Overview of the Progress in the LIT Theme 1119 during 2019–2020

(Written Report)

Gheorghe Adam (LIT-JINR and IFIN-HH), on behalf of the theme leaders

• **Title of the theme:** 05-6-1119-2014/2023, "*Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data*"
Priority: 1
Leaders: Gheorghe Adam, Petr V. Zrelov
Deputies: Ján Buša, Ochbadrakh Chuluunbaatar
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.

• *Characteristics which single out the theme 1119 in the JINR Topical Plan of Research*

The *overwhelming feature* of the research done within the theme 1119 during the present Seven Year Plan for JINR Development is the *work done in close cooperation* with research groups from all JINR Laboratories and Member State institutions. This assumes the use of the existent expertise of the LIT staff for the solution of challenging problems, in over 40 JINR projects, which ask for advanced research in computational mathematics and physics, directed to the creation of new mathematical methods and algorithms for the numerical or symbolic-numerical solution of topics arising in experimental and theoretical physics studies, their implementation into software packages. This subject area includes a wide spectrum of investigations approved for completion in JINR within the seven year period 2017–2023 in high energy physics, nuclear physics, physics of condensed matter and of nanostructures, biophysics, information technologies, the solution of which is inseparable from the use of computing. Such subject matters of the outmost importance in JINR are the NICA project, the neutrino program, the superheavy and exotic nuclei physics, the IBR-2 neutron based investigations.

The large scale computing is done on the Multifunctional Information and Computing Complex (MICC), primarily on the HybriLIT heterogeneous computing platform (which involves the training and test cluster HybriLIT and the "Govorun" supercomputer) and on the emerging Big Data distributed infrastructure.

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

The Covid-19 pandemic forced us to change substantially, for a while, the form (place and style) of the scientific work. While over 90 percent of the LIT staff involved in the solution of the theme 1119 tasks were passed at work at the distance, the pace of the scientific effort remained at a high level. New forms of communication, like the scientific webinars, came to the first plan. Striking examples are the webinar held on 21-st April 2020 by Prof. V. V. Korenkov, leader of the

Big Data analytics within this theme and the 5-th Collaboration Meeting of the BM@N Experiments at the NICA Facility with significant participation from theme 1119 (seven reports).

• *Five kinds of achievements got within the theme 1119*

The research done within theme 1119 involves four activities which agglutinate the different subject matters solved: (a) Mathematical and computation methods for simulation of complex physical systems; (b) Software complexes and mathematical methods for processing and analysis of experimental data; (c) Numerical methods, algorithms and software for multicore and hybrid architectures and Big Data analytics; (d) Methods, algorithms and software of computer algebra and quantum computing.

The analysis of the progress got by the research done within these four activities identifies five kinds of achievements, which are detailed below:

(1) *Contributions to the advancement of the JINR research as a whole;*
(2) *Advances to the solution of cooperation tasks with JINR conducted research projects;*
(3) *Software packages implemented in general purpose computing libraries;*
(4) *Contributions to the JINR excellence in the worldwide research landscape;*
(5) *Grow up of the scientific competence in using the JINR computer tools.*

(1) *Contributions to the advancement of the JINR research as a whole*

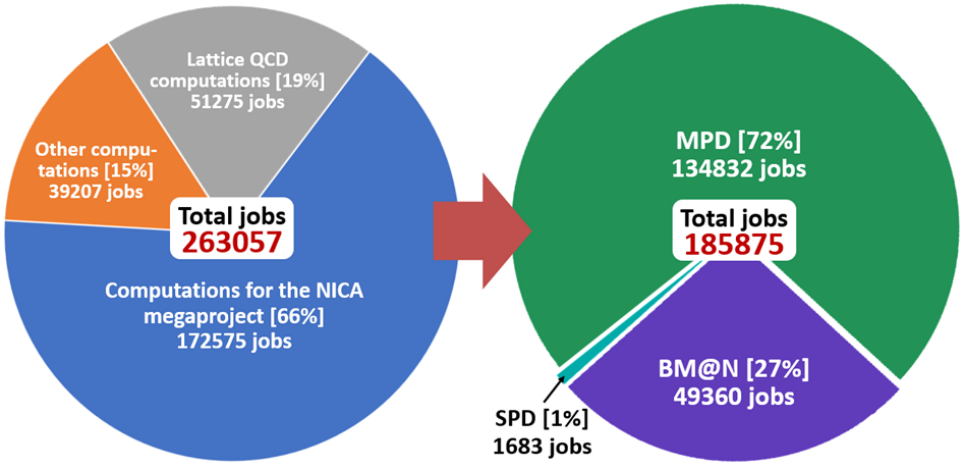
The staff involved in the theme 1119 brings its specific contribution along this direction in close cooperation with the staff engaged in the LIT theme 1118 (on JINR computing infrastructure) and its MICC (Multifunctional Information and Computing Complex) project. Our activity is focused on the development of mathematical methods, algorithms and software on the heterogeneous computing platform which involves the HybriLIT cluster (now learning and testing polygon) and the "Govorun" supercomputer (overseen by D. Podgainy and O. Streltsova) http://hlit.jinr.ru.

We solve specific tasks concerning the creation of ***basic software enhancing the availability and capabilities of the high performance computing* (HPC) *facilities, primarily the "Govorun" supercomputer, cornerstone of the JINR scientific computing.*** Through the three main components of the "Govorun" heterogeneous structure, applications are developed for HPC with distributed memory (in the CPU Intel Gold component – **SkyLake**), HPC with shared memory (in the CPU Intel Phi component – **KNL**), HPC and, especially, neural network methods based on machine learning and deep learning (in the GPU NVIDIA accelerator component – **DGX**). Computer programs using MPI, OpenMP, CUDA, OpenCL parallelization techniques are currently implemented on the "Govorun". Therefrom, the essential task resolved within theme 1119 concerns the *design, development, implementation, and maintenance on "Govorun" of a user friendly environment*. An ecosystem was created and is extended for the solution of ML/DL (Machine Learning / Deep Learning) tasks (see https://jhub2.jinr.ru for the computation component and https://jhub.jinr.ru for the development component). An HPC environment was also created for the development of parallel algorithms and applications, especially for the future experiments at the NICA facility [1].

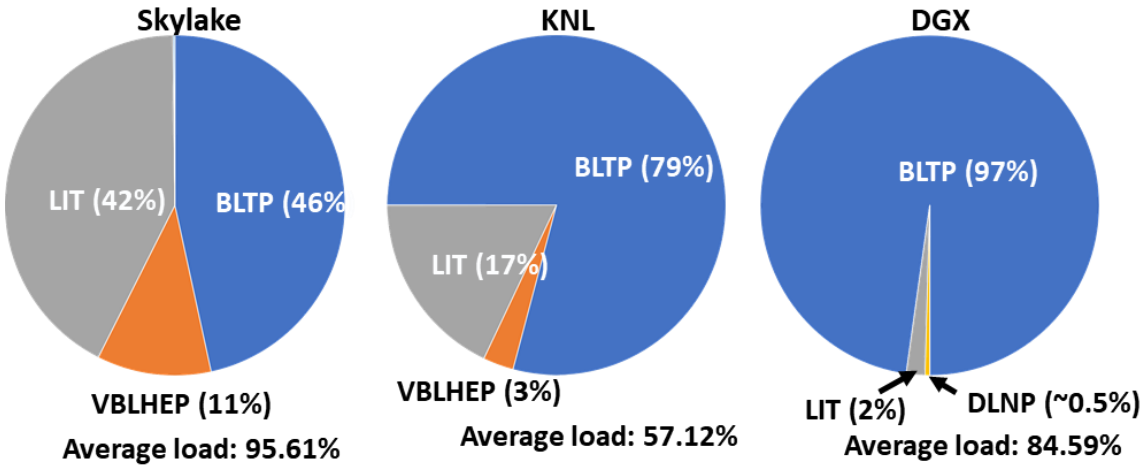
The operation of the first stage of the "Govorun" supercomputer made it possible to carry out resource-intensive computing in lattice quantum chromodynamics, improvement of the efficiency of modeling the dynamics of relativistic heavy ion collisions, the speed up of the event generation and reconstruction for the mega-science experiments of NICA project, to carry out calculations of the radiation safety of JINR experimental facilities, to significantly accelerate the research in the field of radiation biology and other scientific and applied problems. A number of 157 registered users made intensive HPC in the frame of the following 24 topics of the JINR Problem-Topical Plan: VBLHEP – 1065, 1066, 1087, 1088, 1097, 1107, 1108; BLTP – 1117, 1135, 1137, 1138; DLNP – 1099, 1100, 1123; FLNP – 1105, 1121, 1122, 1128; FLNR – 1129, 1130, 1131; LIT – 1118, 1119; LRB

– 1077. The results of these scientific studies have been published in more than fifty leading world scientific journals.

Statistics on the use of supercomputer components in different JINR projects (left) and the share of computations done for the NICA mega-science project are illustrated in this figure



Statistics of using all components of "Govorun" per partitions (06.2018 – 10.2019)



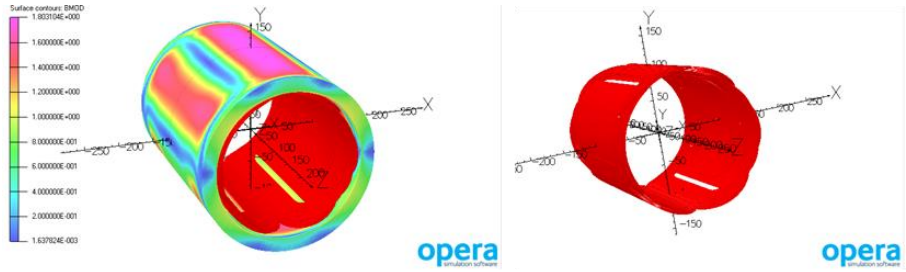
(2) *Advances to the solution of cooperation tasks with JINR conducted research projects*

This concerns the bulk of the activity done in cooperation for the solution of computing tasks raised by different research projects.

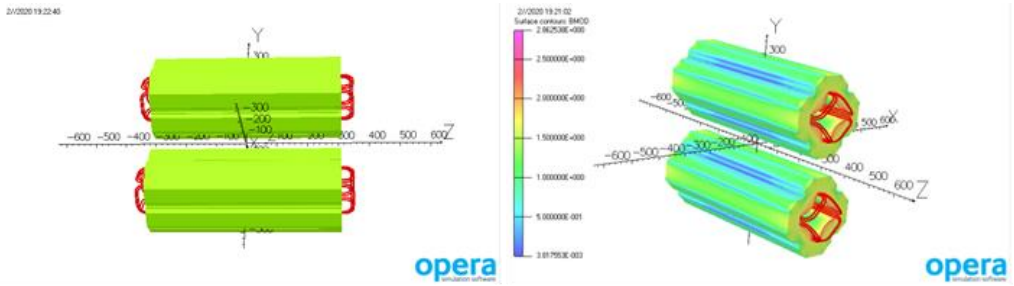
2.1. Selected results on magnetic field modeling

Intense current research involves ***three-dimensional computer simulation of magnetic systems*** *in the framework of NICA (JINR) and FAIR (GSI) projects for the validation of the magnetic field uniformity in the working areas of the new physical magnets* [2]*; case studies for the design of the magnet prototype of the future SPD setup at NICA* [3,4]*.; modeling the CBM 3D shielding dipole magnet at GSI to accommodate the modifications proposed in the conception of the CBM experiment in the options MUCH and RICH* [5–8]*; design of new medical purpose cyclotrons* [9].

• Instances of work done in 2020 in the framework of the NICA project for the 3D modeling of the collider multipole corrector and quadrupole magnet are given in the figures below where the magnet parameter influence on the field distributions in the magnet working areas is illustrated.

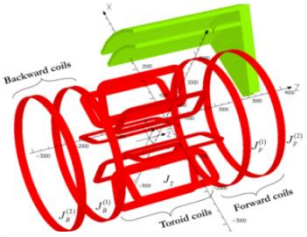


NICA Collider Multipole Corrector Modeling



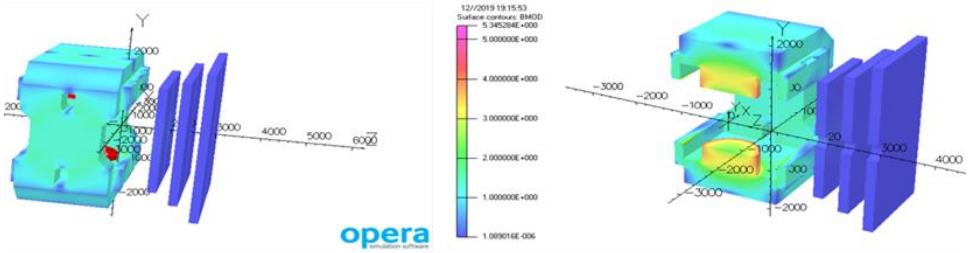
NICA Collider Quadrupole Modeling

• The 3D calculations for the SPD detector magnetic system of the NICA project are done in cooperation by researchers at JINR (Dubna) and Moscow State University. The figure at the right illustrates the basic "hybrid" configuration of the NICA SPD magnetic system which should be basic in further work.



"Hybrid" configuration

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



The CBM dipole magnet system modeling. MUON option

• **The development of discontinuous hp-adaptive schemes** with parallel algorithms of two-level domain decomposition methods enabled highly-precise 3D projection-grid solutions with proved convergence [10,11]. 3D computations for finding optimal configuration of a magnetic device with highly-uniform magnetic fields for experiments with neutrons were continued as part of the collaboration with co-workers from FLNP.

2.2. Progress in Big Data Analytics

Development of the concept and step-by-step implementation within the Big Data approach of a scalable software-analytical platform for the collection, storage, processing, analysis, retrieval

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

Particular attention is paid to new promising areas in the creation of distributed data warehouses (“Data Lake”), the integration of Big Data and supercomputer technologies, and “machine learning” methods. In 2019, a distributed prototype of a “lake of scientific data” was created based on centers in Dubna, Moscow and Gatchina [12]. Using the prototype, the cache system was tested using both synthetic tests and real-life LHC experiments.

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

In Big Data analytics, the mathematical and algorithmic support of information processing plays an important role. Within the framework of the theme, there are carried out research and development of methods such as dynamic quantum clustering, locality-sensitive hashing [13], mathematical methods for organizing computation chains, etc. The results are tested on the created prototype of the analytical platform.

2.3. Solving scientific problems investigated at experimental facilities

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.

