through lecturership were particularly important.

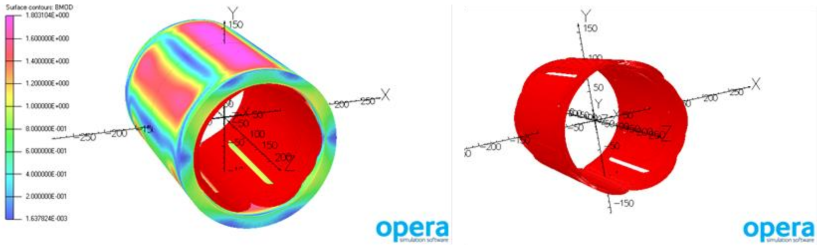
1. Mathematical and Computation Methods for Simulation of Complex Physical Systems

1.1. Selected results on magnetic field modeling

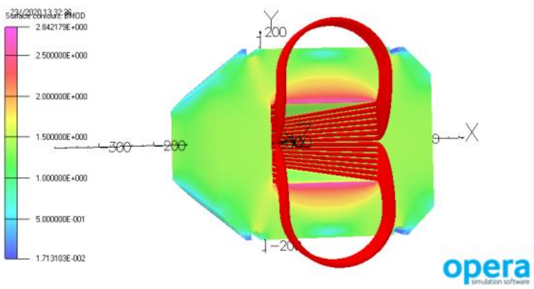
Intense current research involves ***three-dimensional computer simulation of magnetic systems*** *in the framework of NICA (JINR) and FAIR (GSI) projects for the validation of the magnetic field uniformity in the working areas of the new physical magnets*; *modeling the CBM 3D shielding dipole magnet at GSI to accommodate the modifications proposed in the conception of the CBM experiment in the options MUCH and RICH*; *improvement of* ***design tools for new medical purpose cyclotrons***.

● The OPERA 3D modeling of magnetic systems for the NICA collider

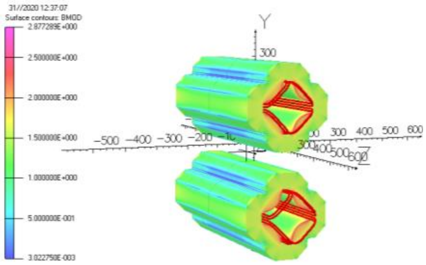
Instances of the work done by P.G. Akishin in the framework of the NICA projects, in collaboration with VBLHEP, for the 3D modeling of various classes of magnets are given in the figures below, where the field distributions in the magnet working areas are illustrated.



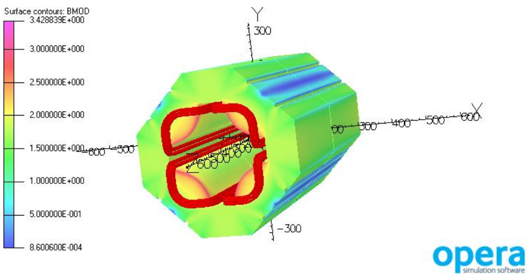
NICA Collider Multipole Corrector Modeling



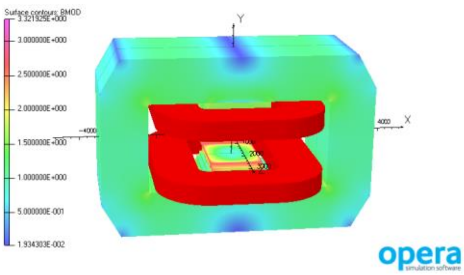
The vertical output dipole (NICA)



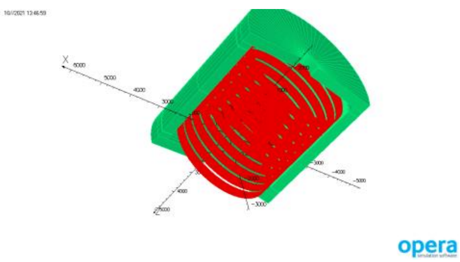
The collider quadrupole magnet model (NICA)



The final focus lens model (NICA)

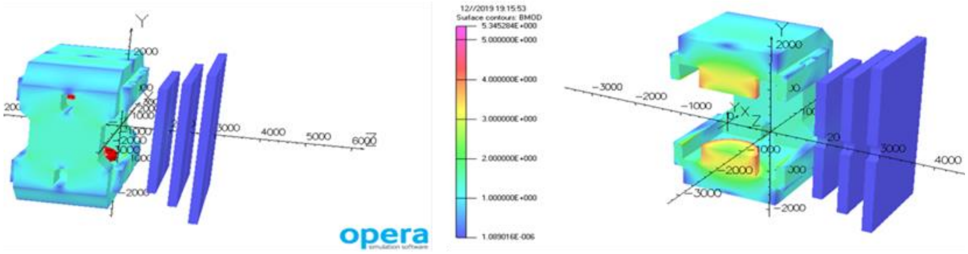


The Opera3d SP41 magnet model (BMN)

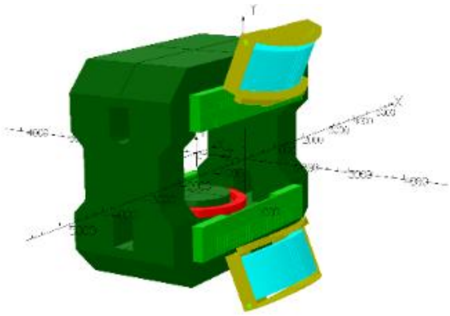


The solenoid SPD magnet model

• **Modeling the CBM dipole magnet at GSI** [5, 6]. The modifications proposed in the conception of the CBM experiment such as to include the muon detection have asked for the buildup of dipole magnets with shielding. P. Akishin has realized the magnet modeling in two possible options (MUCH and RICH). The three-dimensional magnetic system simulation for the MUON option is illustrated below.



The CBM dipole magnet system modeling. MUON option



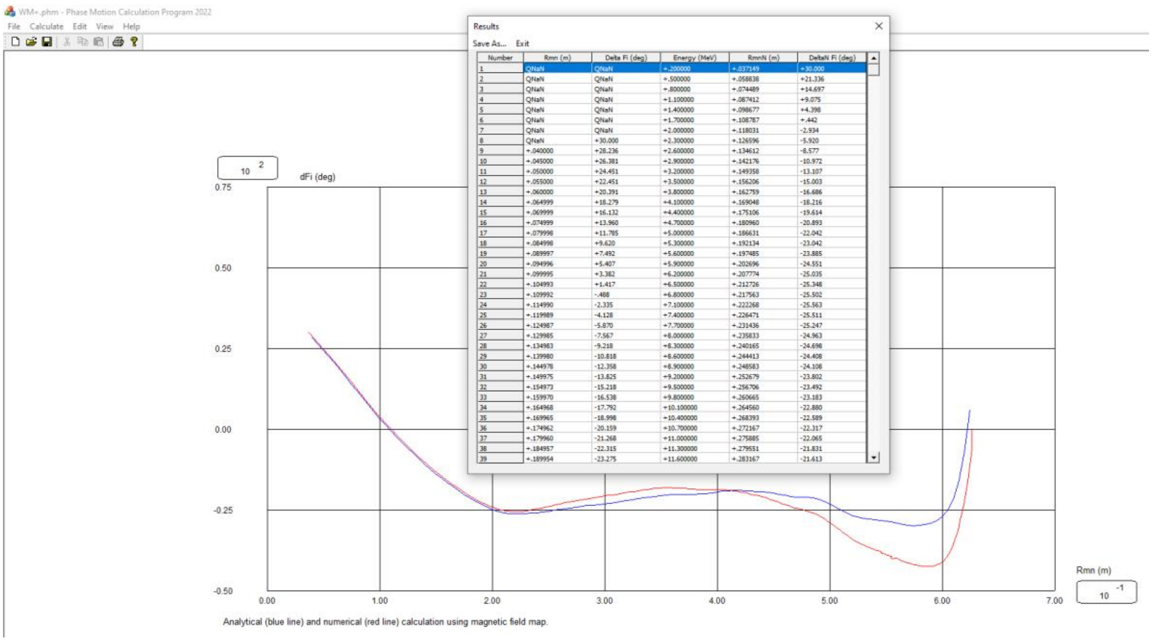
The CBM dipole magnet for RICH option (FAIR)

The main results reported in [7] showed that:

• The CBM magnet with laminated yoke and poles increases significantly the stray field value in the vicinity of the RICH photodetector.

• The design of the shielding box with a “wing” and a back wall allows decreasing the stray magnetic field value by a factor of ~1.8. The optimization of the “wing” location requires systematic simulation on the background.

● **Improvement of design tools for medical purpose cyclotrons**



Phase motion: AIC-144 multipurpose isochronous cyclotron (INP PAS, Krakow, Poland) main operating mode. The experiment 13.12.2019: p, Frf = 26.26 MHz, Ek=60.7 MeV, Kext=30±5 %.

Studies done in cooperation with colleagues from DLNP and from Poland have resulted in numerical theoretical definition of high resolution working regime for the AIC-144 multipurpose isochronous cyclotron (INP PAS, Krakow, Poland), with accuracy parameters exceeding the best known worldwide ones [8]. The figure above provides an excerpt from the obtained data.

An important HPC parallel package, the design and realization of which was driven by this research, was implemented in the PROGRAM LIBRARY JINRLIB:

• **EORP 2020** – Equilibrium Orbit Research Program (April 06, 2020) [9] – software package for computing closed equilibrium orbits in magnetic fields of an isochronous cyclotron by solving the equations of motion.

The work directed to the conceptual development of a new medical purpose cyclotron, SC230, in DLNP, asked for several related developments in MLIT.

One of them concerned the implementation of improved dedicated modules of the COMSOL Multiphysics package, enabling both better solutions of the magnetostatic related problems and their efficient use within the HybriLIT heterogeneous platform [10].

The conceptual design of the proposed SC230, as a compact superconducting isochronous cyclotron for proton therapy, ask for solution of combined dynamic analysis problems involving both magnetic and electric fields. Two kinds of basic problems have been solved [11].

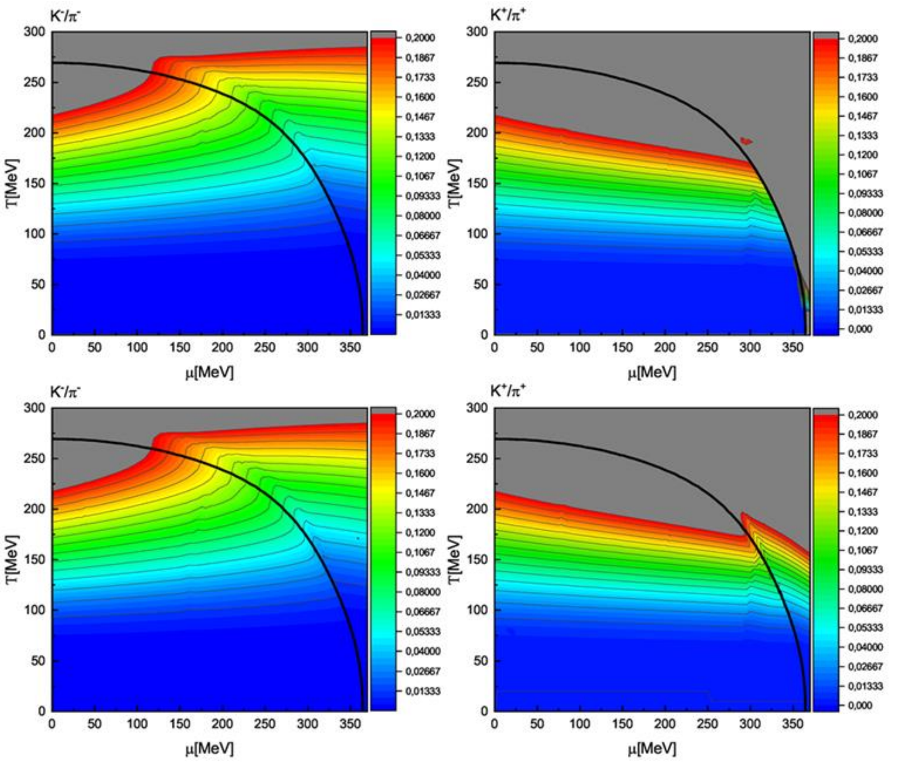
1.2. Selected numerical modeling of physical systems and processes

1.2.1. *NICA driven numeric-theoretical studies in dense hadronic matter*

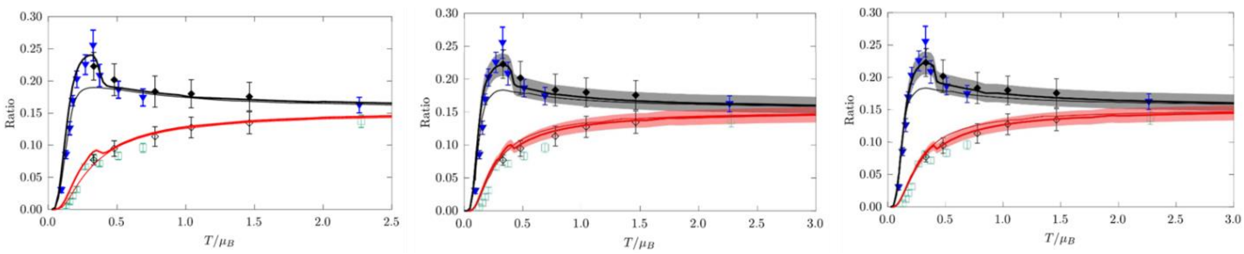
Theoretical and numerical analyses of the available experimental data on heavy ion collisions in the energy range of the NICA collider with an emphasis on the features of nuclear interactions in the observed characteristics are carried out.

• **Horn effect investigations in different PNJL based models** [12–16].

• The Beth–Uhlenbeck approach [12, 13] shows that, in terms of phase shifts in the K^+ channel, an additional low-energy mode could appear as a bound state in the medium, since the masses of the quark constituents are different.



The K^-/π^- and K^+/π^+ ratio in the T-μ_q plane. The two upper panels correspond to full phase shifts while the two lower panels show phase shifts when the anomalous mode is removed. Only the interval of ratios relevant for a comparison with the experimental data is shown [13].



Dependence of the ratios K^+/π^+ (black lines) and K^-/π^- (red lines) on T/μ_B along the chemical freezeout line. Left panel: for the PNJL+g_V model within the BU approach. Central panel: for the EPNJL+g_V. Right panel: for the EPNJL model. The shaded region corresponds to the variation in fitting μ_π to RHIC and LHC data with their uncertainty band at high T/μ_B [15].

• **The computation of the pion damping width in hot nuclear matter**, taking into account all possible pion-pion scattering modes, was made at the HybriLIT cluster by a new algorithm and C++ code for calculating multidimensional collision integrals based on Monte Carlo method [17–20].

• **Suggestions for experiments with usage of the Spin Physics Detector (SPD) and perspectives of the first stage of the SPD Programme at NICA Facility** [21].

• **Hadron Modifications in Dense Baryonic Matter**

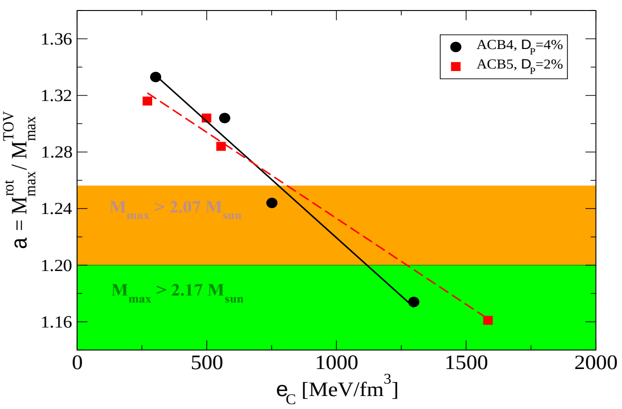
A description of the structure of hadrons within the Strongly Correlated Quark Model is given. Specific changes of the properties of mesons and baryons in a dense nuclear medium are found to occur. In such a medium, the nucleons may be transformed into delta isobars, hyperons and their excited states, and mesons are produced mainly through vector resonances. In addition, the properties of vector mesons, consisting of light quarks, change dramatically: the decay width increases, while the mass value decreases. Such modifications in the nuclear medium, especially in the NICA energy range, can lead to observable effects like strangeness increase, the "horn effect", the increase of the dilepton invariant mass spectra in the range 0.2–0.7 GeV [22].

• Accretion-induced collapse to third family compact stars as trigger for eccentric orbits of millisecond pulsars in binaries and astrophysical aspects of general relativistic mass twin stars have been recently reviewed [23, 24].

• Study of strongly interacting nuclear matter by means of the extended sigma-omega model has been pursued by a Bayesian analysis of state-of-the-art multi-messenger astronomical observations [25, 26].

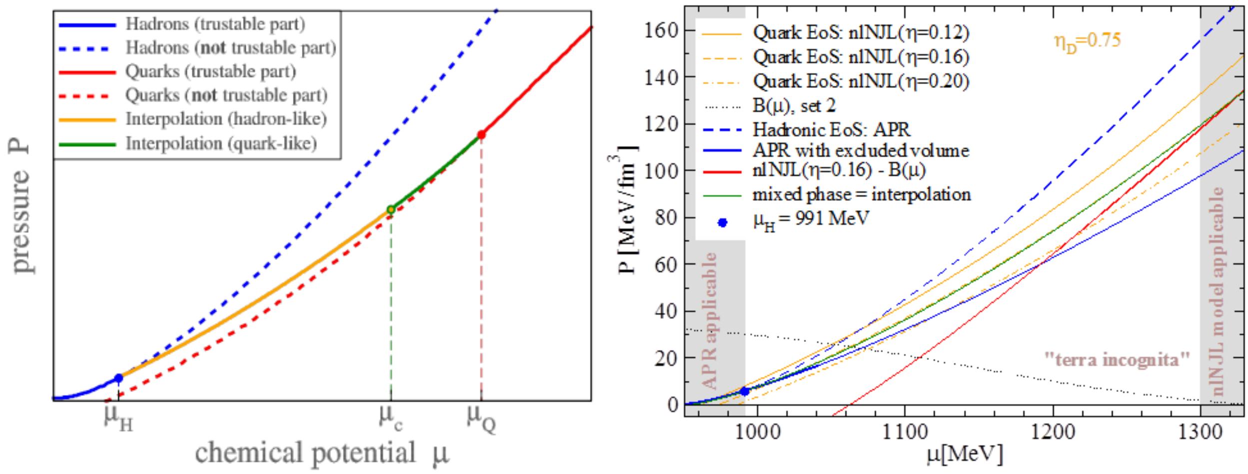
• **Alternative possible mechanism of the emergence of GW170817** was investigated on the basis of a Bayesian analysis enabling the selection of the most probable equation of state under a set of constraints from compact star physics [27].

• **Constraints for the dense matter equation of state**, related to the observation of the binary neutron star merger GW170817, have been derived [24]. The relation between maximum compact star masses of fastest rotating and static configurations in dependence on central energy density of compact star configurations have been quantized.



Dependence of the ratio between maximum compact star masses of fastest rotating and static configurations on central energy density of compact stars for two different models of nuclear matter equation of state, ACB4 and ACB5, having strong phase transition and allowing third-family compact stars.

• **Bayesian analysis of multimessenger M-R data with interpolated hybrid EoS** [28]



Left panel: A hybrid equation of state that joins a soft nuclear equation of state with a stiffer quark matter equation of state by interpolation in the intermediate region between μ_H and μ_Q for $n(\mu_H) = n_0$ and $n(\mu_Q)$=2.5..5 n_0. The dotted curves indicate where the extrapolations of the nuclear and quark matter equations of state become unreliable.

Right panel: Pressure vs. chemical potential for the nlNJL EoS (orange lines) compared to that of the APR EoS (dashed blue line) shows that no reasonable Maxwell construction is possible. When a nucleonic excluded volume is applied to APR (solid blue line) and a density-dependent bag pressure B(μ) (black dotted line) to the quark matter EoS, a Maxwell transition point is obtained and a mixed phase construction (green solid line) can be performed which would correspond to an interpolation between APR and nlNJL.

New thermodynamically consistent two-zone interpolation construction was developed to get hybrid equation of state (EoS) for stellar nuclear matter. It allows systematic study hybrid EoS even when the hadron and quark phases have no equilibrium point (no reasonable Maxwell construction possible). The construction realizes a smooth crossover behavior transition between both phases, due to the assumption that the nature of the transition is a mixing of phases.

The possible microphysical underpinning of the two-zone interpolation construction may be viewed as a shortcut that replaces three microphysical effects: (1) stiffening of the nuclear EoS due to quark substructure effects (quark Pauli blocking modeled, e.g., by a baryon excluded volume), (2) softening of the quark matter EoS at low densities due to confining effects (modeled, e.g., by a medium-dependent bag pressure) and (3) mixed-phase effects due to the occurrence of finite-size structures (pasta phases).

• **Simulation of the evolution of neutron stars** through neutrino and photon emissions, done within an exotic model involving a fraction of light dark matter (LDM), is found to result in cooling patterns that could be distorted by the LDM presence [29].

► **Chemical freeze-out of light nuclei in high energy nuclear collisions** [30–31]

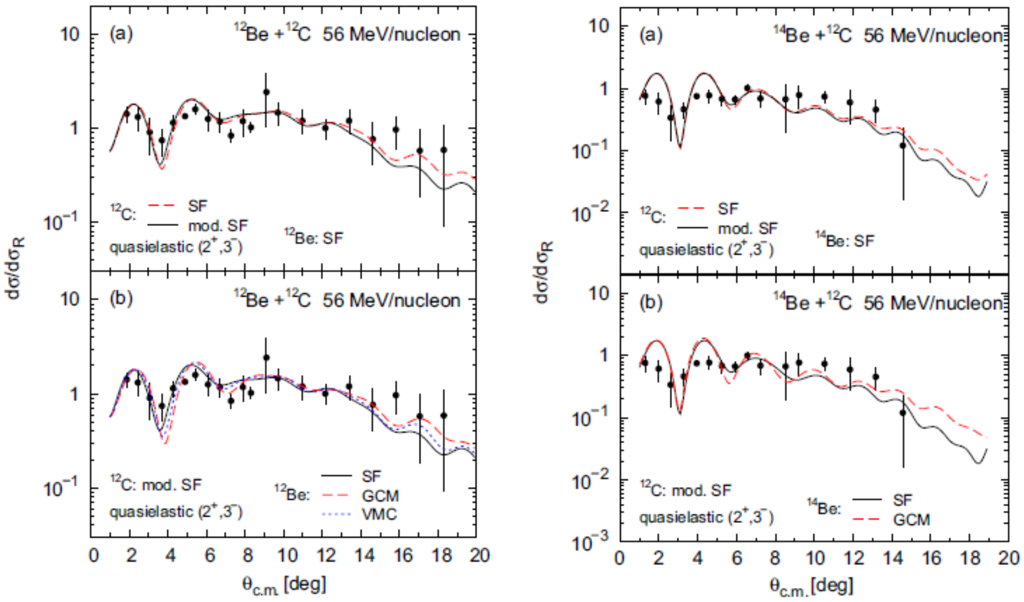
1.2.2. *Numerical modeling of nuclear systems and processes*

Contributions to the worldwide JINR priorities in low energy nuclear physics are brought within a threefold effort able to valorise the existing complementary expertises: in FLNR – experimental investigations devoted to the creation and study of new superheavy elements and of exotic nuclei; in BLTP – formulation of theoretical models and hypotheses able to provide the understanding of the experimental data and to propose new lines of investigation; in MLIT – design and implementation of new high performance computing packages able to provide detailed and efficient mathematical solutions of the simulated processes. The description of results on mathematical modeling of the nuclear systems and processes is covered in the present section. That of the development of packages aimed at providing accurate and efficient solutions to the emerging mathematical problems is covered in Chapter 3.

► ***The breakthrough made by the efficient computer implementation*** of the formulated microscopic optical potential model within BLTP – MLIT collaboration, enabled detailed numerical investigations (on the Govorun supercomputer), pending during decades, previously measured nucleon-nucleon and pion-nucleon scattering processes.

• **Numerical analysis** [32–35] **of differential cross-sections for the elastic scattering of exotic nuclei** ^{12,14}Be by carbon and proton targets at energies of 56 MeV/nucleon and 700 MeV, respectively, is carried out. The influence of the inelastic channel and the choice of a model for the distribution density of nucleons in ^{12,14}Be nuclei on agreement with experimental data is investigated.

For the density of ^{12,14}Be nuclei in the form of the symmetrized Fermi function, parameters are obtained that improve the agreement of the ^{12,14}Be+^{12}C differential scattering cross sections with experimental data. The combined C++ / Fortran complex of computer programs created for this purpose using MPI and OpenMP parallel programming techniques provides a 5-times decrease in computation time when calculating on the MICC LIT HybriLIT cluster.

