Scientific report on the completion of Theme 1119 on 2017–2019

Gheorghe Adam, LIT-JINR & IFIN-HH

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

2. **Abstract**

The present report summarizes the most important achievements obtained during 2017–2019 within the JINR research theme 05-6-1119-2014/2019, "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data".
The organization of the presentation selects a few selected examples from the multitude of specific tasks solved within the theme 1119.

3. **Introduction**

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

The period covered by the present report corresponds to the first three years of the seven-year plan for the development of JINR 2017–2023. Within the broad research effort deployed in JINR, the expertise of the LIT scientists was needed for the solution of computing tasks asked by over 40 JINR scientific projects.

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

The first comes from the rapid pace of evolution of the computing facilities. With the advent of the new supercomputer "GOVORUN" at the end of the first quarter of 2018, *thinking as a computer scientist*, which assumes expert knowledge of several modern programming techniques, has become a basic duty of every LIT scientist. However, this does not alleviate the *need of a deep mathematical expertise* enabling the correct formulation of the problems. Besides that, a *high education level in numerical analysis* is necessary to assess the computational complexity of the problems to be solved. Last but not least, the *profound understanding of the physics side of the problems* is necessary. This has complicated our life, raising as the first priority the need of close cooperation for the solution of real problems.

The work of the experimental setups in heavy radiation fields periodically raises the need for detector reconstruction to add newly acquired expertise. The addition of new features aimed at improving the existing experimental setup frequently asks for radical changes of the algorithm designs and of their implementation into a software code. This feature illustrates the empirical observation that the implementation and maintenance of the software support to a given experiment are needed during the whole lifetime of the experiment itself.

The accumulation of huge amounts of data in the large scale experiments has made more and more difficult the derivation of algorithms able to extract the useful information from the raw data.

To cope with this problem, two fundamentally new approaches are emerging: the quantum computing and the Big Data analytics. While these are mainstreams for the future four year period, they already ask for their consideration in the present days.

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

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

From the wealth of scientific results derived during 2017-2019 within the theme 1119 on the symbolic-numerical and numerical solution of a wide range of topics of interest to the JINR research, the present report will be selectively focused on a few cases of utmost difficulty.

4. From the heterogeneous computing cluster HybriLIT, to the HybriLIT heterogeneous computing platform (involving the training and testing polygon and the "GOVORUN" supercomputer) (overseen by D. Podgainy and O. Streltsova)

The strategic mission of the heterogeneous computing platform HybriLIT [1], under development in LIT-JINR as an indelible part of the Multifunctional Information Computing Complex (MICC) [2], is to provide the coverage the high performance computing (HPC) in JINR.

The starting point of the platform was the HybriLIT cluster which followed a short but rapid evolution driven by the supervision and the key decisions of the LIT management concerning its design and implementation: Modular development based on the most successful new hardware offers on the market and in-house development of an information-computing infrastructure with bilingual support in Russian and English of all web resources to meet the needs of scientist and specialist users from different JINR Member States.

The HybriLIT cluster infrastructure, which reached a top-performance of 142 TFlops in double precision by the end of 2017, has nowadays a twofold role. As a testing polygon, it allows the development from scratch of parallel applications for carrying out computations using computing architectures such as multicore CPUs, Intel Xeon Phi co-processors, and NVIDIA (Tesla K20, K40, K80) GPUs. As an education polygon it provides possibilities to hold tutorials on parallel programming techniques that help students to learn new computing architectures.

The "GOVORUN" supercomputer, inaugurated in March 27, 2018, is a project jointly developed by the Bogolubov Laboratory of Theoretical Physics and the Laboratory of Information Technologies, with the strong support of the JINR Directorate. This project is aimed at sufficient acceleration of complex theoretical and experimental researches in the field of relativistic nuclear physics and condensed matter physics at JINR, primarily the NICA project.

It is a two-component system [3] which includes a CPU-component using the newest Intel architectures (Intel Xeon Phi and Intel Skylake processors), as well as a GPU-component using NVIDIA second generation DGX-1 Volta, with a top summed performance of 500 TFlops in double precision.

A critical issue concerning the efficient use of the "GOVORUN" supercomputer is the creation of an ecosystem for data analysis and machine learning and deep learning (ML/DL) tasks to provide opportunities for the efficient development of mathematical models and algorithms as well as for resource-intensive calculations, including graphics accelerators which significantly reduce the computing time. The conception of such an ecosystem for data analysis and ML/DL tasks was set up and is under active development within the heterogeneous computing platform HybriLIT. It includes two components: the first one is designed for resource-intensive, massively parallel learning tasks of neural networks using NVIDIA graphics accelerators (Fig. 1a); the second is devoted to the design

and implementation of models and algorithms based on JupyterHub – a multi-user platform for working with Jupyter Notebook (Fig. 1b).

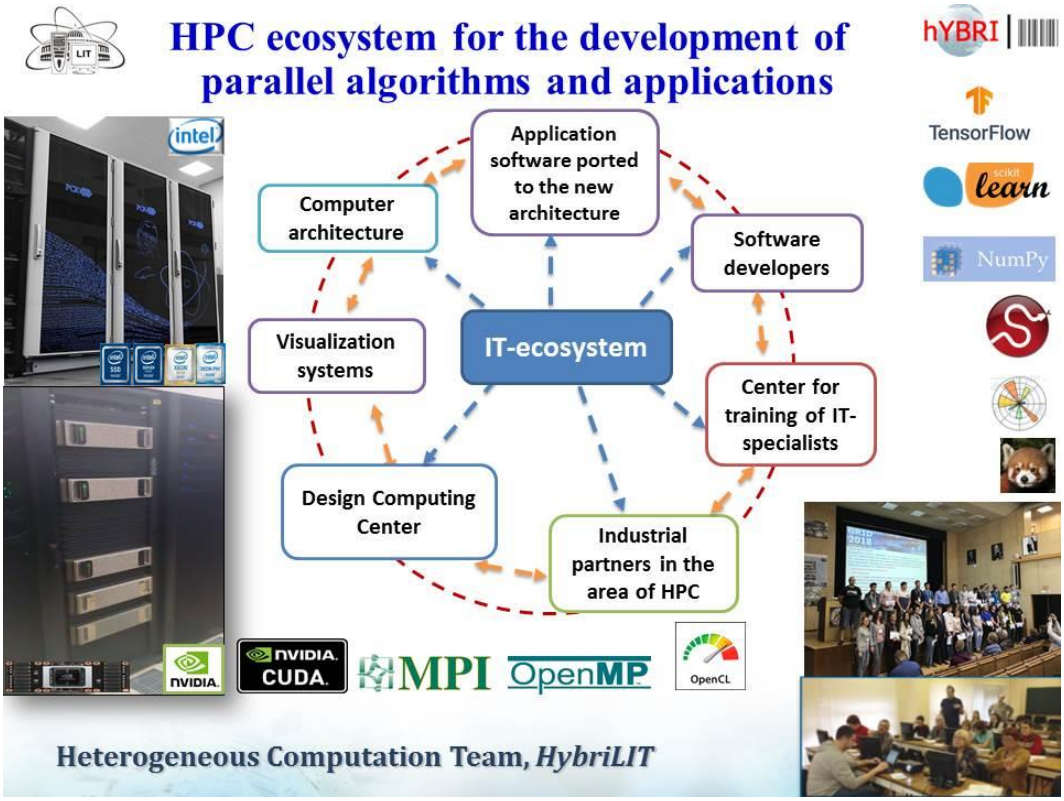


Fig. 1a

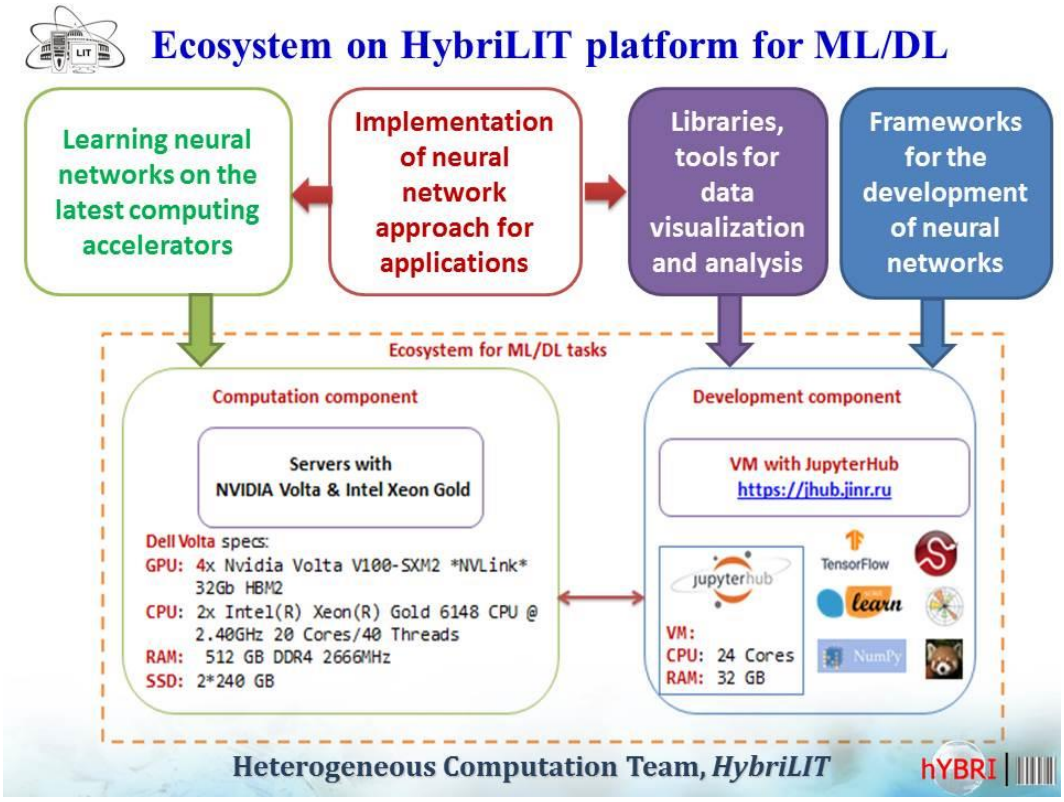


Fig. 1b

5. Selected results on magnetic field modeling within Theme 1119

► Modeling magnetic components of large scale facilities at NICA and FAIR [4-7]

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

Six cases worked out by P.G. Akishin [4] are shown in Fig. 2.

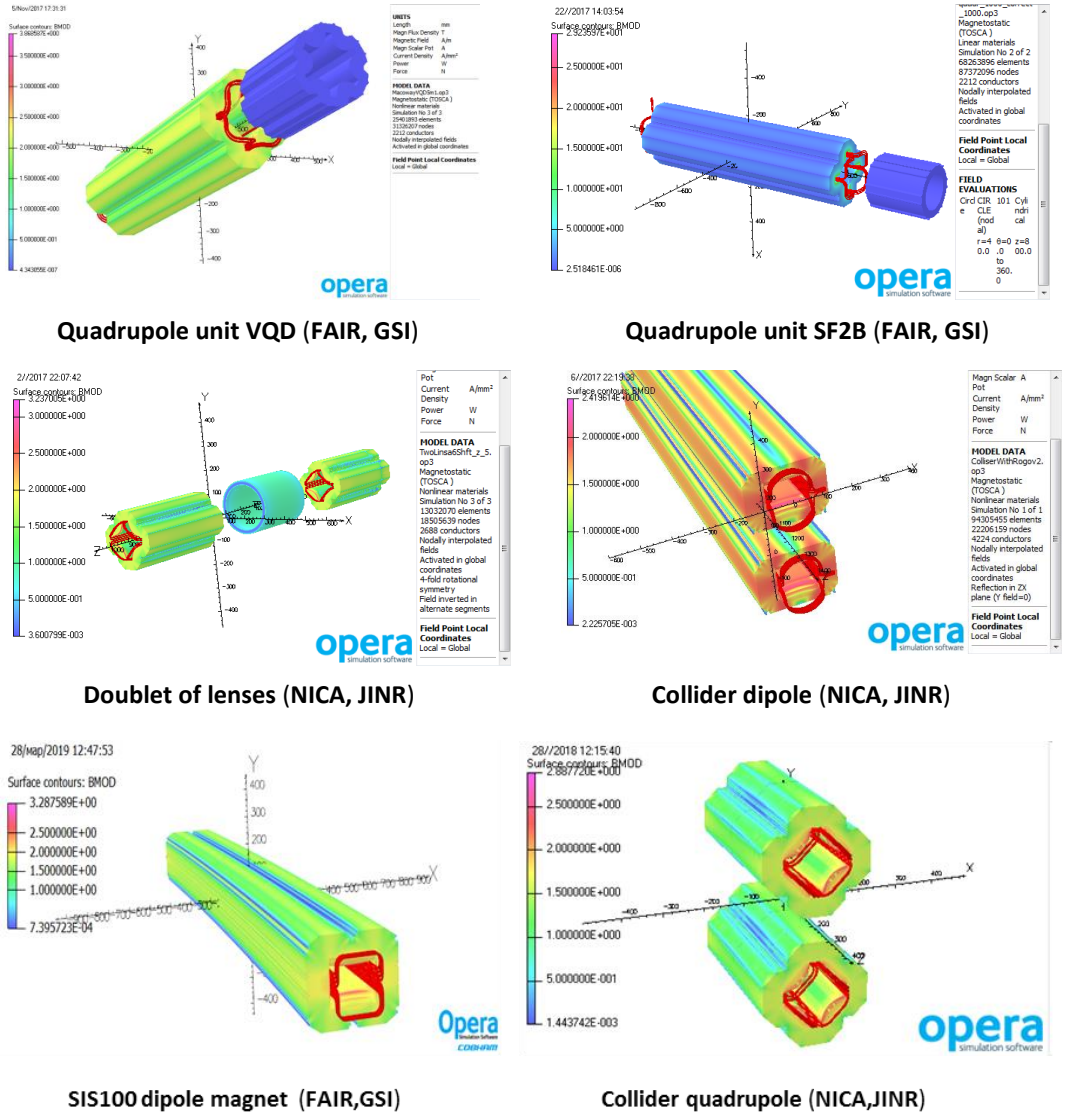


Fig. 2

• The researchers of JINR (Dubna) and Moscow State University are working on the simulation of the behavior of the solution of the magnetostatics boundary value problem in the vicinity of the "corner point" (at the intersection of two regions - vacuum/iron) of a ferromagnetic [6].

Modern accelerator systems and detectors are characterized by complex geometrical configurations of the magnetic field. Often the ferromagnetic/vacuum boundary has non-smooth elements consisting of corner points near which the boundary is formed of two smooth curves crossing at the corner point at some angle. The question then arises about the accuracy of the numerical solution of the boundary value problem in this region, where a significant growth of the magnetic field is possible.