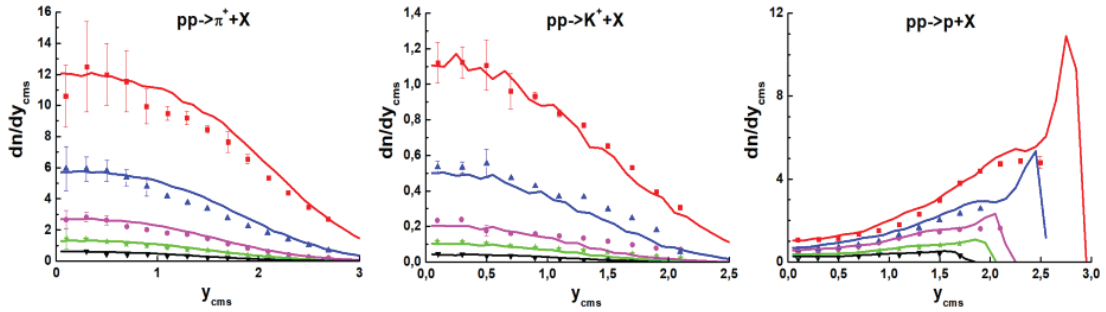
2.3.1. *Upgrade of the GEANT4 package with new modules*

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

- **UrQMD+SMM Modeling**. Parameters of the reactions p, d, He, C+C, Ta, and C+Ne, Cu at momenta of 4.2, 4.5, and 10 GeV/s per nucleon were calculated using the UrQMD model supplemented by the Multifragmentation Statistical Model (SMM). Azimuthal correlations of pions and protons produced in the listed reactions were calculated. Good agreement with

experimental data obtained in VBLHEP on the SKM-200-GIBS and Propane Bubble Chamber installations was achieved [14].

• **Study and development of Monte-Carlo event generators of hadron-nucleus and nucleus-nucleus interactions at high energies** were continued with proposals for the improvement of the HIJING (Heavy Ion Jet INteraction Generator) model. They allow describing experimental data by NA49 and NA61/SHINE collaborations on proton-proton interactions. The modified HIJING model was successfully used to the analysis of the STAR data on nucleus-nucleus collisions at high energies [15] (see figure below). It can be used in MPD and SPD experiments (NICA).



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

• **A model of nucleon coalescence in nucleus-nucleus interactions was implemented in the FTF model of the Geant4 package**. It allowed description of experimental data on properties of produced hadrons in Au+Au interactions at nucleon-nucleon collision center-of-mass energies below 7.7 GeV. This bears significance for the BM@N experiment (NICA).

• **For the first time, production of charmed quarks and hadrons in soft interactions was introduced in FTF and QGS models of the Geant4 package** to account for hard QCD processes at higher energies**.** This allowed description of main properties of D-mesons and Λ_c-hyperons in hadron-nucleus collisions at P_{lab} from 200 GeV/c up to 900 GeV/c. The work was performed in the framework of preparation program of experiments at future accelerator FCC proposed by LHC collaborations for transport and reconstruction of charmed particles. The results can be also used in NICA experiments [16].

2.3.2. *Software support of large scale experiments*

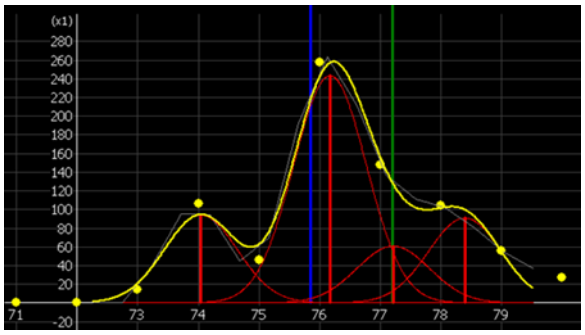
► ***Software support at LHC***: <u>CMS experiment</u>

• **MIP Timing Detector Project** planned for CMS during the High Luminosity LHC era [17].

• **CMSSW** – CMS SoftWare package modules [18]:

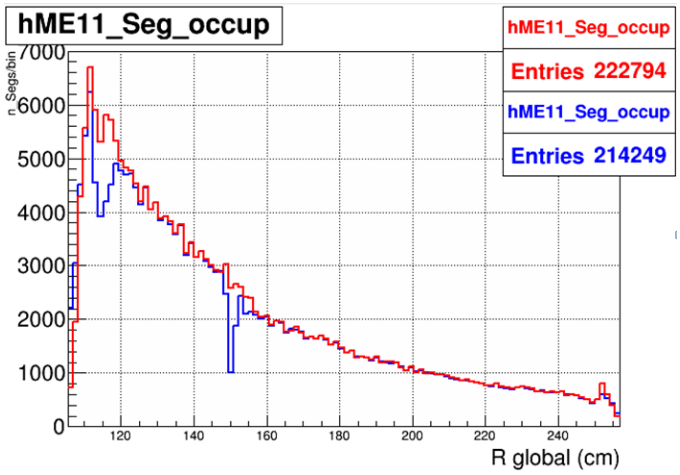
- CSCSegAlgoRU – Segment builder for Cathode-strip chambers of the CMS experiment;
- CSCHitFromStripOnly – delimitation of two overlapped signals;
- CSCRecHitDBuilder – handling of special ME11 chamber geometry

• The development of a new wavelet-based reconstruction algorithm for the strip coordinate was initiated [18] in order to improve the strip coordinate reconstruction for overlapping signals. It is able to separate with high accuracy up to 4 overlapping signals.



An example of the reconstruction of four overlapping signals on a single CSC layer. The green line is the simulated coordinate of the muon; yellow – the initial distribution of the signal; blue – coordinate restored by the standard algorithm; red – overlapping signals recognized by the proposed algorithm.

• The ME1/1 chamber has a special geometry. In connection with the electronics update, the algorithm for reconstructing the coordinates of the particle trajectory on a single layer was tuned. The figure below shows the frequency of segment reconstruction in the ME1/1 depending on the radial R-coordinate (distance to the beam axis) for the standard signal reconstruction algorithm (blue line) and the modified algorithm taking into account the peculiarities of the camera ME1/1 geometry (red line). As it can be seen from the figure, the inefficiency in the strip cut region (R ~ 150 cm) between the two parts of the ME1/1 chamber was eliminated.



Frequency of segment reconstruction in the ME1/1 chamber in terms of R-coordinate. The standard approach is the blue line; the modified approach is the red line.

► ***Software support at LHC***: ATLAS experiment

• Developments are done within three ATLAS projects:

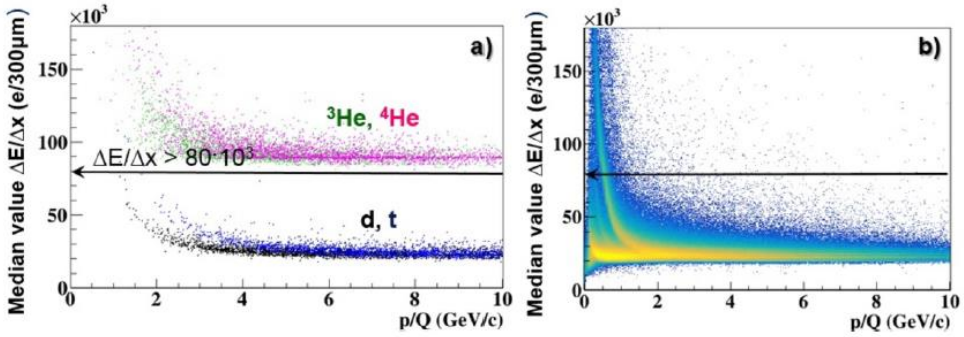
- **TDAQ,** members of CC control and configuration, monitoring groups
  - Improvements in Operational monitoring on users' requests;
  - Modernization of the data visualization service for the network traffic monitoring system in ATLAS (**NETIS**) produced [19].
- **Condition DB**
  - Development of software for converting COOL data to CREST data as part of the ConditionDB enhancement for RUN3 and the creation of Athena user libraries. The CREST server library was included in the official release of the offline ATLAS (Athena) system in December 2019. In 2020 work on creating a script to automatically convert the full amount of data to run the Athena q431 test development of a COOL to CREST conversion algorithm for a large number of IOVs channels and data for one directory. The current version of the algorithm in this case has problems with the amount of memory used. Other work underway: Transition of CrestApi library to the new version of CREST server; Adapting the library API for users; Creating a unit test for the library.
- **Event Index (EI3)** – EventIndex for LHC Run 3 [20]. Work done concerns:
  - Upgrades of a trigger information processing system for indexing in EventIndex for Monte-Carlo data.

- Solving the problems of users working with the EventIndex system (support for EventIndex production, together with F. Prokoshin, DLNP).
- Creation of test environment server for new Event Index prototype (in progress).

► ***Software support at FAIR***: CBM experiment

- **CBMROOT** – First version of "User Requirements Document of the Event Tag Geometry Database for the CBM experiment" is produced and updates based on users' feedback in progress [21,22].

• **The accurate measurement of the yield of hyper-nuclei and their lifetime** in the CBM (Compressed Baryonic Matter) experiment is based on the identification of their decay products including ^{3}He and ^{4}He. The possibility of heavy fragment identification using energy loss method in the STS detector was studied. The ω(k,n) criterion was successfully adapted for the separation of the doubly charged particles from singly charged. The combination of the energy loss method with the ω(k,n) criterion has shown high level of the background suppression without substantial signal loss. The combination of the information from the TOF and STS detectors allowed separating ^{3}He and ^{4}He from the deuteron background [23,24].



Median value ΔE/Δx dependences on the particle momentum for a) signal (^{3}He, ^{4}He), thermal deuterons and tritons and b) UrQMD tracks [23]

• **A simple and effective trigger option for detecting rare J/ψ →$\mu^+\mu^-$ events** in the CBM experiment has been proposed. For its implementation, only information recorded by the coordinate detectors of the MUCH station is required [25,26].

► ***Software support at FAIR:*** PANDA experiment – UrQMD+SMM modeling [27,28].

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

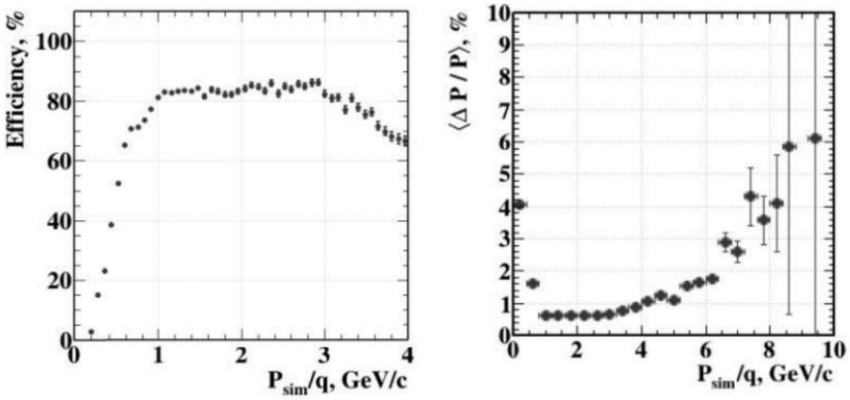
The fixed target BM@N experiment, implemented as part of the NICA-JINR complex, was conceived as a short cut to the more ambitious future fixed target CBM experiment at FAIR, which is being developed from scratch during a two decade slowly evolving process. The buildup of the BM@N setup followed a fast track consisting in the accommodation of a number of performant detectors developed for other international experiments the life cycle of which ended. Since BM@N operates at the already available Nuclotron energies, a primary concern was to assemble the existing detectors into a viable setup and to increase, as fast and as high as possible, the resolution of the resulting facility.

While an in-house team is doing the major part of the software development, the involvement of the LIT staff through theme 1119 into this process has brought very rapid and very high level solutions to a number of tasks, which are detailed below. It is to be stressed that the expertise of the LIT staff was successfully developed, was acknowledged and is in the continuation in high demand within the two large-scale high-energy projects, CMS at LHC and CBM at FAIR.

In the international online Joint JINR Colloquium Seminar "*The Transparent Nucleus: SRC and single nucleon knockout inverse kinematics measurements using a 48 GeV/c carbon beam at JINR*", held on 20 May 2020, Prof. Eli Piasetzky (Tel Aviv University, Israel) has reported the first relevant far reaching high precision physics experiment done at BM@N. At the end of his presentation,

Prof. Eli Piasetzky has explicitly acknowledged, by name and by task solved, the noticeable contribution of the theme 1119 LIT team which made possible this outstanding scientific result at BM@N.

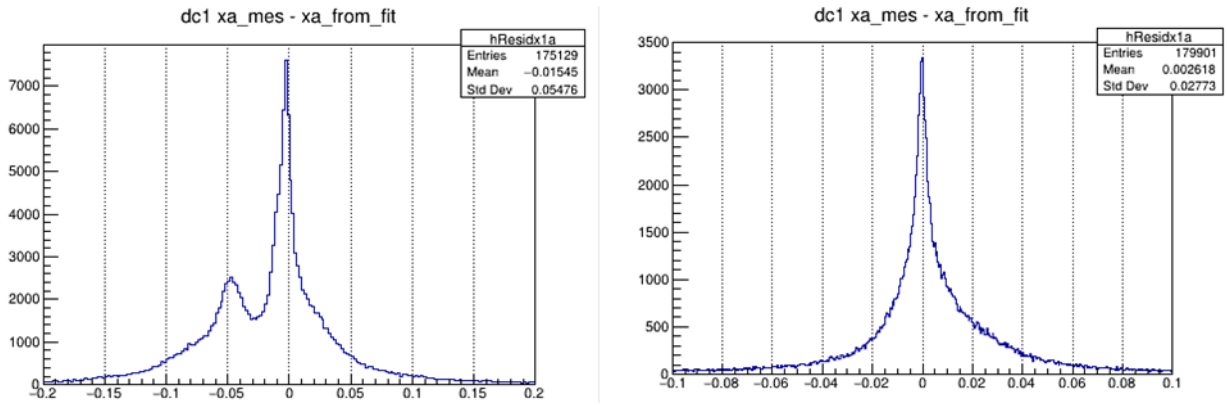
• **Track reconstruction in the BM@N experiment** [29,30]. The reconstruction of charged particle trajectories in the BM@N experiment is one of the most important and time consuming tasks in the event reconstruction procedure. It is developed along requirements following from the two setup configurations defined so far: BM@N, and the Short Range Correlation Program (SRC) at BM@N. Cell-based algorithm is developed and incorporated into the **BmnRoot** software. Instances of tracking efficiency and momentum resolution:



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

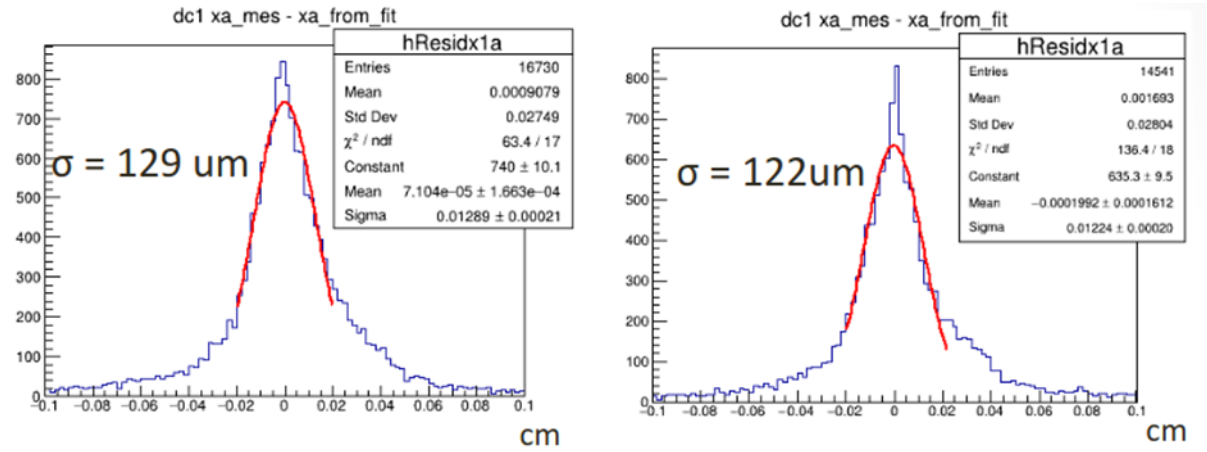
• The usefulness of the **geometry database for the BM@N experiment** and its scope were reviewed ([31], see also [32] and [33] for the latest developments). A workable prototype of the *Geometry Database* was developed. The *Geometry Database* supports storing, updating and retrieving the geometry of BM@N modules. The developed information system includes the database, intuitive and compact GUI tools and API tools as a set of *ROOT* macros. Improvements in application and GUIs based on BM@N users' responses are assumed.