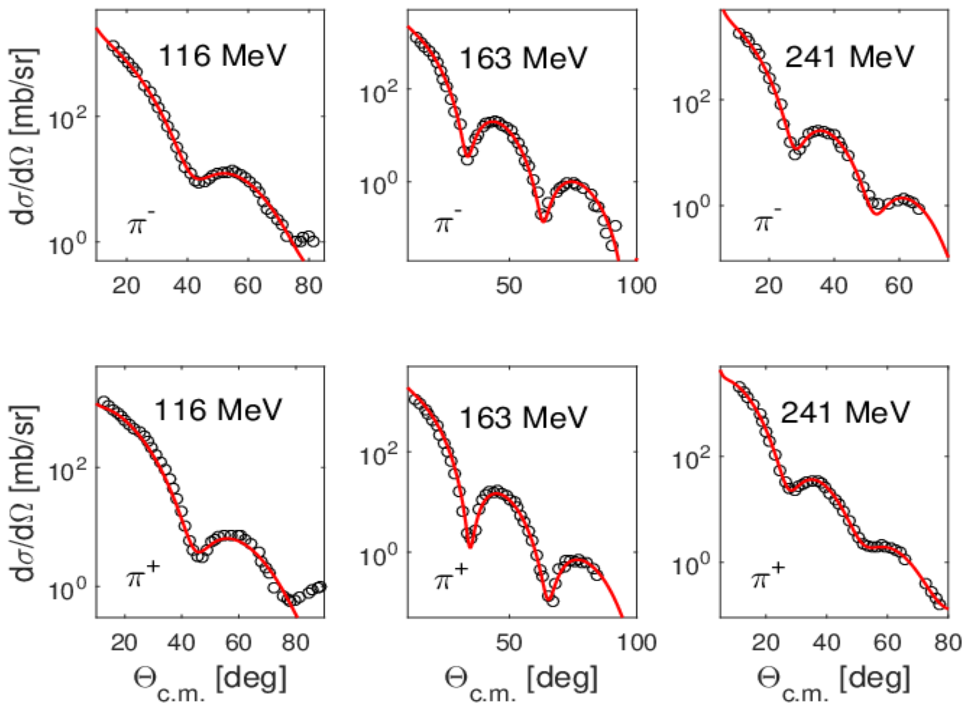


Left: (a) ^{12}Be + ^{12}C quasielastic scattering cross sections at E = 56 MeV/nucleon calculated using the SF density of ^{12}Be and SF (black solid line) and modified SF (red dashed line) densities of ^{12}C. Panel (b) illustrates the calculations with the modified SF density of ^{12}C and using the SF (black solid line), GCM (red dashed line), and VMC (blue dotted line) densities of ^{12}Be. *Right*: (a) Same as left, but for ^{14}Be + ^{12}C. In panel (b) results with SF and GCM densities of ^{14}Be are shown [33].

• **Further numerical analysis of these data and program description** are given in [36].

• **Numerical analysis** [37] **of differential cross-sections for the $\pi^{\pm}$ elastic scattering** on ^{28}Si, ^{40}Ca, ^{58}Ni, ^{208}Pb nuclei in the energy range from 130 to 290MeV. To this end, both the folding optical potential (OP) and the local modified Kisslinger-type OP were calculated, and then the πA cross sections were obtained by solving the Klein-Gordon equation to account for the relativization and distortion wave effects. In the folding OPs, the parameters of the elementary πN amplitude were fitted when describing the πA scattering data, and thus the essential in-medium effect on the parameters of the πN amplitude was established since the pion is scattered not on a free but on a bound nuclear nucleon. Fairly good agreement with experimental data was obtained for both models of optical potentials and their forms turn out to be in coincidence in the region of their surfaces.

• **Numerical analysis** [38] **of differential cross-sections for the elastic scattering** of the pion-nucleus potential. The results obtained in 2022 for $\pi^{\pm}+^{40}$Ca scattering at energies of 116, 163, and 241 MeV (see Figure below) confirm the assessments made on the basis of previous calculations of the influence of the nuclear medium on the pion-nucleon amplitude. The developed approach provides an adequate description of experimental data on pion-nucleus scattering in the region of pion (3,3) resonance energies.



Comparison [38] of the cross-sections of the elastic scattering $\pi^{\pm}$ + ^{40}Ca at energies of 116, 163 and 241 MeV, computed using the microscopic model of optical potential (red curves), with experimental data (circles) from [Q. Ingram, et al., Phys. Lett. B **76** (1978) 173].

● **Numerical analysis [39] of differential cross-sections for the elastic scattering** of the exotic ^{17}F nucleus by ^{12}C, ^{14}N, ^{58}Ni, and ^{208}Pb nuclei at 170 MeV and by ^{208}Pb at various energies yields a good agreement of the theoretical results with the available experimental data. The peripheral character of the ^{17}F scattering was established.

► **Properties of dibaryons in nuclear medium** [40]. For light nuclei with A = 6 (^{6}Li and ^{6}He) in the α+NN cluster model which takes into account dibaryon resonances in the nucleon-nucleon interaction, the basic parameters and wave functions determining the structure and properties of these nuclei are obtained.

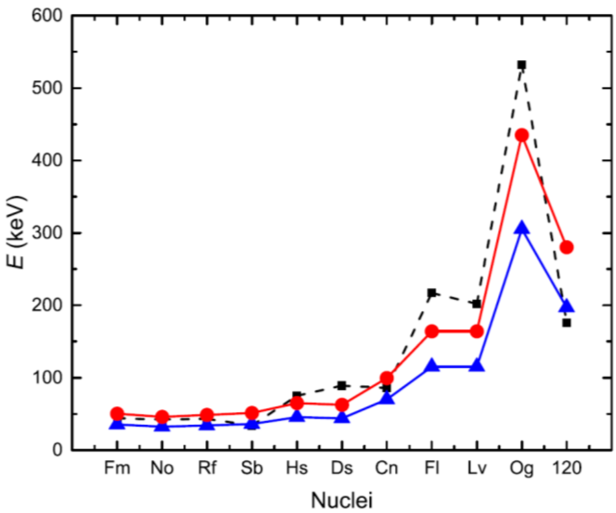
► **Computation of observables of quasiparticle-phonon models for deformed nuclei** (QPMN) is a striking example of long lasting successful MLIT-BLTP collaboration. The QPMN, an articulated nuclear physics model refined in BLTP during several decades, need intricate computations of various obervables that are pinpointed by the worldwide advancement of the study of the deformed nuclei to be of primary interest. N.Yu. Shirikova (MLIT) was the main developer of dedicated code modules, which have been gradually added to a structured package in BLTP. During 2020–2023, five scientific papers have been published with her participation.

● The fine structure of the isovector giant dipole resonance (IVGDR) in $^{142\text{-}150}$Nd and ^{152}Sm [41] provides a systematic investigation of the chain of stable even-mass Nd isotopes representing a transition from spherical to quadrupole-deformed nuclei. The purpose of the investigation was the extraction of the equivalent virtual-photon absorption cross-sections and analysis of their fine structure in the IVGDR region. The wavelet-analysis techniques used allowed for the features of the fine structure to be quantized in the form of characteristic scales. Comparisons between experimental results and model predictions indicate that Landau damping seems to be the main source of the fine structure in both the spherical and deformed nuclei.

● The significant yield of superheavy nuclei in FLNR-JINR has made possible their investigation by gamma spectroscopy methods. In [42] and [43], the understanding of the structure of the even-even superheavy nuclei was proposed to be based on the study of the excitation energy of their first excited 2+ states, $E(2_1^+)$.

In [42], the predictions of excitation energies of the first 2+ states of the chain of even-even superheavy nuclei have pointed to the possibility of using the Godzins phenomenological relation as a sensible tool for the assessment of the variation of $E(2_1^+)$ along this chain.

In [43], detailed predictions of the excitation energies of the 2_1^+ states of the even-even superheavy nuclei from ^{256}Fm to $^{296}_{120}X$, which differ from each other in the number of α particles, are computed. While the results do depend on the model parametrization, sharp increase of $E(2_1^+)$ with A is obtained, to reach a maximum value of 400–500 KeV in ^{284}Fl or ^{292}Og (see figure below).

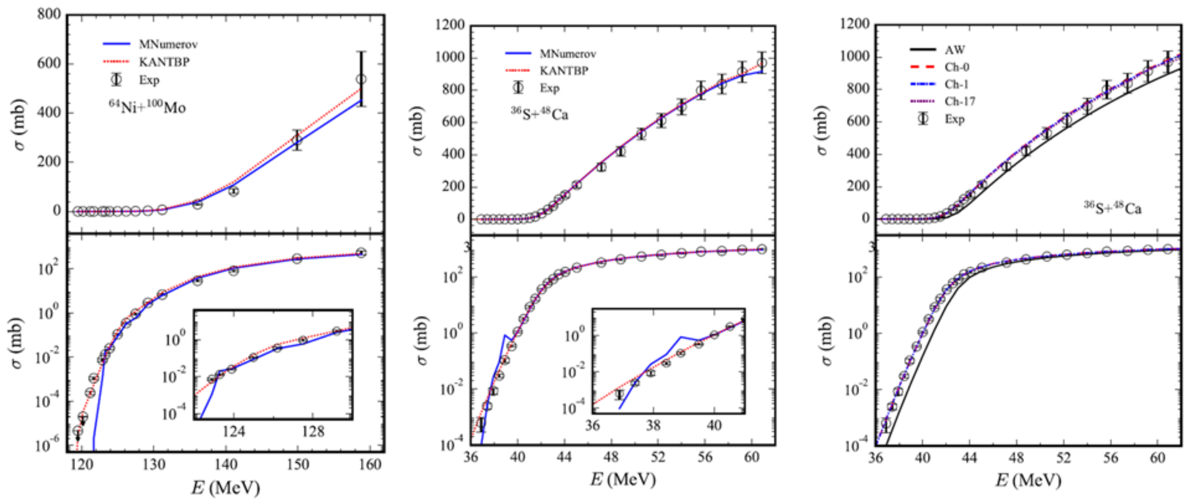


The predicted energies of the 2_1^+ states for different nuclei. Calculations are performed for the microscopic variant of the Grodzins relation (dashed line with squares (black)), the phenomenological Grodzins relation $[E(2_1^+)_{max}$: solid line with circles (red)], respectively $[E(2_1^+)_{min}$: solid line with triangles (blue)] [43].

● The Coriolis mixing in well-deformed even-even nuclei is investigated [44].

● Spin-isospin structure of the nuclear scissors mode [45].

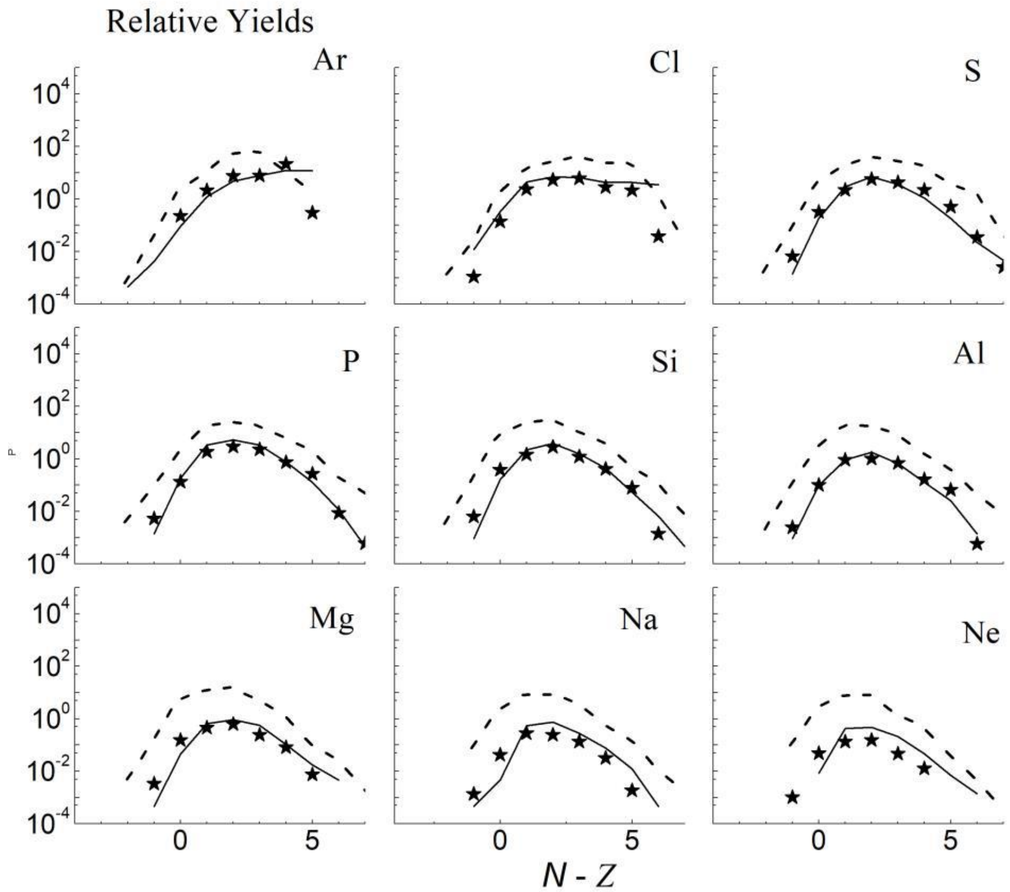
► **Role of the boundary conditions in the near-barrier heavy-ion fusion** [46].



Comparison of experimental fusion cross sections (open circles) with outputs of model calculations. ***Left*** and ***central*** panels: model data of CCFULL (solid line, also labeled as MNumerov) and of authors' KANTBP (dotted line). ***Right*** panel: calculations with standard AW potential and 0 coupled channels are shown by solid lines. Fitted calculations performed with 0, 1, 17 coupled channels are represented by dashed lines (Ch-0), dash-dotted lines (Ch-1), and dotted lines (Ch-17), respectively [46].

A quantum-mechanical description of the near-barrier fusion of heavy nuclei that occurs at strong coupling of their relative motion to surface vibrations was derived. To this end, an efficient finite element method was proposed for the numerical solution of the coupled Schrödinger equations with boundary conditions corresponding to total absorption. The method eliminates the instabilities in the numerical solutions previously noticed at a large number of coupled channels in some reactions. To illustrate the validity of the present approach, the results of fusion cross section of the ^{64}Ni + ^{100}Mo and ^{36}S + ^{48}Ca reactions have been re-examined. The obtained results show a remarkable agreement with the available experimental data. It is found that the experimental data can be well reproduced with a Woods-Saxon potential, without asking for the repulsive cores. It appears that the fusion cross sections at deep sub-barrier energies are sensitive to the potential pocket profile (see figures above).

► **The heavy-ion-induced projectile fragmentation reactions at Fermi energies, realized at the COMBAS setup in FLNR**, yields vast amounts of isotopes far from the valley of stability. The understanding of the production mechanisms of the resulting neutron-rich or proton-rich isotopes is a challenging task the solution of which was gradually articulated such as to include: proper definition of the states of the input nuclei entering the collision; characterization of the dynamical evolution of the density function of the colliding nuclei until the freeze-out point; calculation of the excitation energies of the projectile-like fragments; the understanding of the fragment de-excitation processes, which involve the emission of particles and radiation. Results obtained within this statistical approach to the numerical modeling of the various steps of the solution have been reported in [47–50]. An instance of the obtained results, characterizing the isotope yields from Oxygen to Lithium in the reaction ^{18}O (35 MeV/nucleon) on ^{181}Ta is given in the figure below.

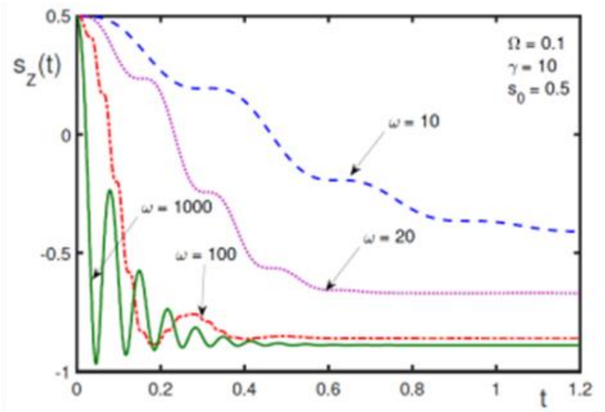


The relative isotope yields [49] in ^{40}Ar (36.5 *A*MeV) + ^{9}Be collissions (stars) in comparison with BNV-SMM calculations (solid curves) and previous experimental data [189] (dashed curves). The isotope names are given in the upper right corner of the pallets.

1.2.3. *Numerical modeling of condensed matter systems*

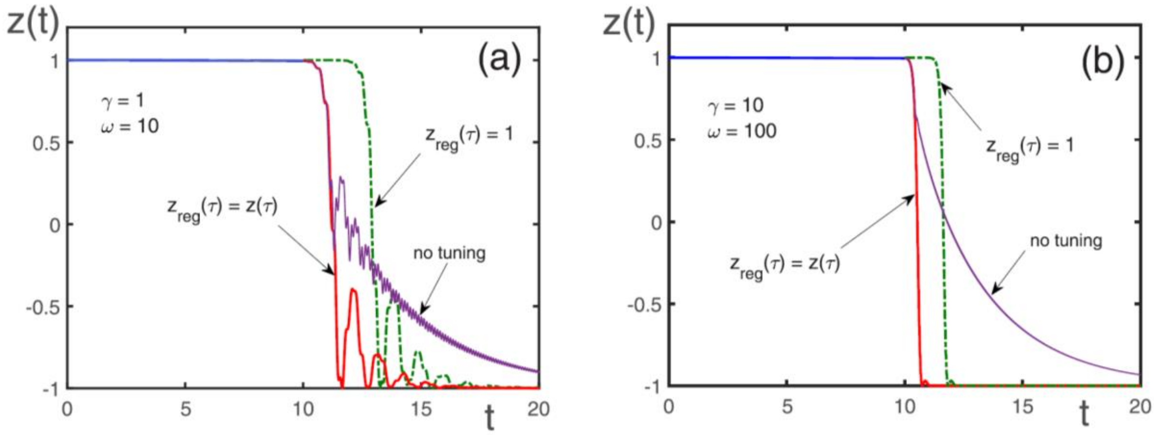
► **Solution of dynamic phenomena in magnetic materials** [51, 52].

● **Ultrafast polarization switching in ferroelectrics** [51]. A method of ultrafast polarization switching in ferroelectrics is proposed and numerically studied in ferroelectrics using the self-acceleration effect of polarization dynamics through the feedback field. The dependence of the polarization switching on the varying frequency ω is illustrated below.



Dependence of the polarization switching on the varying frequency ω for Ω = 0.1, γ = 10, for the initial polarization s_0 = 0.5. Here: ω = 10 (dashed line); ω = 20 (dotted line); ω = 100 (dashed-dotted line); and ω = 1000 (solid line).

● **The fast regulation of the magnetization direction in magnetic nanomaterials**, such as magnetic nanomolecules and nanoclusters is investigated. The method can find applications in the creation of memory devices and other spintronic appliances [52].



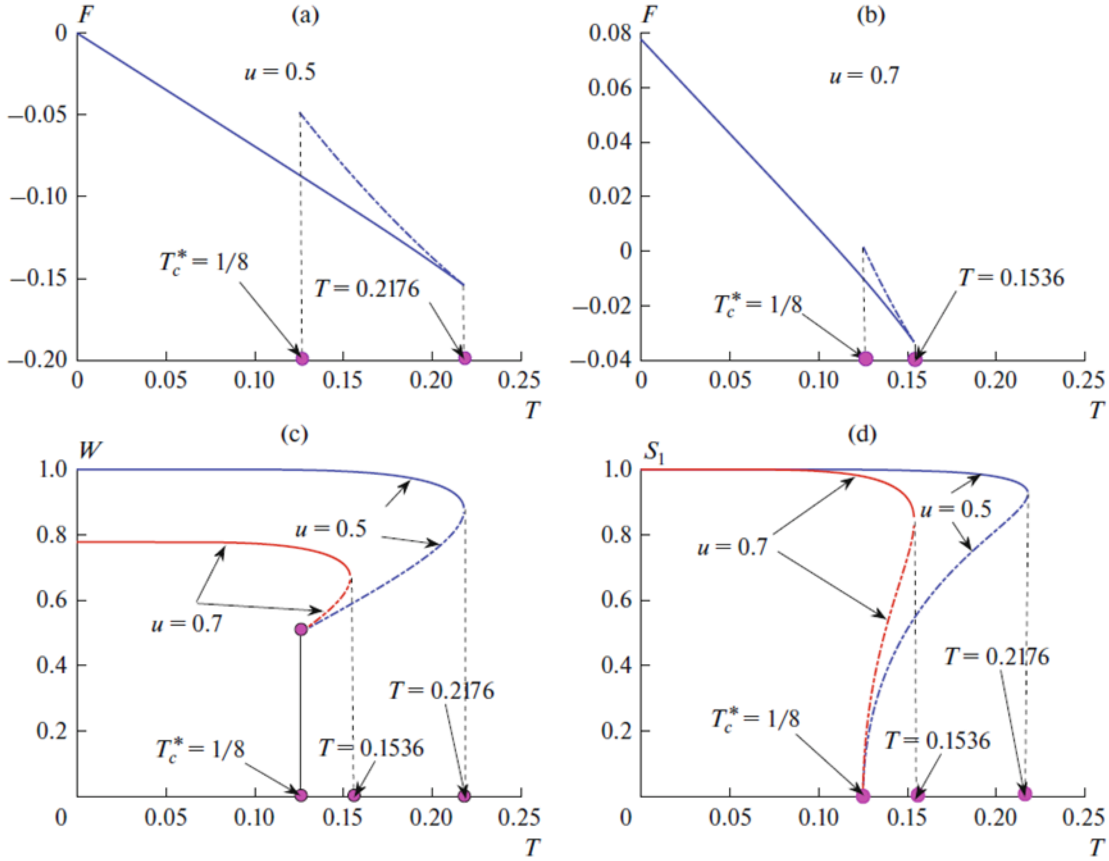
Spin polarization z(t) of a nanocluster or nanomolecule as a function of time under dynamic resonance tuning for different parameters of the system.

► **From Asymptotic Series to Self-Similar Approximants** [53–56]. The method of self-similar approximations proposed and developed by the authors constructs approximate solutions to complicated physics problems, starting from asymptotic series and going through optimized perturbation theory. The method is characterized by low computational complexity and combines simplicity with good accuracy. The multi-scale self-similar extrapolation of non-linear problems [53] allows finding the behavior of solutions at asymptotically large variables when knowing just a few terms of small-variable expansions. The solution of several different problems has been also reported [54–56].

► **Simulation of statistical systems composed of several phases** [57, 58].

● **A microscopic statistical model of a superfluid quantum solid** is developed [57], where inside a crystalline lattice there can exist regions of disorder, such as dislocation networks or grain boundaries. The cores of these regions of disorder are assumed to exhibit fluid-like properties. If the solid is composed of Bose atoms, then the fluid-like aggregations inside the regions of disorder can exhibit Bose-Einstein condensation and hence superfluidity. This microscopic statistical model gives the opportunity to answer which real quantum crystals can exhibit the property of superfluidity and which cannot.

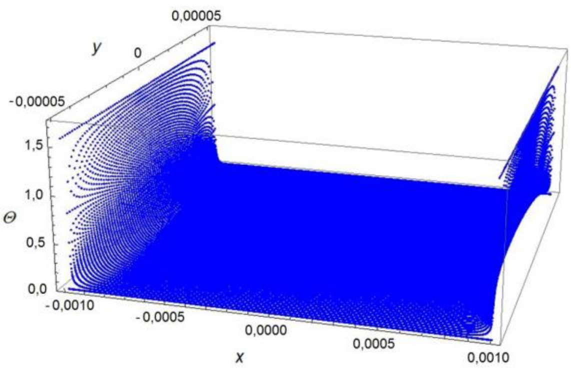
● **The review** [58] considers statistical systems composed of several phases that are intermixed in space at mesoscopic scale and systems representing a mixture of several components of microscopic objects. Heterogeneous materials composed of mesoscopic mixtures are ubiquitous in nature. A general theory of such mesoscopic mixtures is presented and illustrated by several condensed matter models. A mixture of several components of microscopic objects is illustrated by clustering quark-hadron matter.



Two branches of solutions for the thermodynamic potential *F* as a function of dimensionless temperature *T* for the parameters: (a) $u = 0.5$ and (b) $u = 0.7$. The probability *W* of the thermodynamic phase (c) and the order parameter S_1 as a function of temperature (d). The stable branch is shown by solid line and the unstable one is shown by dashed-dotted line [58].

► **Numerical investigation of the water vapour diffusivity in porous media** [59, 60].

► **Simulation of nematic liquid crystal optical waveguide structures** [61–63].

