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

(Annual Report 2023)

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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.

January, 2024

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Main Achievements in the MLIT Topic 1119 during 2023

Extended Abstract

Inside 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 2023 involved 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 work done within the Topic 1119 during 2023 featured a second order phase transition, which may be concisely characterized as change in continuity.

There have been two principal reasons for changes.

On the one side, the planning of the complex scientific activity of the JINR as a whole, which defines the cardinal lines of the strategic scientific goals over seven year periods, reached a milestone. The past seven year period, 2017 – 2023, ended, the new one, 2024 – 2030, seven-year period follows with new challenges for all the scientific community of the Institute.

On the other side, the change of generation in the MLIT Leadership (again with significant features of continuity!), necessarily asked for the rethinking of the most effective ways of enhanceing and articulating the scientific processes within the MLIT, such as to yield maximum benefits for both the MLIT and the JINR as a whole.

The output of this articulated effort, done at all the JINR instances and levels [1–3], resulted in the *continuity decision* of keeping the cornerstone ideas of the Topic 1119 for the next seven year period, 2024 – 2030. With *necessary changes*, however: a new Topic leadership and a new implementation of the research effort, into specific scientific projects, characterized by strong interactions among their team members.

The main features of the activity done within the Topic 1119 have been summarized on the four year report (2020 – 2023) presented at the June 2023 Sessions of the PACs for Condensed Matter Physics [1] and for Particle Physics [2], respectively.

The multi-facetted work carried out within the Topic 1119 asked for the solution of several tasks, which underpinned the timeliness and the importance of the various achievements. Of primary importance was the design, development, implementation, and maintenance of a user friendly computing environment on the MLIT heterogeneous computing platform, which involves the HybriLIT cluster and the “Govorun” supercomputer. Highly needed and appreciated contributions have been brought to the three-dimensional simulations asked by the magnet validation for the future NICA facility, highest-level solutions of specific tasks within the BM@N, MPD and SPD projects at NICA, development of data processing system software for the Baikal-GVD project. The software development, within the JINR contribution, for the CMS and ATLAS Phase 3 projects at CERN, summarize the best results produced within the Topic 1119 for the experimental data processing.

During 2023, the staff of the Topic 1119 co-authored a total number of 153 scientific publications. Among them, 137 scientific papers in prestigious international journals (53 in foreign journals, 84 in Russian journals), 5 monographs or contributions to monographs and 11 publications in scientific collections and periodicals. Co-authorship to 81 CMS Project research papers, 6 DUNE Project research papers, and 5 Baikal-GVD Project research papers, enhance the list of the main scientific papers. The presentation of 20 plenary and 9 oral lectures at international conferences completes the statistics of the contribution to the JINR excellence trough publications.

The MLIT Dissertation Council (DC) has put very high standards to the allowance of scientific degrees. During 2023, the DC afforded the PhD title to two young staff members of the Topic 1119 (N.N. Voytishin and E.I. Alexandrov). Two young staff members defended scientific and qualifying works upon completion of postgraduate studies (V.V. Papoyan, D.R. Badreeva).

An important fraction of the staff of the Topic 1119 contributed to 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.

Unfortunately, not everything went smooth during 2023. Igor Victorovich Puzynin passed away on 17-th July 2023 [4]. This is the heaviest loss of all the JINR, MLIT, and the Topic 1119, in particular. As a creator of the new direction “computational physics” in JINR, I.V. Puzynin has brought, for many decades, an indelible contribution to the algorithmic and software support of theoretical and experimental research based on the effective use of modern computing systems and high-speed networks. He was the initiator of the extremely successful MMCP International Conferences, regularly held during the last two decades, with a significant contribution of scientists all over the world. His memory will be present forever in the MLIT.

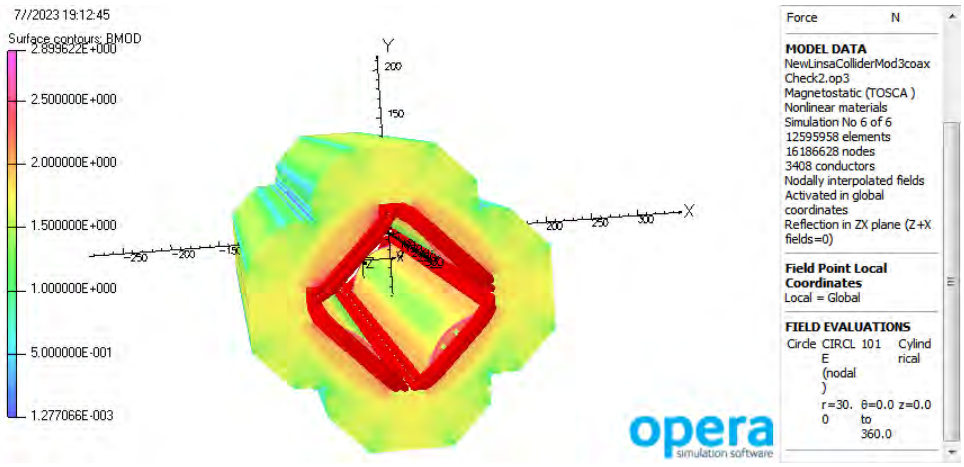
1. Mathematical and Computation Methods for Simulation of Complex Physical Systems

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) project for the validation of the magnetic field uniformity in the working areas of the new physical magnets*; *improvement of **design tools for new medical purpose cyclotrons***.

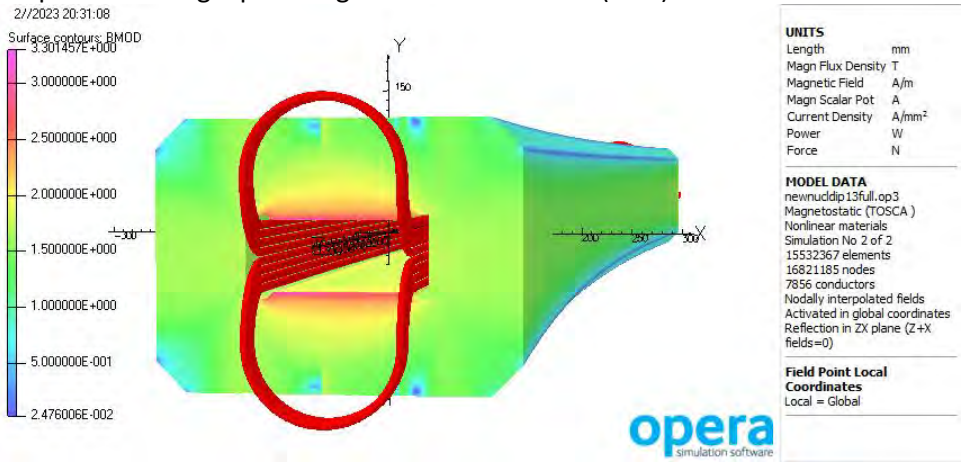
● **The OPERA 3D modeling of magnetic systems for the NICA collider** Instances of the work done by P.G. Akishin in the framework of the NICA projects, in collaboration with VBLHEP, for the 3D modeling of various classes of magnets are given in the figures below, where the field distributions in the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

Based on two-dimensional and three-dimensional modeling of a magnetic system by varying the location of the current windings, the characteristics of the superconducting three-turn quadrupole magnet of the NICA collider were optimized.



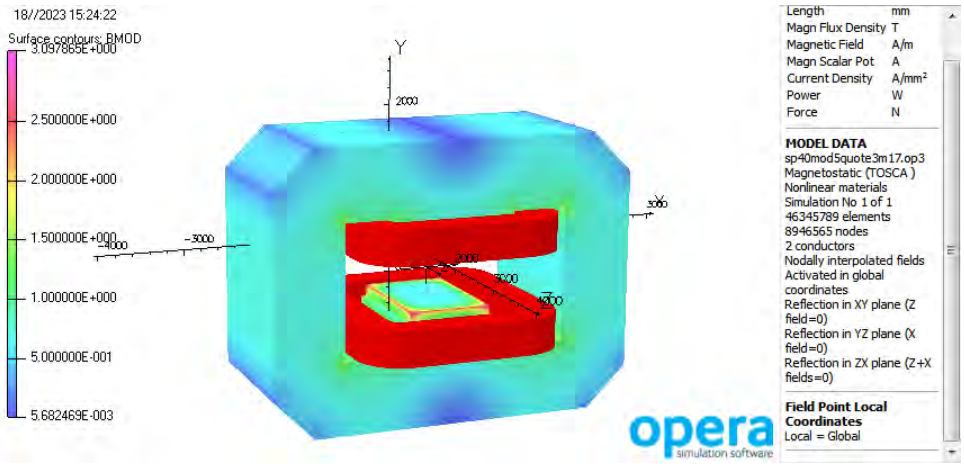
Трехвитковый сверхпроводящий квадрупольный магнит коллайдера NICA
Three-turn superconducting quadrupole magnet of the NICA collider

In order to get the necessary parameters of the magnetic field in the working area, three-dimensional modeling of the superconducting dipole magnet of the Nuclotron (JINR) was carried out.



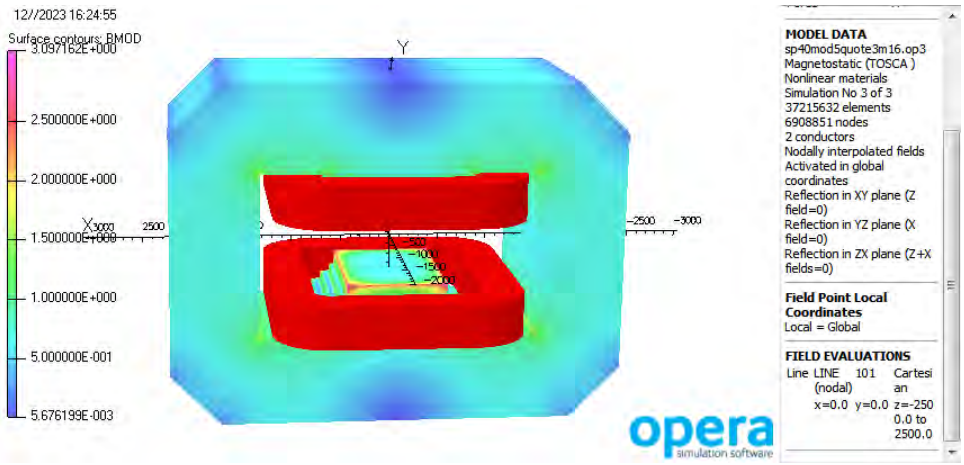
Model of a superconducting dipole magnet of the NUCLOTRON accelerator (JINR)

Three-dimensional modeling of the SP41 magnet of the BM@N experiment (JINR) was carried out. The map of the magnetic field in the working area of the magnet has been prepared.



Opera 3D model of the SP41 magnet of the BM@N experiment (JINR)

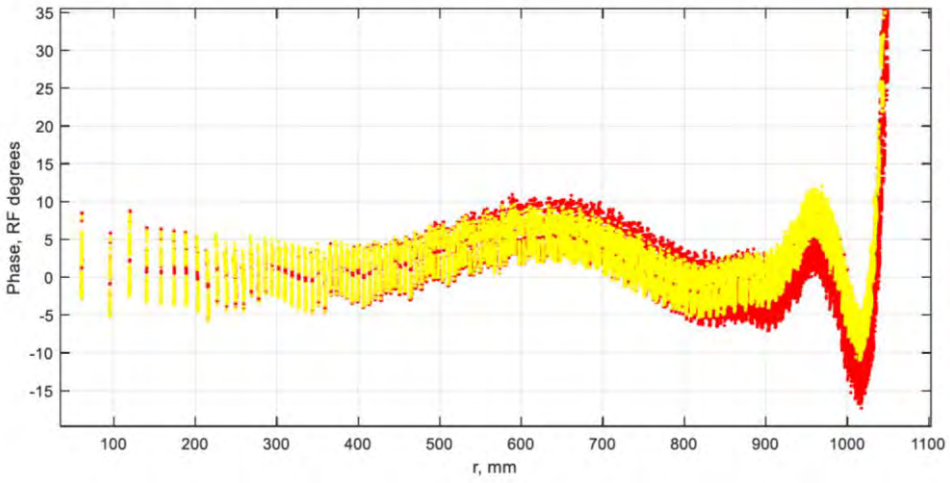
Three-dimensional modeling of the SP40 magnet of the HIPER NIS experiment (JINR) was carried out. The map of the magnetic field in the working area of the magnet has been prepared.