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

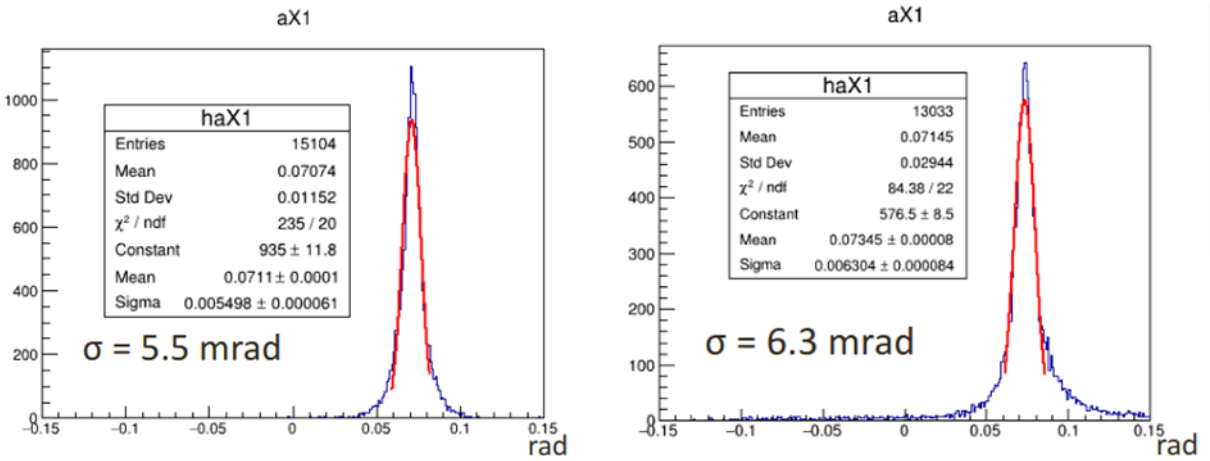


Deviation of coordinates from the fitted segment: *Left* – before internal alignment; *Right* – after

A full reconstruction chain was developed for simulated data in the Drift Chambers of the BM@N Run 7 setup. The achievement of the right tuning of the simulated data reconstruction is proved by the good agreement between the simulated and experimental data (see figures below) [34].



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



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

• **Development of the BmnRoot framework of the BM@N experiment** has been recently reviewed [35]. This is a fundamental step toward a successful accomplishment of the BM@N physics program. The **BmnRoot** framework involves a well-developed and tested software package for simulation, digitization, reconstruction and analysis of collision events and other supporting tasks. The implementation of the software systems is a necessary stage for the successful operation of the BM@N experiment.

► **BMNROOT** development, maintenance and exploitation are done in joint work with colleagues physicists from VBLHEP. This report mentions four kinds of results, summarized below.

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

- BmnDchTrackFinder – Segment builder for Drift chambers,
- BmnDchHitProducer – Hit builder for simulated data for Drift chambers,
- BmnDchHitProducerData – Hit builder for experimental data for Drift chambers – [34]);

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

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

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

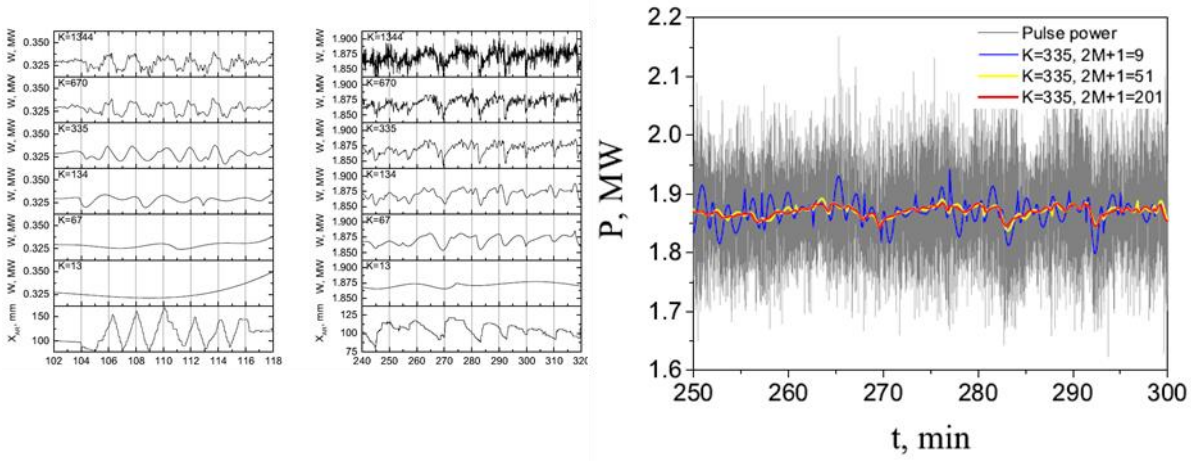
►Design and extensive testing of the new **Monte-Carlo Generator of Heavy Ion Collisions DCM-SMM** [36–38]. The new Monte-Carlo generator, DCM-SMM, is created by the group of authors with the aim to provide the NICA projects with an effective tool for optimizing the detector elements, debugging the event reconstruction algorithms, predicting the efficiency,

calculating the signal-to-background ratio, determining the best criteria for selecting events. The generator DCM-SMM is actively used by the BM@N and MPD detector groups for their needs. Tens of millions of nucleus-nucleus collisions were simulated at the HybriLIT cluster for reactions of carbon (C), argon (Ar) and krypton (Kr) with C, Al, Cu, Pb.

2.3.3. *Computational support of in-house projects in condensed matter physics and radiobiological research*

► **Developments of the Basic Element Method (BEM) and its application to simulations of the IBR-2M reactor noise**. The general mathematical method BEM, proposed and developed by N. Dikusar for the approximation and characterization of functions based on projective geometry representation, has found a valuable application in the processing and characterization of the IBR-2M noise [39,40]. The follow up of the data collected for many years during the IBR-2M life cycle has evidenced the possibility to discard the pure statistical noise from the low amplitude slow variations connected to the ageing processes taking place in the active core of the reactor.

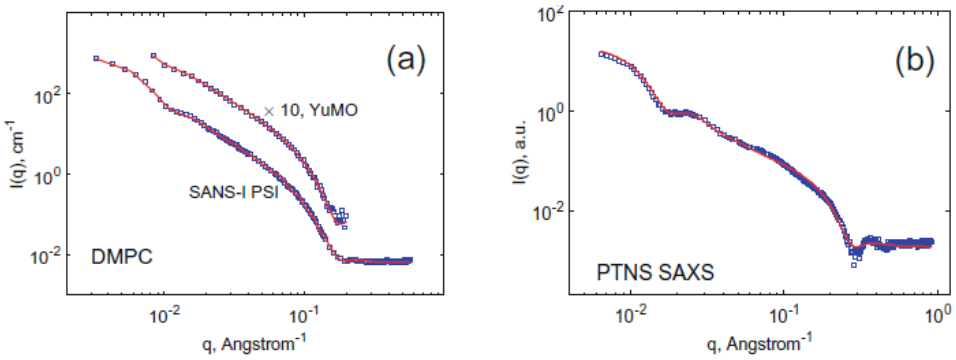
The figure below illustrates an instance of data processing both for static and dynamic states of the reactor. Algorithm speed is adequate for real-time monitoring.



Left and **centre**: Different approximating curves and positions of the automatic regulator (bottom).
Right: Approximating curve as a function of the method parameters [39]

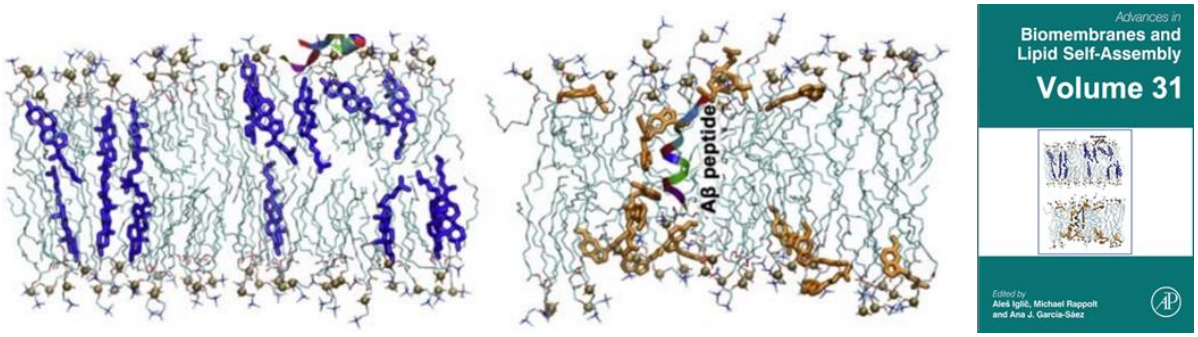
► **On the initial approximation of charged particle tracks in detectors with linear sensing elements** [41]. We provide a method that allows finding initial approximations of straight segments of track in space using four linear sensing elements. This method is especially helpful if there are no parallel elements in the setup. The procedure can also be used as a first approximation to the case of finding curved tracks.

► **Parallel implementation of the method of separated form factors** [42,43]. The distinctive feature of this collaboration is that it provides mathematical modeling for offline data processing for a given type of compound, rather than to data acquisition modeling. The procedure of fitting the parameters of the separated form factors (SFF) model to the experimental data of SANS and SAXS collected at FLNP on various polydispersed vesicular systems, including the phospholipid transport nanosystem, was carried out. To increase the computational performance, the procedure of fitting the parameters of the SFF model to the experimental data of SANS and SAXS is implemented on the HybriLIT cluster using MPI techniques.



(a) Theoretical and experimental SANS spectra of the polydispersed DMPC ULV system in D_2O. SANS data got at spectrometers YuMO (Dubna) and SANS-I PSI (Villigen). (b) Theoretical and experimental SAXS spectra of polydispersed population of PTNS ULVs in the 20% maltose concentration solvent.

► **Interactions in the model membranes mimicking preclinical conformational diseases** [44]. Although a complete understanding of the physicochemical processes taking place in biomembranes is not fully established, the understanding of the lipid bilayer elasto-mechanical properties provides a foundation for better insights into the structure-function relationships that most certainly take place in complex biomembrane systems. The study addresses the mechanism of the Alzheimer disease. The cover of the volume is illustrated with results from this report.



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

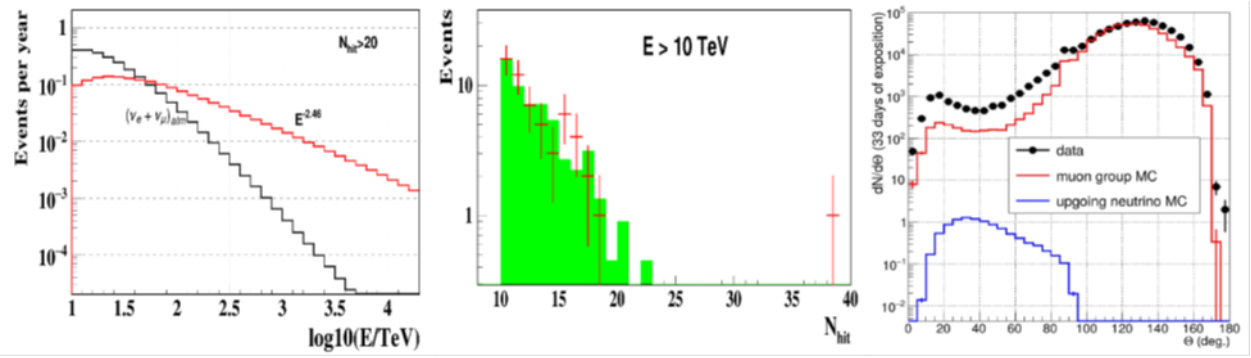
► **SAS – package for small-angle neutron scattering data treatment**. The online data processing at the YuMO spectrometer (channel four of the IBR-2 reactor) is done by means of the SAS package. This package was intensively upgraded during the second half of the past year and the beginning of 2020. The program allows to combine the data referring to the same sample, to calculate the spectrometer resolution function for the given experiment conditions, to carry out data correction on dead times of neutron detectors, and to subtract a background substrate from detector data, to carry out the normalization of the obtained spectrum on standard vanadium scatterer, to subtract background sample data. (For further details, see Sec.(3)).

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

2.3.4. *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 [45], change of the ambient light field [46], 3D monitoring of water parameters [47]. An intricate multistage data processing of recorded data [48] is shown in the figure below.



Left: Energy distributions of events expected for one year observation from astrophysical fluxes with $E^{-2.46}$ spectra and IceCube normalization, and from atmospheric neutrinos. *Centre*: Measured distribution of hit optical modules multiplicity in cascade-like events with energies above 10 TeV and the expected one from atmospheric muons (green histogram). *Right*: Zenith angle distributions reconstructed with data sample of muon-like events (dots) and with MC atmospheric muons (red) and neutrinos (blue).

2.3.5. Support of Experimental Data Processing and Analysis in Nuclear Physics

► **Reliable statistical inferences under low statistics and incomplete observation** [49].

The nonparametric methods are most suitable for tasks facing the uncertainty or complexity of models and the small statistics of the analyzed data. The proposed nonparametric "median/mean" criterion for testing a rather large class of data distributions for purity is suitable for use. This is especially important for the small data statistics and the lack of the a priori information about the parameters of the distribution function.

►**Ion fragmentation reactions**

• **Boltzmann–Vlasov transport approach description of heavy-ion fragmentation reactions** at low and intermediate energies for the production of the hot, excited primary fragments, followed by a statistical decay of these to arrive at the measured cold fragments. While the isotopic distributions are reasonably well-described by this microscopic model, there are larger differences in the velocity distributions. These seem to be due to too small fluctuations in the transport calculation and to the presence of more direct reaction processes in the data [50].