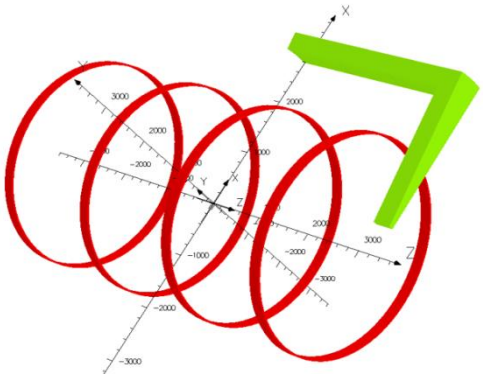


Fig. 3. Set of coils

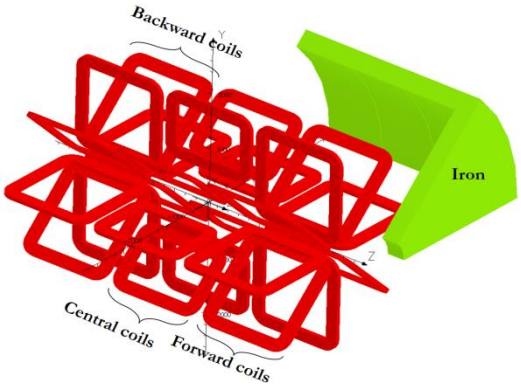


Fig. 4. "Toroidal" configuration

At present, the problem of the design of magnetic detectors providing high fields (over 1 T) is relevant, that is why it is particularly important to know accurately enough the field distribution everywhere inside the detector in order to consider side effects.

The 3D calculations for the SPD detector magnetic system of the NICA project are discussed in [7]. Three basic configurations of the NICA SPD magnetic systems are considered (Fig. 3-5): set of coils, "toroidal", and "hybrid". The model parameters are presented, the maps of magnetic fields are obtained, and the maps of integrals by trajectories are constructed. The "hybrid" configuration is chosen as basic in further work.

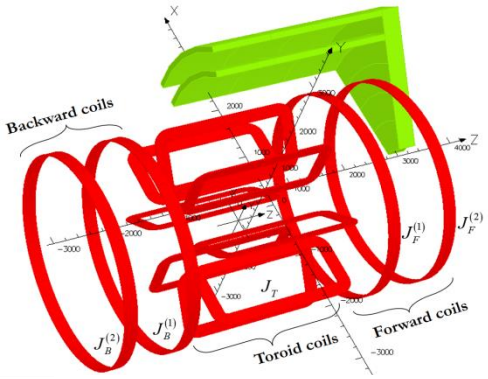
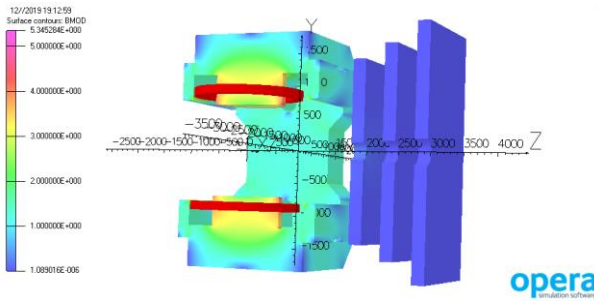


Fig. 5. "Hybrid" configuration

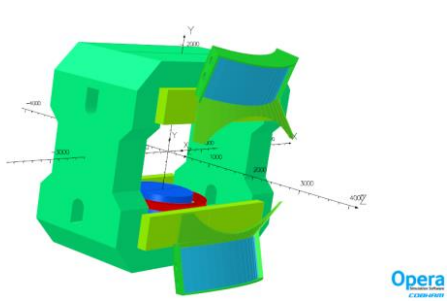
► **Modeling the CBM dipole magnet at GSI** [8, 9]

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) (Fig.6).



CBM dipole magnet, MUCH option (FAIR,GSI)



CBM dipole magnet, RICH option (FAIR,GSI)

Fig. 6

► **Modeling magnetic field configuration inside the SC202 cyclotron for proton therapy** [10,11]

Codes for SC202 beam dynamics simulations were improved with new algorithms where the magnetic field components outside the median plane are calculated up to fourth order (Fig. 7). Scripts were written for producing 3D magnetic field maps, 3D electric and magnetic field maps from RF cavity simulations in CST Studio and for reading them into the MATLAB workspace. MATLAB, being a matrix-oriented tool, allowed us to implement an equilibrium orbit search algorithm for a large number of particles with different energies with a good calculation speed.

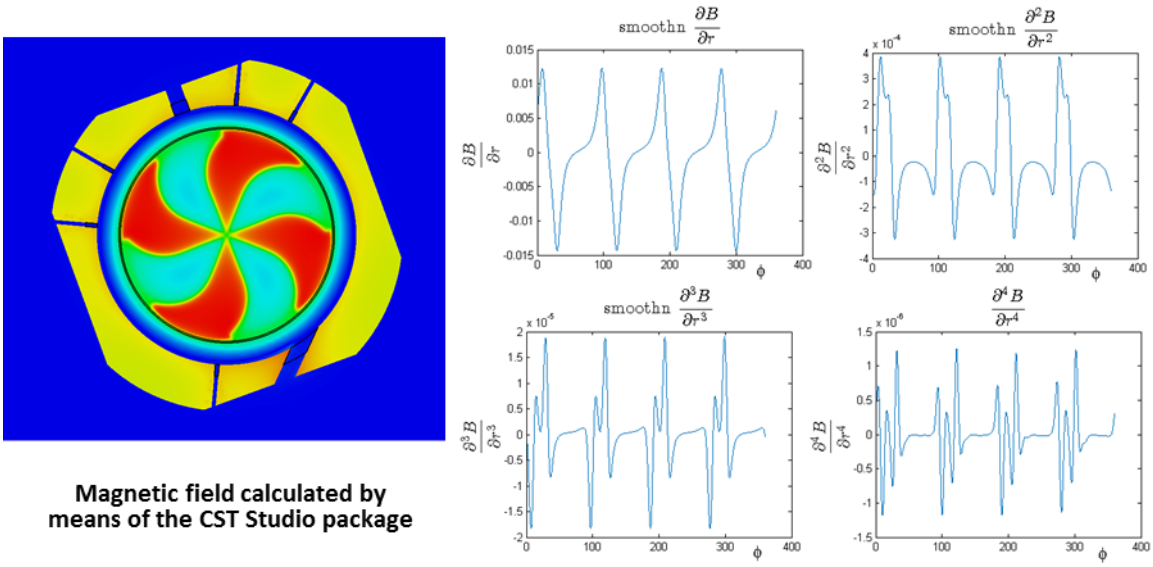


Fig. 7. Derivatives of the magnetic field in the median plane adjusted with smoothing algorithms

► **COMSOL Multiphysics solution of the magnetic field configuration inside the SC202 cyclotron for proton therapy** [12,13]

The simulations of the magnetic field distributions in the superconducting dipole magnet with a nonlinear magnetization (JINR–Hefei, China collaboration) were optimized based on the A-formulation of the magnetostatics with COMSOL Multiphysics. The V-formulation of the magnetostatics was developed by taking into account the nonlinearity of the magnetization and the superconductivity nature of the coil, and was verified by numerical modelling on the HybriLIT platform and experimental measurements of the field maps (Figs. 8-9).

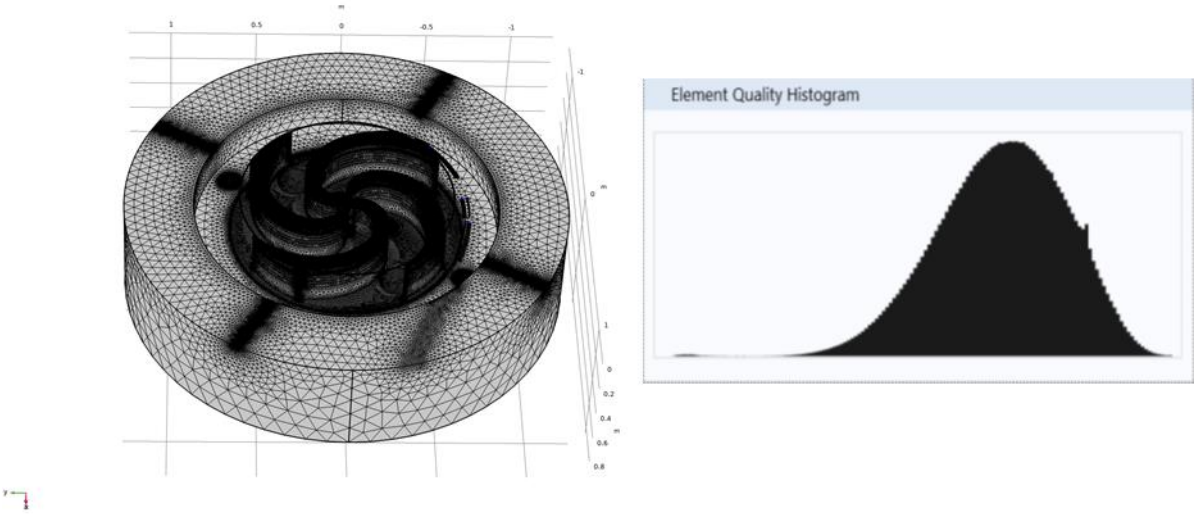


Fig. 8. To achieve the required accuracy of calculations, it was necessary to generate a finite element grid consisting of 18 445 665 tetrahedral elements. Computations were done on the HybriLIT platform.

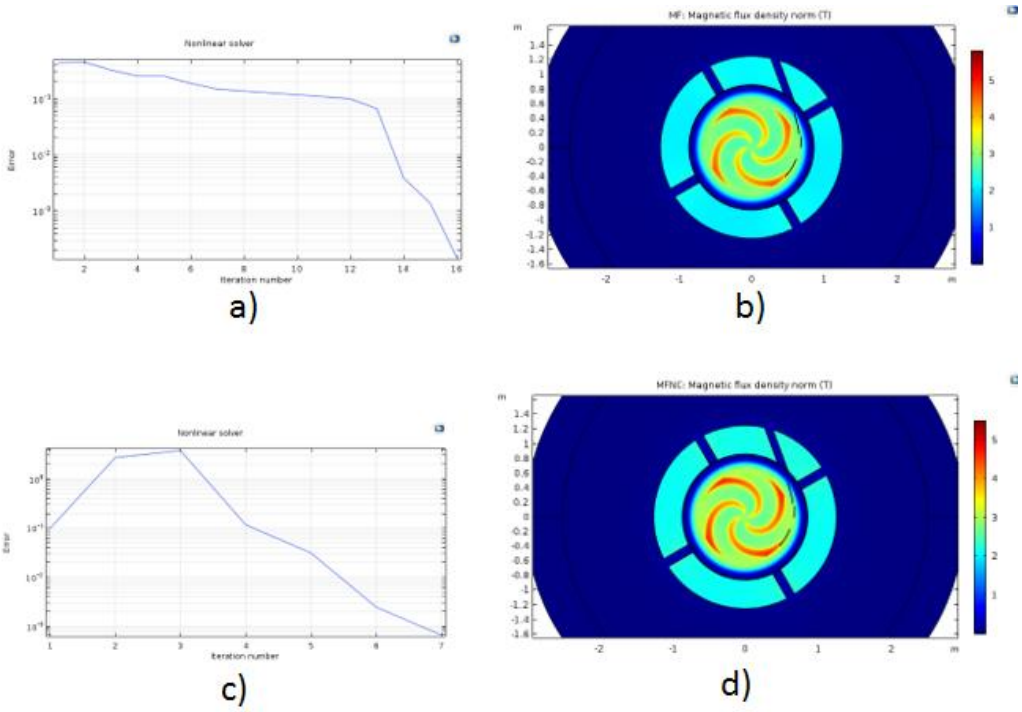


Fig. 9. Comparison of the results of the magnetic field map calculation in the median plane made in the COMSOL Multiphysics based on the A- formulation (a, b) and V- formulation (c, d) of the magnetostatic equations: (a, b): Degrees of freedom (DOF) − 21 801 942, Solution time − 18h17m16s, Physical memory − 94.48GB; (c, d): Degrees of freedom (DOF) – 3 237 238, Solution time − 19m51s, Physical memory − 28.33 GB.

6. Selected results on the development of mathematical models within Theme 1119

► Simulation of reactions with exotic nuclei using the microscopic optical potential model [14]

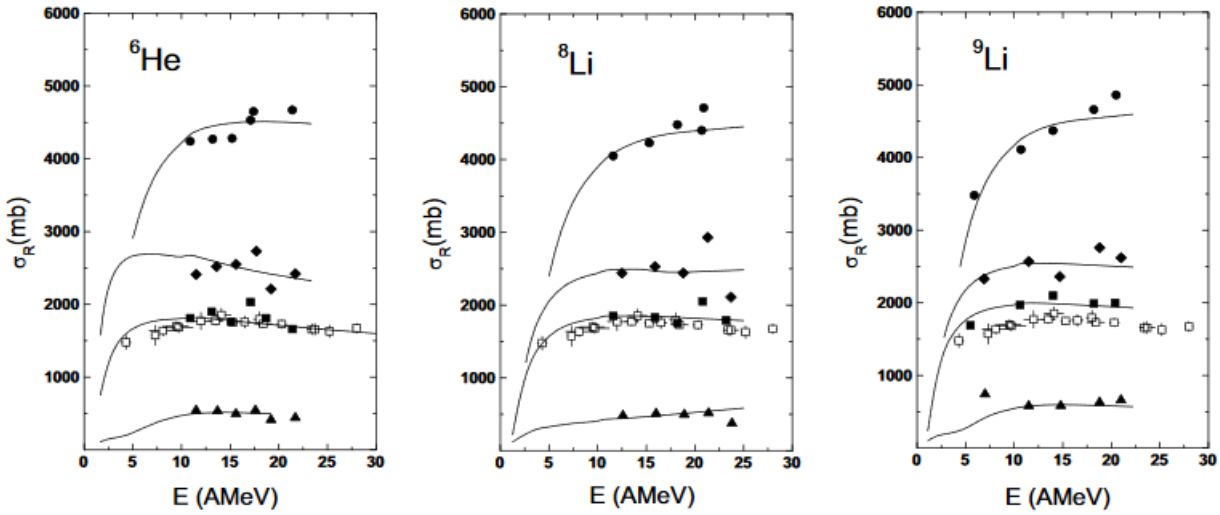


Fig. 10. Calculations of total reaction cross sections of ^{6}He, ^{8,9}Li with different targets. Projectiles are shown at left top corner of each figure. Lines show results of calculations, points – experimental data (black triangles: ^{9}Be target; black squares: ^{28}Si target; black diamonds: ^{59}Co target; black disks: ^{181}Ta target; for comparison, empty squares on ^{6}He + ^{28}Si reaction experimental data from an earlier work are shown)

Based on the hybrid model of a microscopic optical potential using three models of ^{12,14}Be nuclei density, calculations of the observed physical characteristics of the scattering of these nuclei during the interaction of these nuclei with a carbon and proton target were carried out. A good agreement with the experimental data on the scattering of ^{12,14}Be + p at energy of 700 MeV was obtained. It was

shown that adequate reproduction of the differential scattering cross sections of ^{12,14}Be + ^{12}C at an energy of 56 MeV/nucleon required consideration of the contribution of inelastic channels. The momentum distributions of ^{8}B breakup fragments in the reactions of this nucleus with other nuclei and the total cross sections for the reactions of ^{6}He and ^{8,9}Li with other nuclei in a wide range of atomic masses and energies were calculated on the basis of the microscopic approach (Fig. 10). A parallel version of the program package for the microscopic optical potential is available from the JINRLIB [15]

► **Developments of the Basic Element Method (BEM) and its application to simulations of the IBR-2M reactor noise** [16-19]

The technique and algorithms for digital processing of plane curves (closed, with free ends and with self-intersection points) with the aim of obtaining their analytical form were developed.