Model of the SP40 dipole magnet of the HIPER NIS experiment (JINR)

● In order to achieve a quality of calculation similar to the finite-element analysis of three-dimensional magnetostatic problems in terms of magnetic vector potential, but at lower computational cost, it has been proposed to use for modeling of the same problem a combination of magnetic vector and total scalar potentials. It was found that this mixed formulation can provide a substantial reduction in the computational cost as compared to its vector counterpart for a similar accuracy of both methods [5].

● **Improvement of design tools for medical purpose cyclotrons.** The future MSC230 isochronous cyclotron, devoted to proton therapy and life sciences research, is projected by a large team, DLNP centered. The use of the virtual prototyping (VP) design method to this aim, asked for the creation of appropriate computational tools. A Matlab-based platform that encapsulates distributed VP components (such as analysis and tracing programs) and provides a mechanism for their interaction was created. Besides the CAD (Solidworks) and various CST Studio modules, the newly created and actively optimized CORD (Closed ORbit Dynamics) software and beam dynamics software were used. Based on the modeling results, a report was prepared at the RUPAC'23 Conference. The results of tracing a proton beam from the ion source to the exit from the MSC230 cyclotron have been presented [6].



Phase motion of the beam during acceleration, taking into account (yellow color) and without taking into account (red color) the magnetic field of the accelerating system [6]

1.2. Selected numerical modeling of physical systems and processes

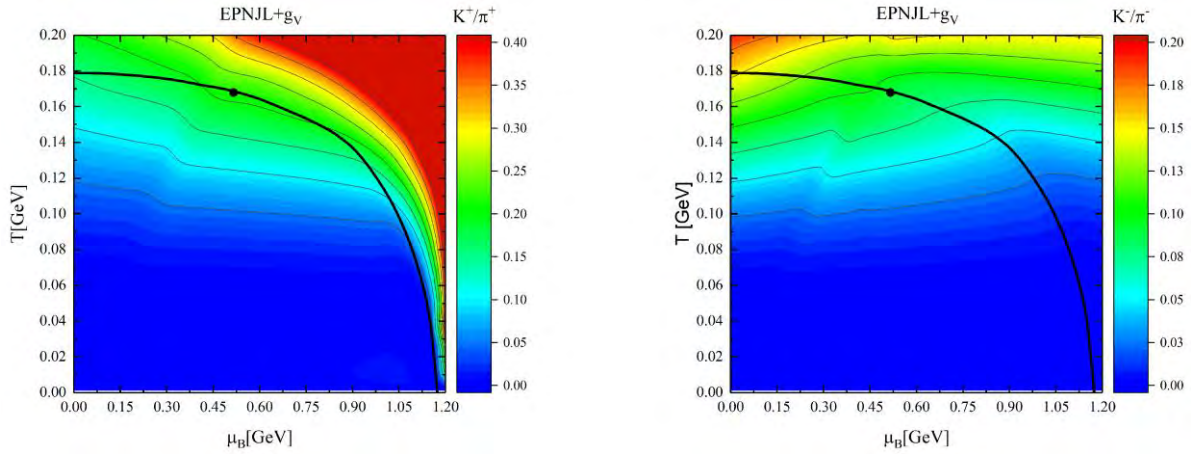
1.2.1. *NICA driven numeric-theoretical studies in dense hadronic matter*

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.

• **Cancellation of the sigma mode in the thermal pion gas** [7]. The pressure of the interacting pion gas has been calculated using the Beth–Uhlenbeck approach to the relativistic virial expansion with Breit–Wigner phase shifts for the σ- and ρ-meson resonances.

• **Two-photon decay of a neutral pion at finite temperature** [8]. Computation of the $\pi^0 \to \gamma\gamma$ decay width at high temperatures in the framework of the Nambu–Jona–Lasinio model requires the calculation of an integral with singularity $1/(x-c)$. The most suitable method must be found that can effectively bypass the singularity and allow obtaining an answer with minimal error and high computation speed. In this work, non-adaptive and adaptive methods based on Gauss–Kronrod quadrature formulas and the Monte Carlo integration method enabled the derivation of the temperature behavior of the two-photon pion decay width.

• **New results within the EPNJL model** [9]. The applicability of the effective models to the description of baryons and the behavior of ratios of strange baryons to pions is discussed. In the framework of the EPNJL model, the Bethe–Salpeter equation is used to find masses of baryons, which are considered to be in a diquark-quark state. Baryon melting is discussed at a finite chemical potential, and a flavor dependence of the hadronic deconfinement temperature is pointed out. It is shown that the description of the diquark-quark state at finite chemical potential is limited due to the occurrence of Bose condensate. This effect is strongly manifested in the description of light diquarks and baryons. Both the Λ^0/π^+ and Ξ^-/π^+ ratios show a sharp behaviour as functions of the T/μ_B variable, where T and μ_B are calculated along the melting lines.



Contour graphs for the K^+/π^+ and K^-/π^- ratios obtained with the Beth–Uhlenbeck approach of the EPNJL model with gV=0.6gS. The black lines show the phase transition (crossover) lines. It can be seen that when shifting along the phase transition line from low to high temperatures, the trajectory shows a quick enhancement and then a fall for K^+/π^+ and a smooth increase for K^-/π^- (Figure 4 [9])

• **Hadron modifications in dense baryonic matter**

• A systematic study of hybrid neutron star equations of state (EOS) consisting of a relativistic density functional for the hadronic phase and a covariant nonlocal Nambu-Jona-Lasinio (nlNJL) model to describe the color superconducting quark matter phase is provided [10]. Changing the values of the two free parameters, the dimensionless vector and diquark coupling strengths eta_V and eta_D results in a set of EOS with varying stiffness and deconfinement onset. The favorable parameters are obtained from a systematic Bayesian analysis for which the multimessenger constraint on the neutron star radius at 14Msun and the combined mass-radius constraint for PSR

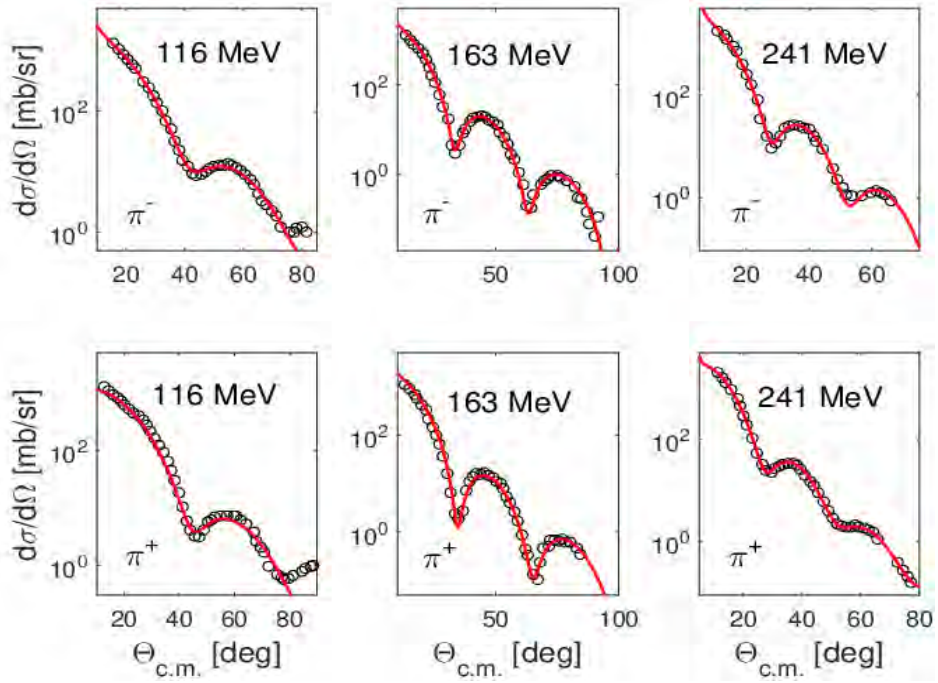
J0740+6620 from NICER experiment are used as the constraints. Additionally, the transition from hadronic matter to deconfined quark matter is constrained to occur above nuclear saturation density. Hybrid stars modeled with these favorable parameters are compatible with the NICER results for the radius of the highest known mass neutron star, PSR J0740+6620. A lower limit for the maximum mass of hybrid stars as a function of the vector coupling strength is obtained.

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** [11] **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.

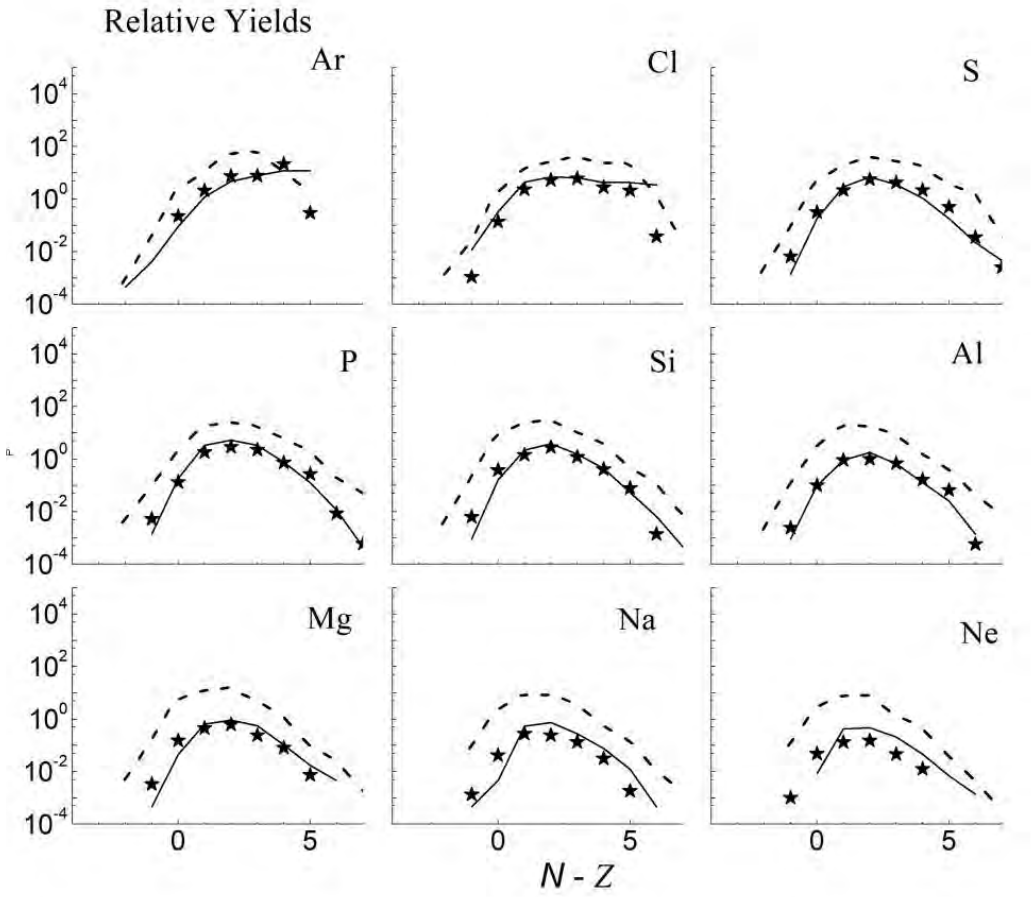


Comparison [11] of the cross-sections of the elastic scattering $\pi^{\pm}$ + ^{40}Ca at energies of 116, 163 and 241 MeV, computed using the microscopic model of optical potential (red curves), with experimental data (circles) from [Q. Ingram, et al., Phys. Lett. B **76** (1978) 173]

● **A review of the pion-nucleus scattering data** for a number of target nuclei based on a microscopic model of the pion-nucleus potential has been published [12]. It is shown that the developed approach provides an adequate description of experimental data on pion-nucleus scattering in the energy region of the pion-nucleon (3,3) resonance. Moreover, it allows the study of the influence of the nuclear medium on the pion-nucleon scattering.