• **Modeling total reaction cross sections of neutron-rich light nuclei measured by the FLNR COMBAS fragment-separator** [51,52]. The total reaction cross sections for projectile nuclei from ^{4}He to ^{12}B at the energy range 10-50 AMeV and ^{28}Si target measured at COMBAS are compared with model predictions based on the Kox formula and MOMDIS calculations.

• Monte-Carlo studies within the EXPERTroot framework for modeling experimental results on the elastic scattering of ^{15}N ions on ^{11}B as well as the analysis of the systematic errors arising from the derivation of the elastic scattering cross-section from experimental data have been done [53].

2.3.6. Machine learning on high-performance computing infrastructures at JINR

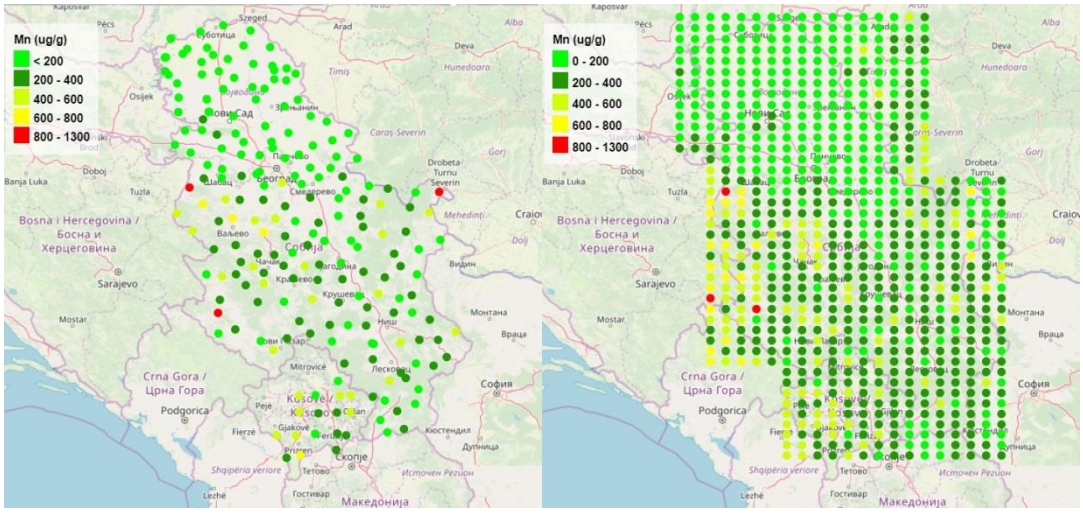
• **Event reconstruction in GEM detectors.** New effective tracking methods based on graph neural network (GNN) are actively developed and tested for the GEM detector of the BM@N setup at NICA. This approach is well-adapted for solving the known fake hit problem inherent to strip detectors like GEM with help of minimum branching tree algorithms [54–57]. Primary event processing for the future cylindrical GEM (CGEM) tracker of the **BESIII *drift chamber***, which involves cluster finding and 3d-coordinate hit reconstruction, is reported [58].

• **Disease detection on the plant leaves by deep learning** [59,60].

Models enabling the identification of the most appropriate deep learning architecture and data training were studied. Ways to avoid pitfalls were identified. A special database of the grape

leaves consisting of four set of images was created. A deep Siamese convolutional network developed to solve the problem of the small image databases yielded over 90% accuracy [59].
The created special database of healthy and diseased grape leaves was further extended and a special classification model based on a deep Siamese network followed by k-nearest neighbors (KNN) classifier was developed. The implementation of a novel architecture with a deep Siamese network as feature extractor and a single-layer perceptron as a classifier results in a significant gain of accuracy, up to 96% [60]. Using of a deep Siamese neural network as feature extractor allows reaching 99% of the recognition accuracy on the test subset of images.

• **Development of new methods for predicting air pollution with heavy metals** [61–63].
Motivation, basic principles and architecture of the Data Management System (DMS) of the UNECE International Cooperative Program (ICP) Vegetation are presented. DMS consists of a set of inter-connected services and tools implemented and hosted at the JINR cloud infrastructure. It provides its participants with a modern unified system of collecting, analyzing and processing of biological monitoring data. The figure below illustrates a pollution case study done in collaboration with the sector of neutron activation analysis of the FLNP, the coordinator of the ICP Vegetation program.



Mn pollution in Serbia. Left – real data. Right – model prediction

• **Use of deep neural tracking to face the tracking crisis challenge in detector environments, such as HL-LHC Run-4 and MPD-NICA**. A few model results have been reported (**TrackNETv2** [64], **GraphNet** [65], LOOT [66]).

(3) ***Software packages implemented in general purpose computing libraries***

We notice submissions to the PROGRAM LIBRARY JINRLIB (two new packages and two major upgrades) and two publications in Computer Physics Communications, the last one in this series being implemented in the 2019 and 2020 releases of the MAPLE computer algebra system.

► Implementations in the PROGRAM LIBRARY JINRLIB of important HPC parallel packages.

• **EORP 2020** – Equilibrium Orbit Research Program (April 06, 2020) [67] – software package for computing closed equilibrium orbits in magnetic fields of an isochronous cyclotron by solving the equations of motion.

• **Split –** a parallel implementation of the numerical solution of a system of algebraic equations with a tridiagonal matrix using partition algorithm and MPI technique (April 27, 2020) [68].

• **SAS** – package for small-angle neutron scattering online data treatment [69]. A number of six major upgrades in-between August 2, 2019 and January 30, 2020 provide substantially improved online processing of the spectra measured on the YuMO setup.

• **DFM-POTM** – parallel calculation of the double folding nucleus-nucleus potential (New addition: OpenMP and major upgrades of the interface to the user, April – July, 2019) [70]. The DFM-POTM package implements the calculation of a nucleus-nucleus optical potential of elastic scattering within the double folding model (DFM). The package includes three constituents: - serial C++ version, - parallel MPI version, - parallel OpenMP version. All codes provide the same outcome. For convenience, the input parameters in DFM-POTM, DFM-POTM_MPI and DFM-POTM_OpenMP are introduced via the input file with arbitrary name which should be indicated in the run command.

► Package publications in the CPC Program Library:

• Comp. Phys. Comm., CPC Program Title: **PBCAVE**; Published: 28 Nov 2019; Version 1; **PBCAVE: Program for exact classification of the mesh points of a protein with possible internal cavities and its application to Poisson–Boltzmann equation solution** [71]. The principal contribution of the program is the analytic approach to the setting of dielectric constant for all discretization points of a grid in the computational domain according to their locations with respect to the molecular surface allowing also taking into account possible cavities. Assigned values of dielectric constant are used in a solver of the linear Poisson–Boltzmann equation for a protein–water system using a finite difference method. The associated paper [72] provides detailed technical description.

• "The MAPLE package **TDDS** for computing Thomas decompositions of systems of nonlinear PDEs" [73]. Published under GNU LGPL license, *this code has become part of the annual releases of the* MAPLE *in* 2019 *and* 2020. TDDS (Thomas Decomposition of Differential Systems) computes a decomposition of a polynomially nonlinear differential system into a finite set of differentially triangular and algebraically simple subsystems whose subsets of equations are involutive. Detailed technical description is provided in the associated paper [74].

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

An overall statistics of the scientific output of the theme 1119 staff for the period under consideration points to the publication of 206 articles in refereed journals (among them, 35 in highly ranked journals such as Nature Physics, Phys. Rev. Lett, Phys. Rev. A, B, C, Phys. Rev. Res., Comp. Phys. Comm., Chem. Phys. Lett., Eur. Phys. J. A, D, Physica D, J. Phys. G, ZhVM & MF (Rus.), Mat. Mod. (Rus.), TMF (Rus.), ZhETF and Pis'ma v ZhETF (Rus.)); five monographs; five papers in scientific collections; 18 electronic publications; four JINR preprints; two textbooks on MPI parallel programming. An additional number of 150 papers were published in the frame of the CMS collaboration.

The subject matters of these publications cover almost all the topics foreseen in the research plan of the theme 1119. *A selective enumeration concerns:*

- *Mathematical modeling and derivation of algorithms for numerical solution of a wide range of problems: QCD-motivated models for describing properties of nuclear matter at NICA energies; near-barrier heavy-ion fusion; new molecular dynamics algorithms aimed at explaining long-range structural changes of materials under heavy ion and nanocluster irradiation; numerical methods for describing equilibrium and nonequilibrium properties of mesoscopic systems of trapped atoms; numerical investigation of nonlinear multiparameter processes in complex physical systems under external fields, including optical and self-assembled atomic lattices, models of superconducting structures, localized states in condensed media, the ballistic electron transport through the rippled graphene with curvature induced spin-orbit interaction, simulation of gas-hydrodynamic processes in porous media, stable solitons in a nearly PT-symmetric ferromagnet with spin-transfer torque; new method for solving the Gross-Pitaevskii equation with a PT-symmetric complex potential; modeling the reflection of neutrons from layered nanostructures, studies of magnetic films as*

structures consisting of vector micro-objects; nuclear-physical processes based on a hybrid model of microscopic potential, including reactions with light exotic nuclei.

- Mathematical modeling, derivation of algorithms, and rigorous solution of numerical analysis topics the state-of-the-art solution of which is unsatisfactory for resolving current theoretical and experimental problems investigated in the JINR and partner institutions: digital processing of plane curves (with application to fast neutron noise analysis of the IBR-2M reactor), two-rule quadrature for the computation of observables, new symbolic-numerical schemes using finite element method, non-canonical Bargmann-Moshinsky basis; interpolation Hermite polynomials in d-dimensional hypercube; compact three center wave function constructed by use of irreducible representations of the D_{3h} point group for solving the ground and five excited states of the equilateral triangular H_3^+ molecule; Compton ionization of hydrogen atom near threshold by photons; kinematically complete experimental study of Compton scattering at helium atoms near the threshold.

- Solution of massively parallel, resource-intensive problems raised by the theoretical and experimental physics: discontinuous hp-adaptive schemes for finding optimal configuration of a magnetic device with highly-uniform magnetic fields for experiments with neutrons (collab. FLNP); derivation of constraints for the dense matter equation of state to explain observations of the binary neutron star merger GW170817; *Landau mass parameters of the extended σ-ω model for neutron star matter (collab. LIT, BLTP, Wigner Institute – Hungary), interactions in model membranes mimicking preclinical conformational diseases (collab. LIT, FLNP, LRB – journal cover 2020); model description of the interaction of atomic and molecular hydrogen, hydrogen anion and water molecule with an external ultrashort laser pulse; MPI implementation of the method of separated form factors for data analysis in polydispersed vesicular systems (collab. FLNP); HPC of physical observables in spintronics; HPC for design optimization of a pulsed cryogenic cell; single ionization of helium by fast proton impact, etc*.

- Solutions of difficult problems of computer algebra: constructive models for the description of finite quantum systems; functional equation methods for reduction of Feynman integrals; table-based representation of polynomials in the computations of involutive and Gröbner bases; parametric occurrence of multiple steady states in biological networks.

- Creation of algorithms and programs possessing strong consistency property, for symbolic-numerical solution of systems of nonlinear PDEs; algorithmic linearizability for nonlinear ODEs.

- Solutions of problems related to quantum computing: entanglement production by statistical operators; mid-range order in trapped quasi-condensates of bosonic atoms; classicality indicator of an arbitrary N-level quantum system; quantum teleportation of two-qubit Bell states; entanglement sudden death and birth effects in two qubit maximally entangled mixed states under quantum channels; robustness of entanglement under quantum decoherence channels.

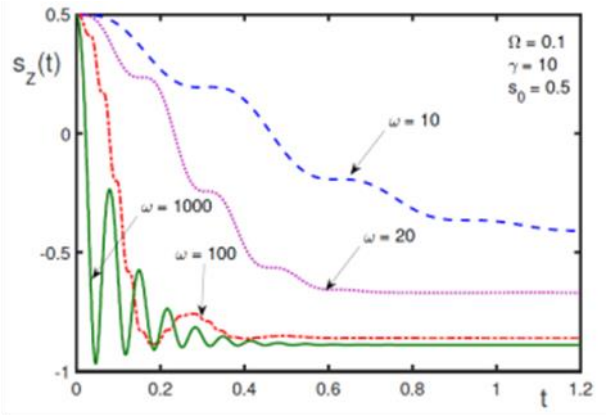
A few selected examples are given below emphasizing the main feature of the research done.

4.1. Selected results on the development of mathematical models

► **Description of the phase transitions in field theory by self-similar approximants** [75]. A self-similar approximation theory was developed for the description of phase transitions in quantum field theory covering: (i) Influence of the coupling parameter strength on the critical temperature of the O(N)-symmetric multicomponent field theory; (ii) Calculation of critical exponents for the phase transition in the O(N)-symmetric field theory; (iii) Evaluation of deconfinement temperature in quantum chromodynamics. Good agreement with numerical calculations (Monte-Carlo, Pade-Borel summation, lattice data) is reported.

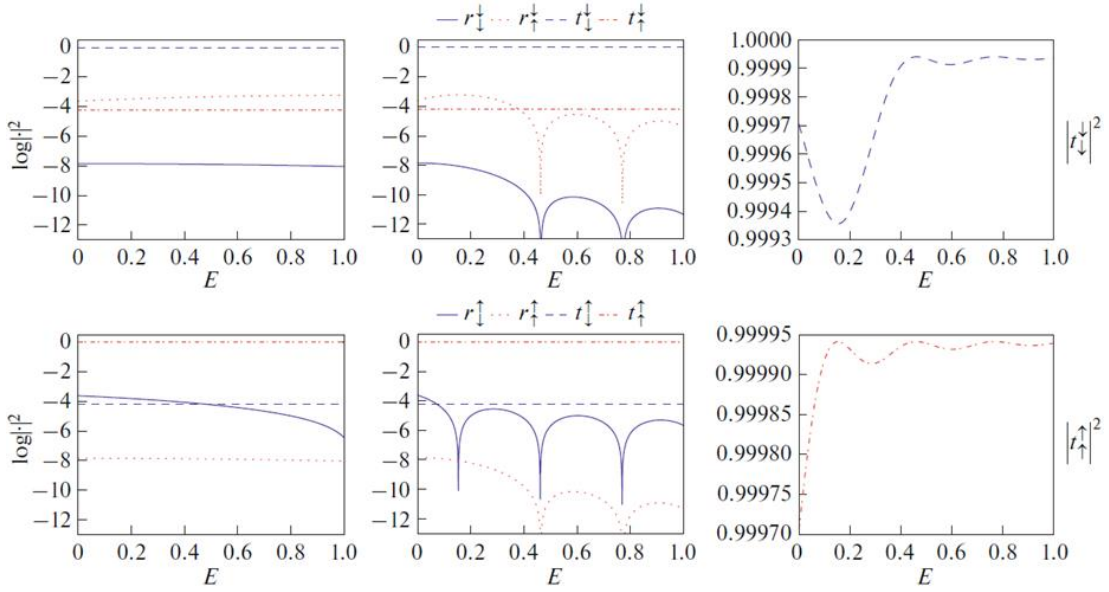
► **Ultrafast polarization switching in ferroelectrics** [76,77]. A method of ultrafast polarization switching in ferroelectrics is suggested. The basic idea of the method is to employ the effect of

self-acceleration of polarization dynamics due to a resonator feedback field. The dependence of the polarization switching on the varying frequency ω is illustrated below.