A technique and algorithm for calculating informative features that are invariant to geometric transformations of 2D curves defined by the coordinates of measured points have been developed.

The BEM method was used for the processing and analysis of the IBR-2M noise (Fig. 11), both for static and dynamic states of the reactor. Algorithm speed is adequate for real-time monitoring.

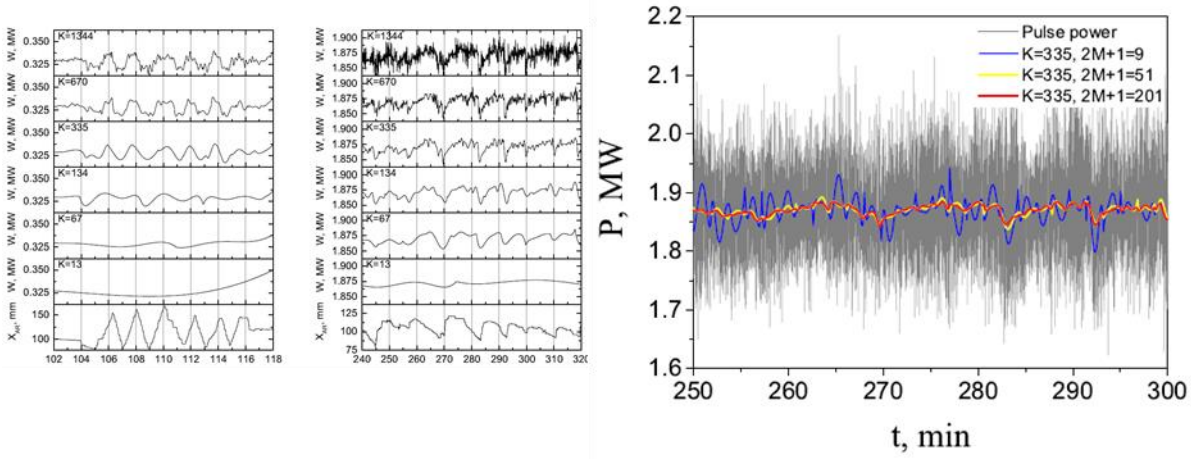


Fig. 11. **Left** and **centre**: Different approximating curves and positions of the automatic regulator (bottom). **Right**: Approximating curve as a function of the method parameters

► **NICA driven numeric-theoretical studies** [20-24]

• 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 Nambu–Jona-Lasinio model with Polyakov loop. The main idea of the work [20] was to show 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 [25] the fast increase in the $K+/\pi+$ ratio and its decrease at further increasing energy was interpreted as a sequence of the chiral symmetry restoration and deconfinement effect.

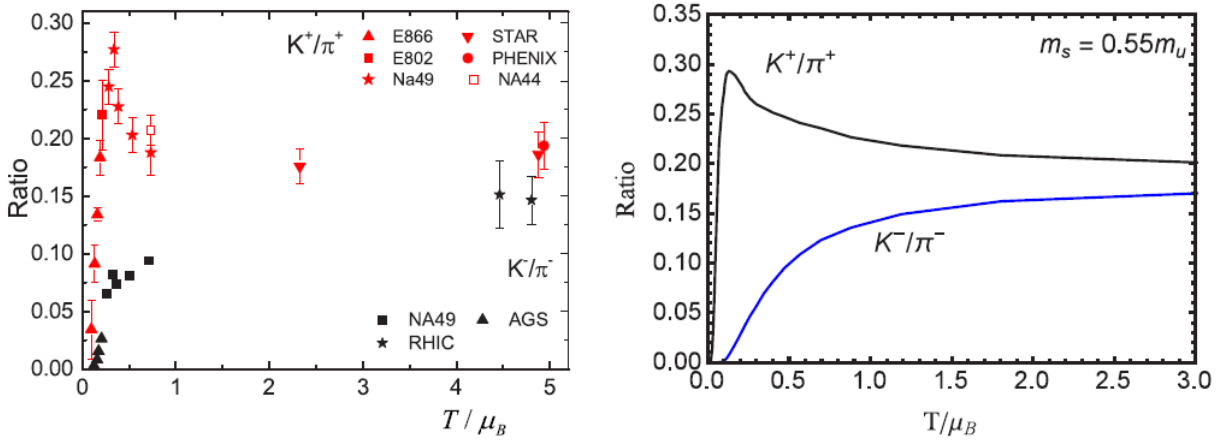


Fig. 12. Dependence of the ratios K^+/π^+ and K^-/π^- in terms of T/μ_B: experimental data (left) and simulation results (right).

The PNJL model gives a schematic description of the chiral phase transition, the deconfinement transition and meson properties at finite temperature and density. By using the model, it was shown that the splitting of kaon and antikaon masses appears as a result of the density variation. It may explain the difference in the $K+/\pi+$ ratio and the $K-/\pi-$ ratio at low energies. When the temperature and the baryon chemical potential are chosen at the phase diagram line, the system is in the phase-transition region, and the chiral condensate is still not destroyed. The main difference between the choice of T and μ_B along the line is whether we are in the crossover region or in the first-order transition region. It is also shown that the increase in the ratio $K+/\pi+$ appears near the critical endpoint and can be considered as a critical region signal (Fig. 12).

• The stability of solutions of the third family for hybrid compact stars with a quark core corresponding to the emergence of high-mass twins with respect to the softening of the phase transition using a design imitating the effects of 'pasta' structures in the mixed phase was investigated. A parametrized class of hybrid models of the equation of state based on the relativistic mean-field model was considered for both the hadronic and quark phases of matter. The effect of the construction of phase transition with a mixed phase consists in the appearance of additional pressure near the critical point belonging to the coexistence of the hadronic and quark phases of matter. The value of the relative additional pressure of about 6% at which the solution corresponding to the third family of compact stars disappeared was found. It was shown that at least the heavier star from the registered merger of a pair of neutron stars GW170817 could be a member of the third family of hybrid stars (Fig. 13) [22]. This result was included in the "BRIEF REVIEW OF THE TOPMOST SCIENTIFIC RESULTS OBTAINED IN 2018 AT THE JINR", JINR Publishing Department, 2019-1, p. 26.

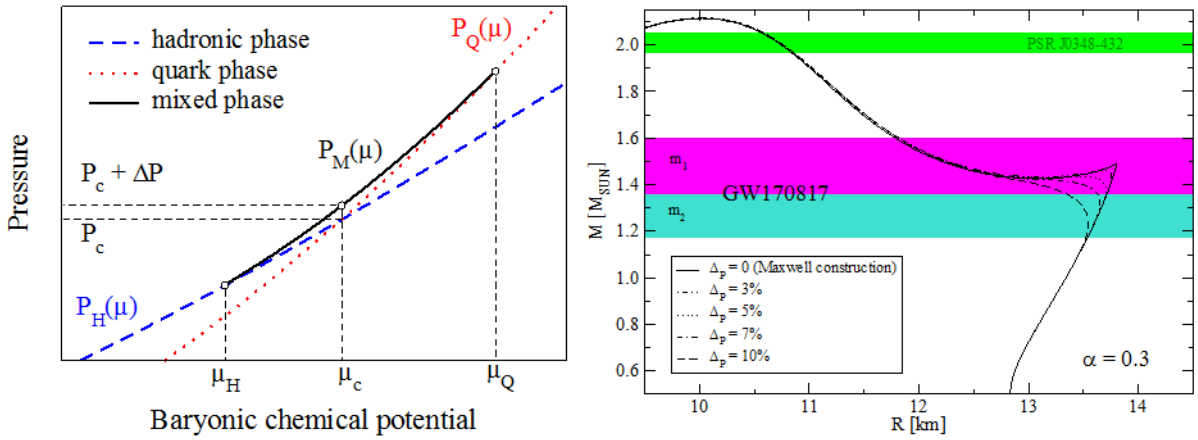


Fig. 13. Left: The three points of the interpolation function serving to the definition of the mixed phase. Right: The impact of the mixed phase in the mass-radius diagram of compact stars. At least one companion of the GW170817 could belong to the third family and both of them could have mixed phase in their interior

►HybriLIT/GOVORUN Enable Implementation of Efficient Numerical Methods for Hardly Solvable Problems [26-33]

• **The method of separated form factors** (SFF) is an effective method for studying the structure of polydisperse systems of phospholipid vesicles emerging from the analysis of small-angle scattering data. In this approach the basic parameters of the vesicular system are determined by minimizing the discrepancy between the experimental data of the small-angle scattering intensity and the results of SFF calculations. The minimization procedure is based on the generalized method of the least squares implemented in the FUMILI program of the JINRLIB library. The efficiency of parallel implementation was tested on the HybriLIT cluster using the parallel MPI version of the program PFUMILI [34]. An acceleration of calculations with a factor of 6–9 was obtained, depending on the number of experimental points. The assessment of the structural parameters of the vesicles of the phospholipid transport system was made on the basis of the numerical analysis of small-angle

neutron scattering data obtained on the YuMO small-angle spectrometer at the Frank Laboratory of Neutron Physics.

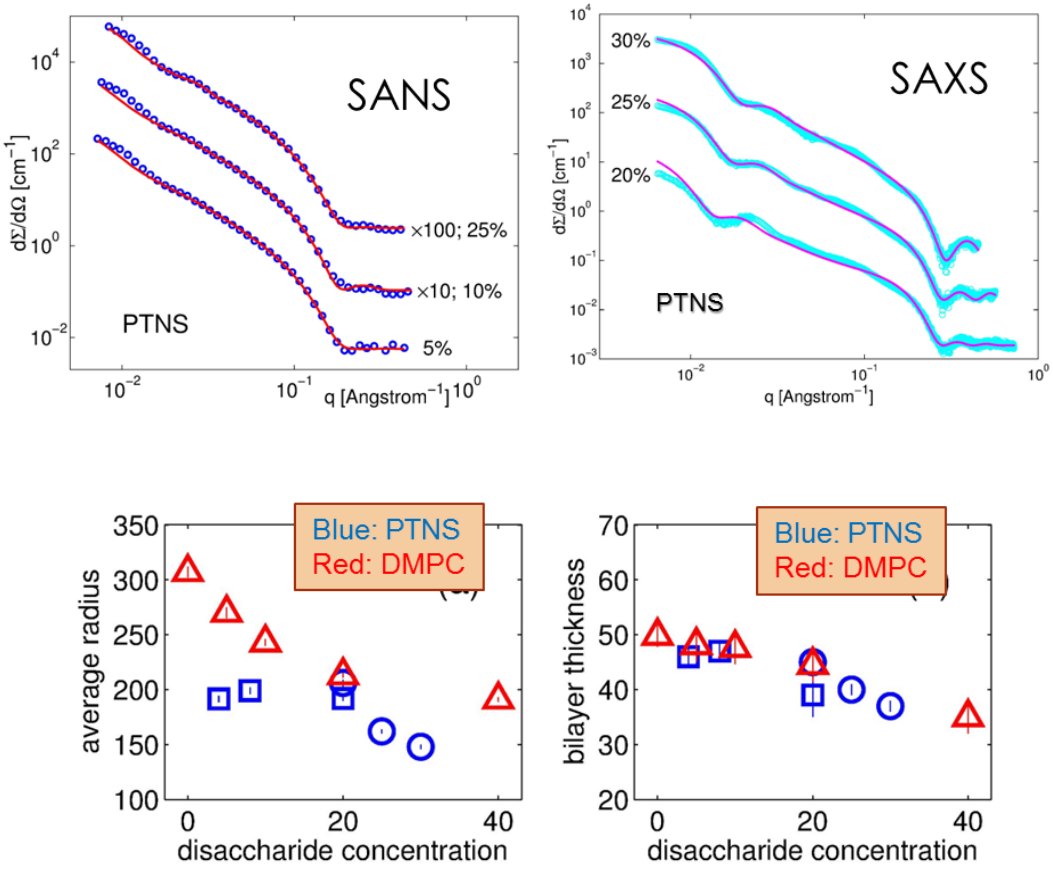


Fig. 14. Basic parameters of the Phospholipid transport nanosystem (PTNS) in water solutions of maltose (down) were estimated from joint analysis of SANS and SAXS data in terms of maltose concentration (up).

Phospholipid unilamellar vesicles (ULVs, liposomes) are important in medicine. Data collected by SAXS and SANS methods on ULVs are analyzed within the Separated form factors model (SFF), using ADE minimization & parallel MPI programming (Fig. 14).

Online interface was developed http://sff-sans.jinr.ru/

• **High-performance calculations of physical observables of a hydrated electron** have been carried out within the modified dynamical polaron model. The calculations have been performed on the GOVORUN (Dubna) and AVITOHOL (Sofia) supercomputers. Agreement of the numerical results with the experimental data is obtained [31].

Methodological calculations have been carried out to analyze the efficiency of the MPI implementation of the iterative local minimization method within the PFUMILI package [34] in order to fit the parameters of the RFF model using the small-angle scattering data on the HybriLIT cluster. The obtained acceleration is about 10 times.

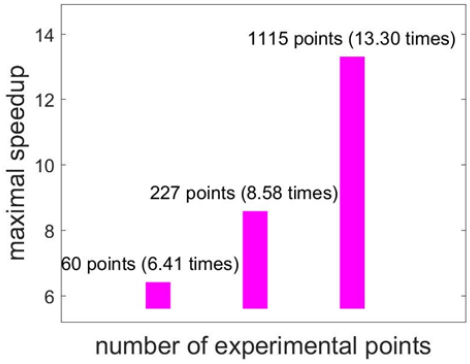
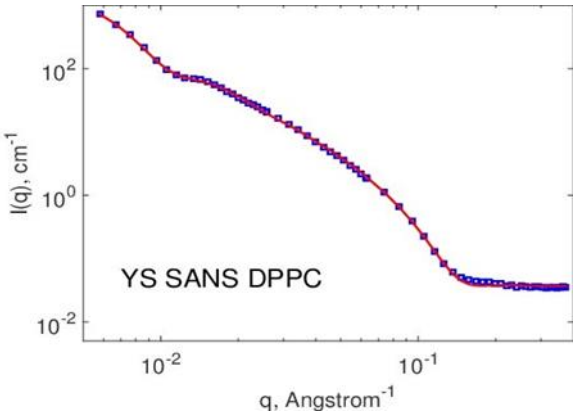


Fig. 15. Maximum speed-up achieved on the HybriLIT cluster for different numbers of experimental points

The estimations of basic parameters of the PTNS ULVs within the SFF analysis of the YuMO SANS data have been made (a case of the 20% concentration in the water solution). The calculation confirms the small size of the PTNS vesicle in comparison with the “classical” ULVs of DMPC and DPPC.