● **Numerical analysis** [13] **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.

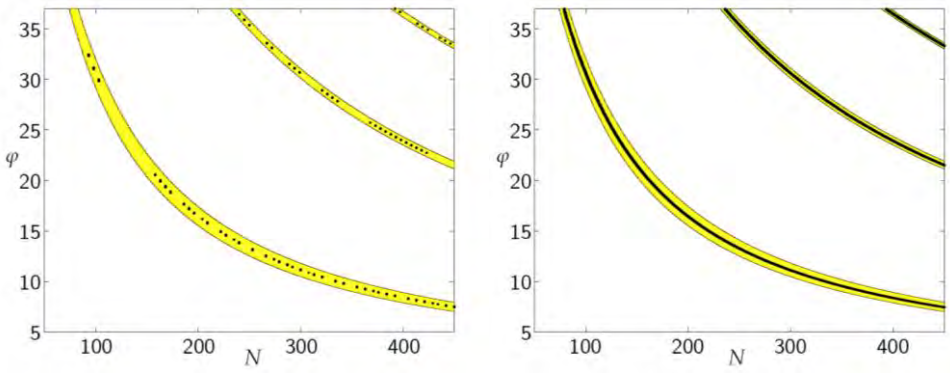
► **The heavy-ion-induced projectile fragmentation reactions at Fermi energies, realized at the COMBAS setup in FLNR**, yields vast amounts of isotopes far from the valley of stability. The understanding of the production mechanisms of the resulting neutron-rich or proton-rich isotopes is a challenging 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 [14–18]. 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 [16] in ^{40}Ar (36.5 *A*MeV) + ^{9}Be collissions (stars) in comparison with BNV-SMM calculations (solid curves) and previous authors' experimental data (dashed curves). The isotope names are given in the upper right corner of the pallets

1.2.3. *Numerical modeling of condensed matter systems*

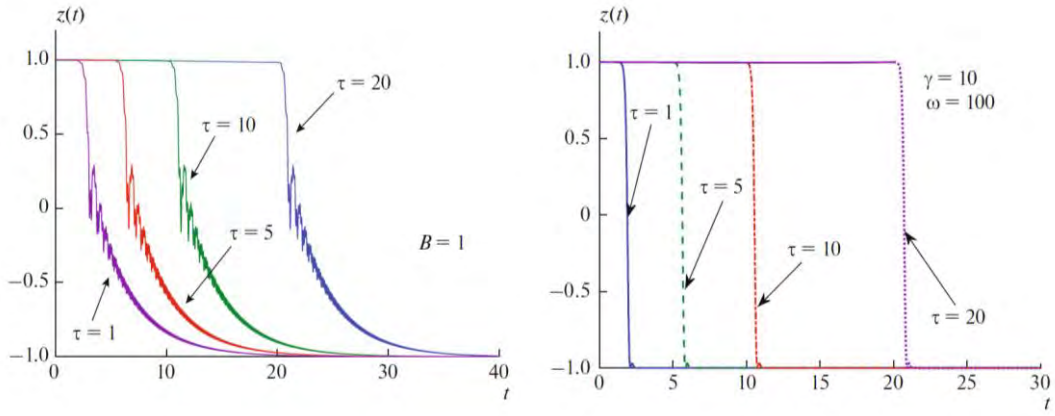
► **Numerical investigation of ballistic electron transport** through a corrugated (rippled) graphene system with a curvature-induced spin–orbit interaction [19]. The corrugated system is connected from both sides to two flat graphene sheets. The rippled structure unit is modeled by upward and downward curved surfaces. The cooperative effect of N units connected together (the superlattice) on the transmission of electrons, incident at arbitrary angles on the superlattice, is considered. The set of optimal angles and corresponding numbers of N units that yield the robust spin inverter phenomenon are found.



The spin inversion probabilities $P_{N,} \geq 0.99$ (yellow domain) as a function of number units N= 50, …, 450 in the superlattice for angles φ = 5°, 5.01°, …, 37°, for R = 12 Å, at the incident beam energy E = 0.1 eV (left) and E = 1.0 eV (right) [19]

► **Solution of dynamic phenomena in magnetic materials**.

• **Numerical simulation of magnetic nanomaterials** [20]. Numerical simulation of models describing the properties of magnetic nanomaterials that can be used to create devices for processing and storing information has to accommodate two contradictory properties of the nanomaterials: on the one hand, the ability to keep the magnetization frozen (information is stored) for a long time, and on the other hand, to have the ability to sharply change the magnetization, which is necessary for quickly erasing memory and rewriting new information. Methods for solving this dilemma have been proposed and studied, based on the creation of a trigger resonance, tuning a dynamic resonance, and the quadratic Zeeman effect.



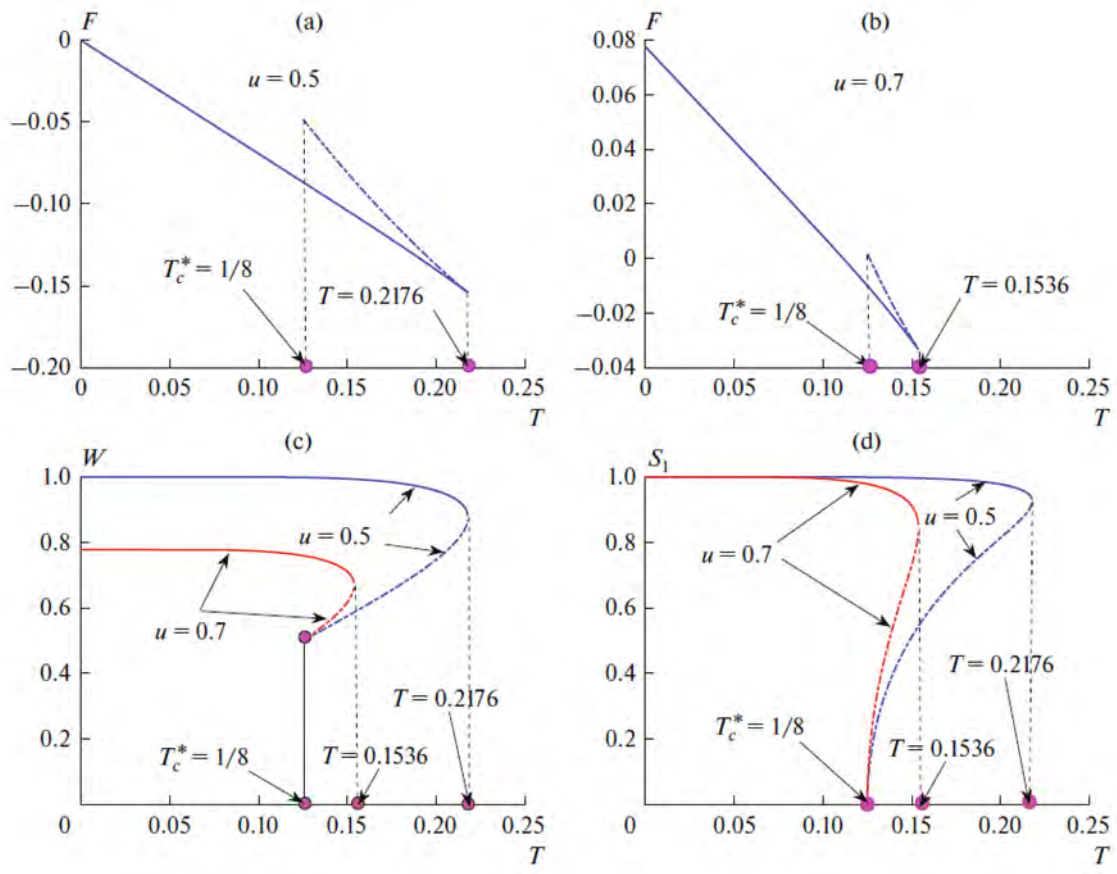
Longitudinal spin polarization z versus the dimensionless time t for different material parameter values (small values – left; large values – right). Dynamic resonance tuning starts at different delay times [20]

► **Simulation of statistical systems composed of several phases** [21, 22].

• **A microscopic statistical model of a superfluid quantum solid** is developed [21], 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** [22] 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 [21]

► **Numerical investigation of self-organization processes in superconductors** [23]. A numerical study was carried out of self-organization processes with the formation of spontaneous patterns in superconductors in the intermediate mixed phase and a search for signals of the coexistence of superconductivity of the first and second types.

• A numerical study and search for signals of phase transitions in quasi-two-dimensional systems of charged particles locked by a centrally symmetric potential were carried out based on the classical molecular dynamics (MD) method [24].

► **Dynamic model of the polaron**. **The review paper** [25], summarizes the results of numerical studies of the process of electron hydration based on the dynamic polaron model. The computational algorithm and software implementaton were optimized to take into account the

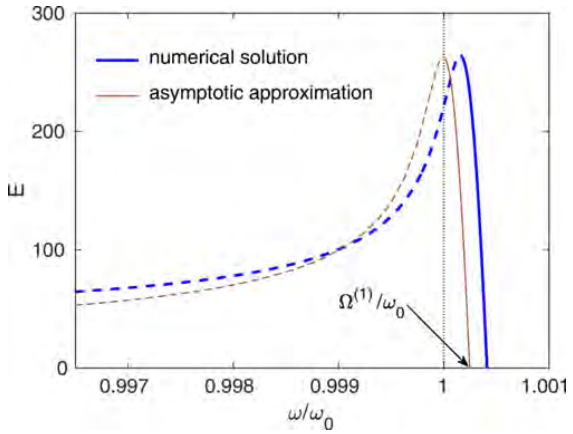
influence of the Coulomb potential. It resulted in a good agreement of computed and experimental data that could not previously be reproduced.

► **Solving nonlinear problems of mathematical physics: Integrability and trajectory confinement in symmetric waveguide arrays** [26]. Completely integrable two-, three-, and four-dimensional necklaces of PT-symmetric waveguides were discovered. In addition to being completely integrable Hamiltonian systems, necklaces are characterized by the complete absence of singular modes.

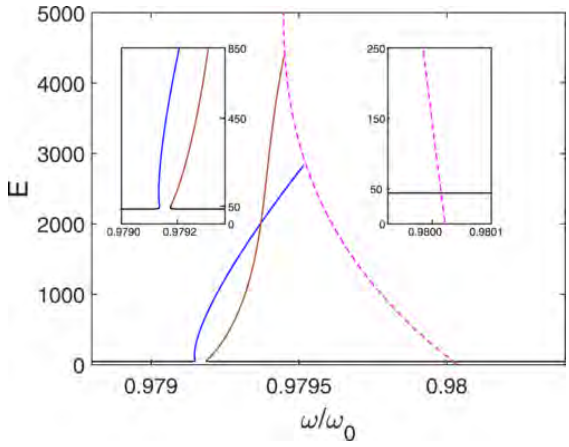
► **Investigations on the Klein-Gordon oscillon** [27, 28].

● Insight into the spatio-temporal structure and bifurcation of the three-dimensional relativistic oscillons is got by studying time-periodic solutions in a ball of a finite radius. The standing waves associated with the resonances are born in the period-multiplication bifurcations of the Bessel waves with higher frequencies. The energy-frequency diagram for a sufficiently large ball displays sizeable intervals of stability against spherically-symmetric perturbations [27].