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

► **Ballistic electron transport through rippled graphene with curvature induced spin-orbit interaction** [78]. We have analyzed the spin dependence of the transmission (t) and reflection (r) of electrons through the corrugated graphene structure at arbitrary incidence angles. The spin-orbit interaction induced by the curvature has a sizeable impact on the scattering of electrons with different initial polarizations. Numerical results point to the reflection of electrons having the same spin polarization with the incoming ones. There is also a transmission of electrons with the opposite spin polarization, while of significantly smaller magnitude as compared to the transmission of the electrons with the same spin polarization. Ripple dependent quantization rules evidence the possibility of specific energy enhanced transmission of the incident electrons.

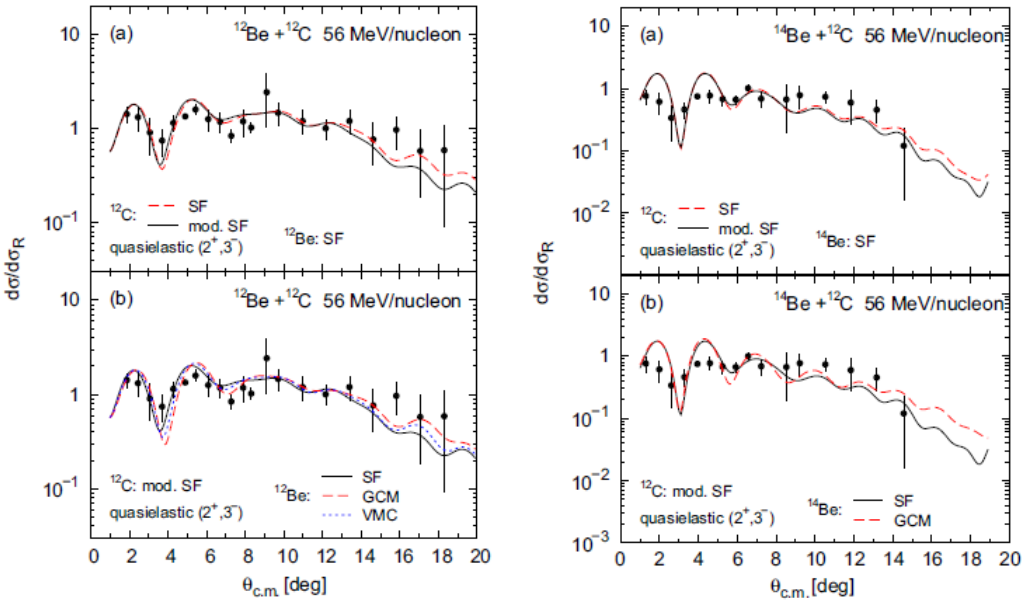


Transmission (t) and reflection (r) probabilities in terms of the incoming electron energy *E* (eV) and the electron spin.

► **Superexchange interactions in oxides with face-sharing ligand octahedral** [79]. Using *ab initio* wave-function-based calculations, we provide valuable insights with regard to the magnetic exchange in 5d and 4d oxides with face-sharing ligand octahedra, $BaIrO_3$ and $BaRhO_3$. Surprisingly strong antiferromagnetic Heisenberg interactions as large as 400 meV are computed for idealized iridate structures with 90° Ir-O-Ir bond angles and in the range of 125 meV for angles of 80° as measured experimentally in $BaIrO_3$. These estimates exceed the values derived so far for corner-sharing and edge-sharing systems and motivate more detailed experimental investigations of quantum magnets with extended 5d/4d orbitals and networks of face-sharing ligand cages. The

strong electron-lattice couplings evidenced by our calculations suggest rich phase diagrams as a function of strain and pressure, a research direction with much potential for materials of this type.

► **Simulation of reactions of exotic nuclei with microscopic optical potential model** [80–84]. Microscopic optical potentials and differential cross-sections for the elastic scattering of the exotic nuclei ^{12,14}Be on ^{12}C nuclei at 56 MeV/nucleon and on protons at 700 MeV were calculated using different density models. The need of taking into account the inelastic channel (quasielastic scattering) is proved. The calculated momentum distributions of the ^{12}Be fragments arising in the reaction of the ^{14}Be nucleus breakup in the interaction with ^{12}C are in good agreement with the experimental data (see figure below).



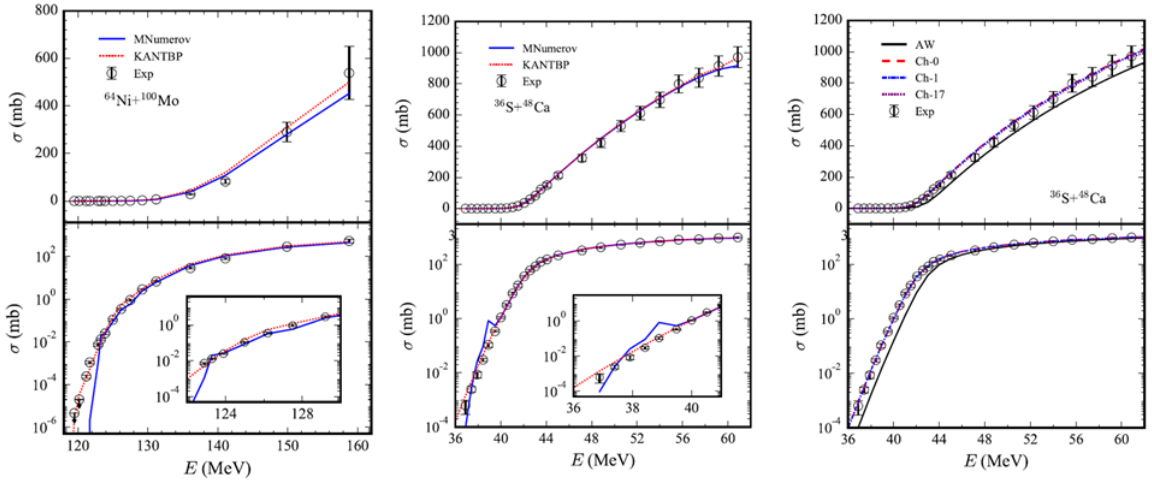
Left: (a) ^{12}Be + ^{12}C quasielastic scattering cross sections at E = 56 MeV/nucleon calculated using the SF density of ^{12}Be and SF (black solid line) and modified SF (red dashed line) densities of ^{12}C. Panel (b) illustrates the calculations with the modified SF density of ^{12}C and using the SF (black solid line), GCM (red dashed line), and VMC (blue dotted line) densities of ^{12}Be. *Right*: (a) Same as left, but for ^{14}Be + ^{12}C. In panel (b) results with SF and GCM densities of ^{14}Be are shown [81].

► **Proton induced pre-equilibrium reactions to the continuum as a test to the reaction mechanism** [85]. Pre-equilibrium proton induced emissions of light complex nuclei with energies in the continuum are considered as an intra-nuclear nucleon-nucleon multistep statistical reaction with typical double-differential cross sections and especially analyzing power distributions. The interplay between the knockout and pickup mechanisms as final step of the pre-equilibrium reaction and its dependence on the energy of the projectile are investigated.

► **Excitation energy dependence of the moments of inertia of well deformed nuclei** [86]. The moments of inertia of the γ-vibrational states of several rare earth nuclei and of the 1+ states of ^{156,158}Gd and ^{160,162,164}Dy are calculated and compared with experimental data. It is shown that both the blocking effect and the Coriolis coupling between quasiparticles and the rotating core contribute significantly to the increase of the excited states' moments of inertia in comparison to the ground state value. In the case of the 1+ states the contribution of the Coriolis interaction of quasiparticles and the rotating core can be considerably larger than the blocking effect. This is one reason for the very large value of the moment of inertia of some 1+ states which can exceed the rigid body value.

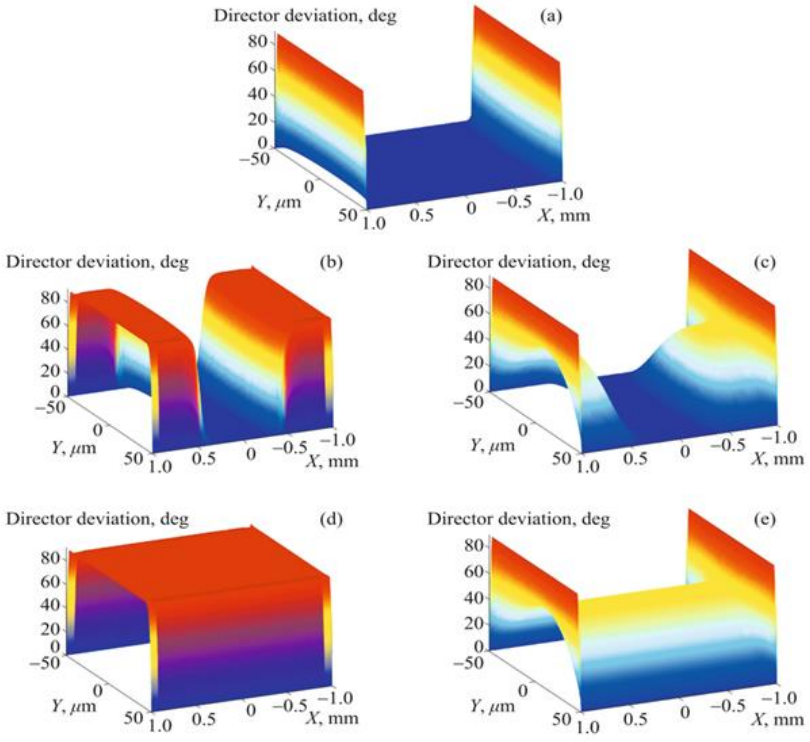
► **Role of the boundary conditions in the near-barrier heavy-ion fusion** [87]. A quantum-mechanical description of the near-barrier fusion of heavy nuclei that occurs at strong coupling of their relative motion to surface vibrations is derived. To this end, an efficient finite element method is proposed for the numerical solution of the coupled Schrödinger equations with boundary conditions corresponding to total absorption. The method eliminates the instabilities in

the numerical solutions previously noticed at a large number of coupled channels in some reactions. To illustrate the validity of the present approach, the results of fusion cross section of the ^{64}Ni + ^{100}Mo and ^{36}S + ^{48}Ca reactions have been re-examined. The obtained results show a remarkable agreement with the available experimental data. It is found that the experimental data can be well reproduced with a Woods-Saxon potential, without asking for the repulsive cores. It appears that the fusion cross sections at deep sub-barrier energies are sensitive to the potential pocket profile.



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

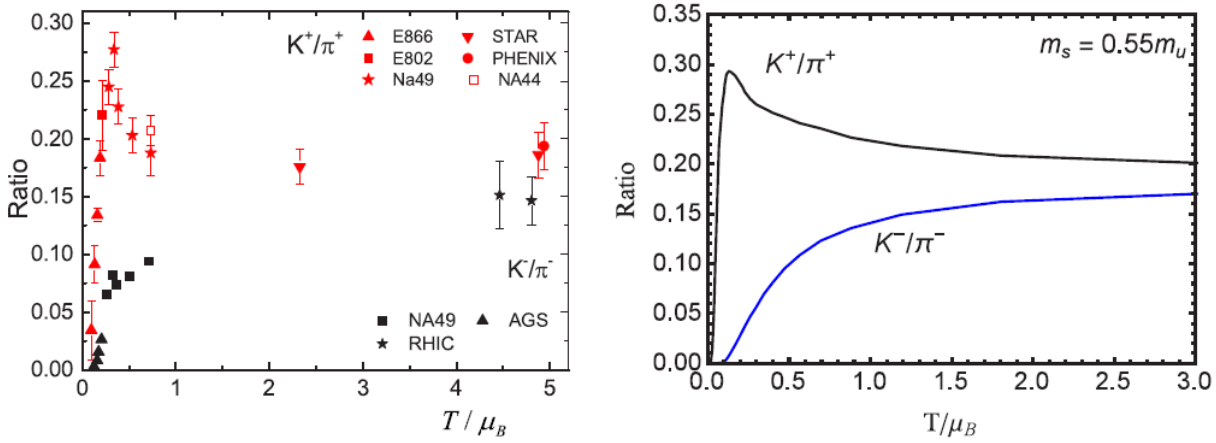
► **Simulation of nematic liquid crystal optical waveguide structures** [88–91]. Numeric and experimental studies of two nematic liquid crystal (NLC) optical waveguide structures (liquid thin waveguide lens and thin film generalized waveguide Luneburg lens) have been made. Results of the two dimensional dynamic model are illustrated in the figure. Better agreement with the experiment is got as compared with the previously used static model.



The director of NLC at the initial state (a) and the change in its orientation for (b, c) strong (1.5×10^6 V m^{-1}) and (d, e) weak (1.2×10^4 V m^{-1}) static electric fields after 6.8 (b), 20 (c), 90 (d), and 300 s (e). The NLC cell is 100 μm thick.

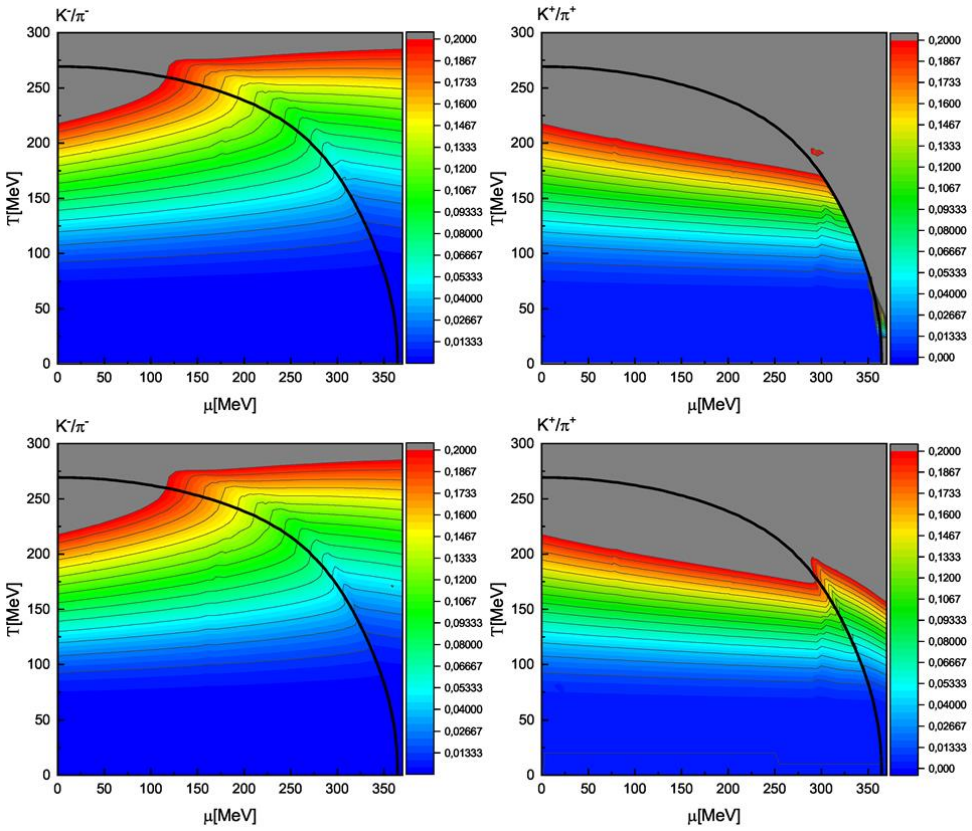
► **Numeric-theoretical studies in dense hadronic matter**

• **First horn effect investigation in the PNJL model** [92–94]. The appearance of a peak in the ratio of the number of strange mesons to nonstrange mesons known as a "horn" was discussed in the frame of the SU(3) Nambu–Jona-Lasinio model with Polyakov loop (PNJL) including the UA(1) anomaly. Former ideas were that the occurrence of the horn at energies 8–10 GeV might be a qualitative change in the state of the environment where kaons and pions were created. In [92] the fast increase in the K^+/π^+ ratio and its decrease at further increasing energy was interpreted as a sequence involving the chiral symmetry restoration and the deconfinement effect.