The SFF analysis of the structure of DPPC ULVs on the basis of the "Yellow submarine" SANS data has confirmed the results of the previous analysis of the YuMO SANS spectrum.

Fig. 16. Theoretical and experimental SANS spectra for the polydispersed DPPC ULV system in D_2O

Numerical simulation of the photoexcited electron states formation in water under the action of ultraviolet range laser irradiation is carried out within the polaron model with a time-dependent calculation of the hydrated electron absorption band width. This framework is shown to reproduce well the experimental data on the light absorption by the hydrated electron in polarized water. Effectiveness of parallel implementation is tested on the HybriLIT cluster (Figs. 17, 18) [31].

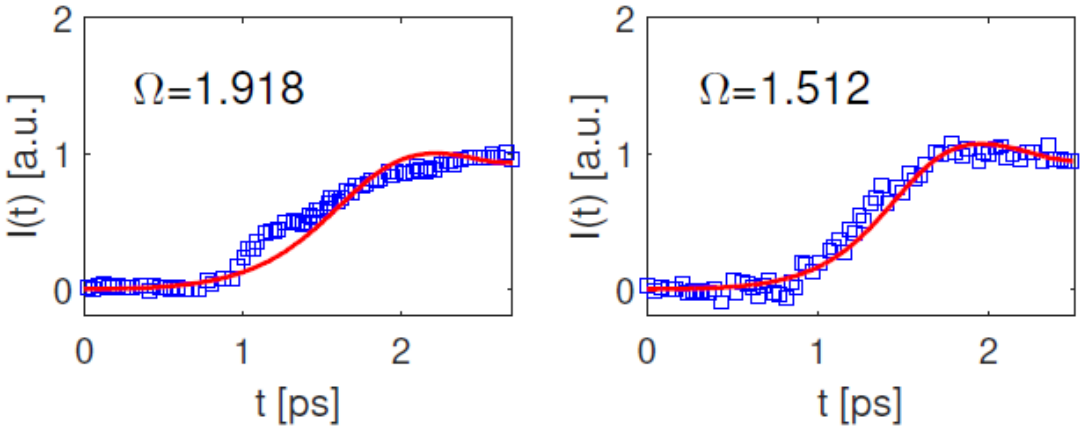


Fig.17. Numerical simulation of the light absorption by a hydrated electron for experimental data derived at light frequencies of the scanning laser Ω = 1.918 eV (left) and Ω = 1.512 eV (right)

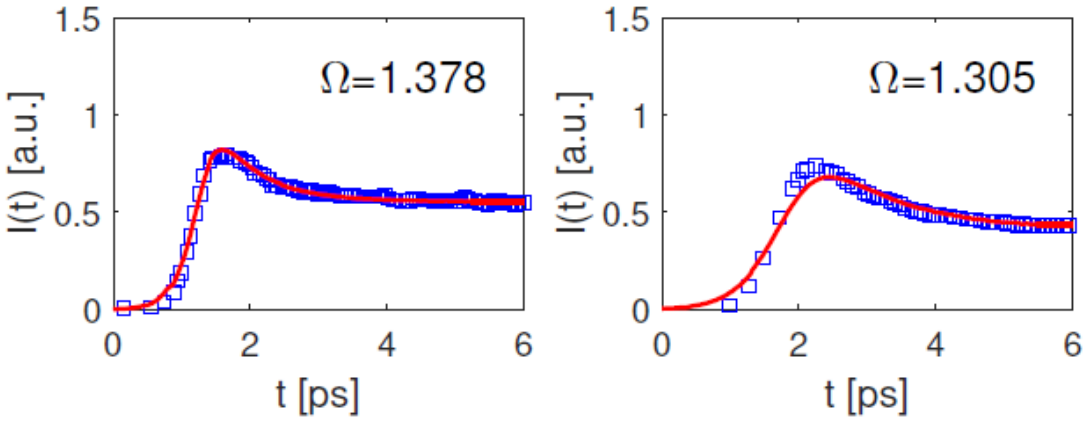


Fig.18. Same as Fig. 17 for experimental data at Ω = 1.378 eV (left) and Ω = 1.305 eV (right)

- **High-performance calculations for solving the optimization problem for designing a pulsed cryogenic cell** [35, 36]

Solving the optimization problem yielding the characteristics of the thermal source of a cryogenic cell, i.e. a multilayer cylindrical sandwich-type configuration designed for a pulsed dosed injection of the working substance into the ionization chamber of the source of multiply charged ions is considered. To solve the optimization problem, an MPI+OpenMP hybrid parallel calculation algorithm based on the brute force method was developed to get the maximum of the integral of

proportionality to the volume of gas evaporated from the cell surface. The algorithm leads to multiple solutions of the initial boundary value problem for the heat equation, which is solved numerically by the alternating direction implicit method (ADI). A method of simple iterations with an adaptive time step has been implemented to solve nonlinear difference equations. [35]. 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 (Fig. 19) [36].

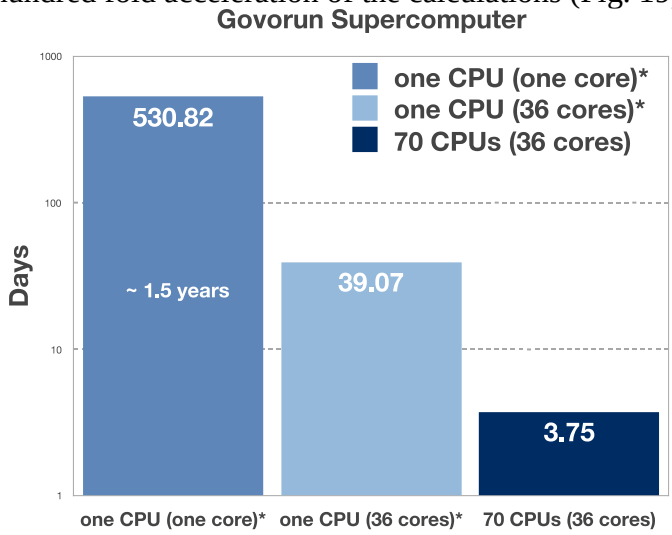


Fig. 19. Time of calculations using the GOVORUN supercomputer

• **Machine learning in high-performance computing infrastructures at JINR** (G. Ososkov, P. Goncharov, A. Nechaevskiy, A. Uzhinskiy)

♦ **Event reconstruction for data processing in high-energy physics** asks for the search of particle trajectories, which are registered as a set of detector responses to a particle passage (hits), and the estimation of track parameters from these data.

Since 2017, studies on the development of new tracking methods using deep learning have been started. A two-stage tracking algorithm for C-C interactions registered by the GEM detector of the BM@N experiment was developed with a track recognition efficiency of 97.5% on the Monte-Carlo simulation data. The drawback of this method was the exceedingly slow of the learning stage.

A new neural network (TrackNET) combining both stages of processing is under development. TrackNET is a deep recurrent neural network as an alternative to the Kalman filter, with the ability to learn necessary parameters from data. Preliminary tests show that the obtained TrackNET accuracy of the reconstruction on the Monte-Carlo simulation data is ~ 98% with a processing speed of 3,483,608 candidates per second for 2xTesla V100 on GOVORUN supercomputer [37].

♦ **Development of new methods for predicting air pollution with heavy metals**, was started in collaboration with FLNP, which is the coordinator of the UNECE International Cooperative Program (ICP) Vegetation in the framework of the United Nations Convention on Long-Range Transboundary Air Pollution (CLRTAP).

The analysis done for large data amounts evidenced the existence of connections between the heavy metal concentrations and data gathered from images provided by satellite projects. The available data have been used to train different statistical models and deep neural networks. Such an approach was successfully used to predict Sb in Norway [38], Mn in Serbia and U in Romania. The figure 20 illustrates one case study.

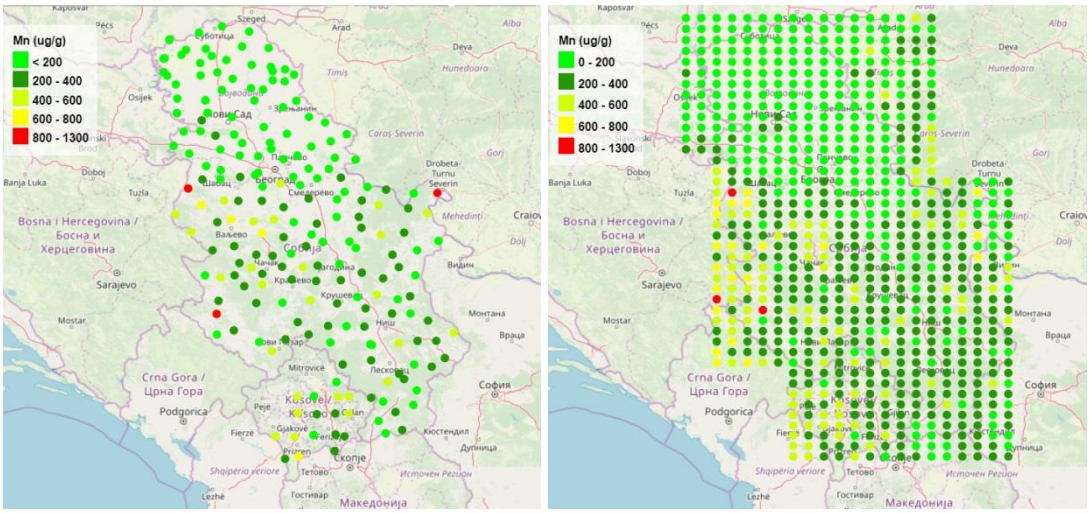


Fig. 20. Mn pollution in Serbia. Left – real data. Right – model prediction

7. Support of Experimental Data Processing and Analysis

New mathematical methods and emerging software for reliable data analysis are developed.

► **Reliable statistical inferences under low statistics and incomplete observation** [39, 40]

This is a permanent problem asked for scrutiny by the low-statistics experiments. The present investigations were particularly important for the rejection of claims made by outer groups concerning the unreliability of the low-statistics data associated to the creation of new superheavy elements in FLNR.

• The analysis of decay chains starting at superheavy nuclei ^{293}Ts and ^{289}Mc presented in [39] considered the spectroscopic properties of nuclei identified during the experiments using the ^{249}Bk+^{48}Ca and ^{243}Am+^{48}Ca reactions studied at the gas-filled separators DGFRS, TASCA and BGS. The analysis of decay data using widely adopted statistical methods and applying them to the short decay chains of parent odd-Z nuclei was done (Fig. 21). It was found that a recently suggested method of analyzing decay chains by Forsberg et al may lead to questionable conclusions when applied to the analysis of radioactive decays. The discussion demonstrates reasonable congruence of α-particle energies and decay times of nuclei assigned to isotopes ^{289}Mc, ^{285}Nh and ^{281}Rg observed in both reactions (Fig. 22).

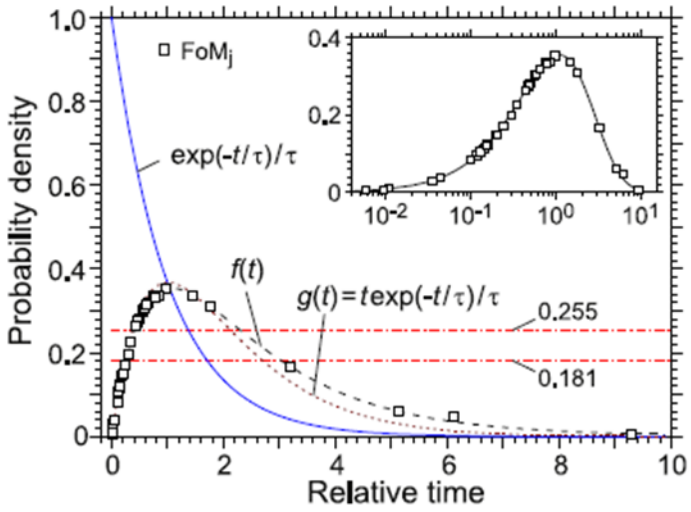


Fig. 21. Individual figure-of-merit values vs relative lifetimes given in τ units (squares), analytic expression for the probability density function f (t) (for 14 events, black dashed line), an 'exponential distribution' g(t) (brown short-dashed line), and 90% confidence interval for arithmetic mean FoM$_{ar}$ values (red dashed–dotted lines). Probability density function exp(−t/τ)/τ for an exponential distribution (blue solid line). FoM$_j$ values and function f (t) are also shown in the inset in logarithmic time scale.