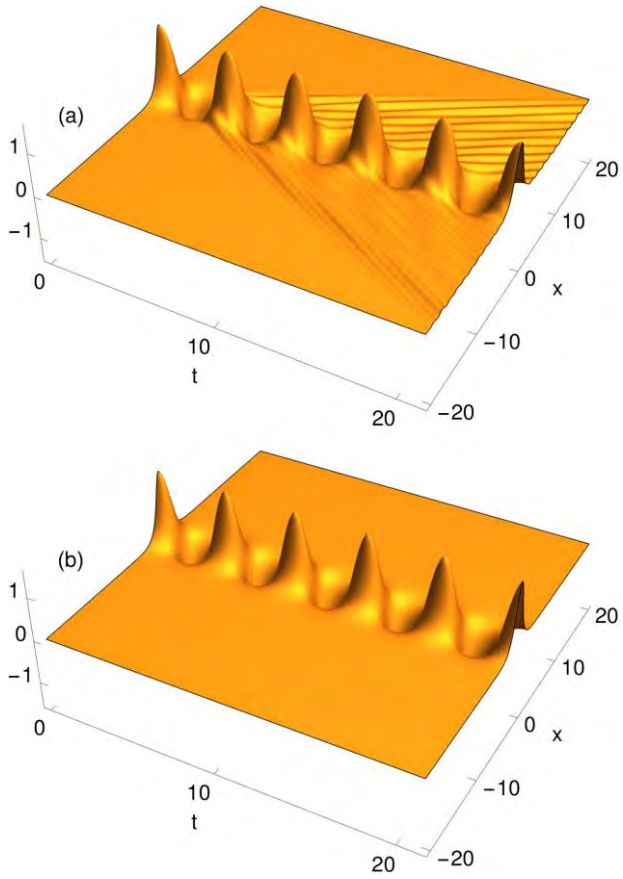
● A multiscale variational description of oscillons is proposed, free from the blow up singularities of the standard approach. In addition to determining the parameters of the oscillon, our approach detects the onset of its instability [28].



The E(ω) dependence near the point of inception of the standing wave in a ball with R=100. Blue (thick) curve: result of numerical continuation. Brown (thin) curve: asymptotic approximation exploiting R−1 as a small parameter. Stable solutions are marked by solid and unstable ones by dashed lines (Fig. 3 [27]).



A fragment of the E(ω) diagram in the vicinity of a 1:2 resonance in the ball with R=150. The blue and brown curves are two slopes of the "spike." The dashed magenta arc emerging from E=0 at $\omega=\Omega^{(114)}/2$ is the 1/2 undertone of the n=114th Bessel wave. (That is, a point (ω,E) on this branch represents the Bessel wave with frequency 2ω.) The insets zooming in on the lower sections of the spike and Bessel branch aim to emphasize the difference in the origins of the two branches (Fig. 7 [27]).



Comparison of the numerical solutions of (a) the Kosevich-Kovalev oscillon with (b) the variational approximation model, at the same ω. Except for the absence of the radiation waves, the variational pattern is seen to be a good fit for the true oscillon (Fig. 3 [28])

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

Results have been obtained for modeling, within the thermal spike model, of ablation processes in materials subject to laser radiation.

► **Numerical simulation of thermal processes occurring in materials under the action of ultrashort laser pulses** [29, 30].

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 [29] explicitely resolved diffusion term and convection term contributions to the relaxation times of both the electron gas and the crystal lattice.

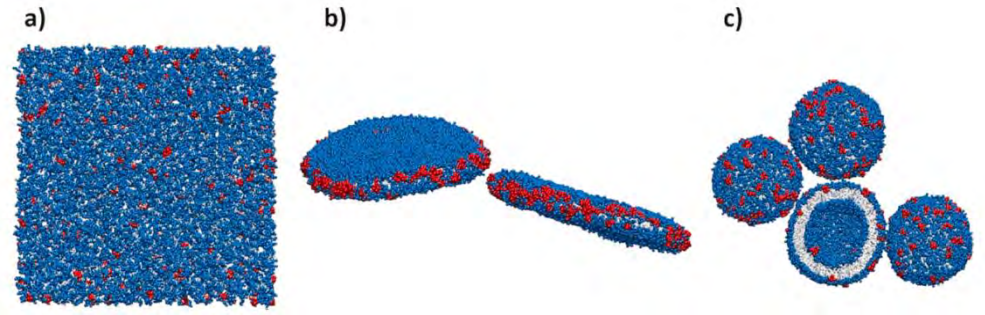
In a second investigation [30], the H-TSM model was formulated for samples of finite thickness. In this case, the sample thickness explicitely enters both the diffusion and convection terms of the heat conduction equations, as well as the source term of the H-TSM model equations and the boundary conditions 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** [31, 32].

• Changes to the membrane thickness and the overall membrane structure**,** with and without $A\beta_{25–35}$ 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 [31].

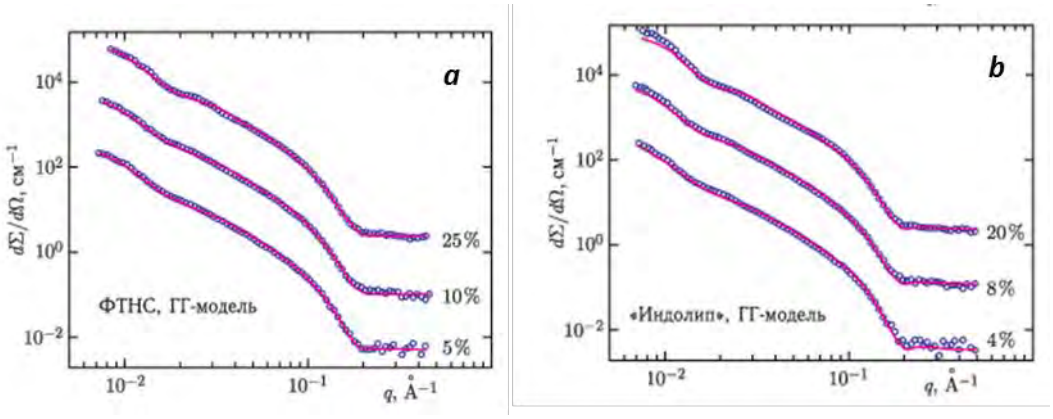
• Further incestigation [32] clarified the interaction of beta-amyloid peptide 25–35 with phospholipid membranes of DPPC from the point of view of a coarse-grained approach, which allows us to consider large vesicular and bicelle-like systems, as well as the influence of the peptide on the morphology of structures, including the formation of vesicles and bicelles. The localization and secondary structures of beta-amyloid peptide in bicelle-like and vesicular systems were assessed. In the case of vesicular systems, modeling of curved membranes was carried out. A study was conducted of the dynamic properties of lipid membranes regulated by the addition of melatonin, cholesterol and beta-amyloid peptide from the point of view of the influence of these additives on the occurrence of a gap in the phonon spectrum.



CG MD snapshots of a) an initial randomly distributed mixture of DPPC lipids, Aβ(25–35) peptides, and water molecules (not shown), b) self-assembled structures of BLSs below Tm after 10 μs simulation, c) self-assembled structures of SUVs above Tm after 10 μs simulation, where one of the vesicles is depicted with its far part sliced through its central plane. The lipid chains are presented in grey, lipid head groups in blue, and Aβ(25–35) molecules are shown in red. Water molecules are not shown for better visualization [32]

► **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.

• 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 [33]. The figure below summarizes the experimental and calculated SANS spectra.

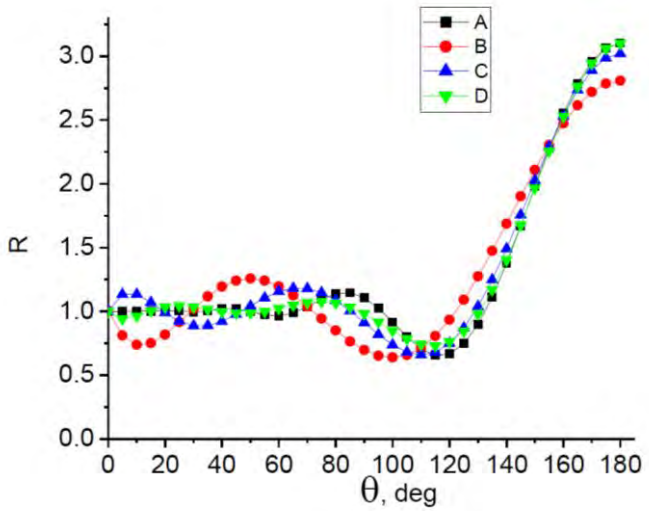


Calculated and experimental SANS spectra on samples of FTNS (***a***) and Indolip (***b***) vesicles in 4, 8, 20% maltose solutions. The calculation was made using the hydrophilic-hydrophobic bilayer model [33]

• **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 [33].

1.2.6. *Numerical modeling of other systems*

► **Comparative study of the energy-loss straggling calculation methods** [34]. Some exact and approximate methods commonly used to calculate corrections to the Bethe stopping formula and the normalized Mott cross section (NMCS), are modified and adapted to the calculation of the energy loss straggling (ELS). It is found that some authors' approximate methods for the ELS calculation show higher accuracy as compared to the conventional approximate method of Lijian–Qing–Zhengming (LQZ). In all the considered cases, the accuracies of the twice modified LQZ method (LQZ_{m2}) and thrice modified LQZ method (LQZ_{m3}) in the ELS calculations are higher than that of the usual LQZ method (see figure).



Dependence of the normalized Mott cross section (NMCS) on the angle θ (deg) for Z = 112 and β = 0.15 [A] in the numerical calculation by various methods: LQZ-method [B] LQZ_{m2}-method [C], and LQZ_{m3}-method [D] [34]

► **Study of the kinetics, mechanism, and reactivity of intermediates of a wide class of redox reactions.** The characterization of a wide class of redox reactions for which the rate-limiting step is the redox decomposition of the intermediate complex is given. The approach was applied to the investigation of the oxidation of oxalic acid (H_2O_x) by cerium(IV) in a sulfuric acid

medium as part of the Belousov–Zhabotinsky oscillating reaction (BZ reaction) catalyzed by cerium ions [35]. Moreover, the thermodynamic and kinetic characteristics of cerium(IV)–citrate complexes formed at the first step of oxidation of citric acid with cerium(IV) are studied [36].

► **Fresh ideas for solving old problems** [37].

The constituent picture of the W and H bosons is considered. Mechanisms for the estimation for the observable value of the cosmological constant in the supersymmetric models at finite temperatures and a connection between bosonic and fermionic statistical sums are defined.

► **On periodic approximate solutions of the three-body problem** [38]. Trivial choreographies are special periodic solutions of the planar three-body problem. In this work, a modified Newton's method based on the continuous analog of Newton's method and a high precision arithmetic for a specialized numerical search for new trivial choreographies is used. As a result of the search we computed a high precision database of 462 such orbits, including 397 new ones. The initial conditions and the periods of all found solutions are given with 180 correct decimal digits. 108 of the choreographies are linearly stable, including 99 new ones. The linear stability is tested by a high precision computing of the eigenvalues of the monodromy matrices.

► **A review of numerical approximation of functional integrals** [39]. The discussion revolves around the most recent outcomes in the realm of approximating functional integrals through calculations. Review of works devoted to the application of functional integrals in quantum mechanics and quantum field theory, nuclear physics and in other areas is presented. Methods obtained by the authors for approximate calculation of functional integrals generated by nonrelativistic Hamiltonians are given. One of the methods is based on the expansion in eigenfunctions of the Hamiltonian. In an alternate approach, the functional integrals are tackled using the semiclassical approximation. Methods for approximate evaluation of functional integrals generated by relativistic Hamiltonians are presented. These are the methods using functional polynomial approximation (analogue of formulas of a given degree of accuracy) and methods based on the expansion in eigenfunctions of the Hamiltonian, generating a functional integral.

► **New approach to the integration of dynamical systems** [40]. Lagutinsky's theory of integration of dynamical systems was reformulated for arbitrary linear systems of hypersurfaces. A certain dynamical system and a certain linear system of algebraic hypersurfaces were considered and an example was constructed showing that the hypersurfaces of the original linear system and the integral level lines may not coincide.