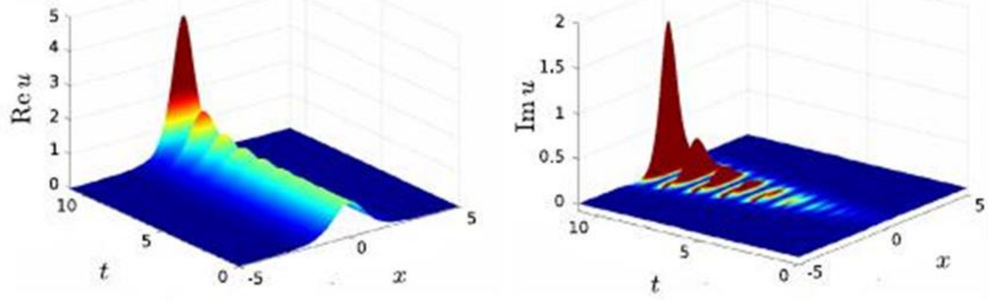


2D director dynamics in 5CB NLC cell [62]

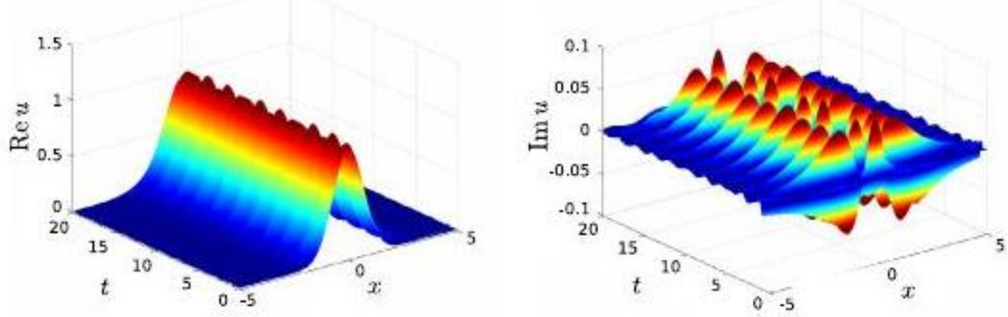
Numerical and experimental studies of two nematic liquid crystal (NLC) optical waveguide structures (liquid thin waveguide lens and thin film generalized waveguide Luneburg lens) were reported [62]. Results of the two dimensional dynamic model are illustrated in the figure above. Better agreement with the experiment is got as compared with the previously used static model.

Numerical modeling of smooth-irregular liquid-crystal waveguide structures (4-cyano-40-pentylbiphenyl) under the action of an external field has made possible the study of the resulting inhomogeneous non-stationary regions, characterized by lack of the orientation of part of the liquid crystal molecules under the action of the field [63].

►**Solving nonlinear problems of mathematical physics: Stable solitons in a nearly PT-symmetric ferromagnet with spin-transfer torque** [64]. The undamped Landau-Lifshitz equation for the spin torque oscillator, a uniaxial ferromagnet in an external magnetic field with polarised spin current driven through it, is PT symmetric in the absence of the Gilbert damping. In the vicinity of the bifurcation point of a uniform static state of magnetisation, the PT-symmetric Landau-Lifshitz equation with a small dissipative perturbation reduces to a nonlinear Schrodinger equation with a quadratic nonlinearity. The analysis of the Schroedinger dynamics demonstrates that stable solitons can exist in one and two dimensions. Near PT-symmetry of Landau-Lifshitz equation is crucial for soliton stability. Illustrations follow:

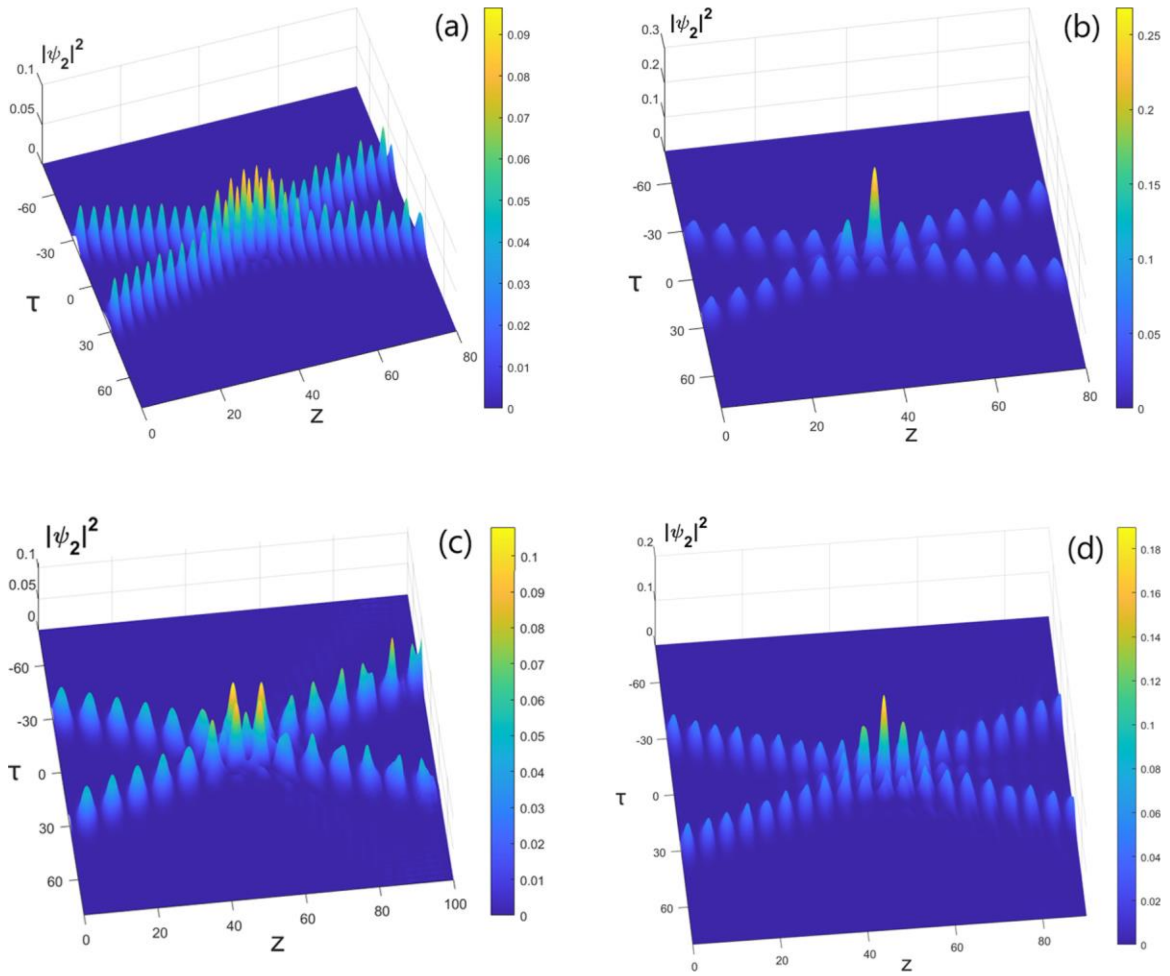


Instability of the fundamental soliton in the presence of damping. The initial condition was in the form of a soliton perturbed by a random perturbation within 5% of the soliton amplitude.



The evolution of the initial condition in the form of a Gaussian. Left panel: Re u; right panel: Im u. The emerging solution is a breather with a small imaginary part and the real part close to the soliton.

► **Gyrating solitons in a necklace of waveguides** [65]. Light pulses in a circular array of *2N* coupled nonlinear optical waveguides are considered. The waveguides are either Hermitian or alternate gain and loss in a *PT*-symmetric fashion. Simple patterns in the array include a ring of *2N* pulses traveling abreast and a breather – a string of pulses where all even and all odd waveguides flash in turn. In addition, the structure displays solitons gyrating around the necklace by switching from one waveguide to the next. Some of the gyrating solitons are stable while other ones are weakly unstable and evolve into gyrating multiflash strings. By tuning the gain-loss coefficient, the gyration of solitons in a non-Hermitian array may be reversed without changing the direction of their translational motion.



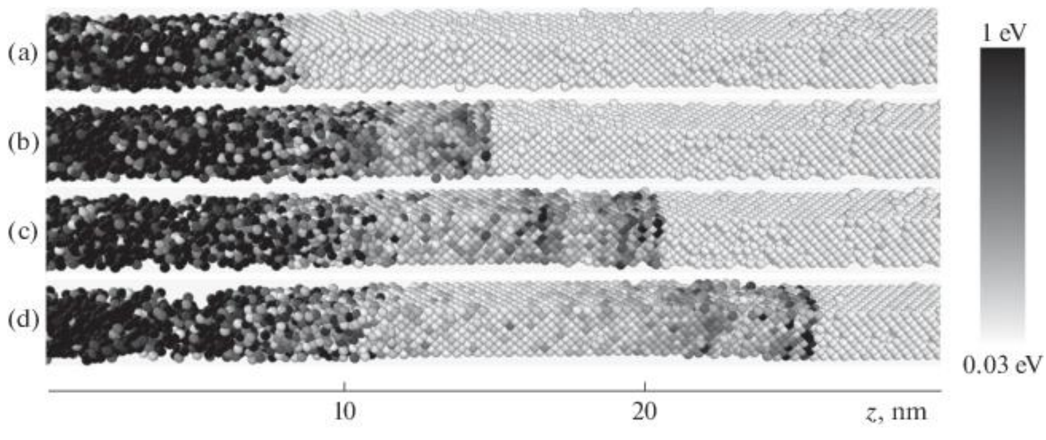
Scattering of gyrating solitons in the necklace of $2N = 6$ waveguides for different model parameter values.

1.2.4. *Numerical modeling of kinetic highly energetic processes in materials*

Results have been obtained for two kinds of complementary investigations: (a) molecular dynamics modeling of the behavior of solid samples of prescribed geometry and nature under bombardment with highly energetic particles or nanoclusters; (b) modeling, within the thermal spike model, of ablation processes in materials subject to laser radiation.

► **Molecular dynamics simulation of metals bombardment by nanoclusters** [66, 67]

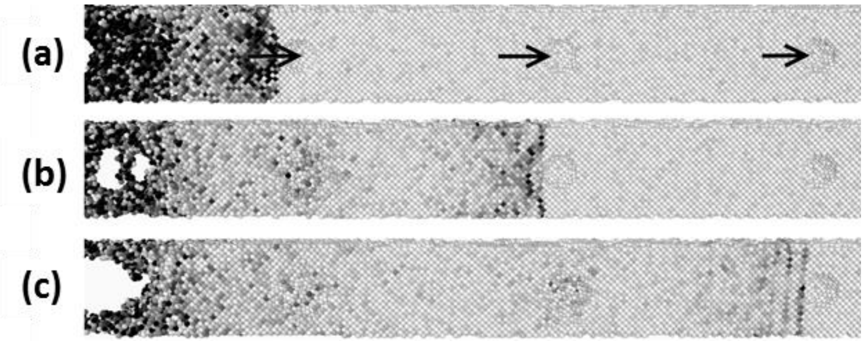
• **Molecular dynamics modeling of effects in metals by nanocluster bombardment** [66].



Dynamics of thermal processes and a shock wave upon irradiation with four copper ions with an energy of 1 keV at the moments of time: 1 (a); 2 (b); 3 (c); 4 ps (d). The target size is 2 × 2 × 40 nm [66].

The results of molecular dynamics modeling of the irradiation of metal targets with pulsed ion beams are obtained (see above) as a function of the ion energy and target size. The results obtained show that, by increasing the energy and power density of the irradiation (the number of particles), it is possible to change the defect structures at different depths of the target.

• **Molecular dynamics modeling of copper nanocluster interaction with metallic targets** [67]. Samples of copper, iron, and nickel with the structure of real crystals with specified pore-type defects, irradiated by copper nanoclusters with energies in the range 1 eV/atom-100 eV/atom, were studied by the method of molecular dynamics in collaboration with colleagues from Bulgaria and Mongolia. Modeling and testing were carried out using a modified LAMMPS package installed on the heterogeneous HybriLIT computing cluster. The numerical simulation investigated the effect of the shock waves on defect structures such as pores in the target. The threshold energies of irradiation by copper nanoclusters, which change the structure of a defect in targets, are obtained. The results obtained show that defects such as pores in an iron target are more resistant to the action of a shock wave compared to copper and nickel samples. Structural changes in the depth of the target depending on the energy of the nanocluster and the size of the target have been resolved. The formation of a hexagonal close-packed lattice near a pore-type defect in a copper target was established as a function of the nanocluster irradiation energy.



Shock wave dynamics in the copper target at times 1.5 ps (a), 4.4 ps (b), and 7.4 ps (c) upon irradiation with a nanocluster of 100 eV/atom. The arrows indicate the location of the pores and the direction of shock wave motion [67].

► **Numerical simulation of thermal processes occurring in materials under the action of ultrashort laser pulses** [68, 69]. The dynamics of the thermal mechanism of laser ablation [68] is described in terms of a one-dimensional nonstationary heat conduction equation. In it, the laser action corresponds to the source in the thermal conductivity equation. The dependence of the maximum temperature on the sample surface and the thickness of the ablation layer on the radiation dose of the incident laser pulse is obtained.

The mathematical formulation of the thermal processes occurring in materials under the action of femtosecond laser pulses [69] is done in terms of hyperbolic equations description of the heat conduction. It was found that the temperature of the sample is influenced not only by the power density of the source, but also by the rate of its change.

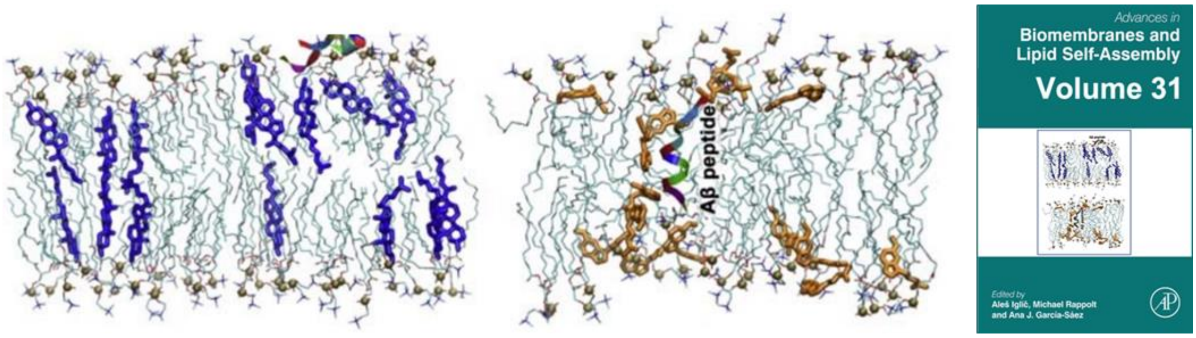
The numerical simulation of the ablation processes in materials under the action of femtosecond laser radiation has been developed further in the frame of thermal spike model (TSM) described by hyperbolic heat conduction equations (H-TSM). Detailed numerical experiments done for semi-infinite materials [70] explicitely resolved diffusion term and convection term contributions to the relaxation times of both the electron gas and the crystal lattice.

In a second investigation [71], the H-TSM model was formulated for samples of finite thickness. In this case, the sample thickness explicitely enters both the diffusion and convection terms of the heat conduction equations, as well as the source term of the H-TSM model equations and the boundary conditions of the problem. The effective velocity of the convective term is defined in terms of the speed of displacement of the up and bottom boundaries of the sample. Detailed numerical experiments evidenced characteristic dependences of the evaporation processes on the sample thickness.

1.2.5. *Numerical modeling in radiation biology*

► **Clarification of the role of the amyloid-beta peptide (Aβ) as a key factor in Alzheimer's disease** [72–75].

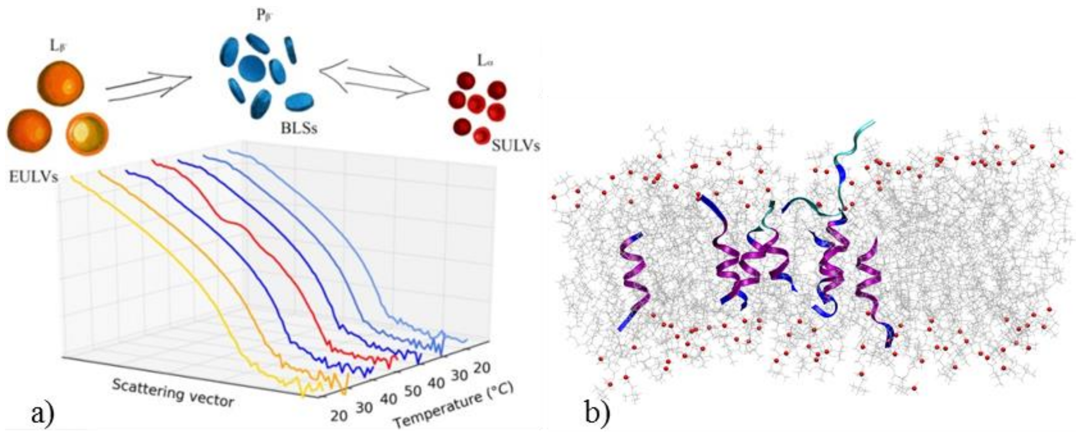
• **Interactions in the model membranes mimicking preclinical conformational diseases** [72].



Snapshots of molecular dynamics simulations depicting the lipid bilayer loaded with cholesterol (left) and melatonin (centre). The interactions of Aβ peptide with more rigid membrane in the former case force its location at the membrane-water interface. In the latter case, Aβ peptide embeds itself within the interior of more fluid membrane. The right snapshot shows the cover of the volume.

Although a complete understanding of the physicochemical processes taking place in biomembranes is not fully established, the understanding of the lipid bilayer elasto-mechanical properties provides a foundation for better insights into the structure-function relationships that most certainly take place in complex biomembrane systems. The study addresses the mechanism of the Alzheimer disease. The cover of the volume is illustrated with results from this report.

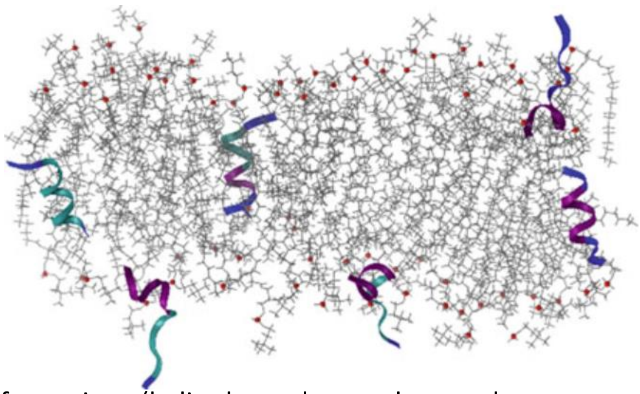
• **Role of amyloid‑beta peptide (25–35) in the reorganization of lipid membranes driven by temperature changes** [73].



a) SANS suggested evolution of the DPPC/$A\beta_{25-35}$ membrane organizations during the temperature changes. The transition from the initial EULVs to BLSs is irreversible, while the BLSs transition to SULVs is reversible. b) Snapshot of MD simulations of the DPPC/$A\beta_{25-35}$ system after 1 μs run.

The understanding of the damaging influence of the amyloid-beta peptide (Aβ) has shifted recently from large fibrils observed in the inter-cellular environment to the small oligomers interacting with a cell membrane. This action was inferred from small angle neutron scattering (SANS), which pointed to the occurrence of a spontaneous reformation of extruded unilamellar vesicles (EULVs) to discoidal bicelle-like structures (BLSs) and small unilamellar vesicles (SULVs). This dramatic change in the overall membrane shape is attributable to parallel changes in its thickness as the Aβ_{25-35} triggered membrane damages and to a consequent reorganization of its structure.

• An overview [74] of the studies of the complex model of biological membranes using a variety of experimental and theoretical methods is done. The effects modulated by the presence of Aβ peptides and, more importantly, the modes of interaction between membranes and peptides are examined. Simulations of the Aβ_{25-35} monomer in an implicit water-membrane environment and explicit DMPC membrane with water models by REMD have shown that the peptide may be present in the membrane in two states – a surface-bound state and a less stable inserted state, between which Aβ can often be interconverted (Fig. 10.10 from [74] illustrates these features, see below):



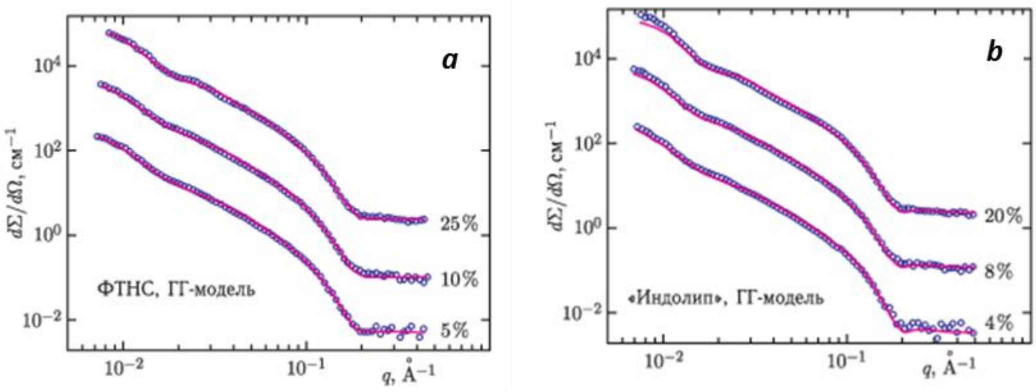
Snapshots of Aβ_{25-35} conformations (helix shown by purple, turn by cyan, and coil by blue colors) and positions in phospholipid membrane (phosphorus atoms shown by red points, rest of the lipids shown by gray color; water was omitted for the simplification of the presentation)

• **Changes to the membrane thickness and the overall membrane structure,** with and without Aβ_{25-35} incorporated, have been investigated over a wide range of temperatures. The results support the previously reported independence of the morphological reformations between bicelle-like structures present in the gel phase and small unilamellar vesicles present in the fluid phase on the charge existence in the system [75].

► **Numerical analysis, in the framework of the separated form factor method, of the structure of phospholipid membranes in vesicular systems by small-angle neutron and X-ray scattering data** is one of the hot topics of modern nano- and biophysics in connection with numerous applications of these objects in medicine, pharmacology, and cosmetology.

• Two program packages have been developed for the effective separated form factors analysis of small-angle neutron scattering data. The MPI-based parallel implementation accelerates calculations by 6–16 times; the Windows-based online interface provides convenient work with the respective local minimization procedure. The perspective of extending this tool within the JINR MICC HybriLIT platform is discussed [76].

• Within the framework of the separated form factor method, an analysis was made of the small-angle neutron scattering (SANS) spectra measured at the YuMO small-angle spectrometer on polydisperse populations of single-layer vesicles of the phospholipid transport nanosystem (PTNS) and Indolip nanodrug in heavy water at three concentrations. The possibilities of obtaining information on the structure of nanodrugs based on PTNS using SANS data are discussed. The basic structural parameters of these vesicular systems, obtained from computer analysis of the SANS spectra, generally agree with the corresponding results of small-angle X-ray scattering (SAXS) data processing. At the same time, the SANS method turns out to be less sensitive in comparison with SAXS as it concerns the detailed account of the structural features of the bilayer of the vesicle envelope. The work was carried out in cooperation with the FLNP [77]. The figure below summarizes the experimental and calculated SANS spectra.



Calculated and experimental SANS spectra on samples of FTNS (***a***) and Indolip (***b***) vesicles in 4, 8, 20% maltose solutions. The calculation was made using the hydrophilic-hydrophobic bilayer model [77].

• **A program package, devoted to the analysis of the structure of vesicular systems** by the model of separated form factors (SFF-Analysis) was implemented on HybriLIT. The program secures a simplified request for resources when starting a task, web monitoring of the calculation process and visualization of results [77].

► **Modeling the COVID-19 pandemic** [78–80]

• **Reduced SIR Model of the COVID-19 Pandemic** [78] A mathematical model of COVID-19 pandemic preserving an optimal balance between the adequate description of a pandemic by SIR model and simplicity of practical estimates is proposed. The presented examples of modeling the pandemic development depend on two parameters: the time of possible dissemination of infection by one virus carrier and the probability of contamination of a healthy population member in a contact with an infected one per unit time. This is in qualitative agreement with the dynamics of COVID-19 pandemic. The proposed model is compared with the SIR model.

• 2020 submission to the PROGRAM LIBRARY JINRLIB of important HPC parallel package:

SIR – SIR-model – the simplest epidemic process model (May 20, 2020) [79]. The simplest 3-state model after the Malthus and Verhulst models, denoted in the literature by the abbreviation SIR (S – susceptible, I – with clinical tests of an infectious disease, R – recovered), with time-dependent coefficients is considered. The model is mapped to current statistics that are in the public domain. Unknown model parameters are found by minimizing the discrepancy between the prediction and available statistics. https://wwwinfo.jinr.ru/programs/jinrlib/sir-model/indexe.html

• **Modeling the multifractal dynamics of COVID-19 pandemic** is done within a mathematical model, which is alternative to other models and free of their shortcomings. It is based on the fractal properties of pandemics only and allows describing their time behavior using no hypotheses and assumptions about the structure of the disease process. The model is applied to describe the dynamics of the COVID-19 pandemic from day 1 to day 699 from the beginning of the pandemic [80].

1.2.6. *Numerical modeling of other systems*

► **Asymptotic solution of Sturm–Liouville problem with periodic boundary conditions for relativistic finite difference Schrödinger equation** [81]. In this paper, Sturm–Liouville problems with periodic boundary conditions on a segment and a positive half-line for the $2m$-order truncated relativistic finite-difference Schrödinger equation (Logunov–Tavkhelidze–Kadyshevsky equation) with a small parameter are considered. A method for constructing of asymptotic eigenfunctions and eigenvalues in the form of asymptotic series for singularly perturbed Sturm–Liouville problems with periodic boundary conditions is proposed. Their solutions allow describing the behavior chains of harmonic oscillators with periodic boundary conditions when they are very far apart from each other. The solutions are relevant for the description of the bounded states of the elementary particles in the quark-gluon plasma.