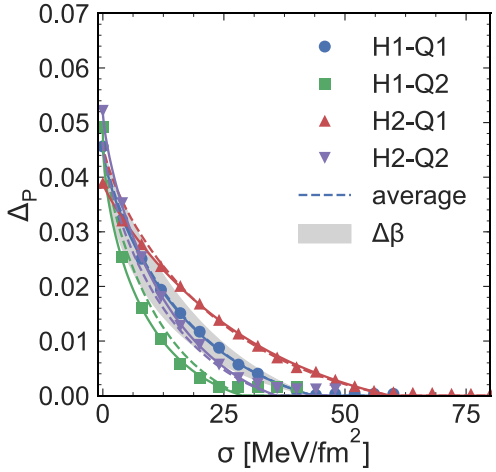
Dependence of the ratios K^+/π^+ and K^-/π^- on T/μ_B: experimental data (left) and simulation results (right).

• Further investigations of the horn effect [95,96] are done in the frame of a 2+1 flavor PNJL model. In order to interpret the behavior of bound states in medium, the Beth–Uhlenbeck approach is used. It is shown that, in terms of phase shifts in the K^+ channel, an additional low-energy mode could appear as a bound state in the medium, since the masses of the quark constituents are different. The comparison with experimental data for the ratios is performed and the influence of the anomalous mode to the "horn" effect in the K^+/π^+ ratio is discussed.



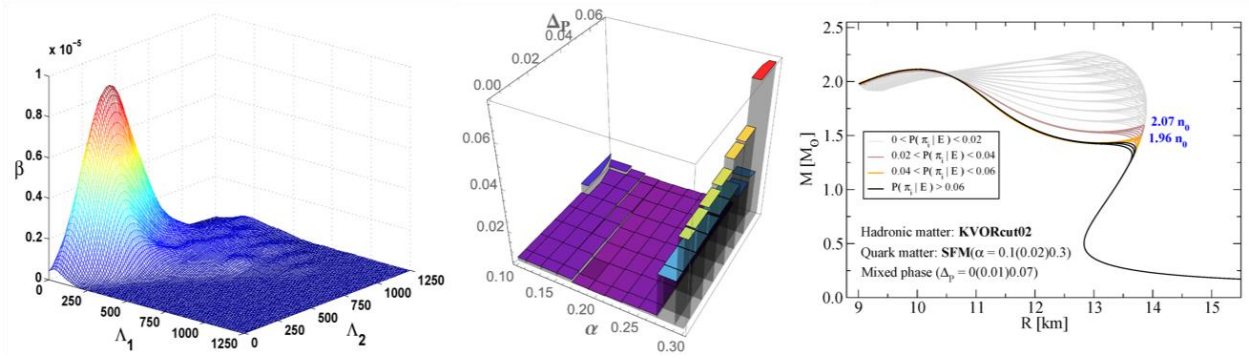
The K^-/π^- and K^+/π^+ ratio in the T-μ_q plane. The two upper panels correspond to full phase shifts while the two lower panels show phase shifts when the anomalous mode is removed. Only the interval of ratios relevant for a comparison with the experimental data is shown.

• The effect of pasta phases on the quark-hadron phase transition was investigated [97–98]. The results of the full numerical solution with pasta phases are compared with those of an interpolating construction used in previous works, for which an adequate description of the numerical results was obtained. The study is extended to neutron star matter in beta equilibrium with electrons and muons and is applied to investigate the effect of pasta phases on the structure of hybrid compact stars and the robustness of a possible third family solution.



Relative pressure shift ΔP at the critical chemical potential μ_c as a function of the surface tension σ of hadron pasta structures for all the combinations of models. Solid lines show the results of the fit with use simple parabolic interpolation method, and the dashed lines are full pasta calculation.

• A Bayesian analysis method for selecting the most probable equation of state under a set of constraints from compact star physics, which now include the tidal deformability from GW170817, has been developed. It has been applied for the first time to a two-parameter family of hybrid equations of state that is based on realistic models for the hadronic phase (KVORcut02) and the quark matter phase SFM(α) which produce a third family of hybrid stars in the mass–radius diagram (see figure below). The parameters of compact stars for these equations of state models like mass, radius and tidal deformability have been inferred and used as empirical data in the newly developed Bayesian analysis method [99].



Left panel: The PDF reconstructed with Λ1–Λ2 data for GW170817 from the LIGO website https://dcc.ligo.org/LIGO-P1800115/public . *Middle panel*: the posterior distribution of models on the parameter space spanned by Δ_P and α. *Right panel*: the compact star sequences in the mass–radius diagram labeled into four probability classes according to the results of the Bayesian Analysis for the posterior distribution of the left panel.

• Accretion-induced collapse to third family compact stars as trigger for eccentric orbits of millisecond pulsars in binaries and astrophysical aspects of general relativistic mass twin stars have been recently reviewed [100,101].

• **Other dense hadron matter reports** [102,103]

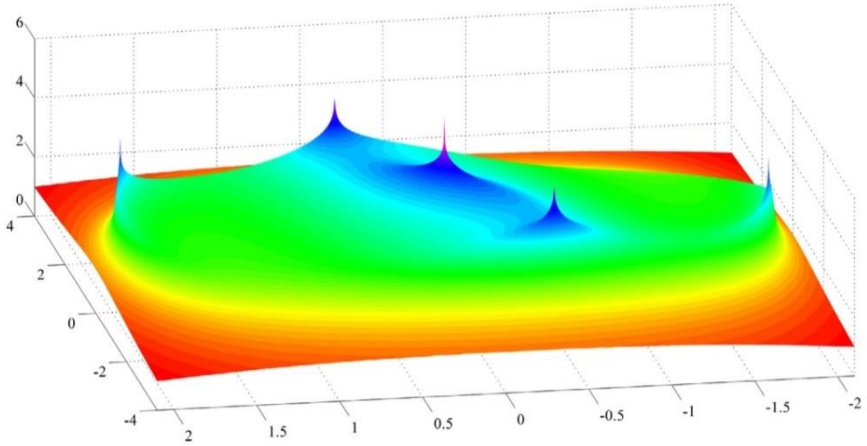
► **Dimesoatom breakup in the Coulomb field** [104]. Momentum and angular distributions of charged meson pairs h^+h^- (h=π,K) from elementary atom (EA) breakup (ionization) in the Coulomb field of a target atom are considered in the Born and Glauber approximations. Exploiting the fact

that the atomic screening of the target Coulomb potential is important at small transfer momenta, while multi-photon exchanges are essential at large transfer momenta, we express the cross sections of EA breakup as a sum of two terms. In the region of modest transfer momenta the cross section is determined by the single-photon exchange (first Born approximation) accounting for the target atoms screening, whereas at large transfer momenta using the unscreened potential allows one to take into account all multi-photon exchanges and obtain the cross section of EA breakup in closed analytical form.

► **Development of methods and analysis of solutions to nonlinear problems of mathematical physics** [105–107].

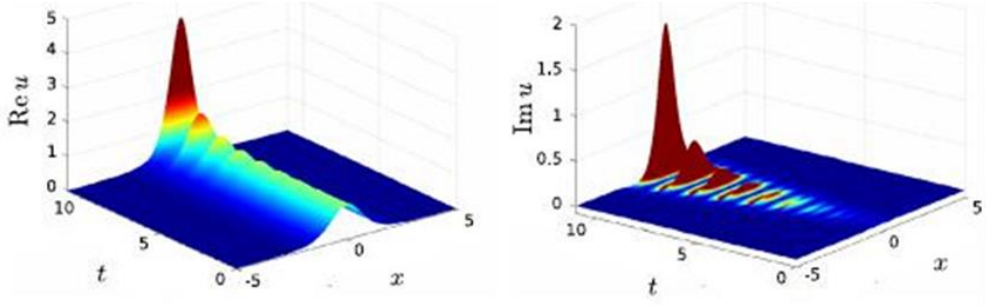
• For the ϕ^4 model of particle and condensed-matter physics, a consistent asymptotic construction of the wobbling kink solution was given. The developed expansion takes into account the coexistence of several space and time scales [105].

• A new approach to the search for localized modes in the scalar and vector nonlinear Schroedinger equations with repulsive nonlinearity was formulated. The new method was applied to the Gross-Pitaevskii equation with a PT-symmetric complex potential, a system of coupled Gross-Pitaevskii equations with real potentials, and the Lugiato-Lefever equation with normal dispersion [106].

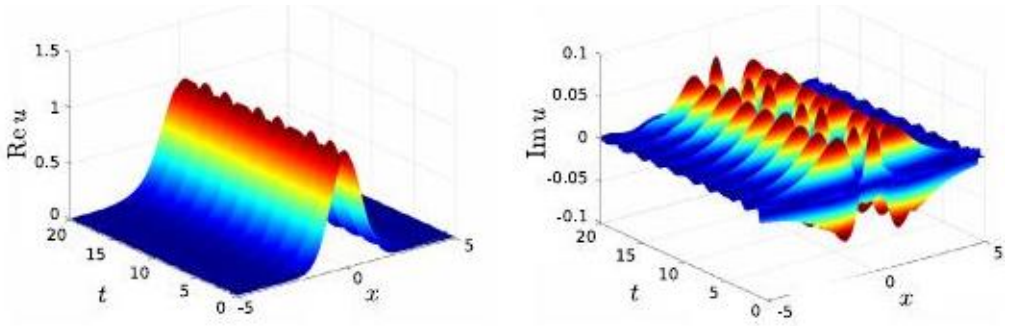


A numerical plot of the function $X^{+}(0; C1, 0, 0, C'_2)$ for the stationary Gross-Pitaevskii equation with a PT-symmetric parabolic potential [106]

• **Stable solitons in a nearly PT-symmetric ferromagnet with spin-transfer torque** [107]. The undamped Landau-Lifshitz equation for the spin torque oscillator — a uniaxial ferromagnet in an external magnetic field with polarised spin current driven through it is PT symmetric in the absence of the Gilbert damping. In the vicinity of the bifurcation point of a uniform static state of magnetisation, the PT-symmetric Landau-Lifshitz equation with a small dissipative perturbation reduces to a nonlinear Schrodinger equation with a quadratic nonlinearity. The analysis of the Schroedinger dynamics demonstrates that stable solitons can exist in one and two dimensions. Near PT-symmetry of Landau-Lifshitz equation is crucial for soliton stability. Illustrations follow:



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



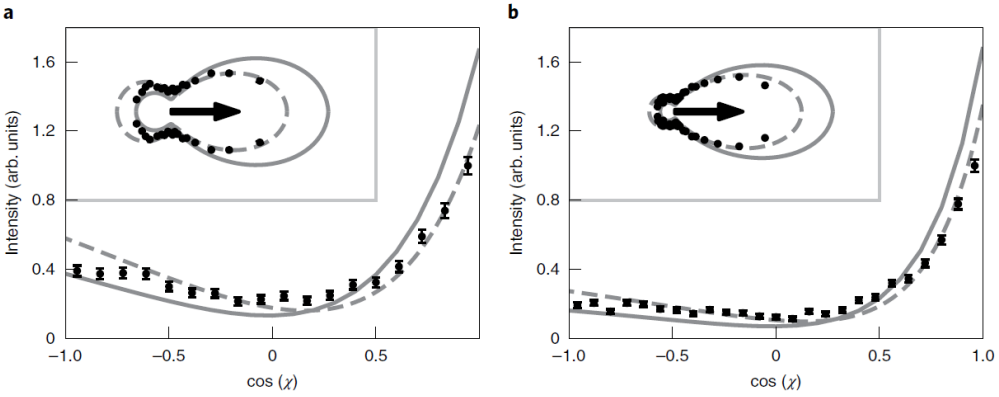
The evolution of the initial condition in the form of a Gaussian. Left panel: Re u; right panel: Im u. The emerging solution is a breather with a small imaginary part and the real part close to the soliton.

► **Progress in photon science** [108] A model based on the replacement of the potential describing the interaction of a single active electron with the nucleus or the nuclei of atoms or molecules, with a potential, separable in momentum space and consisting of several terms is presented. It is used to the description of the interaction of atomic and molecular hydrogen, hydrogen anion and water molecule with an external ultrashort laser pulse. Conditions for the model validity are discussed.

► **Bianchi type-I cosmology studies** [109–112]. Within the scope of Bianchi type-I cosmological model, the role of spinor fields characterized by nonminimal coupling in the evolution of the Universe was studied. Solutions have been found which can generate close universe that at the beginning expands and, after attaining some maximum value, begin to contract and finally end in a Big Crunch.

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

► **Kinematically complete experimental study of Compton scattering at helium atoms near the threshold** [113]. This study, published in Nature Physics, reports high precision experiments on Compton scattering from free atoms by cold-target recoil ion momentum spectroscopy (COLTRIMS), addressing the intriguing low-energy, near-threshold regime, where the classical theory of the Compton effect ceases to be valid. The derivation of a kinematically complete dataset of ionization by Compton scattering of atoms – as opposed to detection of the emitted electron or scattered photon only – provides the essential key to sensitive testing of theories as well as allowing for a clean physics interpretation of the results. Calculations were performed on the supercomputer “Govorun” of JINR. O.C. contributed to theory and numerical simulations. All authors contributed to the manuscript.