► **Properties of the third Vlasov equation** [41]. The third Vlasov equation describes the evolution in time of the distribution function depending on the coordinate, velocity, and acceleration. Such an extension makes it possible to describe the systems with electromagnetic and gravitational radiation and also to construct numerical methods with a higher computational accuracy, as it contains additional motion integrals.

► **Cosmology studies in different universe models** [42, 43, 44]. 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)** [45]. We implement in Maple and Mathematica an algorithm for constructing multivariate Hermitian interpolation polynomials (HIPs) inside a d-dimensional hypercube as a product of d pieces of one-dimensional HIPs of degree p' in each variable, that are calculated analytically using the authors' recurrence

relations. The piecewise polynomial functions constructed from the HIPs have continuous derivatives and are used in implementations of the high-accuracy finite element method. The efficiency of our finite element schemes, algorithms and GCMFEM program implemented in Maple and Mathematica are demonstrated by solving reference boundary value problems (BVPs) for multidimensional harmonic and anharmonic oscillators used in the Geometric Collective Model (GCM) of atomic nuclei. The BVP for the GCM is reduced to the BVP for a system of ordinary differential equations, which is solved by the KANTBP 5 M program implemented in Maple.

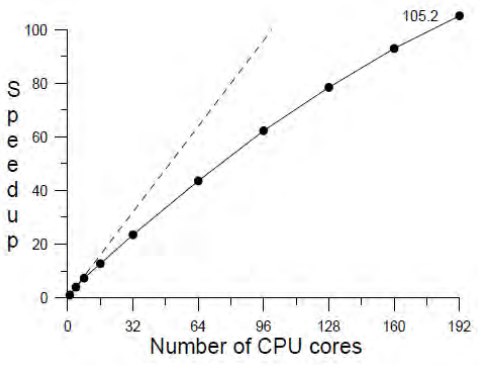
► **Problem adapted multi-scaling quadrature algorithms** [46, 47].

• 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 [46]. 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.

• New algorithmic developments are reported [47] for the recursive algorithms of the Bayesian inference based automatic adaptive quadrature (BAAQ) of the one-dimensional Riemann integrals with the aim at securing robust and reliable automatic decisions at critical steps of the solution path. First, the integrand function conditioning at the ends of a subrange decision tree root is resolved within a Bayesian predictor–corrector algorithm, resulting in decisions characterized by uniqueness and reliability. Second, a new subrange partition strategy enables the highest accuracy available output under cancellation by subtraction. Both types of reported achievements use specific input validation procedures.

• **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 [48]. 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.

• **Multiple precision computation by parallelizing the Taylor series method** [49]. 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.

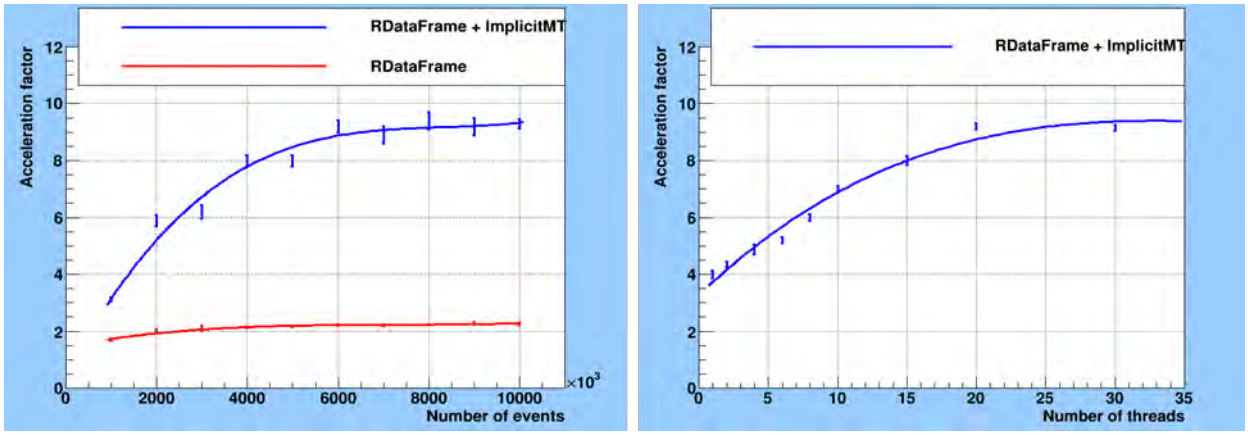
2.1. Parallel ROOT (PROOT) tools for experimental data analysis

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 [50] (see figure below) (see also [86]).



PROOT performance improvement. Left: Dependence of the acceleration coefficient on the number of events; Right: Ibid., on the number of threads [50]

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

2.2.1. *New perspectives to future development of the GEANT4 package* [51].

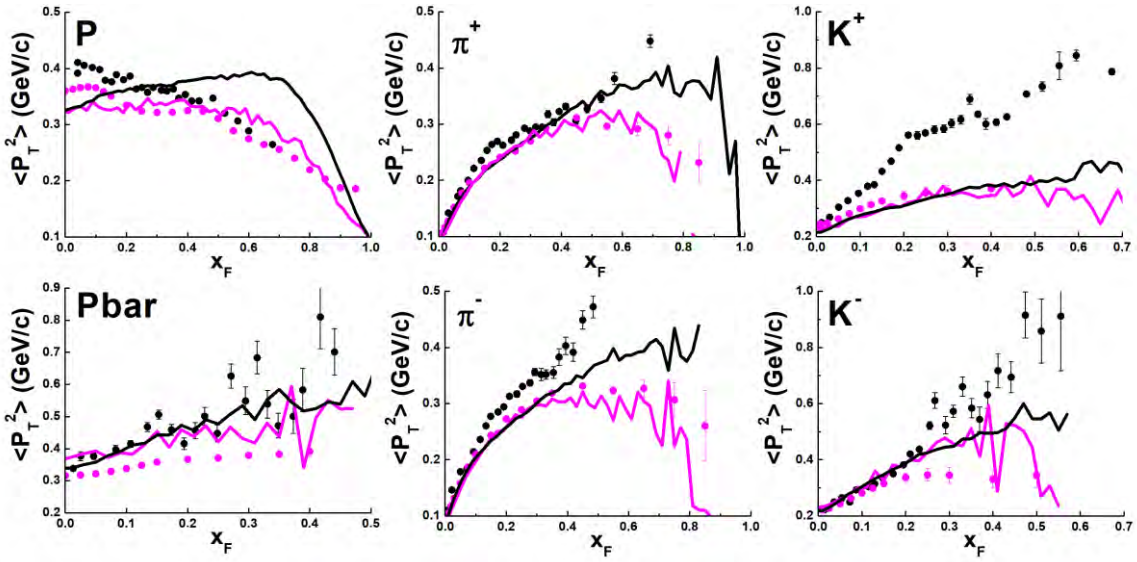
Geant4, the leading detector simulation toolkit used in high energy physics, employs a set of physics models to simulate interactions of particles with matter across a wide range of energies. These models, especially the hadronic ones, rely largely on directly measured cross-sections and inclusive characteristics, and use physically motivated parameters. However, they generally aim to cover a broad range of possible simulation tasks and may not always be optimized for a particular process or a given material. The Geant4 collaboration recently made many parameters of the models accessible via a configuration interface. This opens a possibility to fit simulated distributions to the thin target experimental datasets and extract optimal values of the model parameters and the associated uncertainties. Such efforts are currently undertaken by the Geant4

collaboration with the goal of offering alternative sets of model parameters, also known as "tunes", for certain applications. The effort should subsequently lead to more accurate estimates of the systematic errors in physics measurements given the detector simulation role in performing the physics measurements. Results of the study are presented to illustrate how Geant4 model parameters can be optimized through applying fitting techniques, to improve the agreement between the Geant4 and the experimental data.

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

► **General prospects on Geant4 future** [52, 53].

• **A new method** [52] for studying two-particle transverse momentum (P_T) correlations in soft hadronic interactions is proposed. It is shown that Monte Carlo models: PYTHIA 6 and Geant4 FTF (FRITIOF), give different predictions for the correlations in proton–proton interactions. The correlations are connected with Schwinger's mechanism of particle creation. These correlations can be studied in current and future experiments in high energy physics, in particular, at the Nuclotron-based Ion Collider fAcility (NICA).

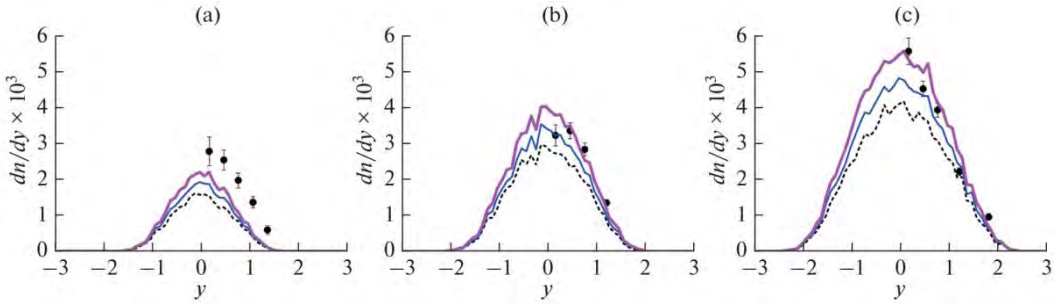


Average P^2_T of $\pi^{\pm}$, $K^{\pm}$, proton and anti-proton as a function of x_F. The points are experimental data without systematic errors at P_{lab} = 158 (magenta points) and 400 GeV/c (black points). The magenta and black curves are Geant4 FTF model calculations at P_{lab} = 158 and 400 GeV/c, respectively (Figure 2 [52])

• **On the future use of Geant4 package at Future Circular Collider experiments** [53]. It is expected that charmed particles will be copiously produced at Future Circular Collider (FCC). Due to relatively long lifetimes of the particles, it will be necessary to consider their interactions with the surrounding materials and materials of the detector. To satisfy these requirements, charmed particle production in soft interactions is studied using the QGS and FTF models of the Geant4 package. Details of these studies are considered in this work.

► **Geant4 FTF model description of the NA61/SHINE collaboration data** [54, 55].

• The latest data of the NA61/SHINE collaboration on the production of Ξ^- and anti-Ξ^+ hyperons in *pp* interactions at P_{lab} = 40–158 GeV/c and inclusive distributions of K^{*0} and ϕ mesons are considered. As was shown in earlier experimental works, Monte Carlo models EPOS 1.99, UrQMD 3.4, and Pythia 6, cannot adequately describe the data. In this work, the yields of particles are analyzed using the Geant4 FTF model and a good description of experimental data is obtained.



Rapidity distributions, *dn/dy,* of ϕ mesons for three beam momenta (40, 80, and 158 GeV/*c*, (a), (b) and (c), respectively). Dots are the data measured by the NA61/SHINE collaboration with statistical errors only. Predictions of the Geant4 FTF model with P_{Vec} = 0.5, 0.6 and 0.7 (for ϕ mesons only) are shown by the dashed line and the thin and thick solid lines, respectively [54]

• It is shown [55] that FTF (FRITIOF) model, used in the Geant4 toolkit for simulations of hadron-hadron, hadron-nucleus and nucleus-nucleus interactions at high energies, describes well the NA61/SHINE collaboration data on π^- meson distributions in ^{40}Ar + ^{45}Sc interactions with centralities 0–5% at $\sqrt{s_{NN}}$ = 5.2, 6.1, 7.6, and 8.8 GeV. At higher energies, $\sqrt{s_{NN}}$ = 11.9 and 16.8 GeV, the model underestimates the experimental data. This is considered as an indication of the formation of the quark-gluon plasma at higher energies in the central collisions of light and intermediate nuclei than in collisions of heavy nuclei ($\sqrt{s_{NN}} \sim 6$ GeV). At the moment, simulations of the hard parton-parton scatterings and the formation of the quark-gluon plasma are not included in the Geant4 FTF model.

► **Data analysis and modeling for the TAIGA experiment** [56–61].