► **Algorithms for calculating dimesoatom breakup cross-sections in Coulomb fields**.

Momentum and angular distributions of charged meson pairs h^+h^-(h = π; K) from elementary atom breakup in the Coulomb field of the target are calculated in the Born and Glauber approximations [82]. A new algorithm is developed to calculate the normalized differential Mott cross section for electron scattering by a Coulomb potential as well as a method for calculating the Mott correction to the Bethe formula for the average ionization energy loss by heavy ions. The results obtained on this basis are compared with the results of calculations by other methods in wide ranges of values of the charge number of the ion nucleus, electron energies, and their scattering angle [83, 84].

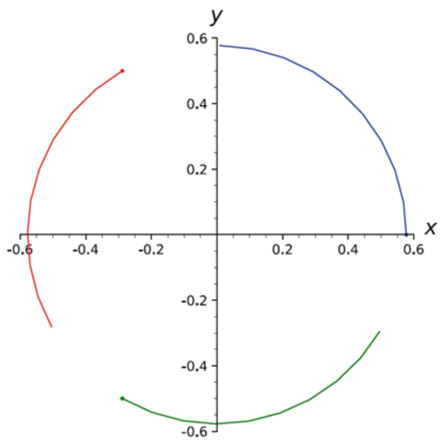
► **Kinetic stabilization of unstable metal oxidation states upon complexation freeze** [85, 86].

► **Modeling of raw material resource depletion processes** [87, 88].

► **Solving a triangulation problem** [89].

► **Fresh ideas for solving old problems** [90, 91].

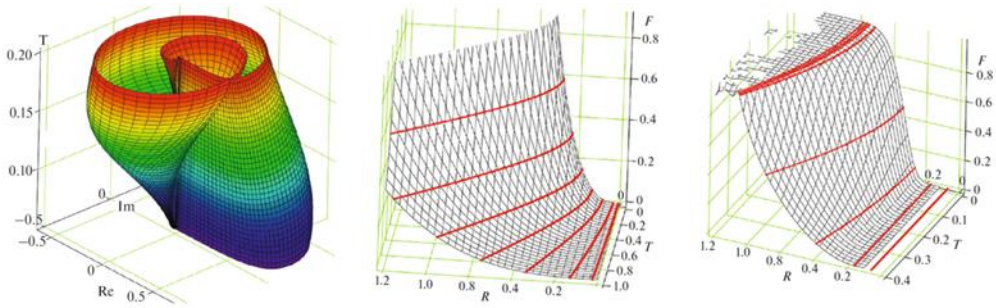
► **On Periodic Approximate Solutions of the Three-Body Problem** [92]. The Lagrange Problem of finding all approximate solutions of the three-body problem at which the distances between the bodies remain constant was reduced to the study of the properties of linear oscillators. In particular, it turns out that the periodicity of the exact solution in the Lagrange case, when the bodies form a regular triangle, is inherited by the approximate solution.



Solution to the three-body problem in the Lagrange case, Δt = 0.1.

► **Approximate evaluation of matrix-valued functional integrals generated by a relativistic Hamiltonian** [93]. An algorithm is derived, which allows to reduce significantly the requested computer resources as compared to other known methods.

► **A method for finding exact solutions of the first equation from the chain of Vlasov equations**, formally similar to the continuity equation, is considered [94]. The equation under investigation is written for a scalar function and a vector field, which depend on the formulation of the problem. Mathematically, the same equation is applicable for describing statistical, quantum, and classical systems. The exact solution obtained for one physical system can be mapped onto the exact solution for another system. Availability of exact solutions of model nonlinear systems is important for designing complex physical facilities, such as the SPD detector for the NICA project. An instantiation of the wealth of results reported is given below.



The left panel shows the evolution of the wave function before the occurrence of the shock wave. The central and right panels illustrate the time evolution of the probability distribution function for a constant initial probability distribution density (no shock wave – center) and for a Gaussian initial distribution with the shock wave (right).

► **Cosmology studies in different universe models** [95–101]. The role of spinor fields characterized by nonminimal coupling in the evolution of the Universe was studied in different Universe models.

1.3. New Ways of Reducing Extreme Inner Problem Complexity

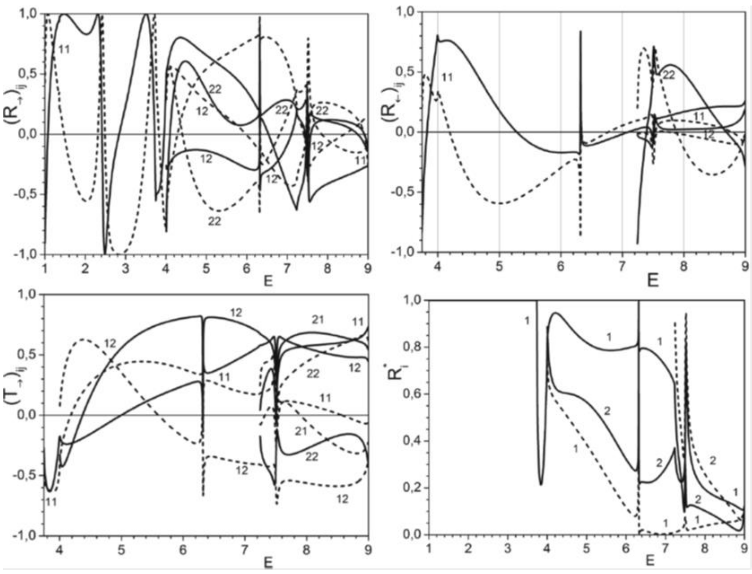
• **New symbolic-numerical schemes using finite element method** (**FEM**) [102], based on analytical Hermite interpolation polynomials in d variables on the standard d-dimensional hypercube and simplex, are developed. They serve to the solution of boundary value problems emerging from physics problems like the quadrupole vibration collective nuclear model.

A special application of the new FEM is the solution of the vibrational-rotational states of the diatomic beryllium molecule with realistic potentials [103]

A specific ingredient of the above schemes is the KANTBP 4M program implemented in the computer algebra system MAPLE for solving, with a given accuracy, the multichannel scattering problem. An upgrade of this program was reported [104].

The FEM and upgraded program KANTBP are used for coupled-channel calculations for heavy ion fusion reactions [105]. The efficiency of the proposed approach is proved by the successful description of experimental data for the sub-barrier and above-barrier fusion cross section of some reaction systems.

• **Symbolic-numeric algorithms for solving problems with complex energy eigenvalues** [106–108].

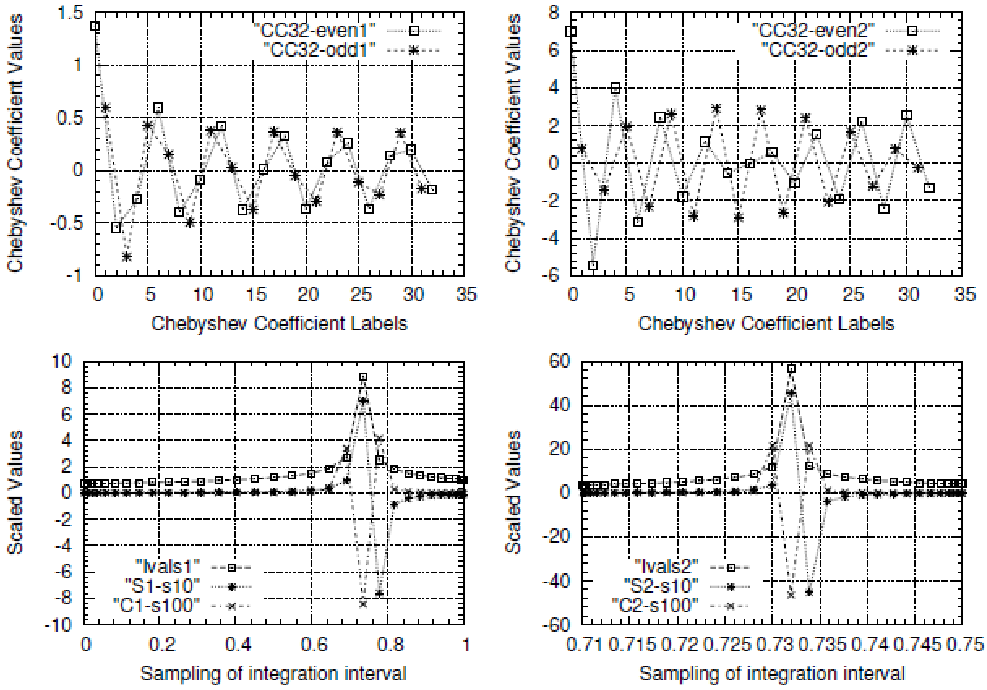


Real (solid curves) and imaginary (dashed curves) parts of elements $(R_{\rightarrow})_{ij}$, $(R_{\leftarrow})_{ij}$, $(T_{\rightarrow})_{ij} = (T_{\leftarrow})_{ji}$ of reflection $\mathbf{R}_{\rightarrow}$, $\mathbf{R}_{\leftarrow}$ and transmission $\mathbf{T}_{\rightarrow}$, $\mathbf{T}_{\leftarrow}$ amplitudes, and reflection coefficients $R^{*}_{i} = (\mathbf{R}^{\dagger}_{*}\mathbf{R}_{*})_{ii}$ at $* = \longrightarrow$ (solid curves) and $* = \longleftarrow$ (dashed curves) as functions of the scattering energy E [106].

The spectra of vibrational-rotational bound, metastable, and scattering states of a beryllium dimer in the ground $X^1\Sigma_g^+$ state, which are important for laser spectroscopy are calculated for the first time using the authors' developed software package KANTBP 5M, which implements the Newton method and a FEM of high order accuracy. The presented approach, implemented in the form of a software package, is a useful tool for studying weakly bound states with eigen-energies close to the dissociation threshold, as well as processes of near-surface diffusion of diatomic molecules.

• **D_{3h} symmetry adapted correlated three center wave functions of the ground and the first five excited states of H_3^+** [109]. An original three-center wave function is constructed by means of the irreducible representations of the D_{3h} point group, which characterizes the symmetry of the planar equilateral triangular H_3^+ molecule. The results of this work and the implementation of the computational techniques open the way to further studies of complex three center systems.

• **Problem adapted multi-scaling quadrature algorithms** [110]. The use of an m-panel rule (CC-32, Clenshaw–Curtis quadrature of algebraic degree of precision m = 32) over macroscopic integration ranges is supplemented with three-point Simpson rules spanned at triplets of successive CC-32 knots. This allows identification and precise characterization of integrand function irregularities through scale insensitive diagnostics (see figure below).

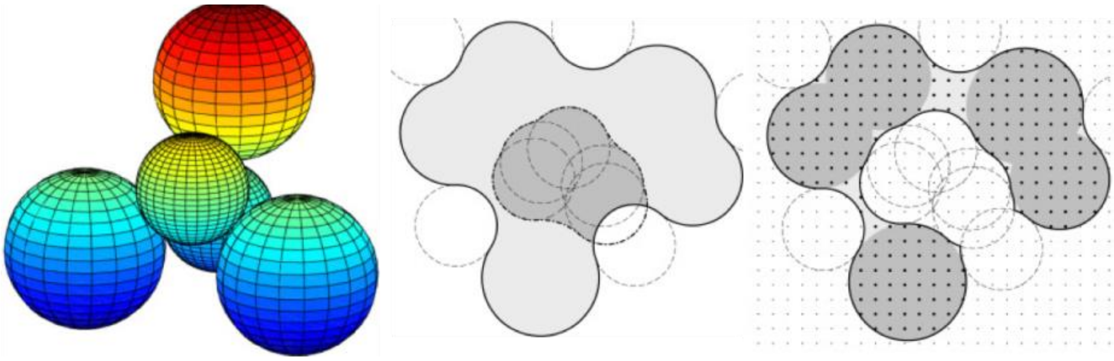


(Top) Case Study 1: CC-32 rule yields Chebyshev expansion coefficients showing irregular behaviour: *Left* – on [0; 1]; *Right* – on [0:71; 0:75]. (Bottom) Three Simpson rule basic elements (Ivalsk): Integrand values k, Sk-s10: Slopes k, scaling factor 10^{-1}; Ck-s100: Curvatures k, scaling factor 10^{-2}) yield Bayesian inference of integrand singularity (k = 1; *left*), confirmed under iteration on the smaller interval (k = 2; *right*).

• **The Bayesian two-rule automatic adaptive quadrature** (B2AAQ) of one-dimensional Riemann integrals is critically driven by the *a priori* input provided by the user. Conditions enabling straightforward elementary input of problem parameters are defined that result in either a single subrange decision tree or a forest of subrange decision trees [111]. This secures a B2AAQ implementation characterized by robustness, reliability and efficiency, together with a significant extension of the flexibility of use as compared to the QUADPACK package, which is the core of the computational integration chapters of the major computer libraries worldwide.

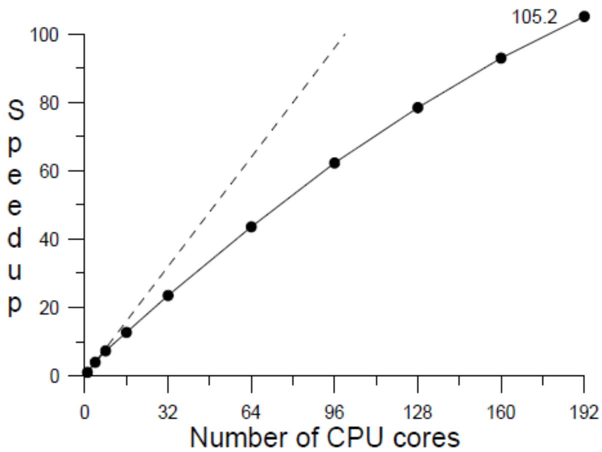
• **A BEM-PC** (Basic Element Method – "Predictor Corrector") of the fifth polynomial order is developed for the numerical solution of the Cauchy problem for ordinary differential equations [112]. The basic building bloks of the method are suitably defined "basic elements", which use four-knot transforms that have been previously proved to be able to suppress the errors and to enable the implementation of stable algorithms for experimental data processing. The advancement of the solution over a tentative step length *h* proceeds through the definition of a predictor spanned by two BEM polynomials of the fifth degree. The validation of the tentative *h* value is controlled by a key parameter *K* ($0 < K < 1$). The new BEM-PC method was empirically shown to be stable down to extremely small step sizes *h*. This feature makes it suitable for the solution of stiff problems.

• **Solving complex protein problems: PBCAVE** [113]. Analytically defined values of the dielectric constant for all discretization points of a grid in the computational domain defined inside a protein. Assigned values of dielectric constant (figure below) are used in a solver of the linear Poisson–Boltzmann equation for a protein–water system using a finite difference method.



A wall triangle of three atoms (large spheres) of a molecule and two touching probe spheres (points in-between are not accessible for probe spheres, hence are in "vacuum") (*left*). Inner and outer molecular surfaces intersections (*middle*). Grid points inaccessible to water depending on the radius of the testing sphere (*right*)

• **Multiple precision computation by parallelizing the Taylor series method** [114]. A hybrid MPI + OpenMP strategy was implemented and tested on the paradigmatic model of the Lorentz system. On a configuration with 192 CPU cores, the 2800-th order computation, with 3510 decimal digits lasted ~ 148 hours, with an acceleration factor of about 105 (see figure below).



2. Software Complexes and Mathematical Methods for Processing and Analysis of Experimental Data

The design, development, implementation, and maintenance of modules of object oriented dedicated scientific libraries are our contributions to the solution of research conducted by JINR at experimental facilities.

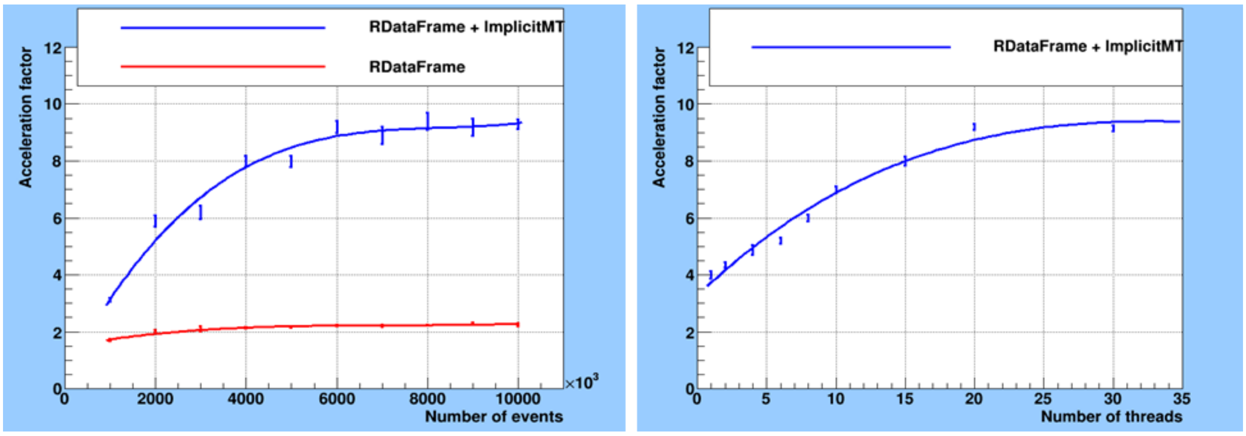
2.1. Parallel ROOT (PROOT) tools for experimental data analysis

The parallel ROOT package (PROOT) is the modernized CERN ROOT package of object oriented (OO) programs and libraries adapted to the multi-core and manycore CPU and GPU hardware, which dominates the landscape of the exising high performance computing (HPC).

While PROOT has become the fundamental tool for the analysis, visualization and storage of the experimental data collected in the high energy physics (HEP) experiments (e.g., FAIRROOT and CBMROOT at GSI, BMNROOT and MPDROOT in the NICA experiments), the question was formulated within the current Topic 1119 if the PROOT package could be used in other physics experiments as well. Investigations done by T. Solovjeva and A. Solovjev have provided an affirmative answer: the PROOT can be an efficient analysis tool for such different experiments as the Baikal-GVD, or small angle scattering (SAS) at the YuMO spectrometer of the IBR-2 facility.

Two kinds of results, reported at the “Parallel Computational Technologies (PCT) 2023” Conference, St. Peterburg, March 28–30, 2023, point to an affirmative answer.

The possibility to get significant acceleration of the data processing has been proved both in terms of the number of processed events and in terms of the number of the threads defined by the PROOT [115] (see figure below) (see also [179]).



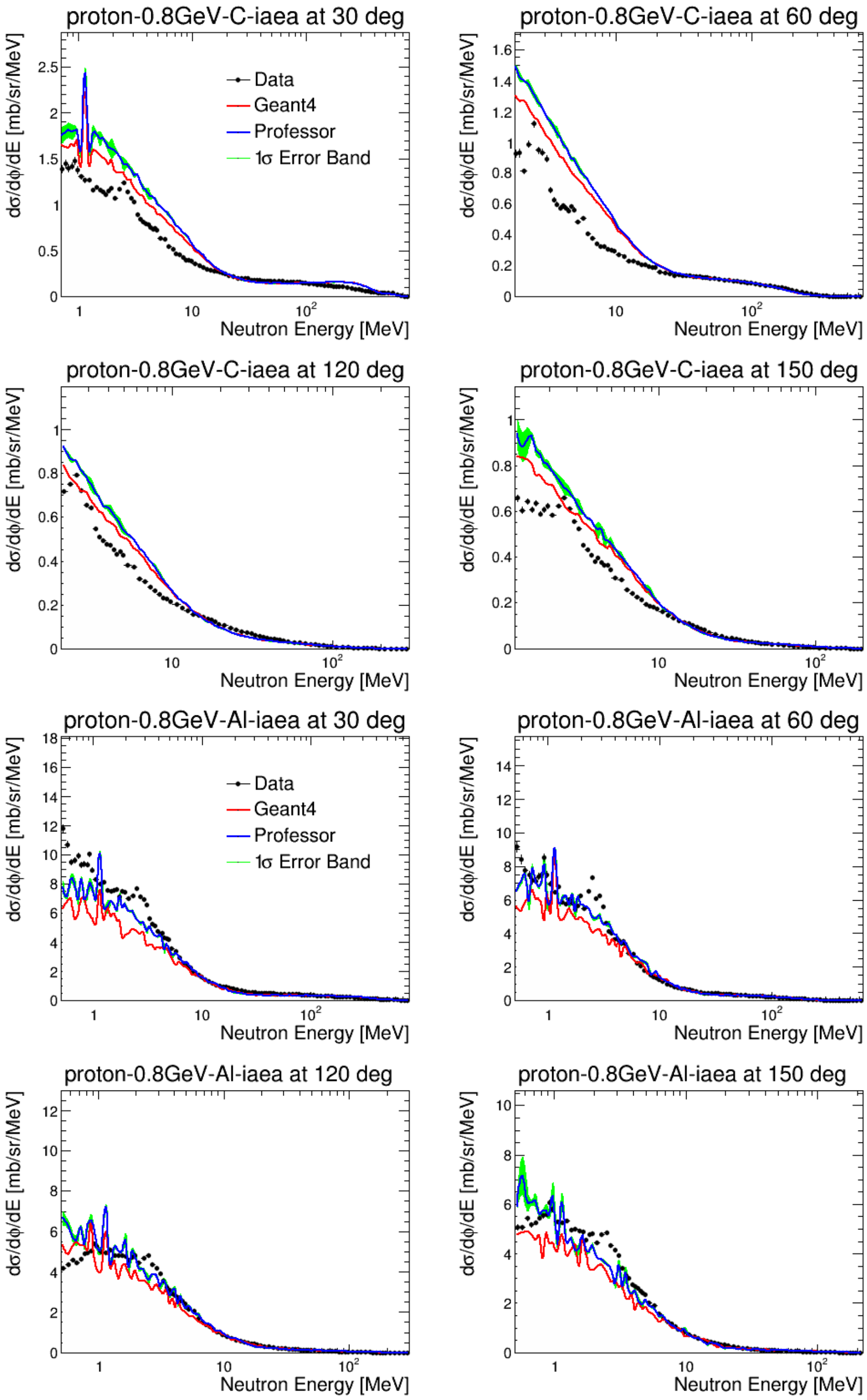
PROOT performance improvement. Left: Dependence of the acceleration coefficient on the number of events; Right: Ibid., on the number of threads [115]

2.2. GEANT4 package for unified simulation of large-scale experimental data

2.2.1. *Upgrade of the GEANT4 package with new modules*

Geant4 provides device independent modeling of experiments in high-energy physics and medical-biological research. For this reason, it is an underlying investigation tool in all the high-energy physics experiments, let they be done at LHC-CERN, FAIR-Darmstadt, Brookhaven, or NICA-JINR. V.V. Uzhinsky continues the long time JINR expertise in modeling high energy and nuclear processes. He is one of the main Geant4 developers, with periodic inclusion of new modules in the validated Geant4 software. *The upgrades include new computing modules (FTF modeling of nucleon coalescence, FTF and QGS modeling of hard QCD processes), Monte-Carlo HIJING generator improvement.*

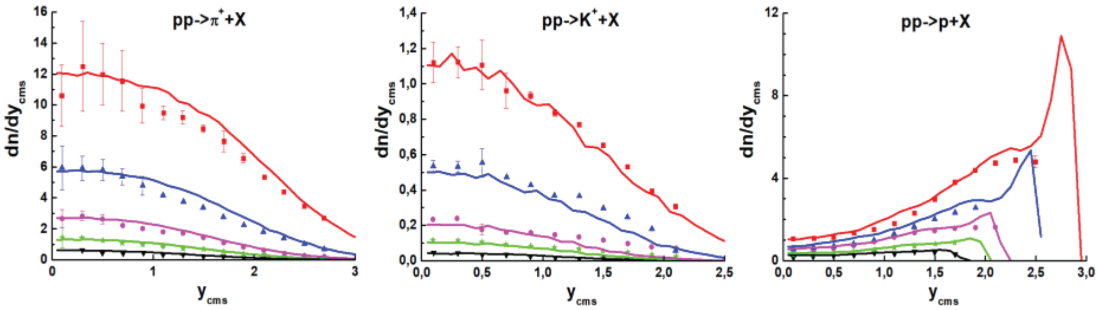
• **GEANT4 parameter tuning using Professor** [116]. A study of the impact of varying parameters in three Geant4 hadronic physics models on agreement with thin target datasets is done together with the description of the fits to these datasets using the Professor model-tuning framework. It is found that varying parameters produces substantially better agreement with some datasets, but that more degrees of freedom are required for full agreement. An example from the wealth of data provided is given in the figures below.



Results of the global Precompound parameter fit, compared to IAEA 0.8 GeV pC --> nX and pAl --> nX data in bins of final state neutron angle. Data points are shown in black; default Geant4 is red and the global fit result in blue; the green band shows uncertainties propagated from parameter uncertainties returned by the fit.