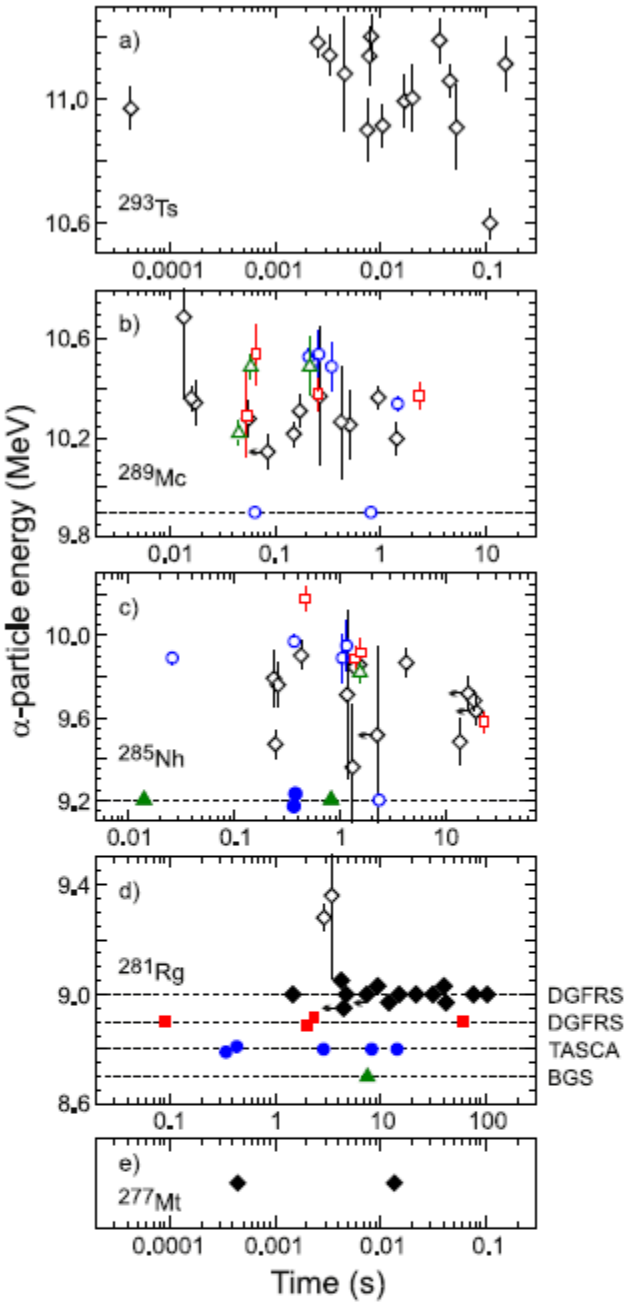


Fig. 22. Relation between measured α-particle energies E_α (with error bars) and decay times of isotopes assigned to ^{293}Ts(a), ^{289}Mc (b), ^{285}Nh (c), ^{281}Rg (d), and ^{277}Mt(e). Results from the DGFRS experiments observed in the reactions ^{249}Bk+^{48}Ca [8–10] (16 chains, the α decays of ^{293}Ts, ^{289}Mc, and ^{285}Nh were missed in 1, 4, and 2 cases, respectively) and ^{243}Am+^{48}Ca [2] (4 chains) are shown by black diamonds and red squares, respectively. Data from the ^{243}Am+^{48}Ca experiments carried out at TASCA [1] (7 chains) and BGS [3] (3 chains) are shown by blue circles and green triangles, respectively. Observed α-decay and SF events are shown by open and closed symbols, respectively. Time intervals for events following a missing α decay were measured from preceding registered events and are shown by arrows (upper limits). Decay times for events with partially measured E_α values (full energy was not registered) or SF events are shown on dashed lines with E_α=9.9 MeV for ^{289}Mc[1], $E_\alpha \approx$ 9.2 MeV for ^{285}Nh [1, 3], and $E_\alpha \approx$9.0MeV [8–10], $E_\alpha \approx$ 8.9 MeV [2], $E_\alpha \approx$ 8.8 MeV [1], and E_α= 8.7 MeV [3] for ^{281}Rg. For spontaneously fissioning ^{277}Mt only decay times are shown.

- **Check of data purity** [41], i.e. absence of impurities, is a necessary condition for the effectiveness of their analysis. A preliminary data testing for purity is a necessary step for a successful analysis. It is desirable that such a test is fast, reliable, and easy to perform. Naturally, it should not require a priori information about the parameters of the data distributions, and at the same time it should be insensitive to their statistics. To a certain extent, nonparametric methods, i.e. “short-cut statistics”, have a reputation of such methods. Their main idea for this case is to use a data characteristic having significantly different distribution functions on pure data and on mixtures.

Here the ratio of the sample median to the sample mean has been taken for the necessary test. It can be used for both the exponential and normal distributions. The confidence intervals for the functions of the ratio distributions have non-intersecting parts for clean data and mixtures, which serves as a basis for the evaluation of the plausibility of hypotheses about the degree of data purity (Fig. 23). The method can also be used for building estimates of the parameters of data distributions and their accuracy, the noise filtration from data and the optimum planning of the experiment.

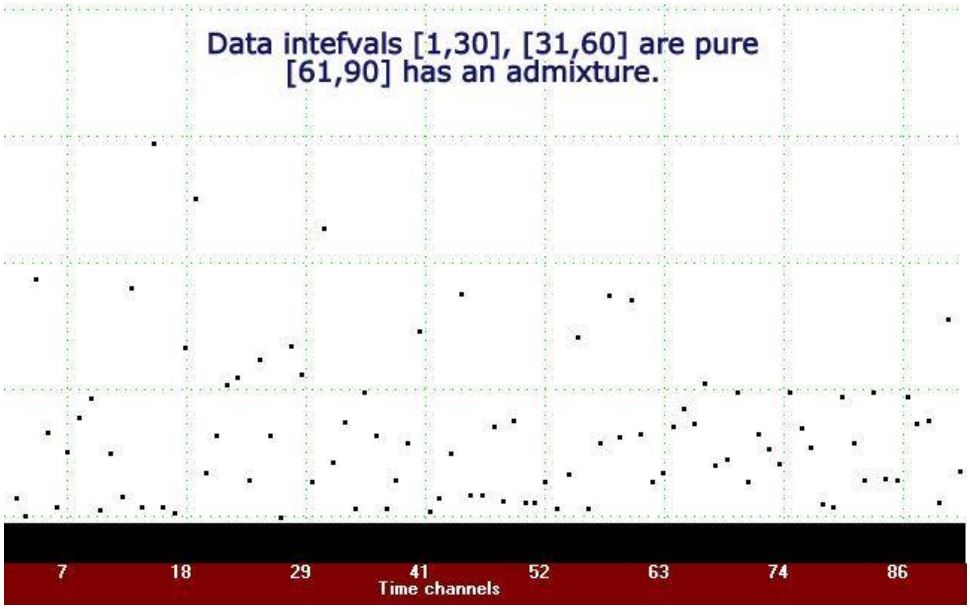


Fig. 23. Three groups of exponential decay data (30 events each) were simulated. Visually, it is difficult to understand what is what, but the test "the ratio of the sample median to the sample mean" gives correct answers: the first two groups are "clean", the 3rd one contains impurities.

►**Automation of on-line data storage on modernized YUMO spectrometer at IBR2-M** [42-49]

An inspection of the JINRLIB software library, maintained both in English and Russian shows that a same LIT author (A.G. Soloviev) has contributed, among others, to the creation of the repeatedly upgraded programs SAS [42] and PSD2SAS [43] (see also the Gitlab page of HybriLIT [44]) which provide online respectively offline information-computing environment for data processing and analysis of the most demanded IBR-2M detector, YUMO. The YUMO upgrade with position sensitive detectors has radically changed the design and implementation of these packages, with new developments foreseen for the near future.

PSD2SAS: Conversion of position-sensitive detector (PSD) data of small-angle neutron scattering spectrometer in isotropic pattern scattering case for automated SAS processing (Fig. 24) is the most recent instance of the modernization process of the YUMO setup (see [44] for detailed discussion).

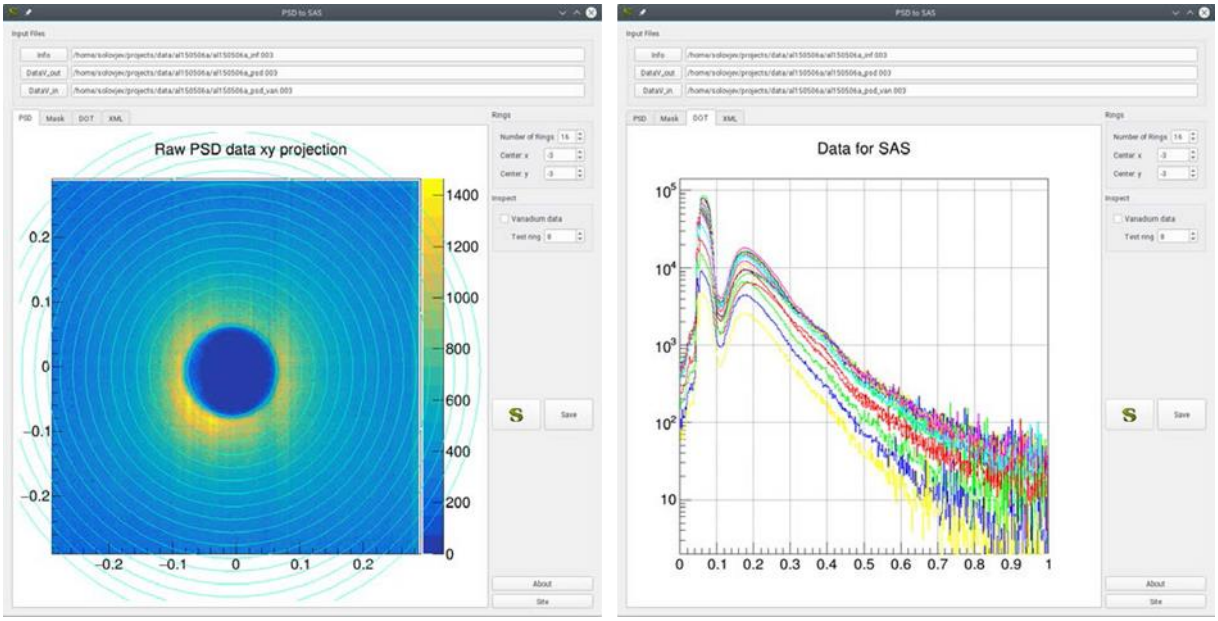


Fig. 24. PSD ring patterns (left) and time spectra (right) for these rings, ready for processing in SAS

►**Heavy-ion fragmentation reactions** at low and intermediate energies were described in a combined method. The first stage, the collision of two ions, was calculated in a transport approach with the use of test-particle method, the second one, the de-excitation of hot fragments, in statistical model. The applicability of the method was studied in a wide range of projectile masses (from oxygen to nickel isotopes) at energies from 35 to 140 MeV per nucleon. The comparison with the experimental data shows that this method describes well enough the isotopic distributions of the fragments. Velocity distributions have smaller width and are shifted to the left as compared to the experimental ones [50].

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

► **Contribution to the upgrade of Geant4 package and applications** [52-54]

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

The JINR scientists (V.V. Uzhinsky-LIT, A. Galoyan-VBLHEP) have continued to develop various modules of Geant4.

• **Improvement of Quark-Gluon String model** (**QGS**) of the Geant4 package. QGS is used by all LHC collaborations for simulations of particle penetration through detector setups at LHC energies. Thus, a correct description of particle interactions with various nuclei is very important for experimental studies. Recently, the NA61/SHINE collaboration has measured the meson resonance production in π^-C interactions at P_{lab} = 158 and 350 GeV/c [51] and found that the data cannot be well described by the well-known cosmic ray interaction models such as EPOS, QGSJet, SIBYLL and DPMjet, see Fig. 25 (left). The QGS model also badly reproduced the data.

The spectra are connected with quark and diquark fragmentation functions. The functions are solutions of integro-differential equations with a predefined kernel. In [52] it was proposed to modify the quark-diquark fragmentation kernel. The obtained results for the new kernel are shown in the Fig. 25 (right). As seen, the QGS simulation results have become closer to the experimental data.

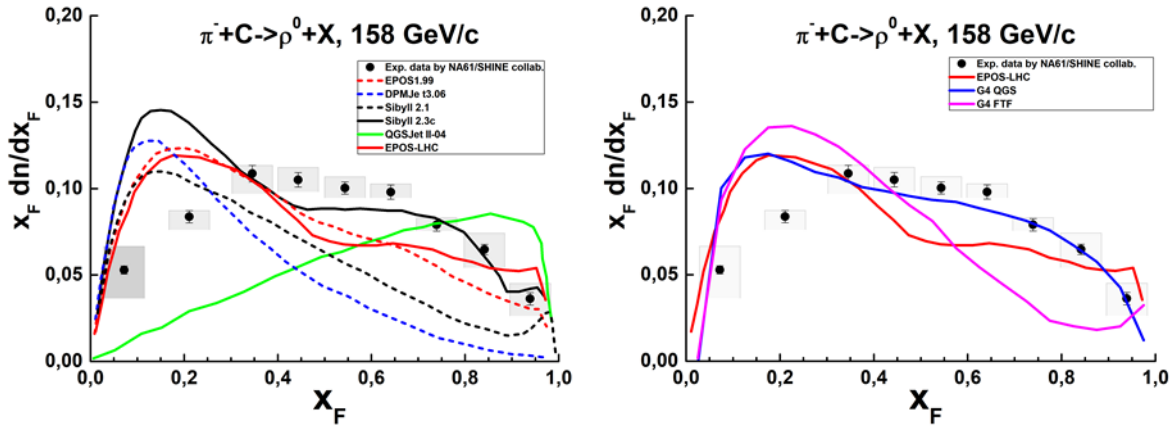


Fig. 25. Mesonic resonance distributions as functions of x_F. The points with statistical and systematical errors are the experimental data [51]. The solid (blue) lines are the calculations of the improved Geant4 QGS model. The long-dashed (purple) lines are the results of the Geant4 FTF model simulations. The short-dashed (red) and dotted (green) lines are the calculations by the EPOS and QGSJet models respectively.

• **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 and compared with the experimental

data obtained in LHEP on the SKM-200-GIBS and Propane Bubble Chamber installations. A good agreement between calculations using UrQMD+SMM and experimental data was achieved [53].

• **Simulation of the birth of strange quark-antiquark and diquark-antiquark pairs within the FTF model of the Geant4 package**. A good agreement between calculations using the improved version of the FTF model and experimental data from the NA61/SHINE collaboration on the production of K-mesons, antiprotons and Λ-hyperons into proton-proton, proton-carbon and π-meson-carbon interactions at different initial energies was obtained. In the framework of the improved FTF model the kinematic characteristics of Lambda-hyperons and K-mesons produced in antiproton-proton interactions were calculated and compared with experimental data at different momentum values of incident antiprotons. A good agreement between experimental data and calculations using the FTF model with new probabilities and rotating quark-gluon strings was achieved. The applicability of the FTF model for the development of the physical program of the Panda Phase0 and Panda Phase1 experiments was shown to hold (Fig. 26) [54].