The background from cosmic protons has been simulated for a simplified model of the OLVE-HERO detector using Geant4. The energy thresholds for various cosmic particles were estimated.

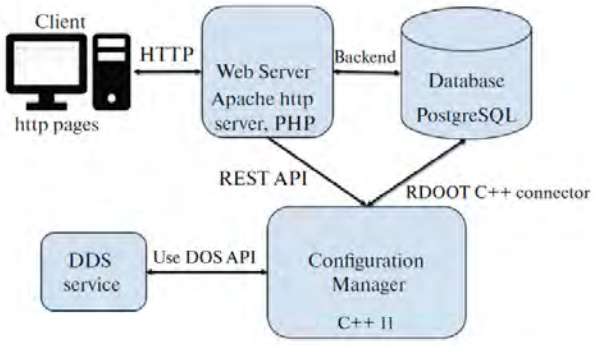
A machine learning model based on a multilayer perceptron was trained and tested for the task of separating hadrons and gamma rays in the TAIGA experiment.

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.

► **The Configuration Information System** (CIS) [62, 63] 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

► ***Excerpts of the work done and results published in* 2023**:

• 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) [64]. At the same time, the Baryonic Matter at Nuclotron (BM@N) experimental setup is completing its configuration to investigate relativistic heavy-ion beam interactions with fixed targets. One of the most important experimental tasks of the BM@N physics program is determination of the equation of state of the high-density baryonic matter. This task can be accomplished via measurements of the (multi)strange hyperon excitation functions, i.e. hyperon yields at different energies, and the collective flows of hadrons. In this paper, the results of the Monte Carlo simulation of the BM@N detector performance for studying strangeness production in heavy-ion interactions are presented.

• **Modeling a Track Detector based on the three-stage GEM chambers** [65]. Stages and aspects of modeling the formation of signal responses are considered for a detector based on the three-stage gas electron multiplier (GEM) used in the track system of the BM@N experiment to plan the first physics session in 2022. The procedure for calculating a map of the electrostatic field in the gas medium of the GEM chamber is described, along with the current parameters required for detailed modeling with the appropriate software tools.

• **The procedure of reconstruction for coordinate detectors of SRC setup** at BM@N was developed for both simulated and experimental data measured in 2018. Multiwire proportional chambers and silicon detectors were located upstream of the analyzing magnet at the SRC at BM@N setup. The developed algorithms were added to the official software. The reconstruction results were compared with the simulation. The main characteristics of the coordinate detectors upstream the analyzing magnet were evaluated and analyzed [66].

• **First physics results of the BM@N experiment** at the Nuclotron/NICA complex are presented on π^+ and K^+ meson production in interactions of an argon beam with fixed targets of C, Al, Cu, Sn and Pb at 3.2 AGeV. Transverse momentum distributions, rapidity spectra and multiplicities of π^+ and K^+ mesons are measured. The results are compared with predictions of theoretical models and with other measurements at lower energies [67].

• **Status of different software developments have been presented at devoted BM@N Collaboration meetings** [68–70].

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

► **Modern analysis framework for the MPD experiment at NICA** [71]. The latest achievements have been presented at the 25th International Baldin Seminar, September 18 – 23, 2023. They involve: Online Visualization of MPD experiment; Offline Software; MPDRoot Framework; Codebase Revamp; QA Engine; MPD Data Lab; Diagnostics & Rapid Development.

2.3.4. *Software support at JINR-NICA*: SPD experiment

► **Development of a specialized computing system and middleware complex: SPD OnLine Filter**. This fundamental task for successful implementation of the SPD experiment, is under active development. Reports have been made at the 10-th International Conference GRID'2023, among others. In the MLIT Scientific Seminar on 20.12.2023, D. Oleynik made a coprehensive presentation of this topic [72]. The general architecture of the software package has been defined, which includes three main systems: a control system of data handling processes, a data management system, and a load management system. Each of the systems is implemented as a set of problem-oriented microservices. Initial prototyping of each of the systems was carried out,

interfaces were determined both between microservices and between subsystems. The primary requirements for the hardware infrastructure of the computing complex have been determined.

► **Distributed Storage and Computing Environment for the SPD Experiment**. This fundamental task for successful implementation of the SPD experiment, is under active development. Reports have been made at the 10-th International Conference GRID'2023, among others. In the MLIT Scientific Seminar on 20.12.2023, A. Petrosyan made a coprehensive presentation of this topic [73]. The SPD facility, being under construction at the NICA collider, will generate large data streams, which, after initial filtering, will need to be stored and processed. Given the expected amount of this data, both JINR resources and external resources provided by the collaboration participants are supposed to be used in organizing storage and processing. The report presents the status of work on the organization of the distributed storage and processing environment of SPD experiment data.

► **Addressing Difficult Data Analysis Topics in the SPD NICA Experiment.** The following four references, [74–77], prepared under the supervision of Prof. G.A. Ososkov, address several topics expected to be critical for the success of the SPD experiment.

• **Efficient Elimination of False Track Filtering Issues** [74]. This paper introduces methods for parallelizing the algorithm to enhance the efficiency of event recovery in Spin Physics Detector (SPD) experiments at the Nuclotron-based Ion Collider Facility (NICA). The problem of eliminating false tracks during the particle trajectory detection process remains a crucial challenge in overcoming performance bottlenecks in processing collider data generated in high volumes and at a fast pace. In this paper, we propose and show fast parallel false track elimination methods based on the introduced criterion of a clustering-based thresholding approach with a chi-squared quality-of-fit metric. The proposed strategy achieves a good trade-off between the effectiveness of track reconstruction and the pace of execution on today's advanced multicore computers. To facilitate this, a quality benchmark for reconstruction is established, using the root mean square (rms) error of spiral and polynomial fitting for the datasets identified as the subsequent track candidate by the neural network. Choosing the right benchmark enables us to maintain the recall and precision indicators of the neural network track recognition performance at a level that is satisfactory to physicists, even though these metrics will inevitably decline as the data noise increases. Moreover, it has been possible to improve the processing speed of the complete program pipeline by 6 times through parallelization of the algorithm, achieving a rate of 2000 events per second, even when handling extremely noisy input data.

• The paper [75] presents an application of the TrackNET model to the simulated data of the SPD tracker and preliminary results of the performance study.

2.3.5. *Software support at LHC:* CMS experiment

► ***Excerpts of the work done and results published in* 2023**

► **New physics following from CMS experimental data**. The meaning of the output of the CMS experiment done at LHC, in which the JINR scientists play a key role, is far from been exhausted by the straightforward analysis of the raw data. The following four papers explore new perspectives toward a new physics [78–81].

2.3.6. *Software support at LHC:* ATLAS experiment

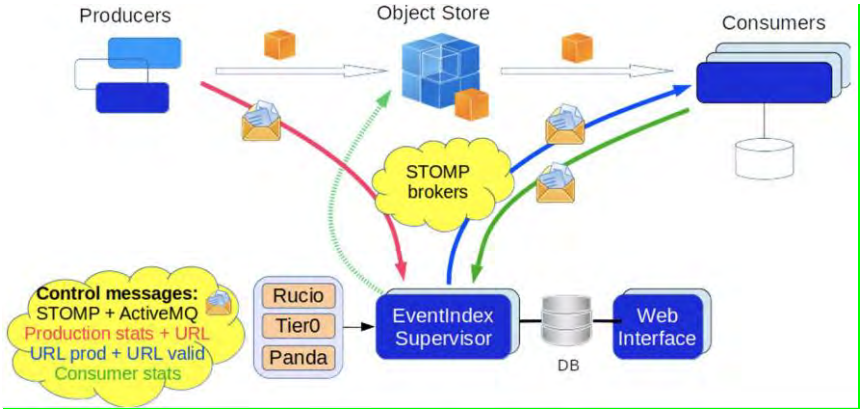
Developments are done within three ATLAS projects, which will be active till 2024.

• **The tasks resolved during 2023 within the ATLAS experiment included** [82]**:**

- **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.
  The CREST project is a new realization of the conditions DB with the REST API and JSON support for the ATLAS experiment. This project allows to simplify the conditions data structure and to optimize the data access. The CREST development requires not only the client C++ library (CrestApi) but also the various tools for testing software and validating data. A command line client realizes a quick access to the stored data. A set of the utilities was used to make a dump of the data from CREST to the file system and to test the client library and the CREST server using the dummy data. Now CREST software is being tested using the real conditions data converted with the COOL to CREST converter. The Athena code (ATLAS event processing software framework) was modified to operate with the new conditions data source [83].
- **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 [82]

2.3.7. *Software support at FAIR:* PANDA experiment

- **Hyperon signatures in the PANDA experiment at FAIR** [84].

2.4. Computational support of JINR projects in radiobiology

A joint MLIT-LRB group (leader O. Streltsova) has designed and implemented a dedicated information system 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–computational system for the BIOHLIT project** comprised:

A prototype of a web service for the "Morris Water Maze" behavioral test was developed, intended to generate a data set for the task of classifying the trajectories of laboratory animals.

An algorithm was developed for tracking laboratory animals in the "Morris Water Maze" behavioral test based on computer vision methods.

Preliminary results on the classification of trajectories based on a convolutional neural network were obtained, which showed the need to both expand the training set and to represent trajectories with characteristic labels.

The prototype of a web service has been developed for the “Open Field” behavioral test, the functionality of which allows solving the problem of tracking a laboratory animal, build a heat map, count the sectors covered and provide the user with summary analytics.

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 most demanded IBR-2 detector, YuMO.

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.

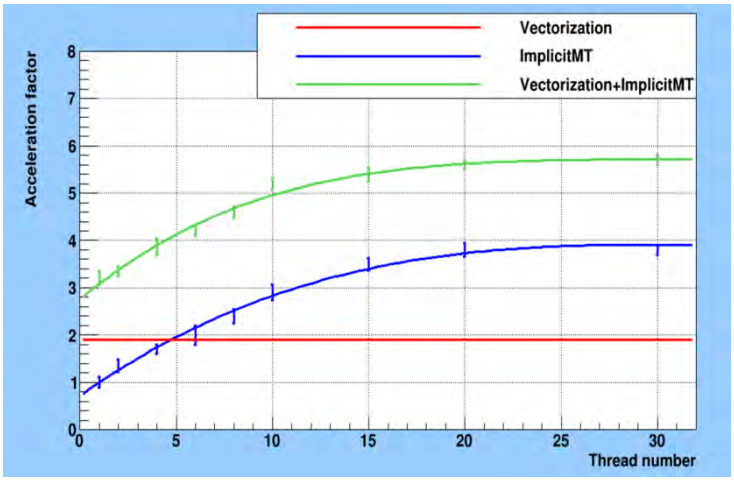
► **The Modernization of the Software for Fitting the Data of the Small-Angle Neutron Scattering Spectrometer YuMO at IBR-2**, is done through the development of a web application.

• **FITTER_WEB** **FITTER_WEB** (http://wwwinfo.jinr.ru/programs/jinrlib/fitter_web/indexe.html) A program for fitting data obtained on a small-angle neutron scattering spectrometer, implemented as a Web application. Version 2.0 [Date of implementation 08.12.2023; Authors: A.G. Soloviev, T.M. Solovjeva]. The FITTER_WEB application is available at http://fitter.jinr.ru.

The FITTER_WEB program is designed to fit experimental data with a selected theoretical multiparameter function. The program uses JSROOT - graphics and ROOT I/O system written in JavaScript, and HttpServer. A special feature of the FITTER_WEB program is the fitting using the resolution function. It implements theoretical SANS models, in which the shape of particles is approximated by simple geometric bodies - balls, ellipsoids, cylinders, prisms. It is taken into account that the molecules of one polymer sample have different molecular weights and sizes that is, they represent a polydisperse system.

• A first paper reporting the FITTER_WEB use is [85].

• A second paper devoted to the new FITTER_WEB use is [86]. The discussed verson 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.