• **Study and development of Monte-Carlo event generators of hadron-nucleus and nucleus-nucleus interactions at high energies** were continued with proposals for the improvement of the HIJING (Heavy Ion Jet INteraction Generator) model. They allow describing experimental data by

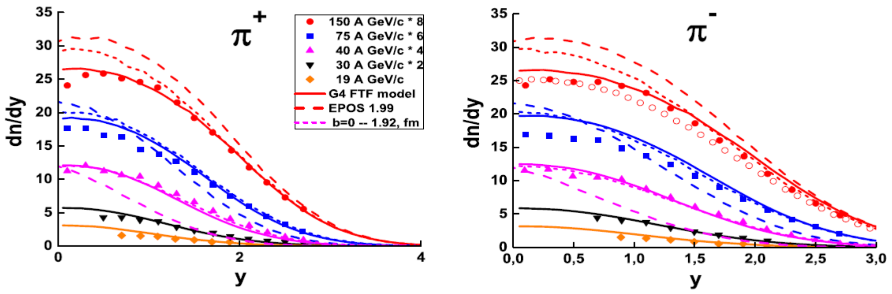
NA49 and NA61/SHINE collaborations on proton-proton interactions. The modified HIJING model was successfully used to the analysis of the STAR data on nucleus-nucleus collisions at high energies [117] (see figure below). It can be used in MPD and SPD experiments (NICA).



Rapidity distributions of particles in pp interactions at 158, 80, 40, 31, 20 GeV/c (from top to bottom, rescaled by 16, 8, 4, 2, 1). Points are experimental data, lines are calculations.

2.2.2. *Use of the GEANT4 package for data handling*

Model descriptions of the latest data by the NA61/SHINE collaboration [118] does a comparison of the HIJING, EPOS 1.99, UrQMD and Geant4 FTF models. It shows that the last is the only one, which describes well the NA61/SHINE data on π^- meson rapidity distributions in ^{40}Ar + ^{45}Sc interactions at $\sqrt{s_{NN}}$ = 5.2 and 6.1 GeV. At higher energies, $\sqrt{s_{NN}}$ =7.6, 8.8, 11.9 and 16.8 GeV, this model underestimates the data by 13%, 14%, 14% and 27%, respectively. The model also describes well the analogous data for ^{7}Be + ^{9}Be interactions at all energies ($\sqrt{s_{NN}}$ = 6.1–16.8 GeV).



Rapidity distributions of π^+ and π^- mesons in ^{7}Be + ^{9}Be interactions. The points are the data measured by the NA61/SHINE collaboration. The Geant4 FTF model calculations are shown by solid lines. Dashed lines show the EPOS model predictions. The short dashed lines are the EPOS calculations for b = 0 – 1.92 fm.

2.3. Software support of large-scale experiments

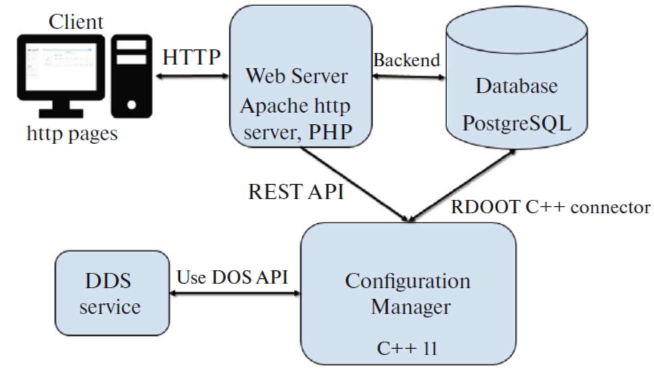
2.3.1. *Software support of all JINR-NICA experiments*

While in-house VBLHEP teams are doing the major part of the software development, the involvement of the MLIT staff through topic 1119 into this process has brought very rapid and very high level solutions to a number of tasks, which are detailed below. A general task concerns:

► **The design of the event metadata system for the experiments at NICA** [119–123]

The new Event Metadata System based on the Event Catalogue has been designed to index events of the NICA experiments and store their metadata. It makes possible the quick search by required conditions and parameters used in various physics analyses for a set of physics events to use in further event data processing. One of the important development tasks is integrating the Event Metadata System with the ROOT-based frameworks of the BM@N (BmnRoot), MPD (MPDRoot) and SPD (SPDroot) experiments. It enables correct multiple access for collaboration members of any role, scalable data architecture, high fail safety and automatic regular backup of the Event Catalogue. The implementation of the information system is a necessary step for accelerating the achievement of scientific results in the NICA experiments.

► **The Configuration Information System** (CIS) [124–126] follows from the implemented Configuration Database, an essential part of the set of information systems developed for the experiments of the NICA project. It provides configuration information for data acquisition and other online processing systems, activating those hardware setups needed in the current experiment session. In addition, the system starts the described software tasks in the required sequence and allows managing them during sessions, including the transmission of messages between tasks and the update of some properties. The architecture of the Configuration Information System, which is shown here, has been implemented using the client-server model, where the server ensures interactions with the Configuration Database, and the client has been developed as a Web application to view and edit configuration parameters by users.

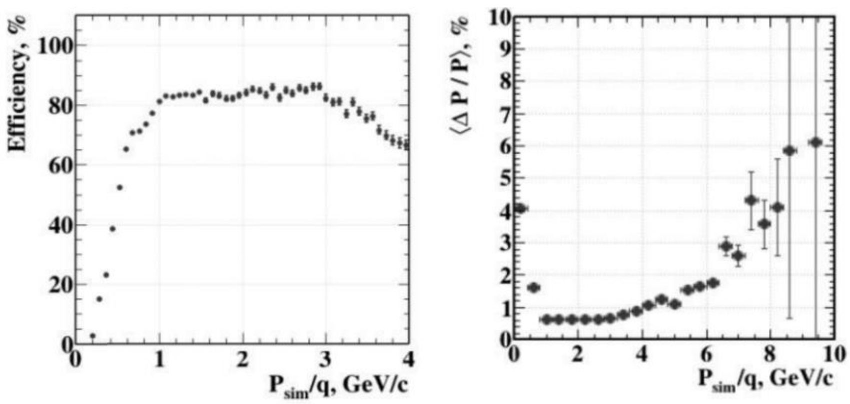


2.3.2. *Software support at JINR-NICA*: BM@N experiment

In the international online Joint JINR Colloquium Seminar "*The Transparent Nucleus: SRC and single nucleon knockout inverse kinematics measurements using a 48 GeV/c carbon beam at JINR*", held on 20 May 2020, Prof. Eli Piasetzky (Tel Aviv University, Israel) has reported the first relevant far reaching high precision physics experiment done at BM@N. At the end of his presentation, Prof. Eli Piasetzky has explicitly acknowledged, by name and by task solved, the noticeable contribution of the topic 1119 MLIT team which made possible this outstanding scientific result at BM@N.

► ***Excerpts of the work done and results obtained in 2020:***

• **Track reconstruction in the BM@N experiment** [127]. The reconstruction of charged particle trajectories in the BM@N experiment is one of the most important and time consuming tasks in the event reconstruction procedure. It is developed along requirements following from the two setup configurations defined so far: BM@N, and the Short Range Correlation Program (SRC) at BM@N. Cell-based algorithm is developed and incorporated into the **BmnRoot** software. Instances of tracking efficiency and momentum resolution:

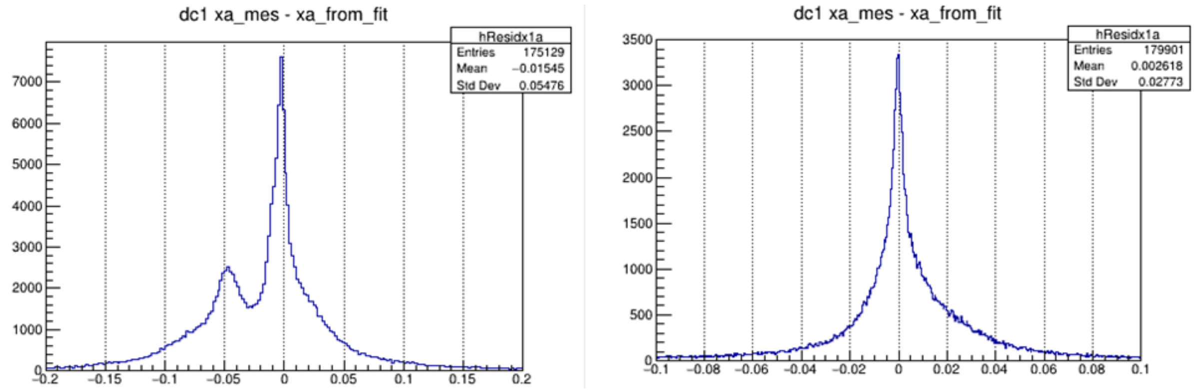


Left panel: tracking efficiency as a function of momentum. *Right panel*: momentum resolution as a function of momentum

• **Geometry update for inner tracker detectors of the BM@N setup** [128, 129] concerned the very important topics on updating the geometry for the inner tracker detectors (GEM and SILICON) of the BM@N setup at the RUN-7 (2018) and the next run (2021-2022) together with the calculation of material budget for these configurations.

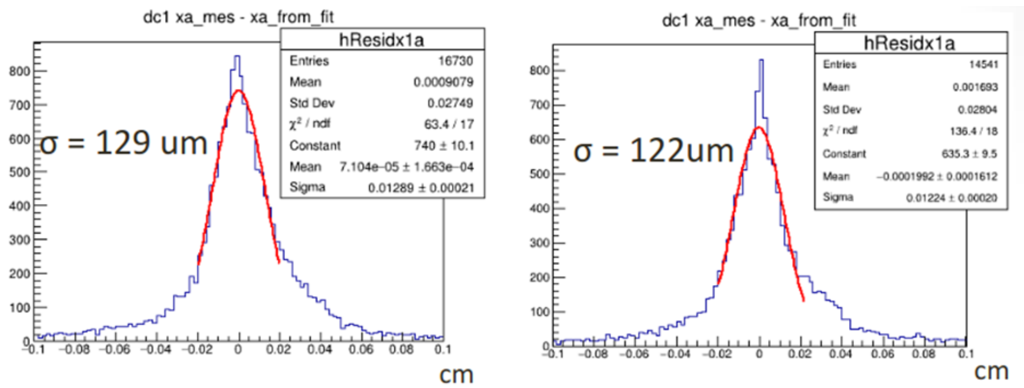
• The usefulness of the **geometry database for the BM@N experiment** and its scope were reviewed ([130], see also [131] and [132] for the latest developments). The *Geometry Database* supports storing, updating and retrieving the geometry of BM@N modules. The developed information system includes the database, intuitive and compact GUI tools and API tools as a set of *ROOT* macros. **The last approach to the geometry data base development** [132] **consists in the design and implementation covering the MPD detector as well**.

• **Alignment of the internal geometry of the drift chambers** (DCH). The presence of individual layers misalignment of the DCH was detected. The elimination of this misalignment increased the efficiency of global tracks reconstruction by more than 1.5 times. The magnitude of the errors of the particle momentum estimation decreased from 7.5% to 4% under the combination of the DCH and GEM data. This fulfills the experimental accuracy requirements (see figure below).

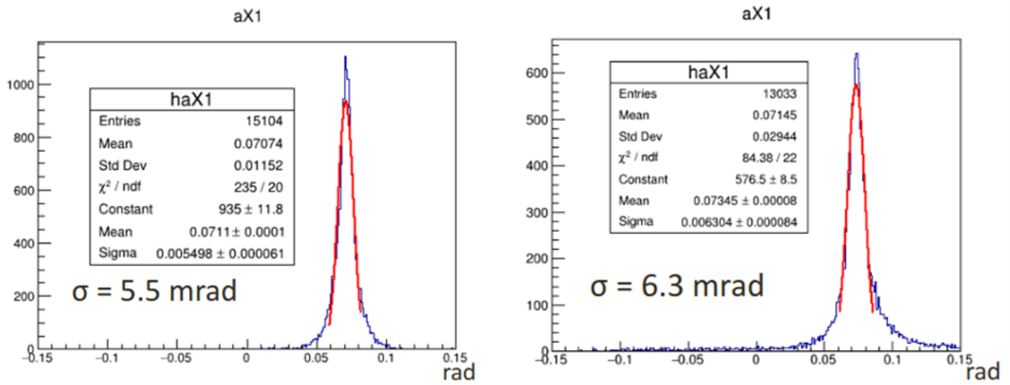


Deviation of coordinates from the fitted segment: *Left* – before internal alignment; *Right* – after

A full reconstruction chain was developed for simulated data in the Drift Chambers of the BM@N Run 7 setup. The right tuning of the simulated data reconstruction is proved by the good agreement between the simulated and experimental data (see figures below) [133].



Spatial resolution in the x plane for the simulated (left) and experimental (right) data



Angular value and resolution for the x coordinate for the simulated (left) and experimental (right) data

• **Development of the BMNROOT framework of the BM@N experiment** was reviewed [134]. This framework involves well-developed and tested software package for simulation, digitization, reconstruction and analysis of collision events and other supporting tasks. This report mentions four kinds of results, summarized below.

• ***DCH*** (***Drift Chamber***) ***detector*** – realization of new code modules:

- BmnDchTrackFinder – Segment builder for Drift chambers,
- BmnDchHitProducer – Hit builder for simulated data for Drift chambers,
- BmnDchHitProducerData – Hit builder for experimental data for Drift chambers – [133]);

• **ROOT Geometries** (description of the detector: its structure and parameters needed for Monte-Carlo simulation and hit-reconstruction procedures) have been generated for each detector of the BM@N setup (GEM, DCH, STS, CSC, Silicon Detector).

• Specific computing intensive **Monte-Carlo simulations** and **realistic simulations** have been done for each detector of the BM@N setup (GEM, DCH, STS, CSC, Silicon Detector).

• **Hit-reconstruction** (to get spatial points, called "hits", from signal obtained with micro-strip readout) has been done for GEM, CSC, and Silicon Detectors.

► ***Excerpts of the work done and results obtained in 2021:***

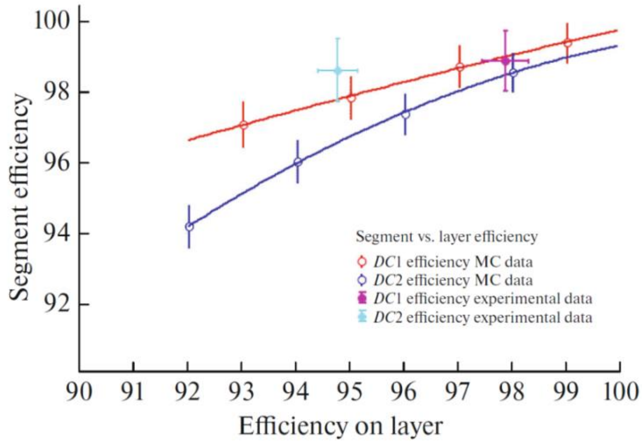
• The first relevant far-reaching high precision physics experiment done at BM@N reports a method of overcoming the complications coming from the initial- and final-state interactions of the incoming and scattered particles in knockout scattering experiments in the quasi-free scattering of 48 GeV c^{-1} ^{12}C ions from hydrogen. The distribution of single protons was studied at BM@N by detecting two protons at large angles in coincidence with an intact ^{11}B nucleus [135, 136].

• **Software developments for BM@N setup configurations.** [137, 138]

► ***Excerpts of the work done and results obtained in 2022:***

• **Preparing software for tracking detectors in the BM@N experiment**, in particular, the software implementation of algorithms for realistic Monte-Carlo simulation and the reconstruction of spatial coordinates from microstrip readout planes, which are used in these detectors, resolved specific technical problems following from the 2022 BM@N run [139].

• **Development of algorithms and programs for recognizing particle trajectories in the BM@N experiment** [140]. The reconstruction of simulated and physical data was done for the Drift Chambers (DCH) and the Cathode-Strip Chambers (CSC), which form the outer tracker of the BM@N experiment. Full compliance with the reconstruction of simulated and physical data was achieved (this concerns: Residuals between the reconstructed hit on the plane and the fitted segment in DCH; DCH segments-slope distribution in x0z-plane; Difference in the segments-slopes of the two chambers; C beam momentum estimation).

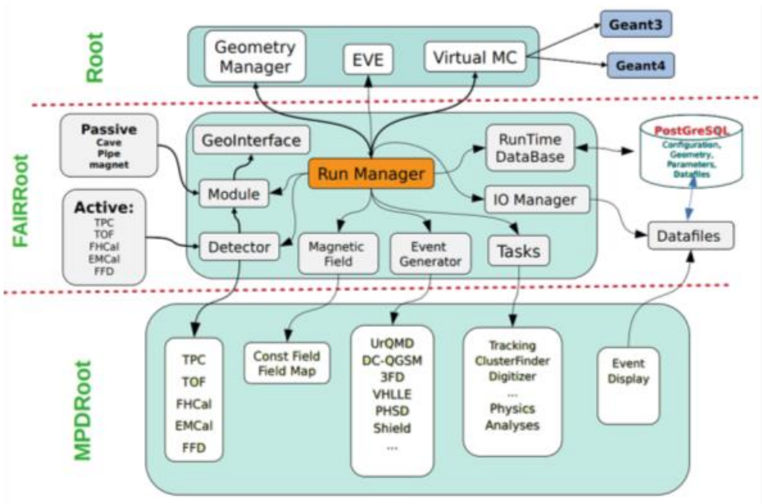


Segment reconstruction efficiency vs. hit-on-layer efficiency. The results for the MC data for the first DCH are shown in red, and the results for the second DCH are shown in blue. The results for the experimental data are in magenta and cyan respectively. The slightly lower efficiency in the second DCH is caused by the presence of the ToF700 system in-between the two chambers [140].

2.3.3. ***Software support at JINR-NICA***: MPD experiment

► Design and extensive testing of the new **Monte-Carlo Generator of Heavy Ion Collisions DCM-SMM** [141–143] (see also [144, 145] for the latest developments). The new Monte-Carlo generator, DCM-SMM, is created by a group of authors with the aim to provide the NICA projects with an effective tool for optimizing the detector elements, debugging the event reconstruction algorithms, predicting the efficiency, calculating the signal-to-background ratio, determining the best criteria for selecting events. The generator is actively used by the BM@N and MPD detector groups for their needs. Tens of millions of nucleus-nucleus collisions were simulated at the HybriLIT cluster for reactions of carbon (C), argon (Ar) and krypton (Kr) with C, Al, Cu, Pb.

► **Unified Software Development for the MPD Experiment at NICA** (**MPDRoot**) [147]



The MPDRoot software framework enables simulation, reconstruction, and physical analyses of the MPD experiment at NICA collider. It must be sufficiently flexible, resilient, robust to be used, developed, and maintainable for the full lifetime of the experiment and the analysis of its data. Effective implementation of build automatization, configuration, and installation of the software (DevOps) for the development and use of the MPDRoot plays crucial role for the success of the whole MPD project in the future. A unified development was presently realized:
• all users and developers are now working with the same package versions of dependencies built in the same unified environment; • quick, user-friendly installation; • no build and configuration required for regular (non-developer) users at all; • nothing but the build of the fresh development branch from git repository is required for developers with much less configuration than previously; • lower probability of installation errors, less time spent on support; • easy updates, less maintenance required; • new commits guaranteed to work on other machines after passing the CI pipeline, eliminates the need for multi-OS testing.

This paper extends results previously reported in [146].

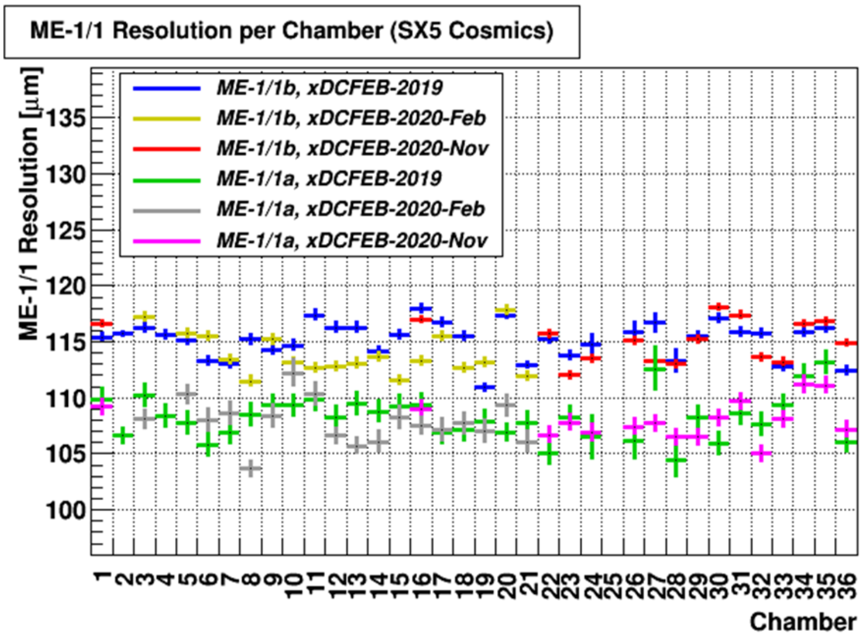
► **Status and initial physics performance studies of the MPD experiment at NICA** [148]**.** An overview of the landscape of the investigation of the QCD phase diagram in the region of maximum baryonic density, where NICA and MPD will be able to provide significant and unique input is given. Detailed descriptions of the MPD set-up, including its various subsystems as well as its support and computing infrastructures, are also provided. Selected performance studies for particular physics measurements at MPD are presented and discussed in the context of existing data and theoretical expectations.

2.3.4. ***Software support at LHC:*** CMS experiment

• **The work done during 2020 within the CMS experiment included:**

- Development, testing and implementation in the official CMS software of algorithms for separating overlapping signals and constructing track segments in cathode-Strip Chambers (CSC).
- As part of the CMS Modernization Phase 2 program, JINR physicists in 2020 participated in the re-equipment of the electronics and cooling system of the CSC muon station ME1/1. Tests of the assembled cameras were carried out on cosmic rays.

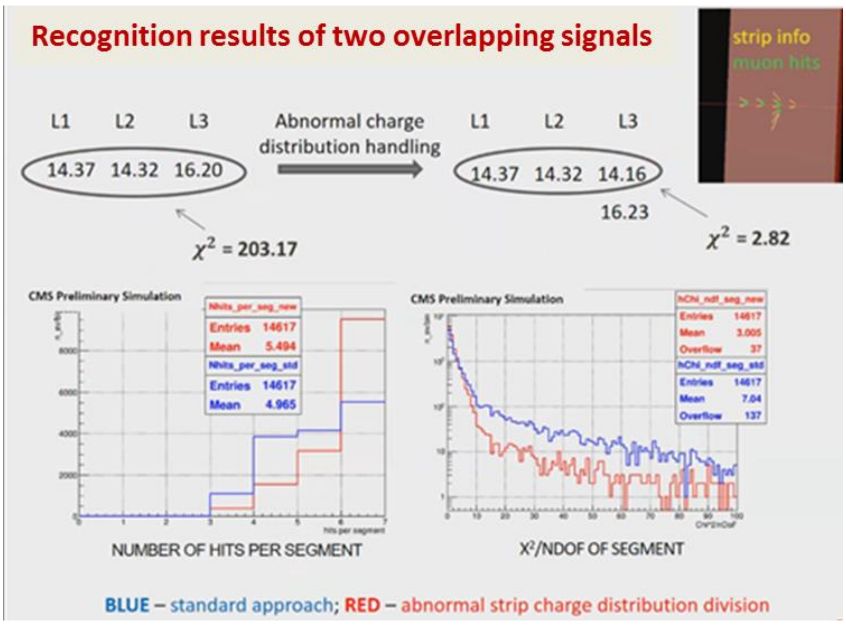
The results on the spatial resolution of the cameras are shown below. The evaluation of the background downloads in CSC are based on the experimental data from LHC. (In collaboration with Mikhail Ignatenko (University of California, Los Angeles, USA)).



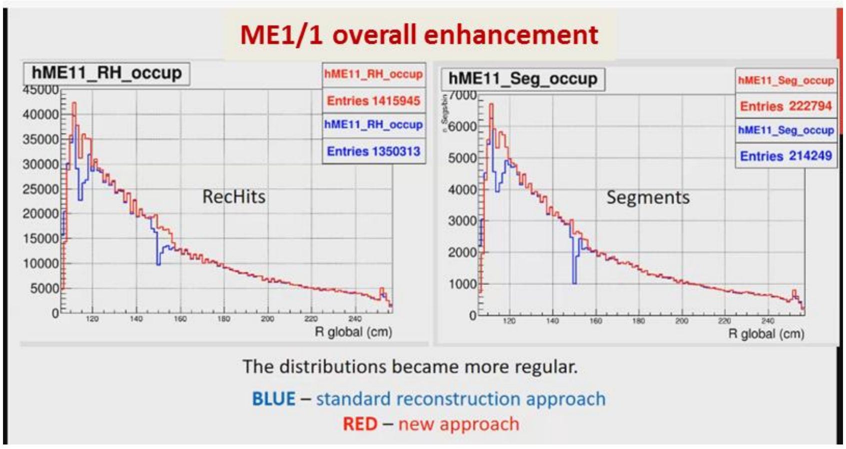
The spatial resolution of the ME-1/1 station cameras on cosmic rays. The results obtained in 2020 are in good agreement with those from 2019.

Apart from the CMS publications with important contributions of the authors from the topic 1119 (V. Palichik and N. Voytishin) [149–159], mention is to be also made of Ref. [160]

- **The work done during 2021 within the CMS experiment included** [161]**:**
  - Improved algorithms for hit reconstruction enhancement in cathode-Strip Chambers (CSC). Significant improvement of the new algorithm is obvious.