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

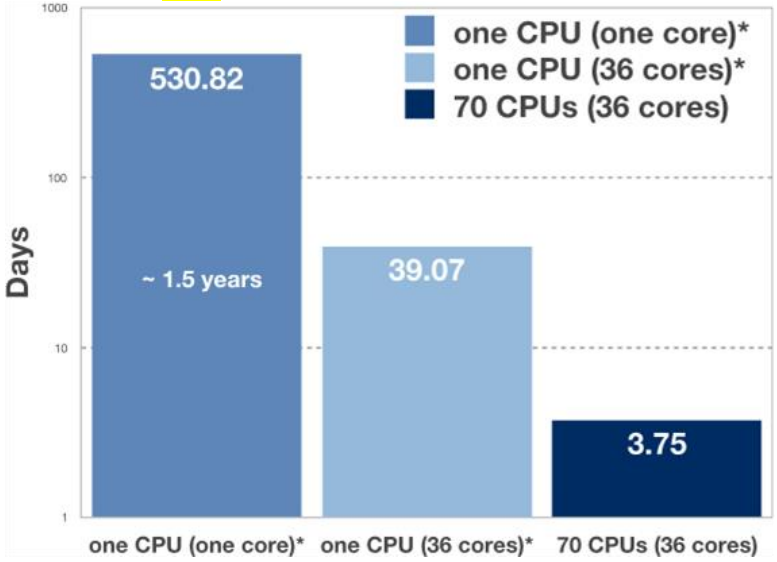
• **Compton ionization of hydrogen atom near threshold by photons in the energy range of a few keV: nonrelativistic approach** [114]. A theory aimed at describing the results of unique experiments on measuring the fully differential cross sections of the Compton single ionization of the helium atom near the ionization threshold at photon energy of a few keV is discussed. Ionization cross sections of the reaction $(\gamma;\ \gamma e)$ at the hydrogen atom are derived due to the theoretical simplicity of the model. Special attention is paid to the study of the kinematic region of the reaction near threshold, where it is expected to obtain valuable information about the initial and final states of the target. Calculations were performed on the Central Information and Computer Complex and heterogeneous computing platform HybriLIT through supercomputer "Govorun" of JINR.

► **MPI and OpenMP computation of nucleus-nucleus optical potential** [115]. Test calculations of the total cross section of the ^{6}He + ^{28}Si scattering at the energy 50 A MeV show that both techniques provide significant comparable speedup of the calculations.

► **JINR cloud driven high-performance calculations using HybriLIT resources** [116,117]. The use of HybriLIT resources within the JINR cloud service for parallel applications is illustrated on the study of superconducting processes in the stacked long Josephson junctions.

• **High-performance calculations of physical observables in spintronics** [118].
The ϕ_0 -Josephson junction model in the "superconductor–ferromagnet–superconductor" system was investigated. For numerical simulation in a wide range of parameters which requires a significant computer time, a parallel MPI/C++ computer code was developed and implemented on the HybriLIT cluster and "Govorun" supercomputer.

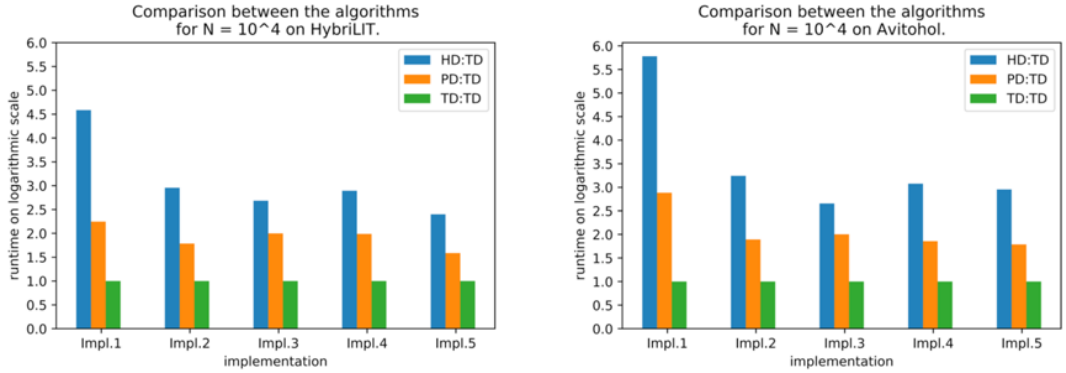
► **High-performance calculations for design optimization of a pulsed cryogenic cell** [119,120]. To solve the optimization problem yielding the characteristics of the thermal source of a cryogenic cell, an MPI+OpenMP hybrid parallel calculation algorithm based on the brute force method was developed [119]. The solution of the optimization problem for a specific cell configuration on the "Govorun" supercomputer has demonstrated a ten- to hundred-fold acceleration of the calculations [120].



Actual computing time (*right column*) and estimated computing times (*left* and *middle columns*) on "Govorun" supercomputer [120].

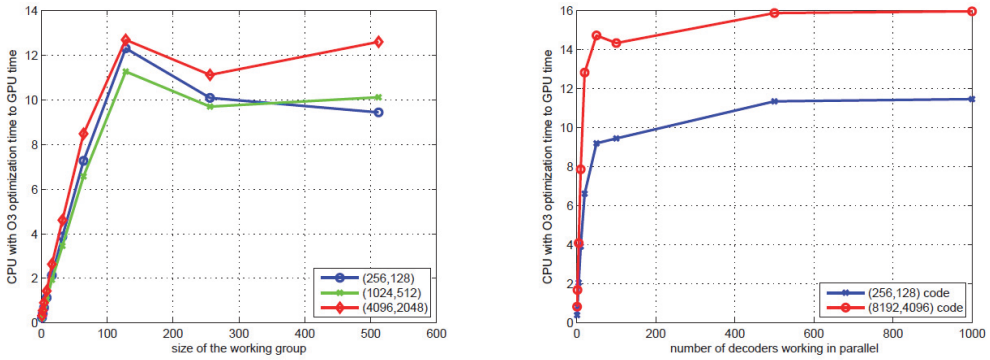
► **Efficient numerical solution of band matrix systems** [121,122]. The authors have reported performance analysis outputs on implementations of three different types of algorithms for solving band matrix systems of linear algebraic equations (SLAEs) got from discretizations of parabolic nonlinear partial differential equations. These algorithms have been implemented on

the “HybriLIT” and “Avitohol” clusters using the GiNaC library of C++ and the SymPy library of Python, considering five different data storage classes.



Comparison between different implementations of the algorithms for solving hepta-diagonal (HD), penta-diagonal (PD) and three-diagonal (TD) SLAEs of size N = 10^4.

► **Efficient Genetic Optimization of LDPC Codes to Improve the Correction of Burst Errors** [123,124]. Reliable bounds of correction capabilities for various code lengths and various redundancies of LDPC (Low Density Parity Check) codes are derived. Outputs of fast parallel solutions run on the HybriLIT cluster and the “Govorun” supercomputer illustrate the method capabilities within various working options (see figure below).

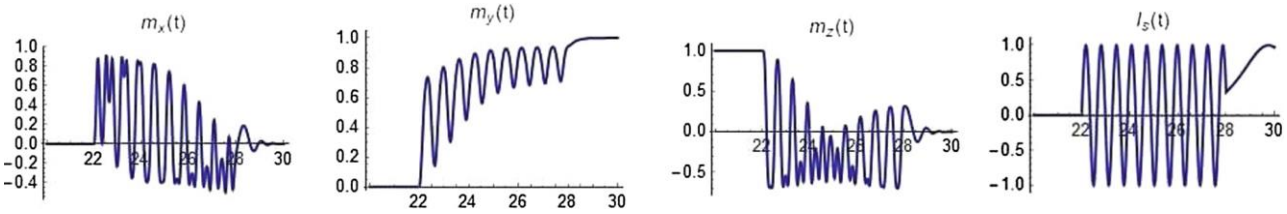


Measured acceleration within the CUDA framework [124]. Acceleration dependence on the block (working group) for 100 decoders running in parallel (left) and acceleration dependence on the number of decoders working in parallel when the size of the working group is 512 (right).

4.3. Numerical solution of difficult mathematical problems with guaranteed output under controlled accuracy

► **Numerical analysis of phase dynamics of stacks of long Josephson junctions** [125–130].

• The dynamics of magnetization, under the influence of a current pulse, in Josephson φ_0 junctions with direct coupling between the magnetic moment and the superconducting current is studied, in collaboration with the JINR BLTP and the University of Plovdiv [125–129]. The study of the time dependence of the magnetic moment for various values of the parameters of the φ_0 transition unveils parameter ranges where magnetization reversal takes place.



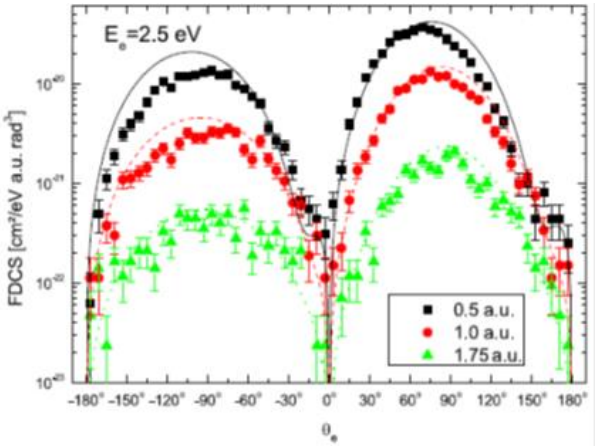
Results of the numerical simulation of the stiff system of equations within the spintronic model

• In usual numerical calculations of the intensity-voltage characteristics of Josephson junctions, the round-off errors may increase in an incontrollable manner. A new computation

scheme is proposed for which bounds of the rounding errors associated to the time and space discretization are kept under control [130]. Theorematic results are established to this purpose and practical experiments on the "Govorun" supercomputer confirm the theoretical results.

► **New Ways of Reducing Extreme Inner Problem Complexity**

• **Single ionization of helium by fast proton impact** [131]**.** Ultrahigh-resolution data on fully differential cross sections for single ionization of helium induced by 1 MeV proton impact are reported. Agreement with theoretical models is discussed. Reasons of discrepancies are investigated.



Experimental angular distribution in the scattering plane for E_e = 2.5 ± 1 eV kinetic energy. Black squares correspond to a momentum transfer q = 0.5 ± 0.15 a.u., red circles to q = 1.0 ± 0.25 a.u., and green triangles to q = 1.75 ± 0.4 a.u. Lines correspond to the model FBA + RHF for q = 0.5 ± 0.15 a.u. (solid black), q = 1.0 ± 0.25 a.u. (dashed red), and q = 1.75 ± 0.4 a.u. (dotted green). [131]

• **New derivation of non-canonical Bargmann-Moshinsky basis** [132–134]. Significantly simplified derivation of non-canonical Bargmann-Moshinsky (BM) basis is reported in connection with the Gram-Schmidt orthonormalization algorithm. Results are used for calculations of components of the quadrupole operator.

• **New symbolic-numerical schemes using finite element method** (**FEM**) [135–137], based on analytical Hermite interpolation polynomials in d variables on the standard d-dimensional hypercube and simplex, are developed. They serve to the solution of boundary value problems emerging from physics problems like the quadrupole vibration collective nuclear model.

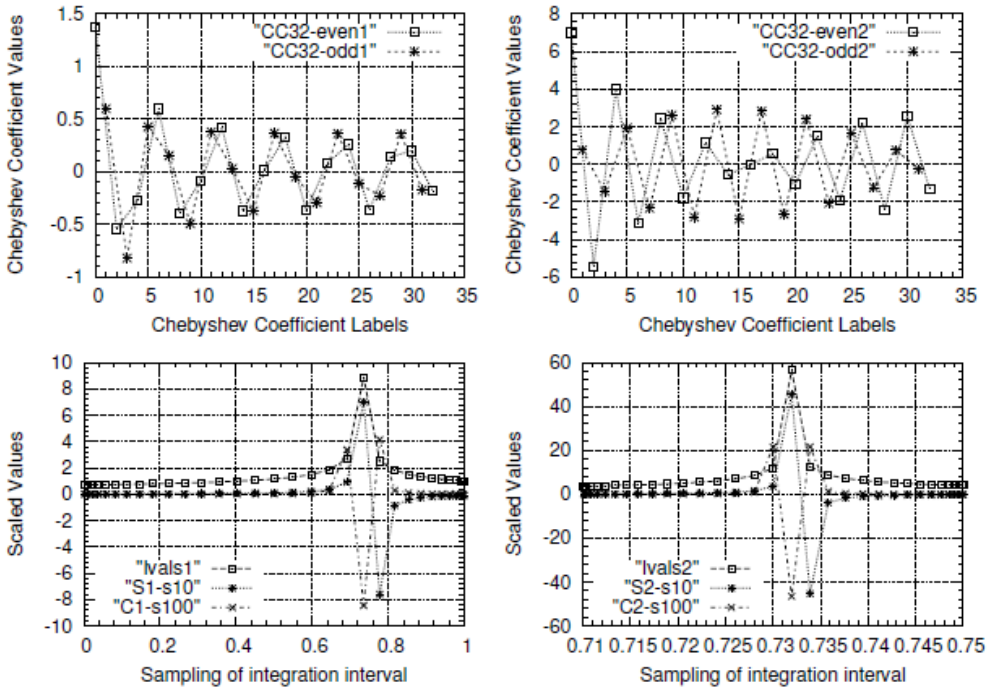
A special application of the new FEM is the solution of the vibrational-rotational states of the diatomic beryllium molecule with realistic potentials [138,139]

A specific ingredient of the above schemes is the KANTBP 4M program implemented in the computer algebra system MAPLE for solving, with a given accuracy, the multichannel scattering problem. An upgrade of this program was reported [140].

• **D_{3h} symmetry adapted correlated three center wave functions of the ground and the first five excited states of H_3^+** [141]. An original three-center wave function is constructed by means of the irreducible representations of the D_{3h} point group, which characterizes the symmetry of the planar equilateral triangular H_3^+ molecule. In contrast to the past large one center or linear combinations of functions of atomic orbitals, the proposed model has the advantage of being well adapted to all internuclear distances, with limited number of basis functions including the electron-electron term. Our functions satisfy, by their very nature, the triangular geometry of the molecule and thus allow the study of the asymptotic behavior of the potential energy curves of the fundamental and excited levels, for which new experimental and theoretical results are needed to confirm astronomical observations. The results of this work and the implementation of the computational techniques open the way to further studies of complex three center systems.

• **Problem adapted multi-scaling quadrature algorithms** [142,143]. The use of an m-panel rule (CC-32, Clenshaw-Curtis quadrature of algebraic degree of precision m = 32) over macroscopic integration ranges is supplemented with three-point Simpson rules spanned at triplets of

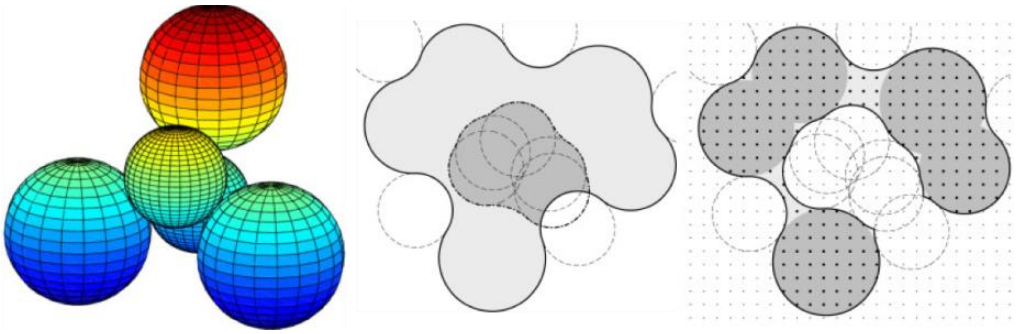
successive CC-32 knots. This allows identification and precise characterization of integrand irregularities through scale insensitive diagnostics (see figure below).