Dependence of the acceleration coefficient on the number of threads [86]

► **Software simulation of condensed matter data** [87]. In this study, neutron diffraction was performed using the time-of-flight technique in the IBR-2M research reactor. The obtained data were refined with the FULLPROF Rietveld suite. The results are different from those obtained from X-Ray diffraction.

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. Instances of the progress obtained during 2023 was reported in [88–92].

- The first observation of the diffuse cosmic neutrino flux with the Baikal-GVD neutrino telescope was reported in [88]. Using cascadelike events collected by Baikal-GVD in 2018–2021, a significant excess of events over the expected atmospheric background is observed. This excess is consistent with the high-energy diffuse cosmic neutrino flux observed by IceCube.
- An analysis of an observed triplet of neutrino candidate events in the Galactic plane is presented, focusing on its potential connection with certain Galactic sources. The coincidence of cascades with several bright and flaring blazars is discussed [89].
- The muons form through the exchange of W-bosons in the interaction between muon- and partial tau-neutrinos near the Baikal-GVD telescope. The muons then propagate to great distances in the lake water. Reconstructing their trajectory allows us to obtain the most accurate estimate of the direction of neutrinos at telescopes of this type. Angular resolution can be as good as 0.5° for fairly long muon tracks. The current state of affairs in analyzing track events at the Baikal-GVD is discussed [90].
- Since 2020, Baikal-GVD has been monitoring IceCube telescope alerts about detecting neutrinos with energies of more than 100 TeV. Results of searching for matches between Baikal-GVD events and IceCube neutrino alerts from September 2020 to April 2022 are presented [91].
- Events from muon neutrinos were identified, the flux of which is consistent with the expectation for the flux of atmospheric neutrinos. The data obtained during the alerts of the ANTARES and IceCube telescopes were analyzed. Candidate events for high-energy neutrinos of astrophysical origin have been obtained [92].

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

- **Review of the some specific features of the detecting of heavy recoils** [93]. Results of the first beam tests of the detection system at the focal plane of the Dubna Gas-Filled Recoil Separator-2 (DGFRS-2), which receives beams from the DC-280 FLNR cyclotron, are discussed.

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 facility 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).

During 2023, the development of the HybriLIT Heterogeneous Computing Platform was continued. The ML/DL/HPC ecosystem was expanded, a testing ground for quantum computing was deployed using the Jupyter platform, platform users were supported and software was updated. The ML/DL/HPC ecosystem is now actively used for machine and deep learning tasks. At the same time, the accumulated tools and libraries can be more widely used for scientific research, including: numerical computations, parallel computing on CPUs and GPUs, visualization of results, accompanying them with the necessary formulas and explanations.

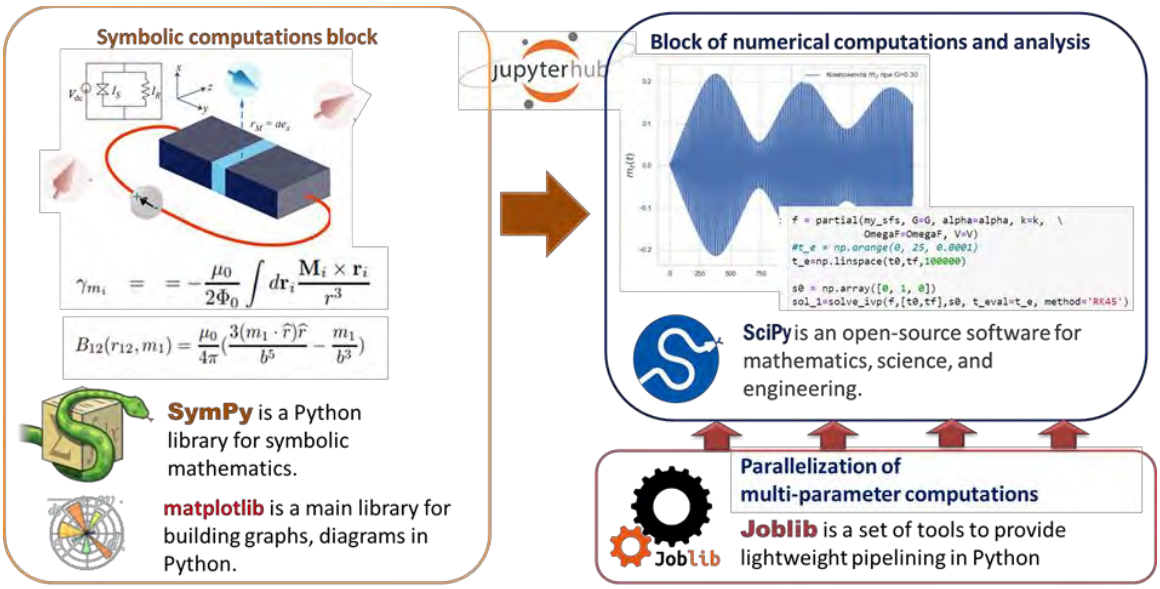
The developments followed three main directions: HPClab component; Computational component; Educational component. An older description of the HybriLIT status was done in [94], while the most recent one is given in the [95].

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 online organization of calculations and scientific visualization** resulted in an ecosystem for modeling the dynamics of a Josephson junction under the influence of external radiation using Python in the Jupyter book environment. Algorithms have been developed to calculate the current-voltage characteristic of a Josephson junction under the influence of external radiation and to calculate the dependence of the width of the Shapiro step on the amplitude. A parallel algorithm for the problem under consideration was implemented using the Joblib library and the efficiency of parallel computing was analyzed. The implementation is available online [96].

► **The investigation of the dynamics of the magnetization in a Josephson ϕ_0-junction on top of Jupyter Book** [97]. 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 [97]

• **A Python based numerical solution** of the calculation of the current-voltage characteristics for the long Josephson junction (LJJ) stack model with inductive and capacitive coupling is considered [98]. From a computational point of view, the problem is reduced to the numerical solution of an initial-boundary value problem for a system of nonlinear differential equations in partial derivatives for different intensities of the electric current. The study is based on the ML/DL/HPC ecosystem of the heterogeneous HybriLIT platform.

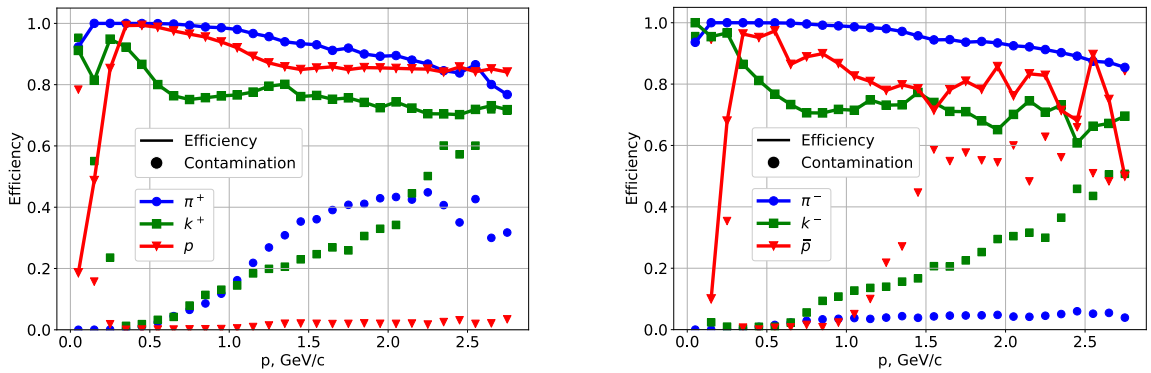
• **Computational environment for mathematical modeling of superconducting nanostructures** was reported in [99].

3.2.2. *Machine learning based solutions for JINR experiments*

► Machine learning on high-performance computing infrastructures at JINR

• **Event reconstruction in GEM detectors** [100]. To solve the problem of the reconstruction of charged particle trajectories in tracking detectors, two neural network algorithms, based on deep learning architectures for track recognition in pixel and strip-based particle detectors, have been developed. These are TrackNETv3 for local (track by track) and RDGraphNet for global (all tracks in an event) tracking. These algorithms were tested using the GEM tracker of the BM@N experiment at JINR (Dubna) and the cylindrical GEM inner tracker of the BESIII experiment at IHEP CAS (Beijing). The RDGraphNet model, based on a reverse directed graph, showed encouraging results: 95% recall and 74% precision for track finding. The TrackNETv3 model demonstrated a recall value of 95% and 76% precision. This result can be improved after further model optimization.

• **CatBoost particle identification in MPD experiment** [101]. The first tests have been achieved of a machine learning application using gradient boosting on oblivious decision trees to particle identification in MPD experiment at NICA. Categorical boosting (CatBoost) implementation of a gradient boosting on decision trees has been used. Particle identification is based on the information provided by the time projection chamber (TPC) and the time-of-flight (TOF) subdetectors. Three different Monte-Carlo datasets of measurements from TPC and TOF were simulated and used within CatBoost classifiers training and testing. A comparison was made with the n-sigma method, which is currently used in MPD software. The gradient boosting shows better efficiency at small and large momentum values ($p < 0.7$ GeV/c and $p > 1.5$ GeV/c). This demonstrated that machine-learning methods are well suited to address the particle identification problem in the MPD experiment.



Efficiency and contamination of a classifier based on the CatBoost library (on the right for particles, on the left for antiparticles) [101]

• **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 [102].

• **AI modeling for Agriculture tasks** [103]. According to the Food and Agriculture Organization, the world's food production needs to increase by 70 percent by 2050 to feed the growing population. However, the EU agricultural workforce has declined by 35% over the last decade, and 54% of agriculture companies have cited a shortage of staff as their main challenge. These factors, among others, have led to an increased interest in advanced technologies in agriculture, such as IoT, sensors, robots, unmanned aerial vehicles (UAVs), digitalization, and artificial intelligence (AI). Artificial intelligence and machine learning have proven valuable for many agriculture tasks, including problem detection, crop health monitoring, yield prediction, price forecasting, yield mapping, pesticide, and fertilizer usage optimization. In this scoping mini review, scientific achievements regarding the main directions of agricultural technologies are explored. Successful commercial companies, both in the Russian and international markets, that have effectively applied these technologies will be highlighted. Additionally, a concise overview of various AI approaches is presented, and our firsthand experience in this field is shared.

3.3. HybriLIT/GOVORUN implementation of efficient numerical methods for hardly solvable problems

► **Modeling single ionization of helium by protons** [104]**.** The parabolic quasi-Sturmian approach, recently introduced for the calculation of ion–atom ionizing collisions, is adapted and applied here to the single ionization of helium induced by an intermediate-energy proton impact. Within the method, the ionization amplitude is represented as the sum of the products of the basis amplitudes associated with the asymptotic behavior of the continuum states of the two noninteracting hydrogenic subsystems (e-, He+) and (p+, He+). The p–e interaction is treated as a perturbation in the Lippmann–Schwinger-type (LS) equation for the three-body system (e-, He+, p+). This LS equation is solved numerically using separable expansions for the proton–electron potential. We examine the convergence behavior of the transition amplitude expansion as the number of terms in the representation of the p–e interaction is increased and find that, for some kinematic regimes, the convergence is poor. This difficulty, which is absent for a higher proton energy impact, is solved by varying the momentum of the auxiliary proton plane wave introduced into the basis function. Fully differential cross-sections are calculated and compared with experimental data for 75 keV protons and the results obtained with the 3C model

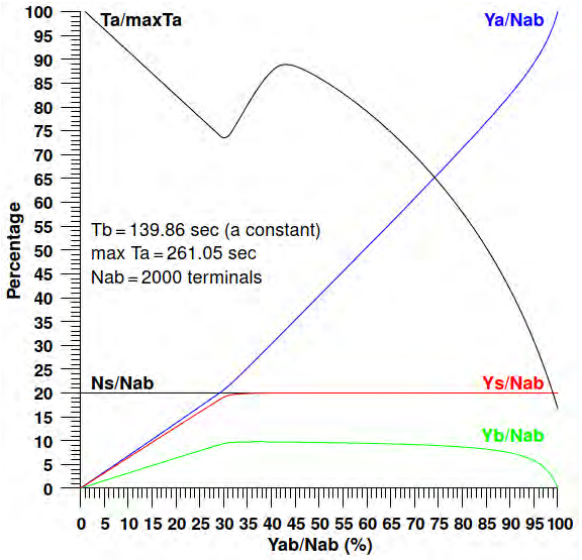
► **MAPLE algorithm for solving the scattering problem** [105]. We present an original algorithm in the MAPLE system for solving the scattering problem in single-channel approximation of the coupled-channel method of the optical model (OM) described by a second-order ordinary differential equation (ODE) with a complex-valued potential and regular boundary conditions. The complex-valued potential consists of the known real part, which is a sum of the nuclear potential, the Coulomb potential, and the centrifugal potential, and the imaginary part, which is a product of the unknown coupling constant $g(E)$, depending on the collision energy E of a pair of ions, and the derivative of the real part of the known nuclear potential with respect to the ODE independent variable.