- Improvement of the processed CSC muon station ME1/1 data



All the improvements have been implemented into the official CMS software and will be used by default starting with the Run3 data taking.

• **The work done during 2022 within the CMS experiment** [162] **dealt with the reconstruction of physical events involving** the development, testing and implementation of a new algorithm for constructing track segments in cathode-strip chambers for the CMS setup. Work on adjusting the reconstruction of tracks and evaluating the operation parameters of the new HGCal CMS detector cassettes in the test module on cosmic muons involved detailed simulation of the test setup, with the determination of the optimal dimensions for the subsequent testing of new detectors.

2.3.5. *Software support at LHC:* ATLAS experiment

Developments are done within three ATLAS projects, which will be active till 2024. Periodic meetings are organized with MLIT participation and reports both at CERN [163] *and at JINR* [164].

• **The tasks resolved during 2020 within the ATLAS experiment included:**

- **TDAQ,** members of CC control and configuration, monitoring groups [165]
  - Improvements in Operational monitoring on users' requests;
  - Modernization of the data visualization service for the network traffic monitoring system in ATLAS (**NETIS**).
- **Condition DB** – Development of software for converting COOL data to CREST data as part of the ConditionDB enhancement for RUN3 and the creation of Athena user libraries. The CREST server library was included in the official release of the offline ATLAS (Athena) system in December 2019. In 2020 work was done on creating a script to automatically convert the full amount of data to run the Athena q431 test development of a COOL to CREST conversion algorithm for a large number of IOVs channels and data for one directory.
- **Event Index (EI3)** – EventIndex for LHC Run 3 [166]. Work done concerns:
  - Upgrades of a trigger information processing system for indexing in EventIndex for Monte-Carlo data.
  - Solving the problems of users working with the EventIndex system (support for EventIndex production, together with F. Prokoshin, DLNP).
  - Creation of test environment server for new Event Index prototype.

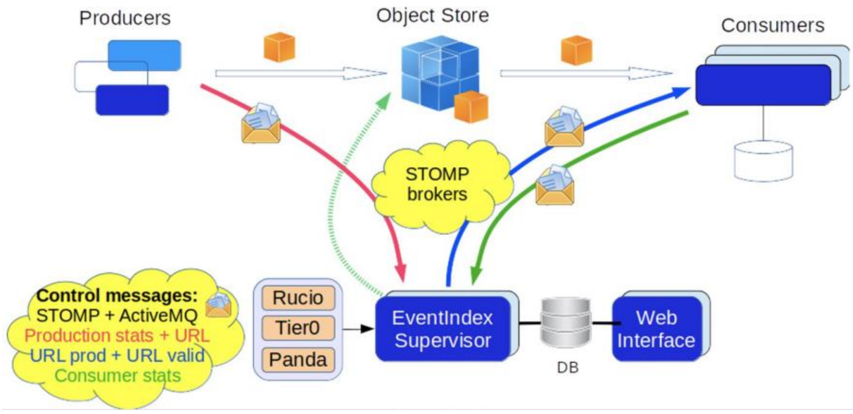
• **The tasks resolved during 2021 within the ATLAS experiment included** [167–169]**:**

- **TDAQ** – The Resource Manager component was reworked such as to fulfil the new rules for maintaining security: using the daq-token mechanism when transferring a username from a client to a server with a call to Access Manager.

- **Condition DB** – The further work on development of software for converting COOL data to CREST data as part of the ConditionDB enhancement for RUN3 resulted in improvement of the corresponding tools.
- **Event Index (EI3)** – EventIndex for LHC Run 3.
  - Participation in the ATLAS EventIndex project continued, a new Event Pickup service was developed that automates the procedure for finding the location of events using the EventIndex and sending tasks to PANDA to receive the requested events.

• **The tasks resolved during 2022 within the ATLAS experiment included** [170]**:**

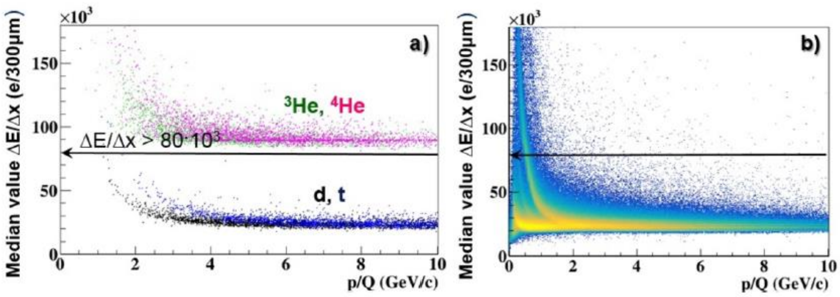
- **TDAQ** – As part of the participation in the work of the TDAQ ATLAS group on software modernization for RUN3-RUN4, modifications of the Resource manager component were carried out. In accordance with the new requirements, the server start algorithm was modified, configuration files associated with resources have been edited to comply with the latest versions of the Configuration components, and changes were made to the daq-token mechanism use according to the results of testing in testbed.
- **Project CREST (ATLAS Condition Database)** – New data types were converted to CREST, algorithm modifications were made to work with new CREST server versions.
- **Project ATLAS Event Index**
  - Participation in the ATLAS EventIndex project continued, work aimed at improving the Event Pickup service is underway, the types of events accepted for processing was expanded, the number of situations requiring expert intervention was reduced.



Architecture of the EventIndex Data Collection system based on Object Store [170].

2.3.6. *Software support at FAIR:* CBM experiment

• **The accurate measurement of the yield of hyper-nuclei and their lifetime** in the CBM (Compressed Baryonic Matter) experiment is based on the identification of their decay products including ^{3}He and ^{4}He. The possibility of heavy fragment identification using energy loss method in the STS detector was studied. The ω(k,n) criterion was successfully adapted for the separation of the doubly charged particles from singly charged. The combination of the energy loss method with the ω(k,n) criterion has shown high level of the background suppression without substantial signal loss. The combination of the information from the TOF and STS detectors allowed separating ^{3}He and ^{4}He from the deuteron background [171].



Median value ΔE/Δx dependences on the particle momentum for a) signal (^{3}He, ^{4}He), thermal deuterons and tritons and b) UrQMD tracks [171].

• **A simple and effective trigger option for detecting rare $J/\psi \rightarrow \mu^+\mu^-$ events** in the CBM experiment has been proposed. For its implementation, only information recorded by the coordinate detectors of the MUCH station is required [172].

2.3.7. ***Software support at FAIR:*** PANDA experiment

– UrQMD+SMM modeling [173, 174].

2.4. Computational support of JINR projects in radiobiology

Starting with 2020, a MLIT group (leader O. Streltsova) has designed and implemented a dedicated information system (IS) on top of the ML/DL/HPC ecosystem developed in the frame of Topic 1119, on the HybriLIT Platfom (Sec. 3.1.).

► **The creation of an information system (IS) for the tasks of radiation biology**, a joint project of MLIT and LRB JINR, is vigorously pursued.

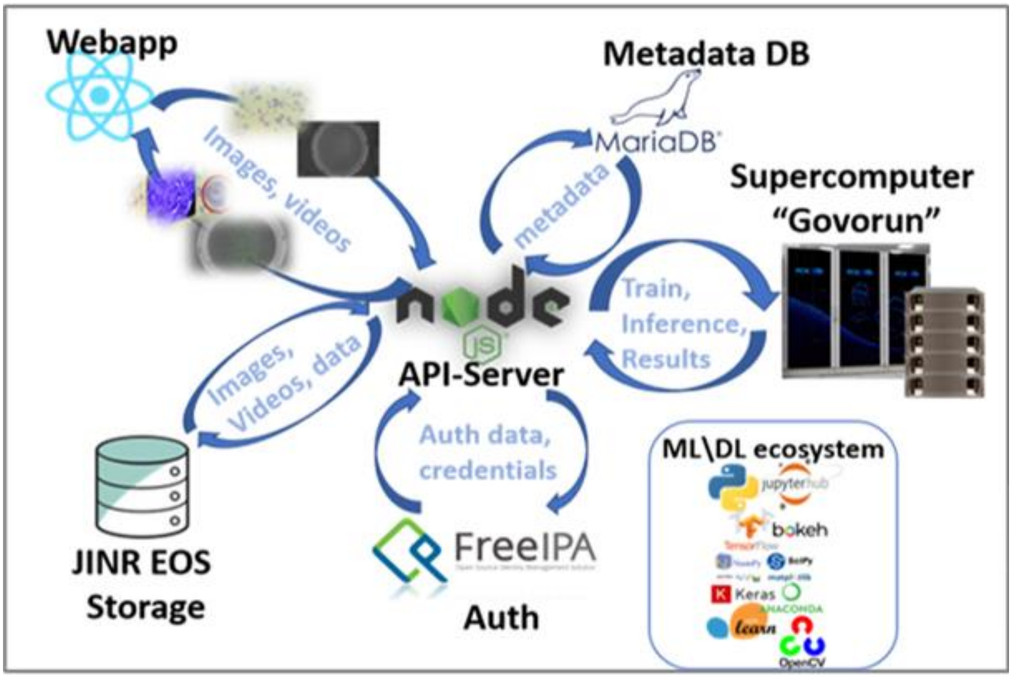
• A first stage concerned the design from scratch of the **IS for radiobiological studies** [175]. The designed IS features secure: storage and access to experimental data and methods of its processing, provision of a set of methods for experimental results systematization and for the detection of hidden patterns that appear in the response of biological systems to the effects of damaging factors, data presentation in a form convenient for complex statistical analysis, opportunities for research automation based on machine and deep learning methods and neural network approaches, a comfortable environment for interaction and collaboration of different research groups.

• The perfection of **the ML/DL/HPC ecosystem** (Sec. 3.1.) enabled quick and substantial IS extension. A module, devoted to the study of the behavioral patterns of small laboratory animals exposed to radiation, enables the automation of the analysis of video data obtained when testing rodents in different test systems, one of which is the "**Open Field"**, based on computer vision methods, together with the method of key points within a neural network approach [176].

• The present, mature IS involves two strong legs comprising:

– **computer vision algorithms** on top of ML/DL technologies;

– **modern IT solutions** for data storage, processing and visualization.



Based on the developed IS, simplification and acceleration were achieved for the following classes of tasks:

– *experimental data processing* is now done by automated morphological classification of the neural cells;

– *data analysis* is done by means of the latest neural network algorithms built upon the existing ML/DL ecosystem;

– possibility of *simultaneous data processing* by different research groups;

– *systematization and development of effective methods* for preventing and countering the negative effects of the ionizing radiation.

The three main steps of the research: acquisition of the experimental data, their analysis and the interpretation of the obtained results, are performed within a complex approach, which is based on elements of the computational HybriLIT infrastructure, shown in the figure above (taken from [194]).

2.5. Computational support of JINR projects in condensed matter physics

The bulk of the experimental condensed matter physics research in JINR is based on the sample probing, on specialized detector systems, with slow neutrons produced by the IBR-2 reactor (FLNP). The IT support by MLIT scientists covers the two most demanded IBR-2 detectors, YuMO and HRFD.

The recent YuMO modernization, consisting in the addition of a system of position sensitive detectors, entailed dramatic increase of the IT support of A. Soloviev and T. Solovjeva, who designed and implemented conceptually new IT solutions.

IT developments, conceived and implemented during 2020 by V.B. Zlokazov, have secured stable, efficient and fast data handling by the high resolution Fourier diffractometer (HRFD).

► **SAS – package for small-angle neutron scattering data treatment**, with periodic updates going until 2023, was implemented in the PROGRAM LIBRARY JINRLIB [177, 178]. The online data processing at the YuMO spectrometer (channel four of the IBR-2 reactor) is done by means of the SAS package. This package was intensively upgraded, corresponding to successive developments or modifications of the YuMO spectrometer. The program allows to combine the data referring to the same sample, to calculate the spectrometer resolution function for the given experiment conditions, to carry out data correction on dead times of neutron detectors, and to subtract a background substrate from detector data, to carry out the normalization of the obtained spectrum on standard vanadium scatterer, to subtract background sample data.

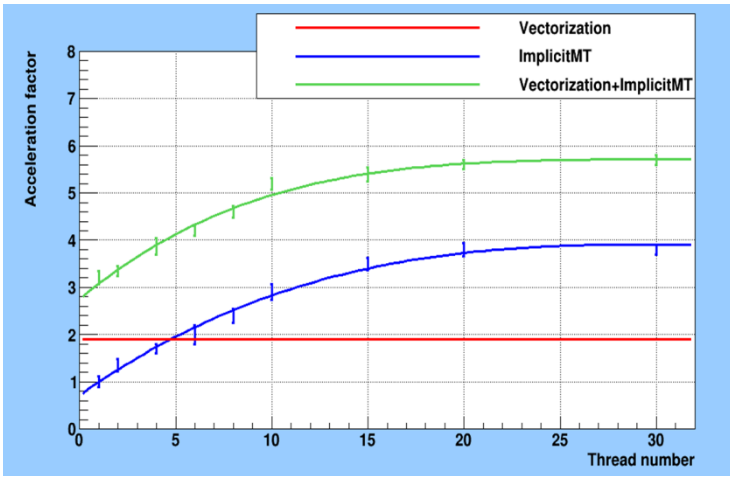
► **Software development based on web technologies** is a promising direction that provides the user with a wide range of opportunities for the processing of experimental data.

Significant advance was achieved in the modernization of the small-angle-scattering YuMO spectrometer at the IBR-2 facility in the FLNP-JINR. Two instances are provided below.

• **FITTER_WEB** **FITTER_WEB JINRLIB**, a program for fitting experimental data obtained on a small-angle neutron scattering spectrometer [178], was implemented as a Web application [Date of implementation: 09.11.2022; Authors: A.G. Soloviev, T.M. Solovjeva]. The program is available in GitLab at the following link: https://git.jinr.ru/yumo/fitter-next

► **The Modernization of the Software for Fitting the Data of the Small-Angle Neutron Scattering Spectrometer YuMO at IBR-2**, is done through the development of a web application.

The present work is devoted to the description of a variant of the programe, which allows separate assessment of the polydispersity and resolution. The inclusion of the polydispersity is an important advance in the online data analysis. Function vectorization and implicit multithreading of the PROOT package increase the speed of the data processing with a factor up to 5.5 [179].



Dependence of the acceleration coefficient on the number of threads [179].

► **Experiments done at the high resolution Fourier diffractometer (HRFD)** include the study of irreversible processes during which the spectroscopic data are quickly changing. The question was quite recently raised on the maximally possible automation of the data processing (the interactive definition of the initial data, visualization of the acquired data, etc.), within different conditions of such experiments. During 2020, offline software was developed and implemented for the batch processing of neutron diffraction spectra measured in real-time in situ mode.

2.6. Software computational support of Baikal-GVD neutrino physics project

The data accumulated in the Baikal-GVD experiment cover a large variety of information which needs intensive computer processing: estimate of the positions of the underwater cubic-kilometer detector components undergoing drift and spatial orientation changes. Progress obtained during 2020 was reported in [180–183].

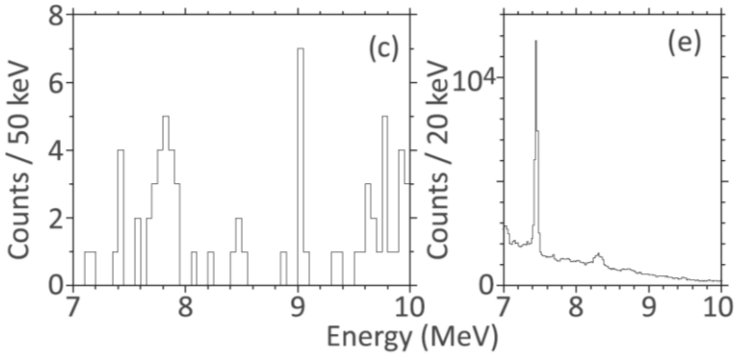
• **Data Processing of the Baikal Neutrino Telescope** needing articulated communication among its different modules was modernized thanks to contributions coming from MLIT. It secures substantial acceleration of the main code of the Cascade Recovery Collaboration, which is important for tracking transient astrophysical neutrino sources [184].

2.7. Support of Experimental Nuclear Physics Data Processing and Analysis

The data collected on FLNR facilities on low energy nuclear processes (creation and characterization of superheavy nuclei, collisions of exotic nuclei with protons and nuclei, nuclear fragmentation, etc.) need, at a rule the development of new theoretical models. The most part of the progress in the development of new mathematical models devoted to this aim, together with illustration of the coverage of specific experimental processes, was provided in section 1.2.2. *of the present report. Description of features related to specific code implementation for high performance computing on the HybriLIT Platform is outlined in section* **3.1.**

► **Reliable statistical inferences under low statistics and incomplete observation** [185].
The development of the described nonparametric methods is indelibly related to the need for the reliable interpretation during the creation and characterization of superheavy nuclei. The main features of such data are the small statistics, their big uncertainty and complexity. The proposed nonparametric "median/mean" criterion for testing a rather large class of data distributions for purity is suitable for use in the analysis of the small data statistics characterized by the lack of a priori information.

► **The interpretation of the statistical data collected during the first experiment at the Superheavy Element Factory in FLNR** evidenced a **high cross-section of ^{288}Mc** in the ^{243}Am + ^{48}Ca reaction and resulted in the **identification of the new isotope ^{264}Lr** [186]. The following excerpt from the published data evidences the nonrandom nature of the 7.6–8.0 MeV peak resolved during the experiment (Fig. 1(c)), in agreement with the sharp increase of the number of counts (Fig. 1(e)).



Excerpt from FIG. 1 [186]. *Left*: Fig. 1(c) reports the statistical distribution of the α-like events recorded in the energy range E_α = 7–10 MeV. The structure resolved within the range 7.6–8.0 MeV points to the nonrandom character of the accummulated records. *Right*: Fig. 1(e) presents the spectrum of the summed α-like events registered during all the experiment runs. This feature substantiates the inference made on the data at the left.

►**Ion fragmentation reactions at the FLNR COMBAS fragment-separator** [187–192]

Modeling total reaction cross sections of neutron-rich light nuclei [187]. The total reaction cross sections for projectile nuclei from ^{4}He to ^{12}B at the energy range 10–50 AMeV and ^{28}Si target are compared with model predictions based on the Kox formula and MOMDIS calculations.

Velocity and isotope distributions of light fragments obtained in the projectile fragmentation reactions of ^{18}O at 35 MeV/nucleon on ^{9}Be and ^{181}Ta targets have been analysed. The parametrization of velocity spectra as the sum of two Gaussians representing dissipative and direct components of the reaction is proposed. Shown that the centroids of dissipative component are reasonably well described within the combined BNV+SMM model. The ratio of dissipative and direct modes gives a better insight into mechanism of these reactions [188, 189].

Results of projectile fragmentation reactions of ^{22}Ne (42 MeV/nucleon) on ^{9}Be and ^{181}Ta targets [190] and ^{40}Ar (36.5 MeV/nucleon) on ^{9}Be targets [191] have also been reported. Competition between different reaction mechanisms was evidenced. The obtained production cross-sections have been compared with the empirical parametrization of fragmentation cross-section (EPAX) and heavy-ion phase space exploration (HIPSE) models. Specific limitations of the two parametrization models have been evidenced.

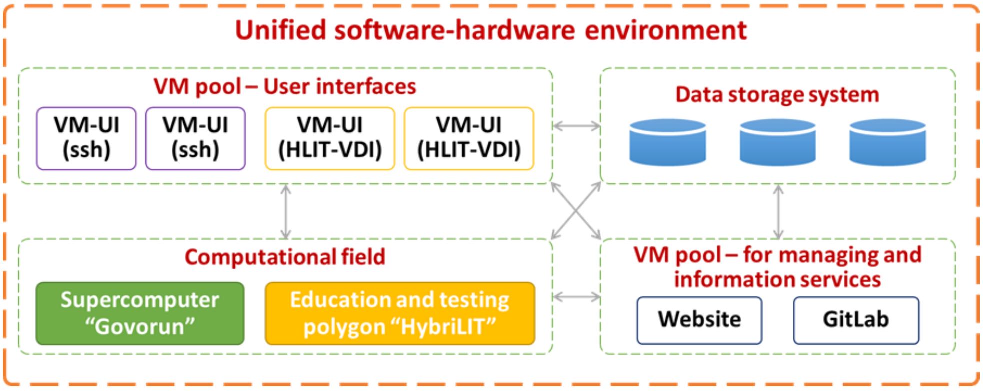
►**Modeling the yield of radioactive isotopes in experimental facilities**. Having in mind the need to get accurate knowledge of the yield of radioactive isotopes in accelerator driven systems, the authors use as their basic simulation tool the JINR developed package CASCADE. Comparison with experimental data and with other simulation methods is made, the obtained results are discussed in detail [192].

3. Numerical Methods, Algorithms and Software for Multicore and Hybrid Architectures and Big Data Analytics

3.1. The ML/DL/HPC Ecosystem on the HybriLIT Computing Platform

Within the Multifunctional Information and Computing Complex (MICC) Project, the HybriLIT Heterogeneous Computing Platform (HCP), which involves the HybriLIT cluster (serving as a learning and testing polygon) and the "Govorun" supercomputer, http://hlit.jinr.ru, is the basic hardware facilities accommodating the implementation of advanced software for the numerical solution of newly developed mathematical methods and algorithms in JINR and, particularly in the Topic 1119. The *design, development, implementation, and maintenance on HybriLIT HCP of a user friendly environment* is a fundamental task, the solution of which is gradualy resolved and refined within the Topic 1119 by a dedicated team (leaders, D.V. Podgainy, O.I. Streltsova).

The expertise gained during the gradual extension of the HybriLIT cluser showed that the design of a *unified, scalable, modular procedure* for the control of the software-information environment is the best solution for the management of the whole HybriLIT HCP [193]. Its modular structure is shown in the figure below [194].



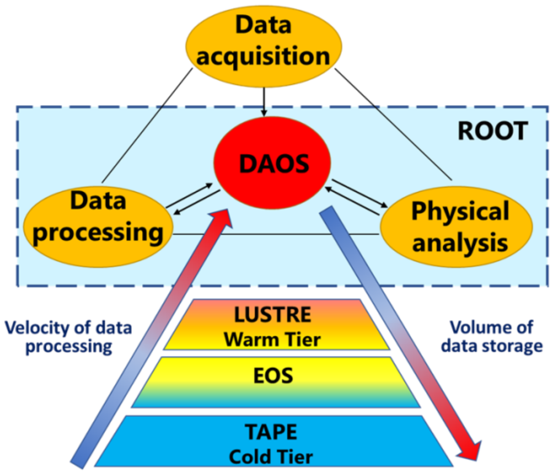
The unified software-information environment of the HybriLIT HCP allows the users to investigate the capabilities of new computer architectures, of IT solutions, to develop and debug their solutions on the learning and testing polygon and, afterwards, to do calculations on the "Govorun" supercomputer. This enables efficient use of the "Govorun" resources [194].

This idea of control procedure was successfully tested twice. The first case was the creation of the HybriLIT HCP, through the addition of the initial "Govorun" supercomputer version, characterized itself by a threefold heterogeneous structure: (i) the CPU Intel Gold component – **SkyLake** – devoted to the implementation of High Performance Computing (HPC) packages with *distributed memory*; (ii) the CPU Intel Phi component – **KNL** – devoted to the implementation of HPC packages with *shared memory*; and, last but not least, (iii) the GPU NVIDIA accelerator component – **DGX** – devoted to the implementation of HPC packages using neural network methods based on *machine learning* and *deep learning* (ML/DL). User friendly access to either of these three possibilities offered by the "Govorun" supercomputer was secured by the in-house development, during the first half of 2020, of *specialized ecosystems*. The ecosystem devoted to the solution of ML/DL tasks involves two specific parts: a *computation component* (see https://jhub2.jinr.ru) and a development component (see https://jhub.jinr.ru). An HPC environment was also created for the easy development of parallel algorithms and applications, especially for the future experiments at the NICA facility [195–197].

The operation of the first stage of the "Govorun" supercomputer made it possible to carry out resource-intensive computing in lattice quantum chromodynamics, improvement of the efficiency of modeling the dynamics of relativistic heavy ion collisions, the speed up of the event generation and reconstruction for the mega-science experiments of NICA project, to carry out calculations of the radiation safety of JINR experimental facilities, to significantly accelerate the research in the field of radiation biology [198, 199] and other scientific and applied problems [200].