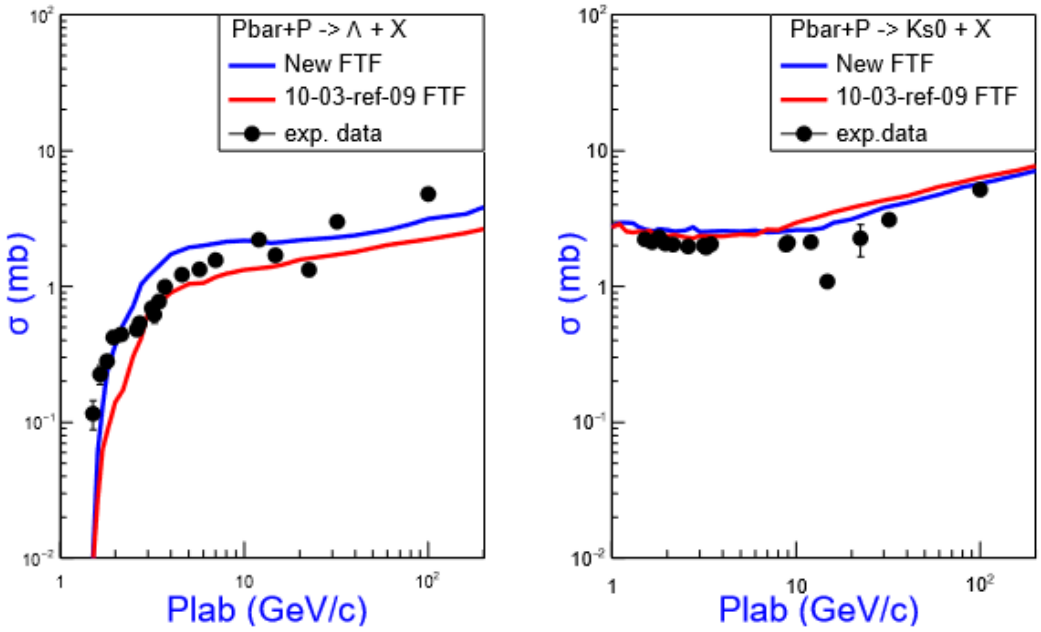
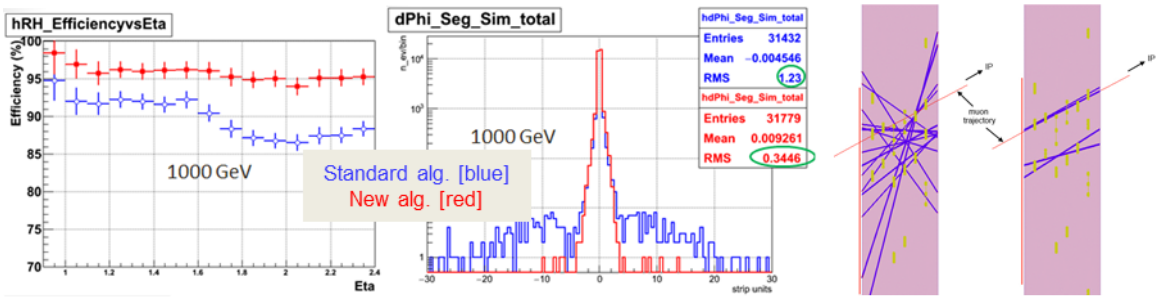


Fig. 26. Inclusive cross sections of Λ-hyperon and K^0_s-meson production in antiproton-proton interactions as function of projectile momentum

► **Contribution to the CMS experiment support** [55-57]

The segment building algorithm [55] for the Cathode-Strip Chambers (CSC) from the CMS experiment was developed with the aim to improve the reconstruction for high hit rates and big backgrounds generated by "hard" muons. The typical efficiency for TeV muons with respect to pseudorapidity is shown in Fig.27-a. It is high and almost constant, while the efficiency of the old algorithm decreases with the increase of the pseudorapidity [55-57]. The comparison of the difference in the azimuthal coordinate of the reconstructed and simulated segments (Fig.27-b) shows that the new algorithm reconstructs segments closer to the actual muon trajectory than the standard one.

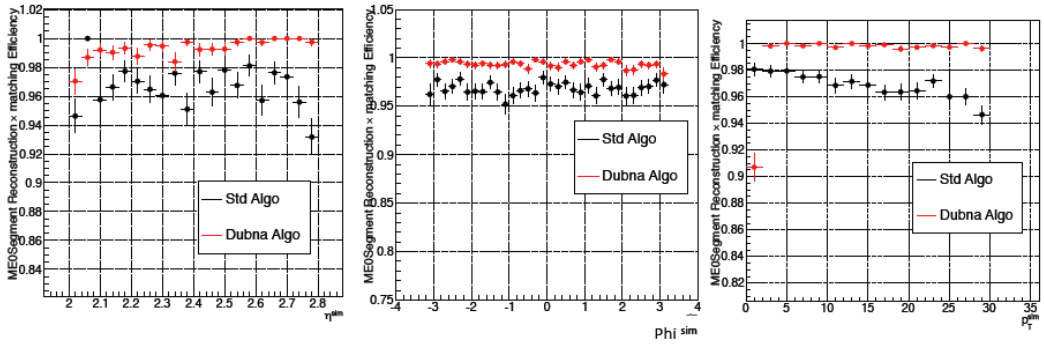
The developed algorithm takes into account the interaction point (IP) while reconstructing segments. As a consequence, the number of fake segments is considerably reduced in comparison with the standard algorithm. An example of a high hit multiplicity event is presented in Fig.27-c. The actual trajectory of the passing muon is drawn as a thin red line and almost coincides in direction with the IP. The reconstruction result of the standard algorithm is visualized on the left side of the picture. A lot of segments (blue lines) were reconstructed and all of them fail to reproduce the direction of the real particle. The new algorithm outputs for the same event are shown on the right part of the picture. Two segments are almost perfectly reproducing the trajectory of the muon and the overall number of segments is lowered to a reasonable amount.



(a) (b) (c)

Fig. 27. (a) – Reconstruction efficiency vs. pseudorapidity (old algorithm – blue, new algorithm - red); (b) – distance in strip units between the reconstructed and the simulated segment (old algorithm – blue, new algorithm - red); (c) – example of high hit multiplicity event (old algorithm – left, new algorithm – right).

Starting with 2017, the new algorithm became the default algorithm used for the reconstruction of real and simulated data. It proved to be effective, stable and robust. It was easily adapted as the reconstruction algorithm for the *new* GEM *detectors* that will be included in the experimental setup for the next major upgrade. The reconstruction efficiencies of the new (red) and the standard (black) algorithms with respect to different parameters are shown in Fig. 28. The new algorithm shows a high (~100%) and constant efficiency, regardless the parameter of interest.



a b c

Fig. 28. Reconstruction efficiency vs. different parameters of the simulated data. a – efficiency vs. pseudorapidity; b – efficiency vs. azimuthal coordinate; c – efficiency vs. transverse muon momentum

► **Contribution to the CBM experiment support** [58-60]

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

• A fast and efficient algorithm has been designed for the reconstruction of muon tracks in the decay J/ψ→μ+μ- registered by the MUCH detector of the CBM experiment. One of the key tasks of this experiment is to study the processes of birth of charmonium in high-energy nucleus-nucleus collisions. The registration of such decays like J/ψ→μ+μ- will be done in real-time. The muon track recognition algorithm is based on the model of cellular automaton (CA) which is used successfully in a number of experiments in high energy physics. The CA model is good because it allows one to reduce the number of recursive operations on the input data array and to perform most of the calculations locally. In this case, the CA elements (“cells") are segments of the broken line from which the approximation of the straight track is built. The track recognition algorithm includes three consecutive stages: calculation of average points; forming segments – the elements of the reconstructed tracks; connection of the segments and track reconstruction. The developed algorithm was included into the package CBMROOT as a dynamically link library under the name of Lx. This

same library is also supplied by algorithms that implement a trigger to select decays J/ψ→μ+μ- and a set of methods for tuning the parameters of the algorithm on model data [58].

• The LIT specialists in cooperation with their colleagues from the international CBM collaboration develop the readout and data acquisition systems of the ring imaging Cherenkov detector (RICH). A detailed analysis of the readout and DAQ prototype has been conducted using the data gathered during the tests of the CBM RICH prototype in the beam conditions at CERN and using the results of the laboratory measurements performed on a specifically developed test stand. The readout and DAQ module prototype consists of a Hamamatsu H12700 MAPMT, PADIWA preamplifier-discriminator boards and a TDC HUB board TRBv3. Calibration techniques were developed and implemented along with the DAQ and analysis code in the CBMROOT framework. Optimization of the readout module components has been performed what allows achievement of best timing characteristics in the high beam rate conditions expected at CBM. The obtained sub-nanosecond time precision allows one to directly measure the time profile of the additional wavelength-shifting films on top of the MAPMT windows and investigate their effect on timing of the full CBM RICH readout chain [59].

• The Geometry Database (Geometry DB) was developed for the CBM experiment. The main purpose of this database is to provide convenient tools for: 1) managing the geometry modules; 2)assembling various versions of the CBM setup as a combination of geometry modules and additional files. The CBM users of the Geometry DB may use both GUI (Graphical User Interface) and API (Application Programming Interface) tools for working with it [60].

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

• **The geometrical database** developed for the CBM experiment was adapted for the BM@N experiment. This application takes into account the specifics of the data flow when modeling the passage of particles through the installation [61].

• **Nuclotron beam momentum estimation in the BM@N experiment** [62,63]

A complex reconstruction algorithm for the Drift Chambers (DC) of the BM@N experiment was developed. The value of correction factors for the drift time of DC was calculated and implemented into the official software as global constants.

The spatial resolution achieved by using the experimental data varies from 180 to 300 μm for different planes of the detector. The efficiency is above 90% for all planes.

The beam momentum was estimated using the data gathered in the recent physical runs of the Nuclotron. All the estimated values and their errors satisfy the expected results, and the desired resolution of 2% was achieved for the working values of the magnetic field integral.

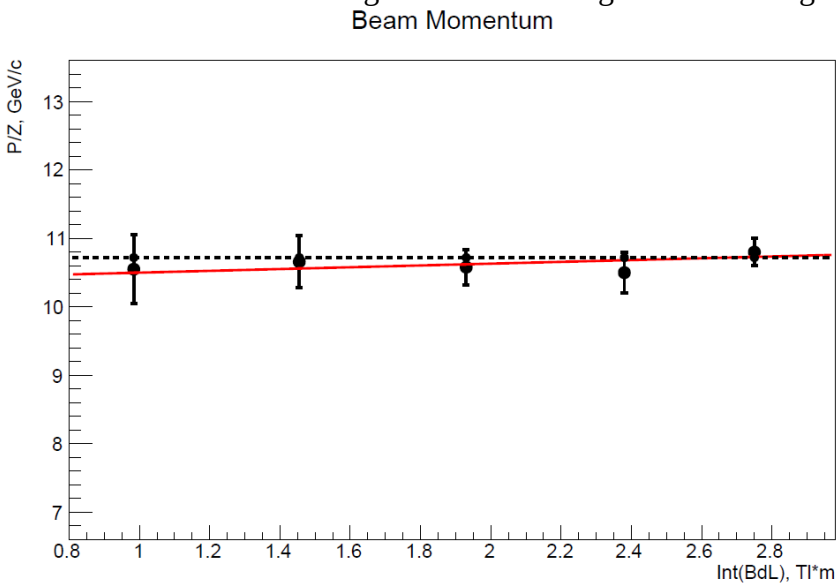


Fig.29. C beam energy 4.5 GeV/nucleon momentum estimation. The dashed line is the nominal beam momentum value. The points are the beam momentum values estimated from the experimental data.

A special macro was developed for the chain used for particle identification in the BM@N experiment. The reconstructed trajectories from tracking detectors combined with the information from Time-Of-Flight detectors allow identifying a large spectrum of particles with high precision. The preliminary results of this identification were reported on BM@N collaboration meetings.

• In the framework of the creation of a system for storing and processing data from the BM@N and MPD experiments included in the NICA complex, a new macro-modeling scheme was developed and implemented as a program using a probabilistic approach to assess various equipment configurations. It determines the probability of loss of information coming from the detectors for each of these configurations and it selects, based on economic factors, the one for which this probability does not exceed the specified limit, and the price is minimal. The program proved its value on calculations of efficiency of the system for data acquisition and storage of the BM@N experiment concerning the price of the investments in the system of the disk memory for the intermediate data storage [64].

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

►**A multifunctional web-based platform for the detection of plant diseases** has been developed, using modern cloud-based organization and deep learning techniques to provide a new level of service to the farming community. The platform includes a web interface designed to manage various databases of agricultural crops necessary for training and testing the corresponding deep neural network, and also provides effective and convenient means for storing, transmitting and retrieving text and photos obtained from farmers. The program, developed on the basis of the deep Siamese convolutional network, was tested on statistics from the developed database of real images of grape leaves and showed efficiency over 90% in recognizing healthy leaves and three common diseases [65].

► **Numerical analysis of the phase dynamics of stacks of long Josephson junctions** was carried out taking into account inductive and capacitive couplings between neighboring Josephson junctions. The influence of the model parameters on the structure of the current-voltage characteristic, the radiation power and the dynamics of the fluxons in individual Josephson junctions inside the stack was studied. The coexistence of a charge traveling wave with fluxon states was demonstrated. The given state can be considered as a new collective excitation in the system of coupled Josephson junctions. It was shown that the observed collective excitation led to a decrease in the radiation power from the system [66].

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

• ***Development of a unified frame for the solution of few particle problems (for bounded, resonant, and scattering states) by embedding the original problem in a different approximation space enables numerical solutions in agreement with the experiment*** for a great many few-particle problems.

Fig. 31 compares a high-resolution experiment done at the University of Frankfurt on electron emissions in fast proton helium collisions with theoretical models from standard scattering theory.

The kinematical conditions are: the proton energy 1 MeV, the transferred momentum 0.75 a.u. and the energy of electron 6.5 eV [67]. The theoretical results were obtained using the first and second Born approximations and the 3C model of the final 3-body state as well as different trial wave functions of the helium ground state. The results were compared with experimental data. Good agreement between the theory and the experiment was obtained with the final 3C state and the probing helium ground state, the wave functions of which include intense electron correlations [68]. It is established that these correlations provide the observed ratio of the binary/recoil peak intensities (Fig. x1). The present study was performed on the HybriLIT computer complex.

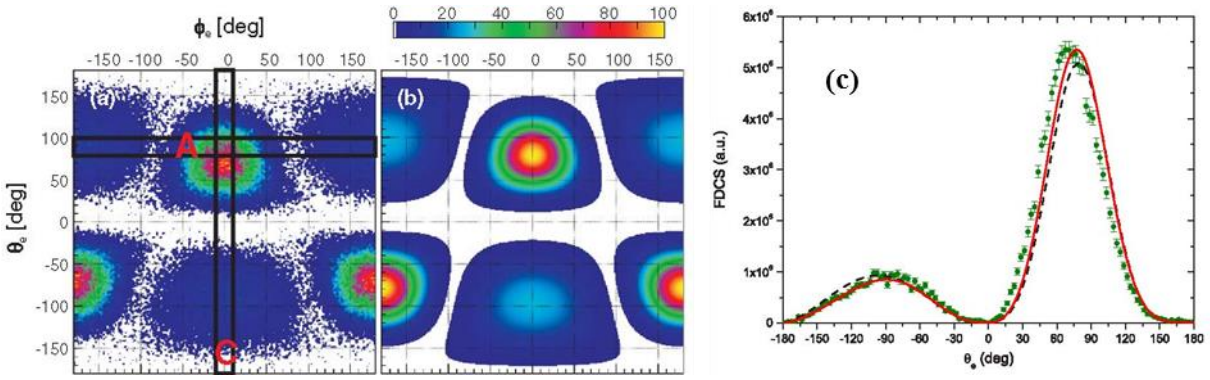


Fig. 30. (a) Measured electron angular distributions for a fixed energy E= 6.5 ± 3.5 eV and a momentum transfer q=0.75 ± 0.25 a.u. The areas marked as A and C correspond to the so-called azimuthal plane and coplanar geometry. (b) Theoretical distribution based on the First Born Approximation (FBA) calculations geometry for E=6.5 eV, q=0.75 a.u. (c) Calculated electron angular distributions in coplanar geometry for E=6.5 eV, q=0.75 a.u.: plane-wave first Born approximation (black dashed line) and 3C model (red solid line) with a strongly correlated function.