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

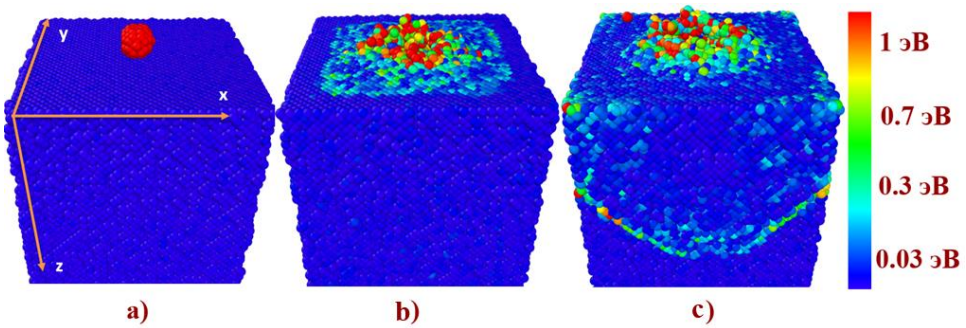
- **Solving complex protein problems: PBCAVE** [72]

Analytically defined values of the dielectric constant for all discretization points of a grid in the computational domain were resolved within the PBCAVE software package [71]. Assigned values of dielectric constant (see figure below) are used in a solver of the linear Poisson–Boltzmann equation for a protein–water system using a finite difference method.

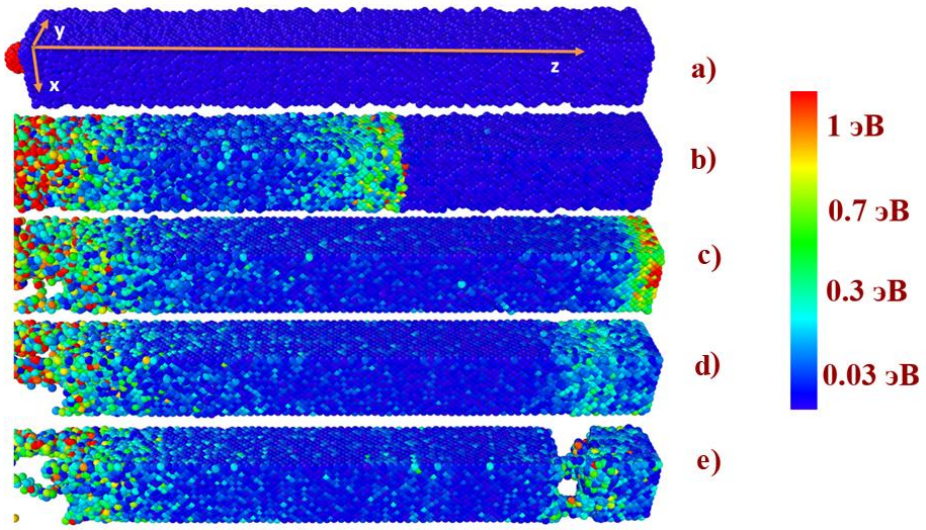


A wall triangle of three atoms (large spheres) of a molecule and two touching probe spheres (points in-between are not accessible for probe spheres and therefore are in "vacuum") (*left*). Intersection of inner and outer molecular surfaces (*middle*). Grid points inaccessible to water depending on the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

- **Molecular dynamics modeling of effects produced in metals by nanocluster bombardment** [144–146]. Molecular dynamic simulations of long-range effects in metal targets irradiated by nanoclusters unveiled in depth occurrence of fusion of high temperature moving regions. The temperature in the fusion region rises sharply, exceeding the melting temperature of the target. As a result, structural changes in the crystal lattice at a target depth exceeding the penetration depth of the nanoclusters can occur.



Dynamics of the propagation of a shock wave and the formation of a crater at the surface of a target when irradiated with a nanocluster of energy 100 eV/atom at instants of time 1 ps (a), 4 ps (b), and 10 ps (c). The calculated region was a parallelepiped with sides 11×11×18 nm, with periodic boundary conditions along x and y, the number of particles in the target was 183,000. On the right, the color scale of the kinetic energies of the particles is given [144]



Dynamics of the shock wave at the depth of the target upon irradiation with a nanocluster of energy 100 eV/atom at instants of time 1 ps (a), 4 ps (b), 7 ps (c), 10 ps (d) and 15 ps (e). The computed area was a parallelepiped with sides 3.6×3.6×51 nm, with periodic boundary conditions along x and y, the number of particles in the target was 40338. On the right, the color scale of the kinetic energies of the particles is given [144]

4.4. Results reported in large-scale collaborations

► **First Measurement of a Long-Lived $\pi^+\pi^-$ Atom Lifetime** [147]. The authors find a lifetime of the $\pi^+\pi^-$ atom which exceeds by three orders of magnitude their own previous result and conclude that the study should be consolidated by new investigations.

4.5. Developments in Computer Algebra and Quantum Computing

► **Development of symbolic-numerical algorithms for solving systems of nonlinear PDEs** [74,148–152]

• The method of triangular Thomas decomposition for polynomial nonlinear systems of partial differential equations described in [74] presents the Maple package implementation of the program TDDS included [73] in the program library of the journal Computer Physics Communications and in the latest versions of Maple. The package was used for algorithmic verification of linearizability for nonlinear (ordinary) differential equations [148].

• Methods and algorithms have been developed for building finite difference schemes for systems of partial differential equations that possess the property of strong consistence [149–152].

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

• **Identifying the Parametric Occurrence of Multiple Steady States for Biological Networks** [153]. We consider a problem from biological network analysis of determining regions in a parameter space over which there are multiple steady states for positive real values of variables

and parameters. We describe multiple approaches to address the problem using tools from Symbolic Computation. We describe how progress was made to achieve semi-algebraic descriptions of the multistationarity regions of parameter space, and compare symbolic and numerical methods. The biological networks studied are models of the mitogen-activated protein kinases (MAPK) network which has already consumed considerable effort using special insights into its structure of corresponding models.

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

To study the constructive models of composite quantum systems, an efficient algorithm was developed [154–158] and implemented for decomposing the representations of the wreath products of finite groups into irreducible subrepresentations [159–162].

• **Methods for the calculation of Feynman integrals** [163,164]. An approach based on the theory of functional equations was developed for the calculation of Feynman integrals and was used to the solution of difficult case studies.

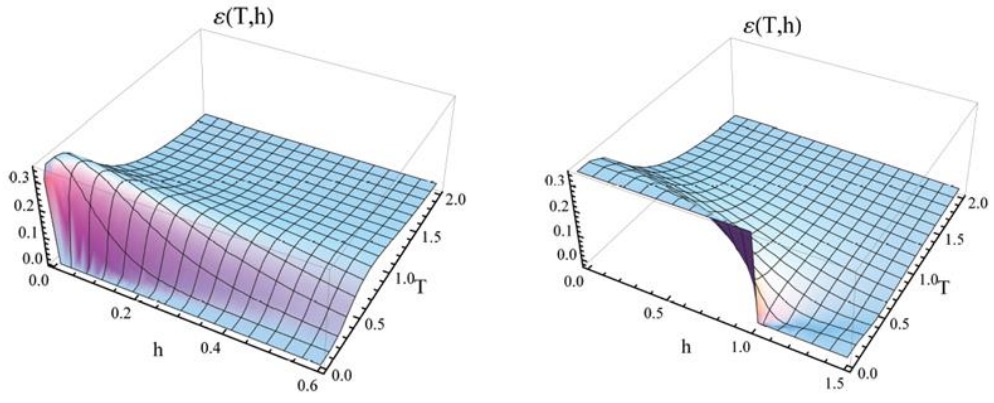
• **GPU resources for the computation of involutive and Gröbner bases** [165].

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

• **Foliations of SL(n) group and the space sl*(n)**. In the papers [166,167] the parameters on a conjugacy class in the Lie group SL(n) and the parameters on a coadjoint orbit in the space sl*(n) dual to the Lie algebra sl(n) were found. In this way the trivialization problems for the foliations of SL(n) group and the space sl*(n) were solved.

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

• **Entanglement production by statistical operators** [168]. Entanglement production by statistical operators, or density operators, is important in quantum measurements and quantum information processing. The measure of entanglement production by statistical operators is defined. Conditions are established showing when entanglement production gets maximal and when it is zero, which is essential for quantum measurements and quantum information processing.



Measure of the entanglement production as a function of dimensionless variables **T** and **h**. *Left*: ferromagnetic coupling (J>0). *Right*: antiferromagnetic coupling (J<0)

• **Mid-range order in trapped quasi-condensates of bosonic atoms** [169]. Finite Bose systems cannot display a genuine Bose-Einstein condensate with infinite long-range order. But, if the number of trapped atoms is sufficiently large, a kind of Bose-Einstein condensation does occur, with the properties of the arising quasi-condensate being very close to the genuine condensate. Although the quasi-condensate does not enjoy long-range order, it has mid-range order. It is

shown that the level of mid-range order in finite Bose systems can be characterized by order indices of density matrices.

• **Classicality indicator of an arbitrary N-level quantum system.** The global indicator for quantization of "classicality-quantumness" correspondence was introduced [170,171] and defined as the relative volume of a subspace with positive Wigner function of the state space of an N-dimensional quantum system, and it was exemplified for the Hilbert-Schmidt ensemble of qubits and qutrits.

• **Quantum teleportation of two-qubit Bell states**. In [172] the results of computational experiments on quantum teleportation of two-qubit Bell states done on five-qubit quantum computer IBM Q are given and compared with such teleportation performed on the classical quantum simulator Feynman written in Maple. Access to IBM Q was provided via the cloud service IBM Q.

• **Robustness of entanglement under quantum decoherence channels.** The robustness of entanglement in two qubits maximally entangled mixed states (MEMS) has been studied under quantum decoherence channels [173].

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

Only educated users can grasp the complex JINR hardware infrastructure. Therefrom, an essential task resolved within theme 1119 concerns the implementation and promotion, in close cooperation with theme 1118, of *an articulated and permanent educational system* with the aim to surpass the huge difficulties associated with the learning curves of the modern computing. The HybriLIT polygon has become the practical center for the education and growth of young specialists both from JINR and JINR Member States. Prominent specialists from JINR and from partner institutions in Russia and abroad are frequently giving lectures and tutorials at HybriLIT. Within the collaboration with Dubna University, the students are using HybriLIT for a twofold purpose: preparation of bachelor's and master's theses and solving tasks within JINR projects.

The International School of Information Technologies "Data Science" is a joint initiative of the Joint Institute for Nuclear Research and the Dubna University. The goal is to train highly qualified IT specialists for the development of megascience projects computing, Big Data analytics, digital economy and other perspective directions. In this frame, the second Summer Computer School "Big Data Analytics Dubna-2019" was organized during 6-13 July 2019 at Dubna University.

The periodical international conferences co-organized by LIT-JINR have become opportunities for intensive tutorials in high demand at associated satellite IT International Students' Schools. In 2019, the associated event to the "Mathematical Modeling and Computational Physics 2019" Conference (MMCP 2019) was the International IT-School "Machine Learning, Parallel and Hybrid Computations & Big Data Analytics" using the ML/DL ecosystem of the HybriLIT polygon (attendance 26 students). At the "27th International Symposium on Nuclear Electronics and Computing, 2019" (NEC 2019) organized by LIT-JINR and CERN, in Budva, Montenegro, the associated third International students school "Big Data mining and distributed systems" was attended by 32 students.

The school of young scientists "High-performance platforms for the digital economy and scientific projects mega-science class" was held at the G.V. Plekhanov Russian Economical University.

A fourth IT-school "Distributed Computing and Big Data", planned on April 2020 at Budva, Montenegro as well, was postponed to the autumn 2020, due to the Covid-19 pandemic.

The developed approaches to creating Big Data analytics platforms are successfully used in the educational process [174–176]. Finally yet importantly, it is worth mentioning the careful preparation of two textbooks for parallel programming [177,178]. These are useful both to the

students of the Dubna University and to all scientists interested in raising their grasp of this difficult but necessary field of reasearh.

• ***Organization of the International Conference MMCP 2019. Participation in other Scientific Conferences***

The Mathematical Modeling and Computational Physics (MMCP 2019) International Conference was held during July 1–5, 2019 at the Congress Center Academia of Slovak Academy of Sciences (SAS) in Stará Lesná, High Tatra Mountains, Slovakia. Together with the permanent organizer of the MMCP conferences, the Laboratory of Information Technologies (LIT) of the JINR, the co-organizers of the tenth MMCP edition have been the Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH), Bucharest, Romania, and four Institutions from Košice, Slovakia (the Institute of Experimental Physics (IEP) SAS, the Slovak Physical Society (SPS), the Technical University (TU), and the Pavol Jozef Šafárik University (PJŠU)). In the tradition of the previous MMCP conferences, it was an open forum to exchange ideas, strengthen personal relations, find incentives for future cooperation, learn and communicate within a wide range of topics. A satellite event of the MMCP 2019 was the abovementioned HybriLIT based International IT-School. The MMCP 2019 was attended by 104 participants from 12 countries. A number of 18 invited and plenary lectures and 74 oral communications (3+23 from theme 1119) were delivered. The Proceedings (revised selected papers) published in EPJ Web of Conferences, Vol. 226 (2020), (Editors Gh. Adam, J. Buša. M. Hnatič), present the 48 contributions which passed all the steps of a high standard reviewing process (19 papers with authors from theme 1119).

The 21-st International Workshop on Computer Algebra (23-24 May 2019) was organized and held in LIT-JINR.

A total of 27 invited lectures and 34 oral contributions have been delivered by authors working in theme 1119 at International Conferences other than MMCP 2019. From them, 10 presentations have been given at the NEC 2019 Symposium (Budva, Montenegro). Other Conferences with participation from theme 1119: ICASC 2019 (Sinaia, Romania), Conf. Series “Mathematics. Computer. Education” (XXVI-2019, Pushchino, RAS; XXVII-2020, DSU), Supervychisleniya & Mat. Modelirovanie (Sarov), POMI Seminars (St. Petersburg), ITTMM 2019 (ИПМиТ), etc.

• ***Perspective of the research within the theme 1119 on the current and the next year***

The Report demonstrates a wide and intensive front of works for the solution of computational physics subjet matters along all the four main activities foreseen in the Topical Plan for JINR Research and International Cooperation within the theme 1119.

Most of the topics covered in the present Report will be continued, new specific subject matters will be solved.

The main lines of our activity will be centered on the support of the overall success of the JINR research and on the contribution to increase of the JINR prestige in the worldwide research landscape.

Work on the organization of national and international schools for students, young scientists and specialists will continue.

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