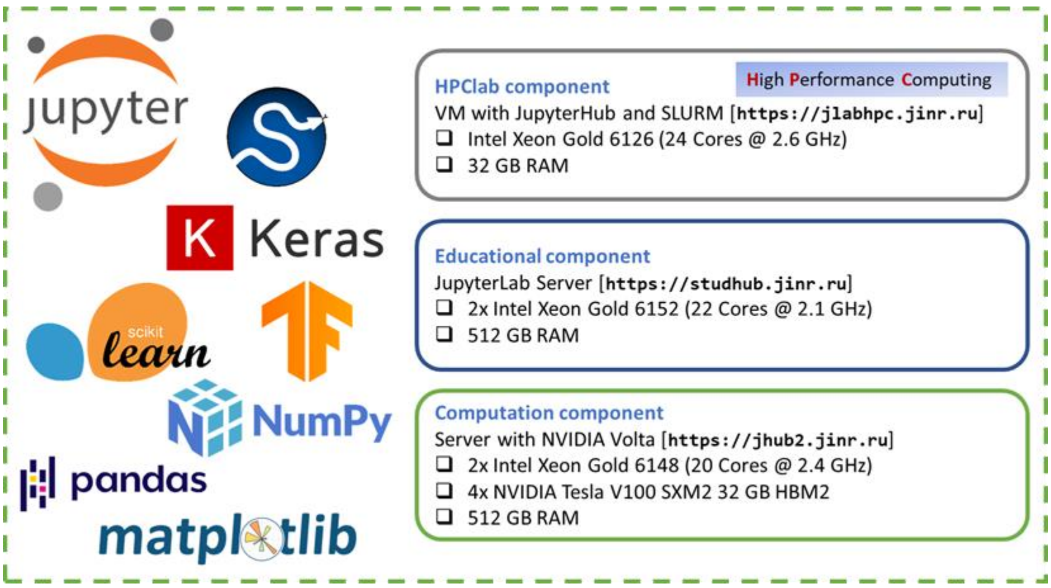
The second successful test of the idea of this control procedure follow the substantial modernization of the CPU part of the "Govorun" supercomputer during 2022. Essentially, this added 32 hyperconverged compute nodes (enhancing the computational field) and 8 distributed storage nodes (for the enhancement and acceleration of the hierarchical storage). With this new structure, a new layer, DAOS (Distributed Asynchronous Object Storage) software, was built upon the existing LUSTRE EOS, making the "Govorun" one of the most I/O efficient supercomputers in the world (48-th place in the current, November 2022 – **IO500** List, https://io500.org/).

Within the new "Govorun" configuration, the data flow for high energy physics experiments is substantially accelerated ([194], see figure below).

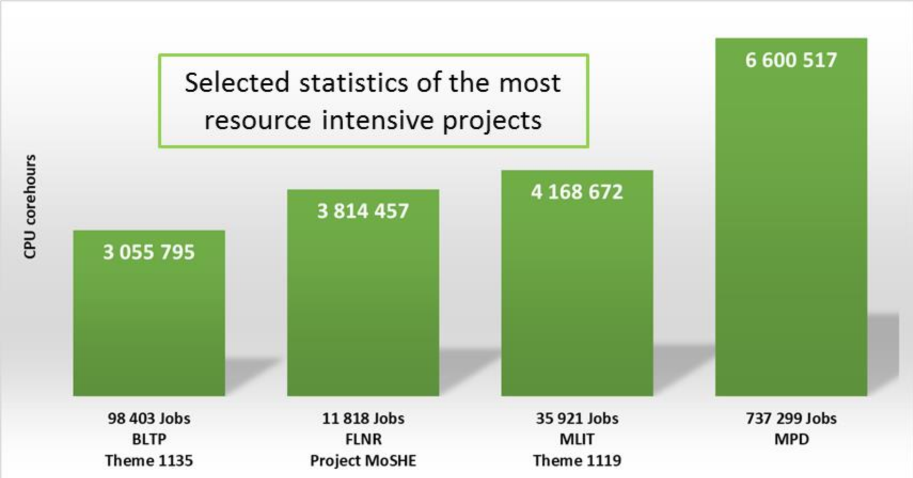


Further evidence on the successful use of the "Govorun" supercomputer in solving JINR tasks is provided in [194].

The main components of the ML/DL/HPC Ecosystem created within the topic 1119 for the solution of "Govorun" supercomputer tasks involve the resources summarized in the figure below [194].



The use of the resources of the "Govorun" supercomputer is asked by all the JINR Laboratories within 25 Topics of the JINR Topical Plan. There are four classes of projects asking for the most intensive use of these resources: the NICA megaproject, the simulations of complex physical systems, the computations of the properties of the atoms of the superheavy elements, and calculations of lattice chromodynamics. The share of these resources is given below [194].

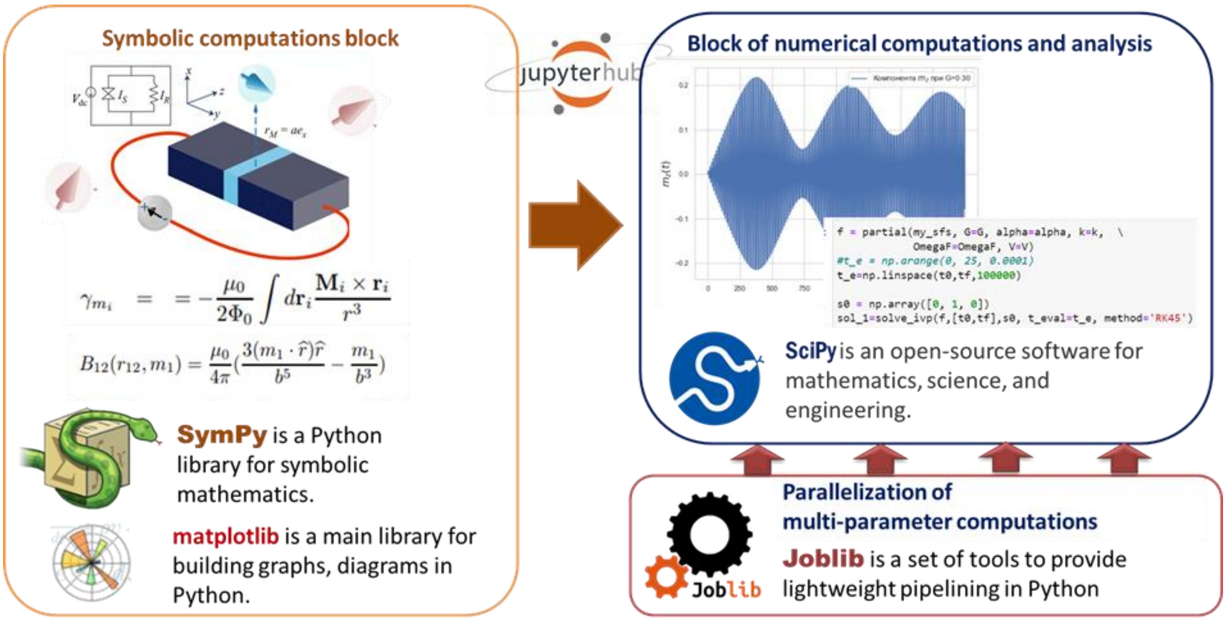


3.2. Developments on top of the ML/DL/HPC Ecosystem

3.2.1. *Extended possibilities of ML/DL/HPC ecosystem use on top of JupyterHub*

► **The overview** [201] discusses opportunities for solving tasks not only in the field of machine learning and deep learning, but also for the convenient organization of calculations and scientific visualization. The ecosystem allows one to develop and implement program modules in Python, as well as to carry out methodical computations.

► **The investigation of the dynamics of the magnetization in a Josephson φ_0-junction** [202]. A methodology for developing software modules, which enable not only to carry out calculations, but also to visualize the results of the study and accompany them with the necessary formulas and explanations is illustrated below.



Scheme of software modules for studying systems with Josephson junctions.

3.2.2. *Machine learning based solutions for JINR experiments*

A summary is made of the progress done under the leadership of Prof. G.A. Ososkov on the possibilities to use ML based methods for the derivation of solutions in JINR experiments.

► **Machine learning on high-performance computing infrastructures at JINR**

• **Event reconstruction in GEM detectors.** New effective tracking methods based on graph neural network (GNN) are actively developed and tested for the GEM detector of the BM@N setup at NICA. This approach is well-adapted for solving the known fake hit problem inherent to strip detectors like GEM with help of minimum branching tree algorithms [203].

• **Use of deep neural tracking to face the tracking crisis challenge in detector environments, such as HL-LHC Run-4 and MPD-NICA**.

During 2020, the previously created program tracking TrackNETv2 through a single training was modified to work with data from the cylindrical GEM (CGEM) tracker of the **BESIII *drift chamber*** with future development of this program to apply to more complex data of the MPD detector at the NICA Collider [204].

During 2021 [205–207]**,** research was continued on the development of fast parallel action programs based on deep neural networks for the reconstruction of elementary particle tracks when processing experimental information from fixed-target detectors (the BM@N experiment) and collider-type experiments (BESIII at the IHEP Beijing and SPD at the JINR NICA collider). In the course of the research, the TrackNETv2 local tracking program and two RDGraphNet and LOOT global tracking programs were further improved, which made it possible to complete the tracking study for the internal cylindrical CGEM detector of the BES-III collider experiment with acceptable accuracy. The results have been published as Conference papers.

During 2022, a particle tracking approach based on deep neural networks for the BM@N experiment and future SPD experiment was developed [208]. Revised algorithms – combination of Recurrent Neural Network (RNN) and Graph Neural Network (GNN) for the BM@N RUN 7 Monte-Carlo simulation data, and GNN for preliminary SPD Monte-Carlo simulation data are presented.

• **Disease detection on the plant leaves by deep learning** [209]
A special database of the grape leaves consisting of healthy and diseased grape leaves was further extended and a special classification model based on a deep Siamese network followed by k-nearest neighbors (KNN) classifier was developed. The implementation of a novel architecture with a deep Siamese network as feature extractor and a single-layer perceptron as a classifier results in a significant gain of accuracy, up to 96%. Using of a deep Siamese neural network as feature extractor allows reaching 99% of the recognition accuracy on the test subset of images.

• **One-shot learning with triplet loss for vegetation classification tasks** [210]

Triplet loss function was successfully used to significantly improve the accuracy of the one-shot learning tasks related to vegetation. The first task is plant disease detection on 25 classes of five crops (grape, cotton, wheat, cucumbers, and corn). The second task is the identification of moss species (5 classes). In both tasks, we used self-collected image databases. Our Siamese network architecture with a triplet loss function and MobileNetV2 as a base network showed the most impressive results in both above-mentioned tasks, with over 97.8 % rate of success of the average accuracy for plant disease detection and 97.6 % for moss species classification.

• **Joint research together with FLNP within the UNECE ICP Vegetation international program for monitoring and forecasting air pollution processes in Europe and Asia** was continued with the implementation of Earth remote sensing data together with machine learning methods for predicting air pollution by heavy metals. The average accuracy of the models exceeded 89%. Models of pollution by aluminum, iron and antimony in the central region of Russia have been constructed [211].

• **Use of machine learning methods for the analysis of nuclear reaction products** [212]**.**

Research carried out jointly with FLNR JINR in the framework of the project to reveal the fine structure in the mass and energy distributions of nuclear reaction products has successfully done neural network analysis of the fine structure in the spontaneous fission fragments of californium ^{252}Cf(sf).

3.2.3. *Other ML/DL/HPC ecosystem based solutions*

► **Genetic Algorithm** (**GA**) **Method: Comparison of Advanced Methods for Picking Path Optimization: Case Study of Dual-Zone Warehouse** [213]. Minimizing the travel distance of a picking tour is often considered an imperative factor in improving warehouse operation efficiency. This paper concentrates on the performance of the GA method and its comparison to other routing strategies such as heuristics, the experienced warehouse picker and the brute-force algorithm under given assumptions. The set of simulations and calculations is based on an industrial case example. The results of the investigated routing strategies under given assumptions (middle size dual-zone warehouse, order size – 15 items, etc.) show the dominance of the brute-force algorithm in comparison to the experienced picker, GA and simple heuristics. It also indicates that GA is an optimization method which needs modification in dealing with picking path optimization problems and under given assumptions could generate better solutions than simple heuristics and comparable to experienced picker. The results also show quite significant sensitivity of GA results on used selection operator, size of population and number of generations.

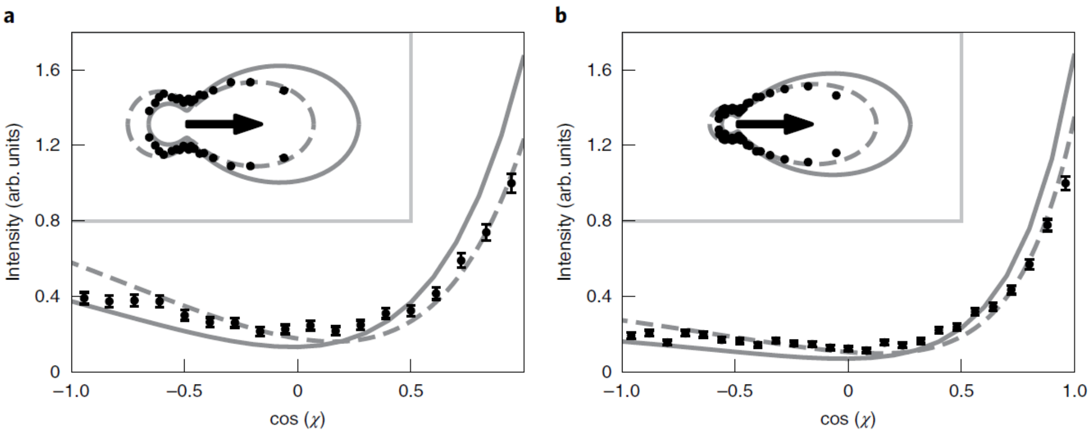
► **Predictive modeling of data storage and processing centers**

• **Probabilistic approach to simulation of BM@N data centers**.

This is an interdisciplinary effort the goal of which is to determine the hardware configuration that will ensure operability of the data storage and processing system with minimum resources. Results have been reported for the software support of the BM@N detector [214, 215].

3.3. HybriLIT/GOVORUN Implementation of Efficient Numerical Methods for Hardly Solvable Problems

► **Kinematically complete experimental study of Compton scattering at helium atoms near the threshold** [216]. This study, published in Nature Physics, reports high precision experiments on Compton scattering from free atoms by cold-target recoil ion momentum spectroscopy (COLTRIMS), addressing the intriguing low-energy, near-threshold regime, where the classical theory of the Compton effect ceases to be valid. The derivation of a kinematically complete dataset of ionization by Compton scattering of atoms – as opposed to detection of the emitted electron or scattered photon only – provides the essential key to sensitive testing of theories as well as allowing for a clean physics interpretation of the results. Calculations were performed on the supercomputer “Govorun” of JINR.



Fully differential electron angular distributions. **a**,**b**, The photon scattering angle is $130 < \vartheta < 170°$. Displayed is the cosine of the angle χ between the outgoing electron and the momentum transfer Q for electron energies of $1.0 < E_e < 3.5$ eV (**a**) and $3.5 < E_e < 8.5$ eV (**b**). Insets show the same data in polar representation, where the arrow indicates the direction of momentum transfer. Black dots are the experimental data. Error bars represent the standard statistical error. The solid and dashed lines are the theoretical curves resulting from Approach I and Approach II, respectively. Theoretical curves are normalized such as to get the same integral of experiment and theory.

• **Compton ionization of hydrogen atom near threshold by photons in the energy range of a few keV: nonrelativistic approach** [217]. A theory aimed at describing the results of unique experiments on measuring the fully differential cross sections of the Compton single ionization of the helium atom near the ionization threshold at photon energy of a few keV is discussed. Ionization cross sections of the reaction ($\gamma;\ \gamma e$) at the hydrogen atom are derived due to the theoretical simplicity of the model. Special attention is paid to the study of the kinematic region of the reaction near threshold, where it is expected to obtain valuable information about the initial and final states of the target. Calculations were performed on the Central Information and Computer Complex and heterogeneous computing platform HybriLIT through supercomputer "Govorun" of JINR.

► **Compton ionization of atoms as a method of dynamical spectroscopy** [218].

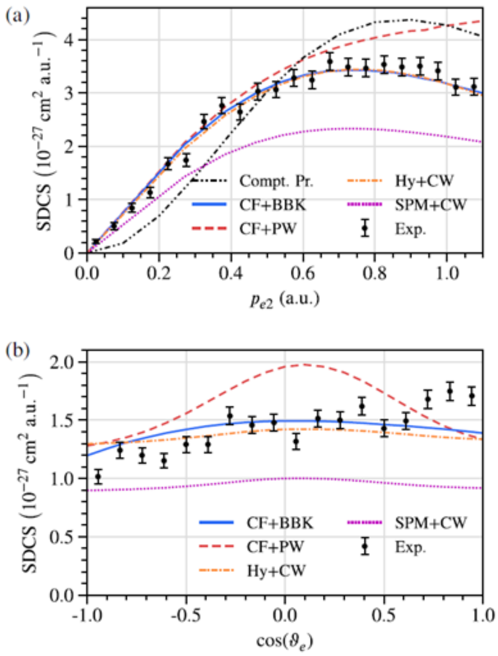
In [216], the possibility to measure the fully differential cross section of the reaction of single Compton ionization of a helium atom without detecting the scattered photon has been demonstrated. In the continuation of this study [218], the use of such reactions for studying the momentum distribution of an active electron in the target atoms is investigated in detail and a comparison of the Compton momentum spectroscopy method with the well-known electron momentum spectroscopy is made.

► **Potential roots of the deep subbarrier heavy-ion fusion hindrance phenomenon.** The analysis of the origin of the unexpected deep subbarrier heavy-ion fusion hindrance in ^{64}Ni+^{100}Mo, ^{64}Ni+^{64}Ni, and ^{28}Si+^{64}Ni reactions is performed based on an improved coupled-channels approach, implemented by means of the finite element method. With the aid of the Woods-Saxon potential, the experimental cross sections and the S factors of these reactions are remarkably well reproduced within the sudden approximation approach. It was found that the inclusion of the off-diagonal elements of the coupling matrix, ignored in the traditional approaches of the coupled channels method when setting the boundary conditions inside the potential pocket and its minimum value, play a decisive role for the derivation of numerical results in agreement with the experimental data. A good agreement is also achieved with the general trend of the experimental data for the S factor of the fusion reaction ^{12}C+^{12}C, which has no pronounced maximum for this system [219].

► **Accurate calculations of Dirac electrons in the two-center Coulomb field: Application to heavy ions.** The relativistic ground state energies of two-center problems for the Dirac equation are calculated with an accuracy of 8-9 digits at an internuclear distance of 2/Z (au) up to Z = 121. The occurrence of false states in the solution of the Dirac equation for the Coulomb problem is eliminated by means of a minimax formulation, which uses independent nonlinear parameters in the large and small components of the basis functions. To date, a test version of the program has been written to find a solution to the problem of unconditional continuous minimax [220].

► **Establishing a new method of dynamical spectroscopy,** complementing the well-known methods like (e,2e) and (e,3e) spectroscopy. The possibility to use double ionization of the helium atom by Compton scattering as a tool for direct spectroscopy of electron-electron correlations has been shown to be a valuable investigation tool [221]. This asked for the development of a non-relativistic theoretical description of the process within the Kramers-Heisenberg-Waller approximation, which has been implemented with a high computational efficiency for rather high photon energies of a few dozens of keV. These developments laid the ground for a new method of Compton scattering, discussed in the next investigation [222].

► **Ion and Electron Momentum Distributions from Single and Double Ionization of Helium Induced by Compton Scattering** of photons with $h\nu$ = 40 keV [222]. The doubly charged ion momentum distribution is found to be very close to the Compton profile of the nucleus in the ground state of the helium atom, and the momentum distribution of the singly charged ion to give a precise image of the electron Compton profile. To reproduce these results, nonrelativistic calculations require the use of highly correlated initial- and final-state wave functions.



Double ionization by Compton scattering of photons at $h\nu$ = 40 keV. Respectively, the single differential cross sections for electron momenta (a) and the emission angle ϑ_e between the electron and incident photon beam direction (b) are shown. The data are integrated over 0.1–1.1 a.u. electron momentum and normalized to the integral of the solid blue line and differ in each panel, respectively. The error bars are the standard statistical error. Colored lines are calculations using different initial and final states. The dash-dot-dotted black line is the momentum distribution of the bound electron [222].

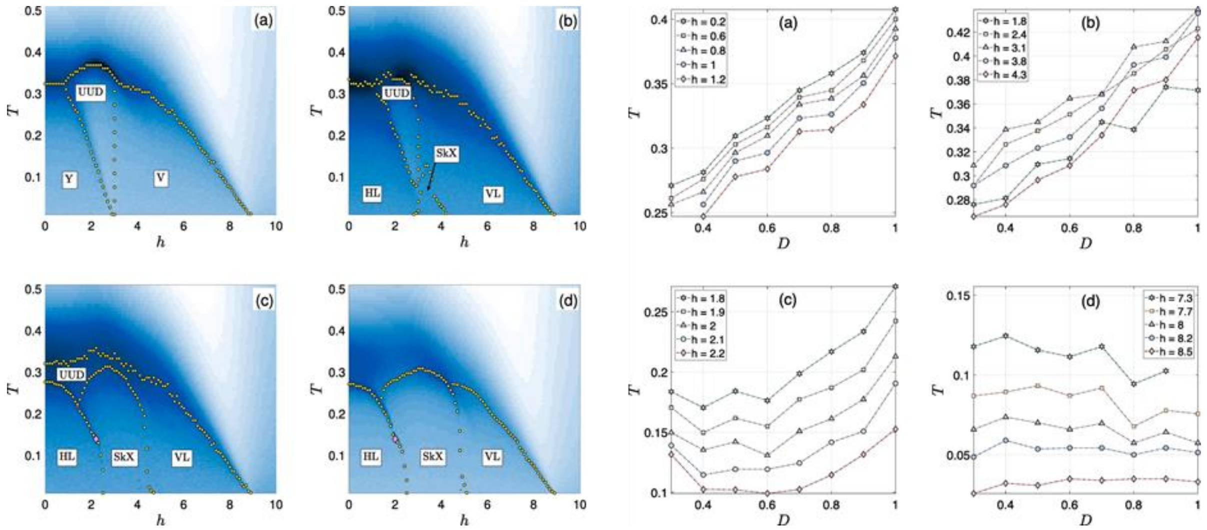
► **The development of new dedicated algorithms and software** was instrumental for the success of these investigations.

• **KANTBP 3.1: A FORTRAN program included in CPC Library** [223]. The program calculates energy values, reflection and transmission matrices, and corresponding wave functions in a coupled-channel approximation of the adiabatic approach. Benchmark calculations for the fusion cross sections of $^{36}S+^{48}Ca$, $^{64}Ni+^{100}Mo$ reactions are presented. As a test desk, the program is applied to the calculation of the reflection and transmission matrices and corresponding wave functions of the exact solvable wave-guide model, and the fusion cross sections and mean angular momenta of the $^{16}O+^{144}Sm$ reaction.

• **Fully symmetric quadrature rules with positive weights, and with nodes lying inside the 3, …, 6–dimensional simplex** (so-called PI-type) [224]. PI-type fully symmetric quadrature rules up to 20-th order on the tetrahedron, 16-th order on 4-simplex, 10-th order on 5-and 6-simplexes are presented. The corresponding programs are implemented in MAPLE-FORTRAN environment.

• **INQSIM** – *a program for converting PI-type fully symmetric quadrature rules on 2-, ..., 6-simplexes from compact to expanded forms* (May 05, 2022) [225]

► **Formation and growth of a skyrmion crystal (SkX) phase in a frustrated Heisenberg antiferromagnet on a triangular lattice, with Dzyaloshinskii-Moriya interaction in the presence of an external magnetic field** [226] are studied. Phase diagrams are built in the temperature-field parameter plane, featuring first-order phase transitions and tricritical points, and their evolution with the increasing DMI strength is studied. It is found that already relatively small DMI intensity can lead to the appearance of the SkX phase at low temperatures in the vicinity of the meeting point of the remaining helical, coplanar up-up-down, and canted V-like ordered phases. By means of a parallel tempering (PT) Monte Carlo algorithm, it is found that the minimum value of DMI, at which the skyrmion phase emerges, $D_t \approx 0.02$, is one order of magnitude smaller than previously reported. Reliable and precise location of the phase boundaries between different phases are found. Part of computations was done on the HybriLIT heterogeneous computing platform. An instance of the obtained results is illustrated below.



Left: Evolution of the phase diagram topology in T-h plane for L=48 and smaller *D* values: (a) D=0, (b) D=0.1, (c) D=0.2, and (d) D=0.3; ***Right***: Transition temperatures as functions of the DMI parameter *D* for selected field values at (a) P-HL, (b) P-SkX, (c) HL-SkX, and (d) P-VL phase transitions.

► **Parallel implementations of packages for the computation of nucleus-nucleus optical potential within the double-convolution model.**

• **The MPI and OpenMP realizations of the package** [227]. Test calculations of the total cross section of the ^{6}He + ^{28}Si scattering at the energy 50 A MeV show that both techniques provide significant comparable speedup of the calculations.

• **OpenMP package for the acceleration of the calculation of the matrix elements** of the dibaryon-induced three-body force potential in light nuclei with A = 6 within the a + 2N cluster model [228]. The theoretical framework is briefly described. The results of test calculations on the MICC HybriLIT platform with an increase in the number of parallel threads are presented and discussed.

► **HPC *Software packages implemented in general purpose-computing libraries***

New submission to the PROGRAM LIBRARY JINRLIB of important HPC parallel package:

• **Split** – *a parallel implementation of the numerical solution of a system of algebraic equations with a tridiagonal matrix using partition algorithm and MPI technique* (April 27, 2020) [229].