• The dependence of the multiply differential cross-section of the (e, 2e) simple ionization of H_3^+, with the incident and ejection energy values, as well as the directions of the ejected and scattered electrons, was studied. The calculations have been performed in frames of the perturbative first Born procedure, which has required the development of equilateral triangular three-center bound and continuum state wave functions. The results explore the optimal conditions and the particularities of the triangular targets, such as the appearance of interference patterns in the variation of the four fold differential cross-section (FDCS) with the scattering angle for a fixed orientation of the molecule. The comparison between the results obtained by two H_3^+ ground wave functions, with and without the correlation term r_{12}, shows that the effect of correlation on the magnitude of the triple differential cross-section is not large, but it produces some modification in the structure of the FDCS [69].

• ***Developing problem adapted multi-scaling algorithms*** [70, 71]

A Bayesian automatic adaptive quadrature solution for numerical integration was proposed which took into account three main factors: refining the automatic adaptive *m*-panel scheme by using quadrature sums adapted to the scales of the length of the integration domain; quick assessment of the problem complexity; the use of a weaker accuracy of the two possible ones (specifications of input accuracy and internal properties of the integrand function). Consideration of the above factors allows achieving the highest possible accuracy of the solution with the minimum possible computation time [70]. Consistent Bayesian inference in the automatic adaptive quadrature over macroscopic integration ranges can be done within a multistage decision process which involves multiscale approaches defined by the resolved integrand features [71].

• ***Molecular dynamic modeling of tffects produced in metals by nanocluster bombardment*** [72-75]

In cooperation with Bulgarian colleagues, LIT researchers developed a continuously-atomic model (CAM) to simulate the interactions of high-energy heavy ions with condensed matter. The CAM is described by two different classes of equations, namely, continuous heat conduction equations of the thermal spike model and by equations of motion of material points of the molecular dynamics method. Within this approach, structural changes in a copper target irradiated by Cu(147) ion nanoclusters were investigated by a model combining the molecular dynamics method with the thermal spike model. The modeling of structural changes predicted the density and the depth of penetration of the nanocluster atoms in the irradiated target in terms of the nanocluster energy. The shape of the source predicted by the thermal spike model was used to describe the dynamics of crater formation under nanocluster bombardment of the target (Fig. 32) [72].

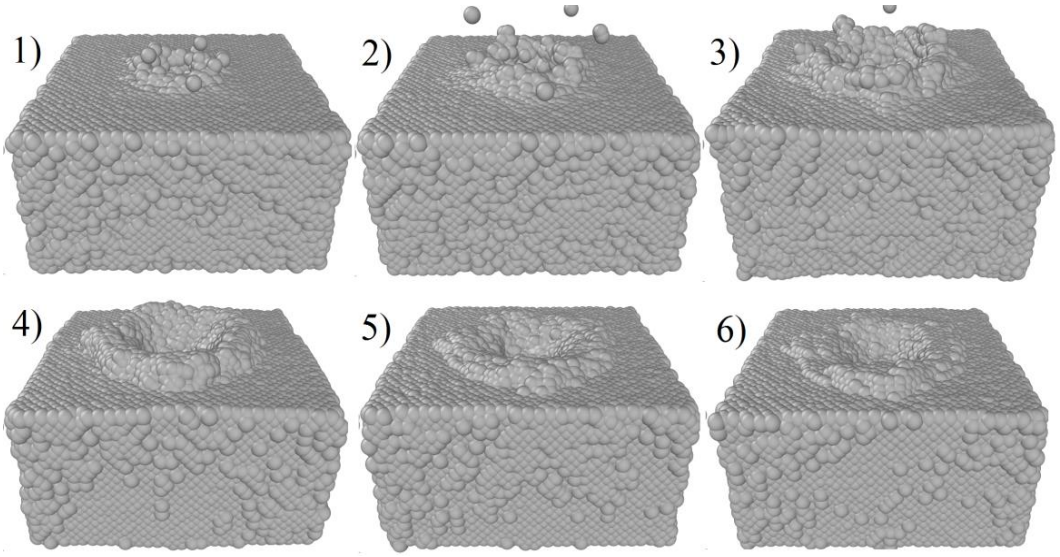


Fig. 31. Dynamics of crater formation as a function of time: 1) – 0.5ps; 2) – 1ps; 3) – 2ps; 4) – 5ps; 5) – 10ps; 6) – 20ps.

Simulations of structural changes at the nickel surface exposed to 100−700 MeV uranium ions have been performed. Dimensions of specific injuries have been obtained in terms of the energy of irradiation at different times. It should be noted that when irradiating the metal sample by high energy ions, the most part of energy is lost in the electron gas and then passed to the crystal lattice, but a certain amount of the energy is accumulated in the electron gas. Therefore, if choosing the initial conditions for the molecular dynamics simulation, this fact must be taken into account. The initial conditions (temperature profiles) can be varied in this case. In addition, the experimental data can be used to refine the initial conditions. In frames of the conducted research one can make the following two conclusions: the technique proposed in this work is well suited to describe the structural changes in the surface layers of the material under irradiation and to obtain more accurate predictions on the structural changes, the use of experimental data is recommended as well as a better use of nonlinear dependence on the temperature of parameters of the thermal spike model [73].

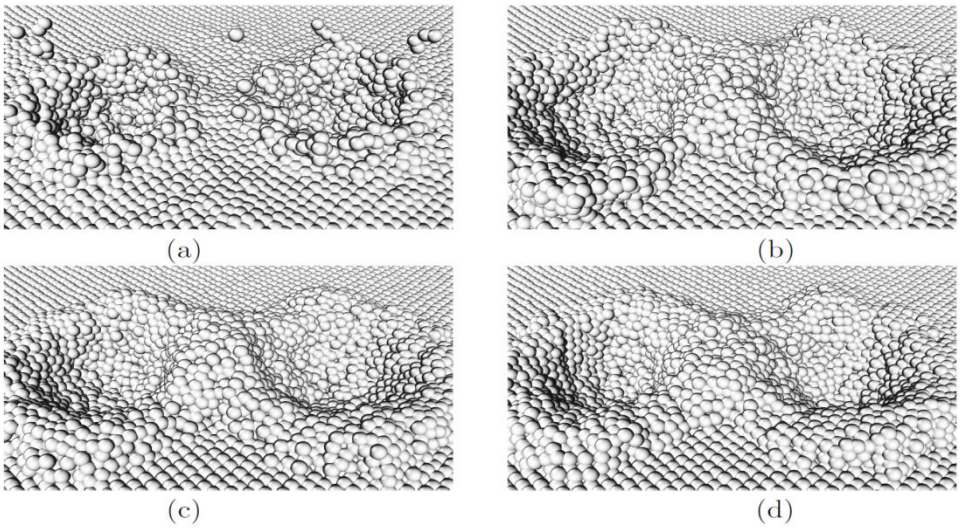


Fig. 32a. Structural changes of the target and formation of craters at its surface when irradiated with two nanoclusters of energy 50 eV/atom at instants of time 1 ps (a), 4 ps (b), 7 ps (c), and 10 ps (d).

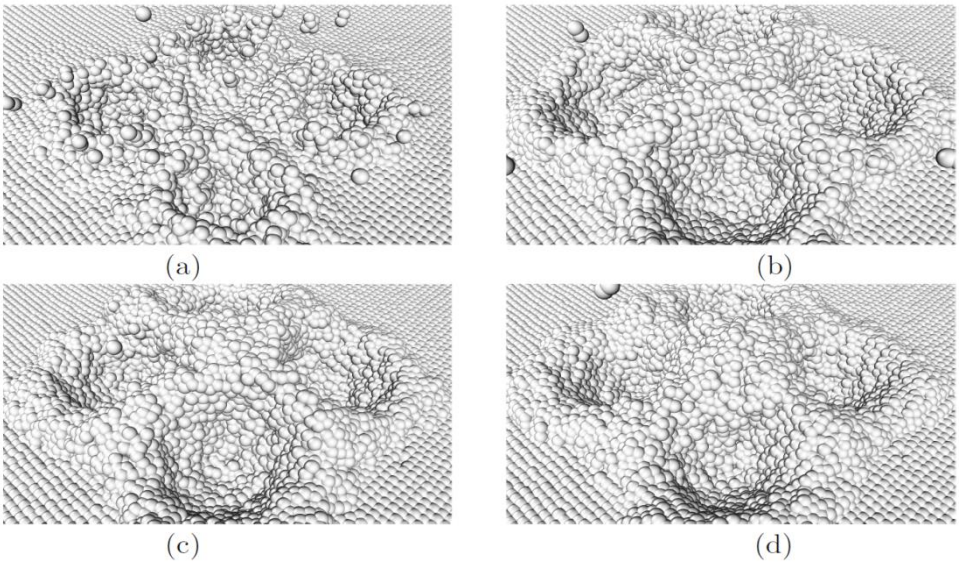


Fig. 32b. Structural changes of the target and formation of craters at its surface when irradiated with four nanoclusters of energy 50 eV/atom at instants of time 1 ps (a), 4 ps (b), 7 ps (c), and 10 ps (d)

Molecular dynamics simulation of the long-range effects in a metal target, irradiated by nanoclusters have shown that, under simultaneous irradiation by several nanoclusters having different areas of interaction with the target surface, fusion of high temperature moving regions occurs in depth. 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 (Fig. 33a, Fig. 33b) [74].

• In order to receive a more effective algorithm for calculation of characteristics for stochastic differential equations (SDE), we propose to use a representation of the transition probability density function (TPDF) for solving SDE by means of a functional integral and methods for approximate evaluation of the arising functional integrals. To represent TPDF by means of functional integral, we propose to use the Onsager-Machlup functional technique. In order to evaluate the arising functional integrals, a method is used which is based on distinguishing among all trajectories a classical trajectory for which the action takes an extreme value, and decomposition of the action with respect to the classical trajectory [76].

10. Developments in Computer Algebra and Quantum Computing [77-92]

► Development of symbolic-numerical algorithms for the construction of high-accuracy finite element schemes [77-82]

• New calculation schemes and algorithms have been suggested for solving a parametric self-adjoint elliptic boundary-value problem with the Dirichlet and/or Neumann type boundary conditions in a 2D finite domain using a high-accuracy finite element method (FEM) with rectangular and triangular elements. The programs complexes implementing the algorithms calculate eigenvalues, surface eigenfunctions and their first derivatives with respect to the parameter and the potential matrix elements – the integrals of the products of surface eigenfunctions and/or their first derivatives with respect to the parameter which appear when reducing the multi-dimensional boundary-value problem to a one-dimensional one by means of the Kantorovich method. The efficiency of the proposed calculation schemes and algorithms is demonstrated in benchmark calculations of the 2D elliptic boundary-value problems describing quadrupole vibrations in a collective nuclear model [77].

• A new method for constructing fully symmetric multidimensional Gaussian quadratures on a simplex was developed. The main idea of the method is to replace the coordinates of nodes with their symmetric combinations obtained by the Viète theorem which simplifies the system of nonlinear algebraic equations. The construction of the required systems of equations is performed analytically using the original author's algorithm implemented in the Maple system. Up to the sixth order the given systems are solved using the built-in PolynomialSystem procedure that implements the

Gröbner basis technique while the systems of higher order are solved using the developed symbolic-numerical algorithm based on numerical methods for solving a system of nonlinear algebraic equations implemented in the Maple-Fortran environment. The obtained quadrature formulas are used to solve self-adjoint elliptic boundary-value problems in the d-dimensional polyhedral finite region by the finite element method of high order of accuracy [80].

• New symbolic-numerical algorithms have been implemented in Maple-Fortran environment for solving self-adjoint elliptic boundary-value problems in a *d*-dimensional polyhedral finite domain in the framework of the high-accuracy finite element method (FEM) [78-81]. The first of them is the generation of multidimensional Lagrange interpolation polynomials (LIP) and two-dimensional Hermite interpolation polynomials (HIP) and the second one is the construction of high-order fully symmetric PI-type Gaussian quadratures with positive weights and no points outside the simplex. The efficiency of algorithms and programs is demonstrated by the calculations of a low part of spectra of exactly solvable problems (Figs. 34 and 35).

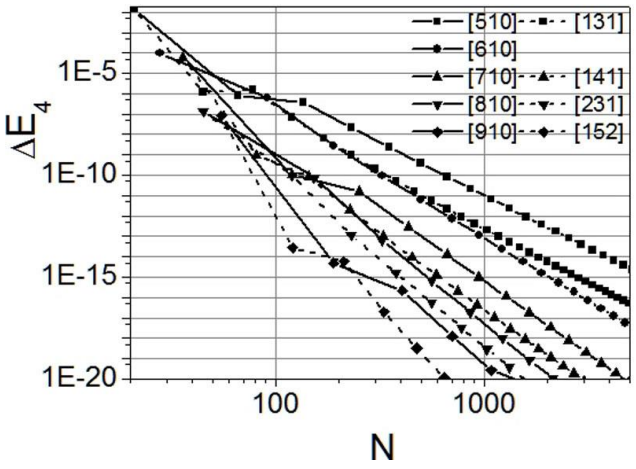


Fig. 33. The errors for the eigenvalue depending on the length of the vector of the algebraic eigenvalue problem for FEM schemes from the fifth to the ninth order of accuracy: using LIP with the labels [510], ..., [910], and using HIP with the labels [131], [141], [231] and [152], for the Helmholtz equation on the equilateral triangle.

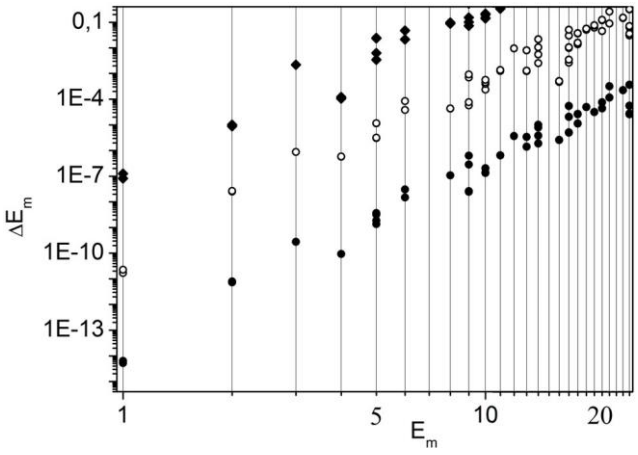


Fig. 34. The error calculated using FEM with sixth-order LIP versus the exact eigenvalue for the Helmholtz equation on the cube. Squares, empty circles and solid circles: the cube is divided into 6, 48 and 384 equal tetrahedrons.

► **Information Processing by Networks of Quantum Decision Makers** [83]

A new model describing the processing of artificial intelligence is suggested. Several decision makers, interacting with each other through information exchange, are considered simultaneously.