► **High-performance calculations of physical observables in spintronics** [106]. The periodic structure of the magnetization reversal (MR) domains is studied within the superconductor–ferromagnetic–superconductor ϕ_0-junction model. The model is described by the Cauchy problem for the system of nonlinear ordinary equations which is numerically solved by means of the 2-step Gauss–Legendre method. Two versions of parallel implementation on the basis of MPI and OpenMP techniques have been developed. Efficiency of both versions is confirmed by test

calculations. The effect of the frequency of the ferromagnetic resonance on the configuration MR domains has been investigated. The calculations have been performed at the HybriLIT Platform of the JINR Multifunctional information and computing complex.

► **Round off error growth estimation in stacks of long Josephson junctions for the Cauchy problems in the uniform l_1 metric** [107]. 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.

► **Assessing the FIFO quality of service of telecommunication system** [108]. In the present paper, arising in a collaboration with Bulgarian colleagues, a method for solving the system of equations with respect to certain dynamic parameters is proposed with the aim at modeling the quality of service in an overall telecommunication system including users and a queuing system with FIFO (first in, first out) discipline.



The average duration of occupation of an A-terminal (Ta), traffic at A-terminals (Ya) and B-terminals (Yb), as well as the switching system traffic (Ys) for a network with queuing with Nab = 2000 terminals and Ns = 400 equivalent connections lines (20% of Nab) [108]

3.4. Progress in Big Data analytics and Artificial Intelligence

• **A simple journal adviser for scientific articles** [109]. A prototype recommendation system for effective scientific information management in the era of big data is presented. Using metadata and keyword filtering, the system is designed to help researchers select the most appropriate journal for publication by analyzing factors such as the number of citations and publication dates. A thematic list of the most significant scientific sources is compiled. The prototype uses machine-learning algorithms to produce accurate and personalized journal recommendations, improving the search for scientific information and increasing the influence of a researcher in the scientific community by publishing articles in the most relevant journals.

• **Results of the development of methods for comparing higher education programs and the needs of the labor market** [110, 111]. Methods were developed by the authors as part of the implementation of an analytical platform for automated monitoring of the labor market and intelligent analysis of personnel against university specialties. Texts of titles, levels of development and indicators of IT-profile competence achievement, as well as vector language models with various architectures and training text bodies were used for the analysis. The results

are mutually compared and the stability of the methods of matching educational competencies and the needs of the labor market is shown.

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

► Solutions of difficult problems of computer algebra

• **Methods for the calculation of one-loop Feynman integrals** [112]. The method for functional reduction of Feynman integrals, proposed by the author, is used to calculate one-loop integrals corresponding to diagrams with four external lines. The integrals that emerge from amplitudes for the scattering of light-by-light, the photon splitting in an external field and Delbrück scattering are considered. For master integrals in d-dimensions, new analytic results are presented. For d = 4, these integrals are given by compact expressions in terms of logarithms and dilogarithms.

► Solutions of problems related to quantum information

• **Constructive models for the description of finite quantum systems** [113]. Mathematical formulation of Bohr's complementarity principle leads to the concepts of mutually unbiased bases in Hilbert spaces and complementary quantum observables. In this paper, we consider algebraic structures associated with these concepts and their applications to constructive quantum mechanics. We also briefly discuss some computer-algebraic approaches to the problems under consideration and propose an algorithm for solving one of them.

• **Constructive versions of Quantum Mechanics** [114]. The standard formulation of quantum mechanics is essentially nonconstructive, since it is based on continuous unitary groups and number fields R and C. This descriptive flaw does not allow one to study some fine details of the structure of quantum systems and sometimes leads to artifacts. Modern problems of quantum physics and quantum informatics require a detailed analysis of the "fine structure" of quantum systems, which cannot be carried out using traditional approximate methods of quantum mechanics. We consider a modification of quantum mechanics based on permutation representations of finite groups in Hilbert spaces over cyclotomic fields.

• **Description of evolution of finite quantum systems by permutation groups** [115]. Two constructive approaches to quantum theory are considered: quantum mechanics based on permutation representations of finite groups, and quantum mechanics of a finite Weyl–Schwinger phase space. We show that both approaches converge to the conclusion that, at a deep level, the quantum evolution is based on permutations of finite sets.

• **Extension of Stratonovich-Weil axioms in Quantum Mechanics** [116]. The statistical model of quantum mechanics is based on the mapping between operators on the Hilbert space and functions on the phase space. This map can be implemented by an operator that satisfies physically motivated Stratonovich-Weyl axioms. Arguments are given in favour of a certain extension of the axioms, provided that there is a priori knowledge about the composite nature of the quantum system.

• **Interrelation between classicality/quantumness and symmetry of states** [117]. Within the phase-space formulation of finite-dimensional quantum systems the interrelation between classicality/quantumness and symmetry of states is pointed out. The argumentation is given that quantum states ordered with respect to their "symmetry" exhibit also the ordering with respect to their "classicality" in a way that can be formulated as: the larger symmetry quantum states possess, the more classical they are.

► **Nonequilibrium Bose systems of trapped atoms and their properties** [118]. **The review** presents the methods of generation of nonlinear coherent excitations in strongly nonequilibrium Bose-condensed systems of trapped atoms and their properties. Non-ground-state Bose–Einstein condensates are represented by nonlinear coherent modes. The principal difference of nonlinear coherent modes from linear collective excitations is emphasized. Methods of generating nonlinear modes and the properties of the latter are described. Matter-wave interferometry with coherent modes is discussed, including such effects as interference patterns, internal Josephson current, Rabi oscillations, Ramsey fringes, harmonic generation, and parametric conversion. Dynamic transition between mode-locked and mode-unlocked regimes is shown to be analogous to a phase transition. Atomic squeezing and entanglement in a lattice of condensed atomic clouds with coherent modes are considered. Nonequilibrium states of trapped Bose-condensed systems, starting from weakly nonequilibrium state, vortex state, vortex turbulence, droplet or grain turbulence, and wave turbulence, are classified by means of effective Fresnel and Mach numbers. The inverse Kibble–Zurek scenario is described. A method for the formation of directed beams from atom lasers is reported.

► **Two kinds of artificial intelligence decisions** [119]. The dynamics of affective decision making is considered for an intelligent network composed of agents with different types of memory: long-term and short-term memory. The consideration is based on probabilistic affective decision theory, which takes into account the rational utility of alternatives as well as the emotional alternative attractiveness. The objective of this paper is the comparison of two multistep operational algorithms of the intelligent network: one based on discrete dynamics and the other on continuous dynamics. By means of numerical analysis, it is shown that, depending on the network parameters, the characteristic probabilities for continuous and discrete operations can exhibit either close or drastically different behavior. Thus, depending on which algorithm is employed, either discrete or continuous, theoretical predictions can be rather different, which does not allow for a uniquely defined description of practical problems. This finding is important for understanding which of the algorithms is more appropriate for the correct analysis of decision-making tasks. A discussion is given, revealing that the discrete operation seems to be more realistic for describing intelligent networks as well as affective artificial intelligence.

► **Quantum Intelligent Control and Robotics**

The group working on this subject matter is perhaps the most proficient in MLIT. Instances of the reported results durin 2023 (*some of which will be published in* 2024) *are provided below.*

• Specific examples from robotics and self-organizing quantum controllers built into on-board control systems unveil the effectiveness and advantage of using intelligent control systems based on soft and quantum computing [120]. Quantum soft computing and quantum fuzzy inference are implemented on a classical processor and simulated on the Govorun supercomputer.

• The technology of knowledge extraction from a physically recorded learning signal using a genetic algorithm allows the formation of objective knowledge bases for fuzzy controllers of intelligent control systems [121]. A comparison of different types of control models based on the TANGO system is carried out. A method for optimal trajectories design as the gain coefficients schedule of the hybrid PID controller is presented. The effectiveness of the end-to-end information technologies application based on soft computing in intelligent control tasks is shown.

• The implementation of information technologies for the design of embedded intelligent control systems based on fuzzy logic, neural networks, genetic and quantum algorithms for the problem of nitrogen pressure stabilization in the cryogenic system of the test stand of the JINR VBLHEP magnet factory was done. The efficiency of the current control system with a built-in quantum controller implementing coordination control was demonstrated experimentally [122].

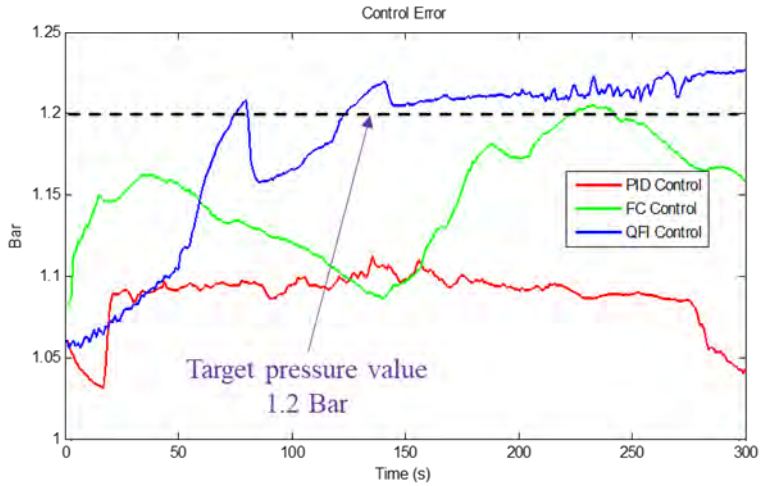
• The new applications of the previously developed quantum intelligent control technology require a significant increase of the number of input parameters. The possibility of implementing a thirty-qubit quantum fuzzy inference on a simulator with classical architecture is addressed. A quantum scheme is presented and the results of the operation of a quantum intelligent regulator for the robust control of the nitrogen flow in the cryogenic system of the booster measuring arm of the NICA accelerator complex are presented [123].

• The review paper [124] discusses the basics of the description and physical interpretation of quantum processes for IT specialists, developers of control systems and robotics, based on the concepts of classical stochastic mechanics and the theory of random processes, introducing additional concepts and their formalized representations, which follow from the accepted classical form, as necessary.

• The information technology approach to the design of a robust intelligent control system based on quantum fuzzy inference is discussed [125]. The application of the developed design methodology is based on quantum self-organization of imprecise knowledge bases of fuzzy controllers. The results of mathematical modeling and physical experiments are compared using the example of an autonomous robot in the form of an "inverted pendulum – moving carriage" system.

• A quantum fuzzy inference gate design provides prepared programmable algorithmic solutions for board embedded control systems. The possibility of neuro-interface application based on cognitive helmet with quantum fuzzy controller for vehicle driving is shown [126].

• **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 [127].



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)

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Details of proposal at: **04.11 Written Proposals**

PAC Recommendation:

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https://www.jinr.ru/wp-content/uploads/Advisory_Bodies/PAC/CMP/57/57_PAC_CMP_rus.pdf (с. 6)

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Details of proposal at: **08.1.MPE**; Oral presentation: **8.1.** S. Shmatov (Slides)

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