There was a new submission in 2021 to the PROGRAM LIBRARY JINRLIB of important HPC parallel package:

• **RK4-MPI** – *parallel implementation of the numerical solution of the Cauchy problem by the 4-order Runge-Kutta method using MPI technology* (March 23, 2021) [230].

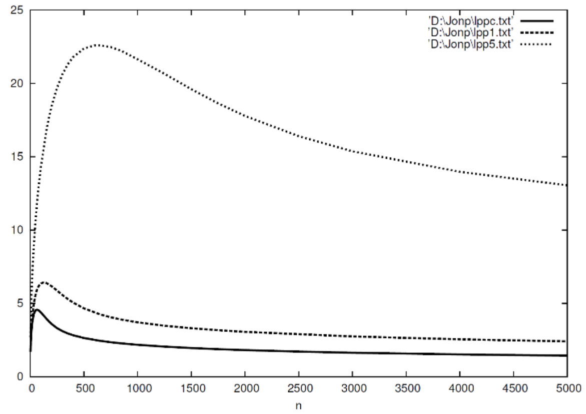
► **High-performance calculations of physical observables in spintronics** [231, 232].
The φ_0-Josephson junction model in the “superconductor–ferromagnet–superconductor” system was investigated. For numerical simulation in a wide range of parameters which requires a significant computer time, a parallel MPI/C++ computer code was developed and implemented on the HybriLIT cluster and “Govorun” supercomputer.

• The periodic structure of the magnetization reversal domains is studied within the superconductor–ferromagnetic–superconductor φ_0-junction model. Two versions of parallel implementation based on MPI and OpenMP techniques were developed. Efficiency of both versions was confirmed by test calculations performed at the HybriLIT Platform [233, 234].

► **Round off error growth estimation in stacks of long Josephson junctions**

• **The analysis of the round off errors i**n usual numerical calculations of the intensity-voltage characteristics (IVC) of Josephson junctions shows that the round-off errors may get out of control. A new computation scheme is proposed together with theorematic results guaranteeing their boundedness [235]. Practical experiments on the "Govorun" supercomputer confirm the theoretical results.

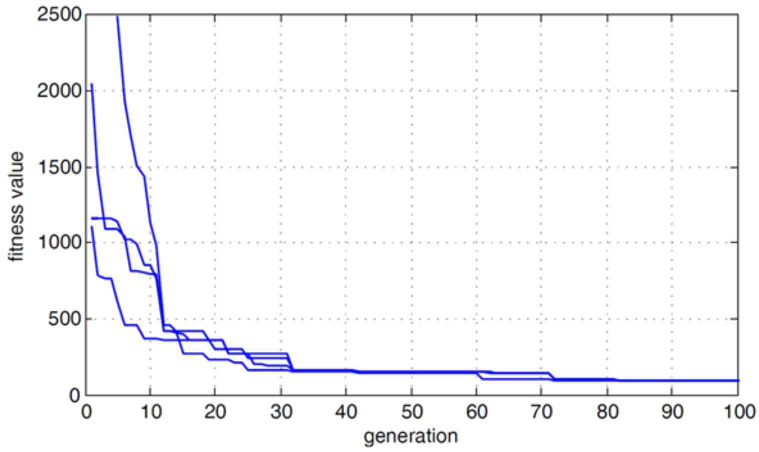
• **Round off error growth estimation done in the l_2 metric** [236].



The figure shows graphs of the growth of a single error in the metric l_2, $t \le 5000\ \tau$, for various τ and h. The bottom graph is for the case $\tau = h = 0.1$. The middle one is for the case $\tau = h = 0.05$, and the upper plot is for $h = 0.05$, and $\tau = h/5$. Comparing these graphs, we see that rounding errors grow fastest in the case of $\tau/h = 1/5$. From here follows the practical advice to use the same grid spacing, $\tau = h$.

• **Round off error growth estimation is done for the Cauchy problems in the uniform l_1 metric** [237]. Specific Cauchy problems are scrutinized, among them the IVC calculations for long Josephson junctions. Theorematic results establish the boundedness of the round off error accumulations in the uniform metric. Calculations done on the Govorun Supercomputer in MLIT using the REDUCE system allow the empirical validation of these results.

► **Efficient Genetic Optimization of LDPC Codes to Improve the Correction of Burst Errors** [238]. Reliable bounds of correction capabilities for various code lengths and various redundancies of LDPC (Low Density Parity Check) codes are derived. Outputs of fast parallel solutions run on the HybriLIT cluster and the "Govorun" supercomputer illustrate the method capabilities within various working options.



Sample optimization tasks. The LDPC code (128, 72) has been selected for the optimization. The convergence of the best fitness value to the optimal solution is illustrated.

3.4. Progress in Big Data Analytics

Development of the concept and step-by-step implementation within the Big Data approach of a scalable software-analytical platform for the collection, storage, processing, analysis, retrieval of relevant information and visualization of results for the MPD, SPD and BM@N experiments at the NICA accelerator and within the JINR neutrino program are foreseen. The use of supercomputer technologies, coupled with "data lakes" and Big Data technologies also provides new opportunities for the development of large-scale mega-science research projects. Further developments concern methods and software for the efficient use of Big Data Analytics for resource-intensive computations on coprocessors and GPUs for modeling, reconstruction and processing of experimental data (installations at the NICA accelerator complex, JINR neutrino experimental programs, LHC experiments).

Particular attention is paid to new promising areas in the creation of distributed data warehouses ("Data Lake"), the integration of Big Data and supercomputer technologies, and "machine learning" methods. In 2019, a distributed prototype of a "lake of scientific data" was created based on centers in Dubna, Moscow and Gatchina. Using the prototype, the cache system was tested using both synthetic tests and real-life LHC experiments.

Time series analysis methods are being developed using Big Data technologies for intelligent monitoring of distributed computing systems, including methods and technologies of machine learning and artificial intelligence for optimizing the functioning of distributed computing of large-scale physical experiments. The prototype of a software and analytical platform for solving current and future JINR tasks using the Big Data mining has been created. Currently, studies of the characteristics and structure of the JINR external network traffic are being conducted on the prototype of the analytical system. The results of these studies are planned to be used to create a system for intelligent monitoring of the JINR information and computing infrastructure, including its part involved in distributed international computing infrastructures. The use of methods developed for distributed systems will allow us to propose new solutions to ensure the security of the computing infrastructures of the experiments.

In Big Data analytics, the mathematical and algorithmic support of information processing plays an important role. Within the framework of the topic, there are carried out research and development of methods such as dynamic quantum clustering, locality-sensitive hashing, mathematical methods for organizing computation chains, etc. The results are tested on the created prototype of the analytical platform.

The development of a platform for streaming and batch processing of big data is underway and it is tested on the example of network traffic analysis [239].

The methods of the intellectual processing of texts in socio-economic applications offer a wide range of applications for Big Data analytics [240]. An instance is the creation of an automated system for collecting, processing and analyzing data from open sources of information aimed at identifying activities related to the collection of funds for the financing of extremism.

The developed approaches to creating Big Data analytics platforms are successfully used in the educational process [241].

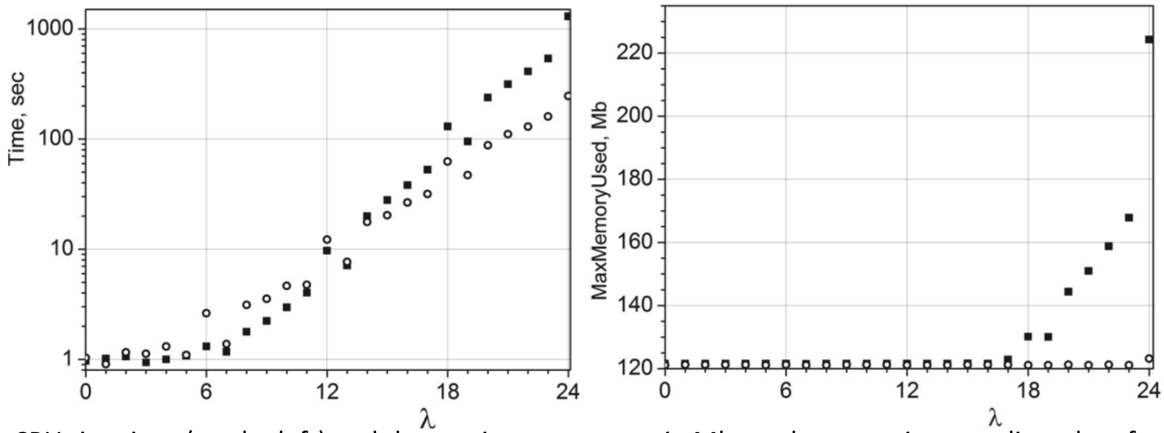
► **Big Data solutions** for automated monitoring and analysis of the labor market in the Russian Federation have been derived and implemented in an analytical platform, which implements a full data processing cycle, resulting in an impressive 20 TB database. The analytical core of the platform is built on the methods and algorithms developed by the authors using natural language processing (NLP) methods, including semantic analysis based on neural network models trained on large text arrays [242].

4. Methods, Algorithms and Software of Computer Algebra and Quantum Computing

► **Development of symbolic-numerical algorithms for solving systems of nonlinear PDEs**

• The method of triangular Thomas decomposition for polynomial nonlinear systems of partial differential equations, previously developed by the authors, was used for algorithmic verification of linearizability for nonlinear (ordinary) differential equations [243].

• **Symbolic-Numerical Algorithm for Computing Orthonormal Basis of O(5) x SU(1,1) Group** [244]. A new universal effective symbolic-numeric algorithm was elaborated and implemented as the first version of O5SU11 code in the Wolfram Mathematica for computing the orthonormal basis of the Bohr–Mottelson(BM) collective model in the both intrinsic and laboratory frames, which can be implemented in any computer algebra system. This kind of basis is widely used for calculating the spectra and electromagnetic transitions in solid, molecular, and nuclear physics.



The CPU time in s. (on the left) and the maximum memory in Mb used to store intermediate data for the current Mathematica session in computation of the overlap integrals and orthogonalization matrices (on the right). Both values are given versus the parameter λ at L = λ in the laboratory (marked by squares) and intrinsic (marked by cycles) frames

► **Solutions of difficult problems of computer algebra**

• **Identifying the Parametric Occurrence of Multiple Steady States for Biological Networks** [245]. A problem from biological network analysis of determining regions in a parameter space over which there are multiple steady states for positive real values of variables and parameters is considered. Multiple approaches to address the problem using tools from Symbolic Computation, together with the progress toward semi-algebraic descriptions of the multistationarity regions of parameter space were reported. The biological networks studied are models of the mitogen-activated protein kinases (MAPK) network which has already consumed considerable effort using special insights into its structure of corresponding models.

• **Constructive models for the description of finite quantum systems**

An algorithm for decomposing permutation representations of wreath products of finite groups into irreducible components is reported. The C implementation of the algorithm is capable of constructing irreducible decompositions of representations of wreath products of high dimensions and ranks [246–249]. The constructive approach to quantum mechanics has been recently analized, from the point of view of physics and cosmology, in Tom Banks, ``*Finite Deformations of Quantum Mechanics*'', arXiv:2001.07662[hep-th] (2020). This author concludes that the quantum models derived within this approach ``*can encompass finite dimensional approximations to all known models of theoretical physics*."

• **Methods for the calculation of Feynman integrals** [250] enabled computation of anomalous dimensions of quark masses in the three-loop approximation.

• **GPU resources for the computation of involutive and Gröbner bases** [251].
The table-based representation of polynomials for the computations of involutive and Gröbner bases of systems of nonlinear polynomial equations is developed. Using this representation implemented in C++, the possibility of effective delegation of some parts of this computational task to the GPU is shown and implemented. This opens up new opportunities for solving complex problems in this field of science.

• **Foliations of SL(n) group and the space sl*(n)** [252]. The parameters on a conjugacy class in the Lie group SL(n) and the parameters on a coadjoint orbit in the space sl*(n) dual to the Lie algebra sl(n) were found. In this way the trivialization problems for the foliations of SL(n) group and the space sl*(n) were solved.

► **Solutions of problems related to quantum information**

• Dynamic **Simulation of Quantum Entanglement in Finite Quantum Mechanics** [253, 254]. In the framework of constructive quantum mechanics, the emergence of geometry from entanglement in composite quantum systems is discussed. It is shown that the 2nd Rényi entanglement entropy may be useful in applying polynomial computer algebra to model metric structures in quantum systems with geometry.

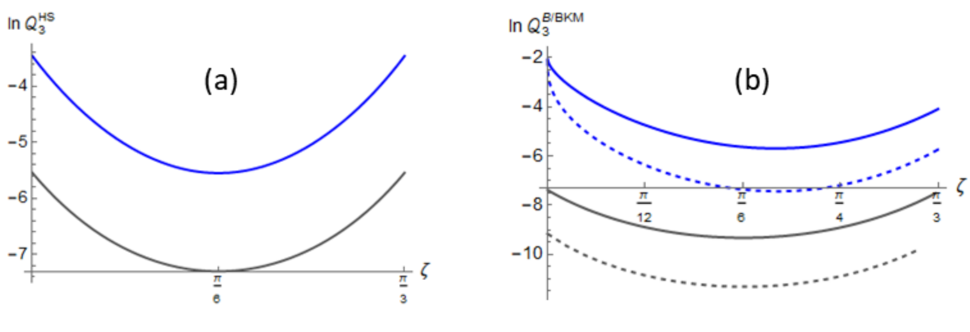
• **Classicality indicator of an arbitrary N-level quantum system.**

The global indicator for quantization of "classicality-quantumness" correspondence was introduced [255, 256] and defined as the relative volume of a subspace with positive Wigner function of the state space of an N-dimensional quantum system. It is exemplified by constructing the global indicator of classicality/quantumness for the Hilbert–Schmidt, Bures and Bogoliubov–Kubo–Mori ensembles of qubits and qutrits.

Assuming that the states of an N-level quantum system are distributed by Hilbert–Schmidt measure, the global measure is defined as the average non-classicality of the individual states over the Hilbert-Schmidt ensemble. A numerical estimate of this quantity is obtained and a proposition is proved, claiming its exact value in the limit of $N\to\infty$ [257].

• Research on the analysis of the quantum information resource of finite-dimensional quantum systems was continued using the method of quasi-distributions in the phase space. Measures of quantumness were introduced, which made possible the quantitative description of the difference between quantum states and the corresponding classical analogue. Based on the negativity property of the corresponding Wigner quasi-distribution, an indicator characterizing the quantumness of the basic systems, qubits and qutrits for various metrics (Hilbert–Schmidt, Bures and Bogolyubov–Kubo–Mori) given on the space of quantum states was calculated [258, 259].

• **The Q_3-indicator of classicality of quantum states** with different symmetries of a 3-level quantum system defined as the probability to find a state with a positive Wigner function within unitary invariant random ensembles associated with the Hilbert–Schmidt (HS), Bures (B) and Bogoliubov–Kubo–Mori (BKM) metrics was studied. The computations of Q_3-indicators for all ensembles showed a same pattern: the states with a "larger" symmetry are more classical [260].



(a) Q_3-indicators for the HS ensemble with $(1)^3$ (gray curve) and (2)×U(1) (blue curve) symmetries; (b) Q_3-indicators for the B (solid curves) and BKM (dashed curves) ensembles with $U(1)^3$ (gray curves) and $SU(2)\times U(1)$ (blue curves) symmetries [260].

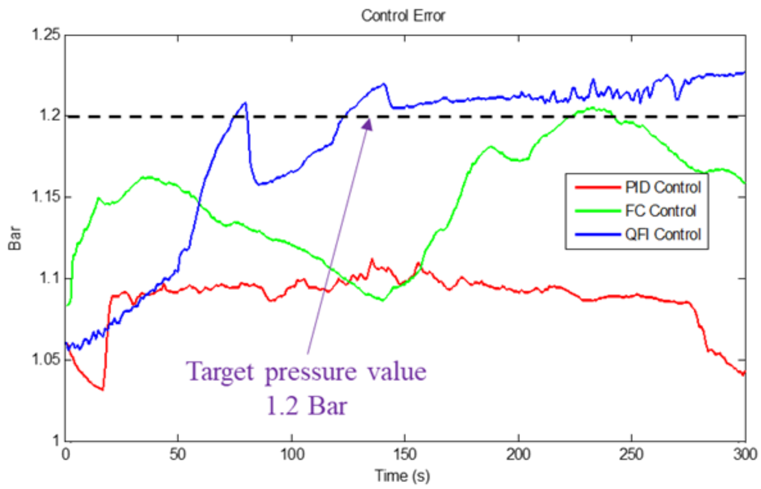
• **Robustness of the entanglement** in two qubits maximally entangled mixed states (MEMS) has been studied under quantum decoherence channels [261].

► **Nonequilibrium Bose systems and quantum information processing** [262, 263]. The Hohenberg–Martin dilemma, assessing the incompatibility between the occurrence of a gapless state and fulfillment of conservation laws, is solved within the Hartree–Fock–Bogolubov method [262]. This enables a new classification of the nonequilibrium states for Bose condensed systems. Numerical calculations yield results in good agreement with experimental data. The possibility of using the Bose–Einstein condensation for generating entanglement production can be employed for quantum information processing [263].

► **Role of collective information in networks of quantum operating agents** [264, 265]. A theory of intelligence networks of quantum operating agents is developed. The role of information exchange between the agents on the network operation is numerically investigated. These studies are important for the creation of human-like artificial intelligence.

► **Quantum algorithms on simulators implemented on supercomputers (SC) of classical architectures** is motivated by the perspectives it offers in the study of the chemical properties of heavy elements, for quantum deep machine learning, in robotics, and other fields. Using the software models QuEST, Qiskit, CuQuantum and the generator of quantum circuits Circ, the current capabilities of the Govorun Supercomputer were assessed. It was found that the dimension of the state vector grows exponentially with the increase in the number of qubits and the possibilities for modeling quantum algorithms are limited to 38 qubits on a CPU, 31 qubits on one GPU, and 34 qubits on eight GPUs [266, 267].

► **The control of the pressure and flow of liquid nitrogen in the superconducting magnets of the cryogenic system of the NICA accelerator complex** was achieved within a newly developed hardware and software platform based on quantum fuzzy controllers embedded into the control feedback loop. The quantum controller demonstrated the highest speed in achieving the target value, low overshoot and accuracy of reaching the control goal compared to other types of controllers (blue curve, in figure below). The performance and efficiency of the developed intelligent system for remote control of the technological process of cooling a superconducting magnet secured a guaranteed achievement of a stable superconductivity zone with more than 50% savings in nitrogen consumption [268].



Controlling the process of achieving the given level of nitrogen pressure by different types of regulators in cooling mode (blue curve – quantum regulator, green – fuzzy regulator, red – PID regulator)

The design of quantum fuzzy controllers is performed using the QSCIT (Quantum Soft Computational Intelligence Toolkit) software toolkit developed by MLIT specialists [269].

<u>Addendum</u>:

Grow up of the scientific competence in using the JINR computer tools

Only educated users can grasp the complex JINR hardware infrastructure. Securing an adequate level of competence in using the JINR computing tools is a *sine qua non* condition for successful highest level solution of the existing scientific challenges.

The grasp of the highest level computing tools of the MICC (Multifunctional Information and Computing Complex) hardware infrastructure implemented in MLIT needs an abrupt learning curve for the novice and continuous preoccupation of the expert for the development and extension of the acquired knowledge. To this aim, *<u>an articulated and permanent educational system</u>* was implemented and promoted by the MLIT leadership who coordinated this activity, done with the participation of the MLIT staff from both Topics 1118 and 1119.

This activity addressed both the MLIT staff and the MICC users from JINR and JINR Member States. Briefly, this education system included three legs:

(*a*) ***<u>Allocation of high-level resources</u>*** to this aim. The HybriLIT polygon has become the practical center for the education and growth of young specialists from both JINR and JINR Member States. Prominent specialists from JINR and from partner institutions in Russia and abroad are frequently giving lectures and tutorials at HybriLIT. Besides direct access admission to computing HybriLIT modules, there have been promoted new forms of online communication (e.g., Github), with the aim to secure effective contacts at distance and feedback.

Within the collaboration with Dubna University, the students are using HybriLIT for a twofold purpose: preparation of bachelor's and master's theses and solving tasks within JINR projects.

In 2020, master classes were remotely held for students from the Czech Republic and Armenia, practical classes were held on the HybriLIT platform for more than 1 000 students within the following courses: “Architecture of Computing Systems”, “Technologies of High-Performance Computing”, “Modern Methods of Analyzing Complex Systems”, “Machine Learning and Data Mining”, “Languages and Technologies of Data Analysis”, “Mathematical Apparatus and Tools for Data Analysis” – using the ML/DL/HPC ecosystem, which allows students to master state-of-the-art technologies for developing parallel algorithms on novel computing hybrid architectures and tools (libraries and frameworks) for the tasks of machine and deep learning.

In 2021, training courses and practical classes on “High-performance Computing and Supercomputer Technologies” and “Machine Learning and Data Mining” were held on the HybriLIT platform. A number of 780 students from Dubna State University and more than 300 students and postgraduates from other universities and JINR Member States were registered on the training and testing polygon. In 2021, nine master and bachelor theses were prepared using the resources of the HybriLIT platform.

In 2022, the resources of the HybriLIT platform were actively used for educational purposes. This direction is connected both with training courses for JINR staff members and practical classes for students of Dubna State University, Tver State University, etc.

In 2022, practical classes on “Architecture of Computer Systems”, “High-performance Computing Technologies”, “Modern Methods for Analyzing Complex Systems”, “Machine Learning and Data Mining”, “Languages and Technologies for Data Analysis”, “Mathematical Apparatus and Tools for Data Analysis” were held using the resources of the education and testing polygon and the ML/DL/HPC ecosystem for more than 800 students, which enabled them to master state-of-the-art technologies for developing parallel algorithms on novel computing hybrid architectures and tools (libraries and frameworks) for machine and deep learning tasks.

(*b*) ***<u>Stimulation of the interest of the young people</u>*** (students and JINR staff) for obtaining ***<u>qualification degrees based on hard work</u>*** (bachelor, master, candidate, doctor) in the field of scientific computing.

A multiscale approach to skilled education has been secured and promoted thanks to individual efforts, which have been encouraged by the MLIT leadership.

Within this effort, the links with high education institutions (the Dubna University, the Russian Economic University, the People's Friendship University, etc.) enabled direct participation to the education process, supervision of bachelor and master degrees.

In this frame, it is worth mentioning the careful preparation of a textbook for parallel programming [270]. This is useful both to the students of the Dubna University and to all scientists interested in raising their grasp of this difficult but necessary field of research.

The participation as lecturers at the INTEREST cycles, organized by the JINR University Centre on a competitive base, for young peoples from all over the world, contributes to the increase of the interest to the JINR as an international institution.

On top of this scale, the existence in MLIT of a Doctoral Council for affording scientific titles of candidates and doctors of science maintenance a vivid interest among the young staff of the Topic 1119 for the recognizance of the outstanding value of their scientific results.

During 2020–2022, three young people from the Topic 1119 staff have passed all the steps to the defense of candidate theses:

1. Alexander Ayriyan (2020), thesis title: "Numerical Modelling of Thermal Processes in Cells for Molecular Injection into Ion Source".
2. Andrey Sapozhnikov (2020), thesis title: "Magnetic system modelling using method of volume integral equations with piecewise-linear approximation of the field within ferromagnetic".
3. Alina Volokhova (2022), thesis title: "Numerical investigation of the observables describing dynamical characteristics in the hydrated electron model and in the filtration of gas condensate mixtures".

(*c*) ***Periodic organization of dedicated events*** (Schools, Courses, Conferences, etc.) with the best available lecturers.

In 2021, the workshop "Distributed Computing and Data Science", within which students attended the training course "Distributed Computing, Machine and Deep Learning for Solving Applied Tasks", and the 3rd IT School for Young Scientists "Modern IT Technologies for Solving Scientific Tasks", in which over 60 students and teachers from universities of the South of Russia (North Ossetia, Kabardino-Balkaria, Chechnya) and from Tibilov South Ossetian State University participated, were held at the North Ossetian State University. Lectures on JINR scientific projects, on information technologies and solutions for scientific tasks being developed at JINR were delivered, master classes and training courses on distributed computing, virtualization and cloud technologies, machine and deep learning algorithms for analyzing complex structured data were conducted.

The International School of Information Technologies "Data Science" is a joint initiative of the Joint Institute for Nuclear Research and the Dubna University [271]. Annual editions have been held in 2019, 2020, 2021. A summary of the last event may be watched at the JINR web site http://www.jinr.ru/posts/international-it-school-data-science-trains-specialists-for-mega-science-projects/

Or on youtube:

https://www.youtube.com/watch?v=5LJ87lkqeoc and pressing the BROWSE YOUTUBE.

The first "JINR Autumn School on Information Technologies" was held in the MLIT on November, 14–19, 2022. The students got acquainted with the JINR program and got the opportunity to choose topics for their final theses. The school was attended by 60 senior students from 13 Russian universities, including universities where the information centers of the JINR operate. Ten lectures were delivered by the members of the Topic 1119 staff; among them nine are available at the School web site [272].

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From the ten lectures delivered by the MLIT staff working in Topic 1119, nine are available at the School web site:

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