A multistep procedure is treated, when the agents exchange information many times. Several decision makers exchanging information and forming their judgement, using quantum rules, form a

kind of a quantum information network, where collective decisions develop in time as a result of information exchange. In addition to characterizing collective decisions that arise in human societies, such networks can describe dynamical processes occurring in artificial quantum intelligence composed of several parts or in a cluster of quantum computers.

The practical usage of the theory is illustrated on the dynamic disjunction effect, for which three quantitative predictions are made: (i) the probabilistic behavior of decision makers at the initial stage of the process is described; (ii) the decrease of the difference between the initial prospect probabilities and the related utility factors is proved; (iii) the existence of a common consensus after multiple exchange of information is predicted.

The predicted numerical values are in a very good agreement with the empirical data.

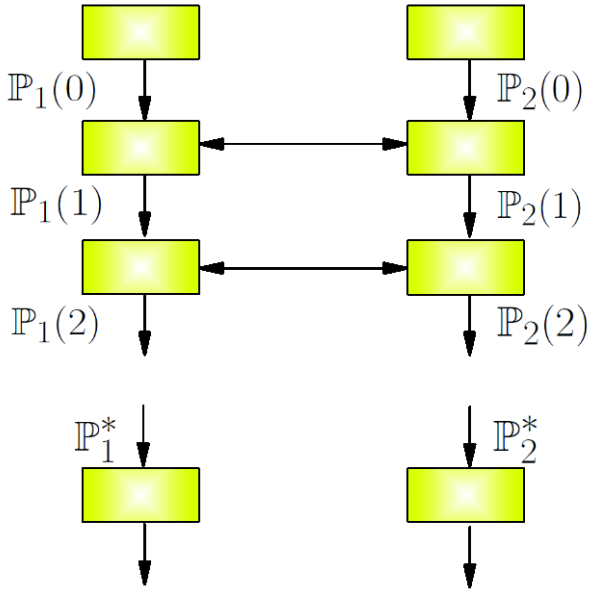


Fig. 35. Dynamics of multistep decision making governed by information exchange between two agents

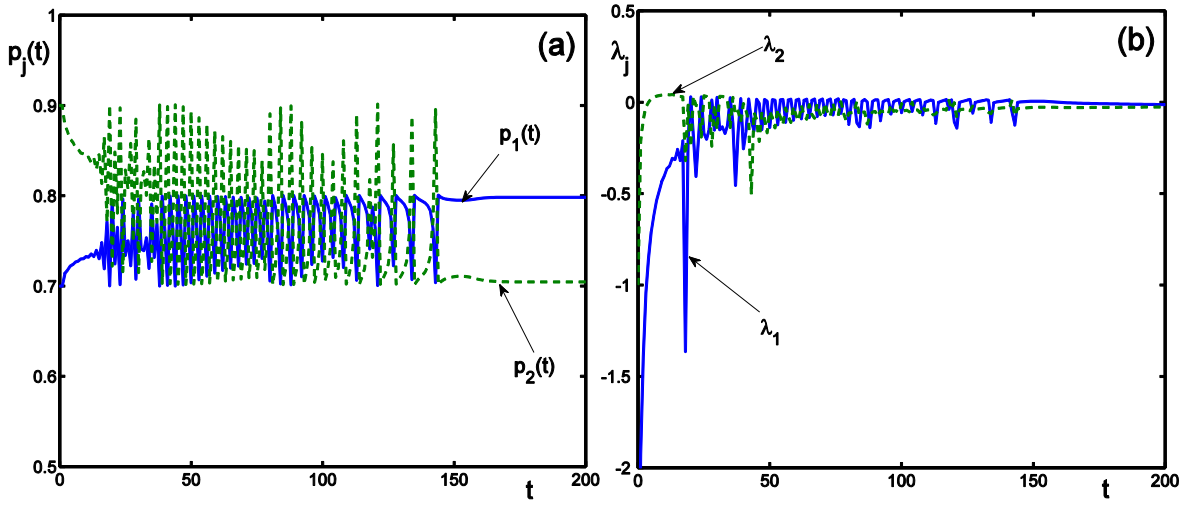


Fig. 36. Reconstructive memory under conflict. Dynamics of the probabilities (a) and the local Lyapunov exponents (b)

► **Description of N-level quantum systems in terms of quasiprobability distributions** [84, 85]. The Weyl-Wigner map between the operators of an N-dimensional quantum system and the Wigner quasiprobability distributions on the corresponding phase space establishes a connection between the quantum and classical representations of the observables.

The classification of Wigner quasiprobability distributions on the phase space realized in the form of a symplectic flag manifold was studied [85]. The Wigner quasiprobability distribution is

constructed in the form of a dual convolution of the density matrix and the Stratonovich-Weyl kernels [84]. It was shown that the moduli space of the Stratonovich-Weyl nucleus is given by the intersection of the coadjoint orbit space of the connected action of the SU(N) group with a unit (N–2)-dimensional sphere. The general approach is illustrated by a detailed description of the module space of 2-, 3-, and 4-dimensional systems. Examples are shown in Figs. 38 and 39.

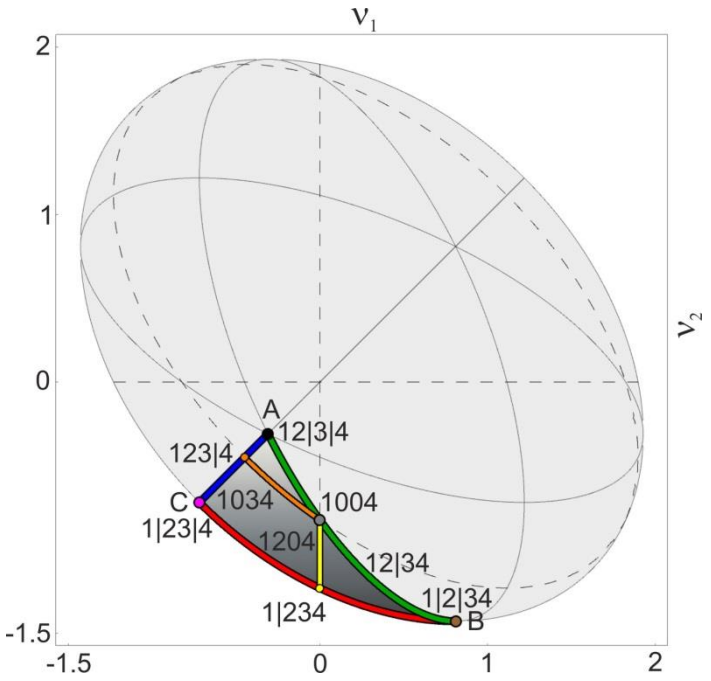


Fig. 37. Mapping of the tiling of $S_2(1)$ sphere by the Mobius triangles (2,3,3) onto a subset of the plane (υ_1, υ_2). The dashed lines represent the degeneracies of the spectrum

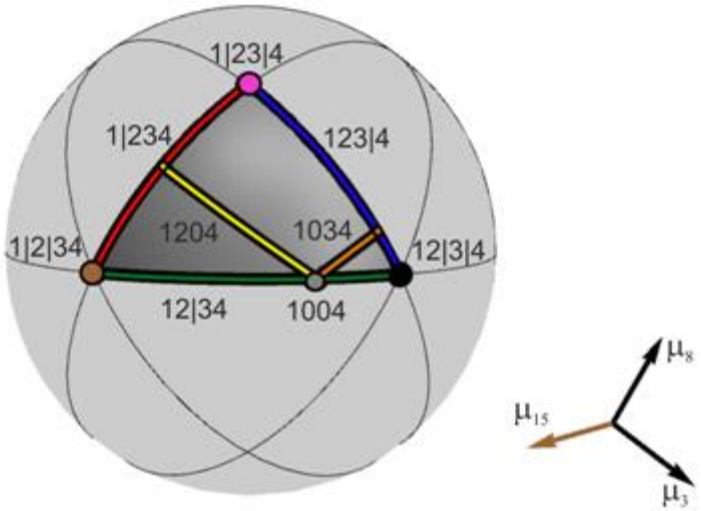


Fig. 38. Quatrit (N=4) moduli space represented by the Mobius spherical triangle (2, 3, 3) on a unit sphere

► Description of finite quantum systems

- A new algorithm for decomposing the irreducible components of the permutation representations of finite groups over zero characteristic fields was proposed. The algorithm is based on the fact that the components of an invariant scalar product in invariant subspaces are projection operators into these subspaces. This makes it possible to reduce the problem to solving systems of quadratic equations. In the zero characteristic, the proposed algorithm significantly exceeds the most

well-known algorithm in the computing group theory called MeatAxe. The current implementation of the algorithm allows splitting representations of dimensions to hundreds of thousands [86].

• A model of quantum evolution has been constructed on the basis of combining methods of computational group theory and Monte Carlo simulation. The model is inspired by the quantum Zeno effect — the most convincing illustration of the role of observation in the dynamics of quantum systems. In the model under consideration, the trajectory of a quantum system is represented as a sequence of observations with unitary transitions between them. Time is assumed to be fundamentally discrete. From a mathematical viewpoint, the observation (measurement) is an orthogonal projection onto the subspace of a Hilbert space that is defined by the "measuring device". Statistics of the results of observations is described by the Gleason theorem (a special case of which is the Born rule). Standard quantum mechanics assumes a single deterministic unitary evolution of a quantum system in the time interval between observations. However, in accordance with the principle of least action, this single evolution appears as the dominant element in some set of "virtual" evolutions. A unitary transition between observations is interpreted as a kind of gauge connection, that is, a way of identifying indistinguishable entities at different instants of time (in discrete time it is impossible in principle to trace the individuality of indistinguishable objects in the process of their evolution), and it is assumed that all possible unitary transformations are involved in transitions between observations with weights corresponding to transition probabilities. This assumption is confirmed by the Monte Carlo simulation that demonstrates a sharp dominance of some of the evolutions over the others. This dominance grows rapidly with increasing size of the symmetry group of states and the dimension of the Hilbert space. The probability of a trajectory of a quantum system is calculated as a product of the probabilities of transitions between adjacent observations. The continuum limit of the (negative) logarithm of this product is an action. Thus, the principle of selection of the most probable trajectory turns into the principle of least action in the continuum limit [87].

► Solutions of difficult problems of computer algebra

• The TDDS software package (Thomas Decomposition of Differential Systems) in the Maple symbolic computation language intended for algebraic analysis of systems of nonlinear partial differential equations is included in the Computer Physics Communications program library and the latest version of Maple (Maple 2018) [88].

• For the first time, the classical problem formulated in 1883 by the outstanding Norvegian mathematician Sophus Lie, was algorithmized in the paper [89]. The problem is to check whether a nonlinear ordinary differential equation solved with respect to its highest order derivative is linearizable by a point transformation of the independent and dependent variables. The algorithm allows not only to check the linearizability but also to obtain a system of partial differential equations for the linearizing transformation whose solution gives the explicit form of such transformation. The paper [89] got the Distinguished Paper Award of ACM (Association for Computing Machinery) (http://www.issac-conference.org/2017/awards.php) at the world symposium on symbolic and algebraic computation (ISSAC 2017, Kaiserslautern, Germany, July 25–28, 2017).

• As examples of algorithmic construction of difference schemes for partial differential equations receiving inheriting their basic algebraic properties on a discrete level, new difference schemes have been constructed for Navier-Stokes equations and Korteweg-de Vries equation. These new schemes demonstrate a good numerical behavior [90].

• The methods of obtaining functional equations for Feynman integrals on the basis of the algebraic relationships for propagators have been improved. The computations of the QCD contributions to the constant of renormalization of the mixed propagator of fermions are performed taking calibration into account [91, 92].

11. Other important developments

• In cooperation with the Plekhanov Russian University of Economics, an automated system for monitoring and predict matching of a compliance of higher vocational education with the needs of

labor market has been developed. To create the system, a significant arsenal of methods and tools of Big Data Analytics and the experience gained in the projects on computing for the ATLAS and CMS experiments at CERN, were used. The task, which lies in the mainstream of the so-called "Digital economy", looks quite complicated so its solution requires new approaches and methods of data science, including methods of semantic analysis and machine learning. The constantly updated information database is generated using open sources. The developed system provides additional opportunities to reveal qualitative and quantitative interrelationships between education and labor market. It is aimed at a broad circle of users including authorities and management of regions and municipalities; management of universities, companies, recruitment agencies; graduates and university enrollees [93].

12. The MMCP International Conferences

Besides the above mentioned aspects of the output of theme 1119, the organization of periodic international conferences is a point deserving consideration.

The International MMCP Conferences (Mathematical Modeling and Computational Physics), organized once every two years, have got a solid international reputation, with the publication of the MMCP Conference Proceedings under a severe refereeing process.

The ninth conference in this series, MMCP 2017, was hosted by LIT JINR on 3–7 July 2017. It was devoted to the 60-th anniversary of the foundation of the Joint Institute for Nuclear Research. Co-organizers of the conference were LIT-JINR, IFIN-HH (Bucharest, Romania), Technical University (Košice, Slovakia), Institute of experimental physics of the Slovak Academy of Sciences (Kosice, Slovakia), Pavol Jozef Šafárik University in Košice (Slovakia).

The scientific topics of the Conference covered a wide range of issues concerning distributed and parallel computing and tools for scientific computing; mathematical methods and application software for modeling complex physical and engineering systems; bioinformatics and computational biophysics; physical processes simulations and related computational methods; computer algebra and quantum computing with applications.

The conference was attended by over 250 scientists and specialists from various scientific centers of Romania, Bulgaria, Germany, Lithuania, Finland, France, Slovakia, USA, Mongolia, Canada and from many Russian research centers and universities such as NRC "Kurchatov Institute", IMPB RAS, ITAM SB RAS, St.-Petersburg University, NSU, RPFU and others.

In total, 212 reports (31 plenaries, 158 orals and 23 posters) were presented. Following a rigorous reviewing procedure, a hundred manuscripts have been accepted for publication in a special issue of the journal EPJ Web of Conferences (Vol. 173, February 2018, Eds. Gh. Adam, J. Buša, M. Hnatič and D. Podgainy).

A satellite student-school "Mathematical modeling for the NICA project" was organized in the frame of MMCP 2017 under the support of the JINR Directorate. The school program included lectures and practical classes as well as master classes.

The tutorials were conducted on the basis of the heterogeneous cluster HybriLIT under the support of the Heterogeneous Computing Team at LIT JINR.

The conference-school was attended by 54 young scientists and specialists of JINR, students of the University "Dubna", Moscow Engineering Physics Institute. MSU, St. Petersburg State University, Tver State University, RPFU, KazNU al-Farabi (Kazakhstan) and others.

The next, MMCP 2019, International Conference will be organized in Stará Lesná, Slovakia, by the same partner institutes, on July 1–5, 2019. Welcome to MMCP 2019!

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