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SCIENTIFIC AND TECHNICAL JUSTIFICATION FOR THE OPENING OF A PROJECT WITHIN A THEME OF THE TOPICAL PLAN FOR JINR RESEARCH

1. General information on the project

1.1 Theme code

05-6-1119-2014/…

1.2 Project/sub-project of a MIP code (for renewed themes)

1.3 Laboratory

MLIT

1.4 Scientific field

Networking, computing, computational physics (05)

1.5 The name of the Project

Methods of computational physics for the study of complex systems

1.6 Project Leader(s)

O. Chuluunbaatar, E.V. Zemlyanaya

1.7 Project Deputy Leader(s)

Yu.L. Kalinovsky, A. Khvedelidze

2 Scientific case and project organization

2.1. Annotation

The proposed project is aimed at the development and application of mathematical and computational methods for modeling complex physical systems studied in the framework of the JINR priority topics and described by systems of dynamic nonlinear, spatially multidimensional integral, integro-differential or differential equations that depend on the parameters of the models. The evolution of the solutions of such systems can be characterized by the occurrence of critical regimes, bifurcations and phase transitions.

Mathematical modeling is an inseparable part of the modern scientific research. It requires an adequate mathematical formulation of the problems in the framework of the models under study, the adaptation of known numerical approaches or the development of new ones to effectively take into account the features of the studied physical processes, the development of algorithms and software packages for high-performance simulation on modern computer systems, including the MICC MLIT resources. Research in the framework of the project will be focused on the following main directions:

I. Development of methods, algorithms and software packages for carrying out numerical studies of interactions of various types in complex systems of nuclear physics and quantum mechanics.

II. Studies of intricate processes in condensed matter and materials under external actions.

III. Solutions of modeling problems in the design of experimental facilities and optimization of their operating modes.

IV. Modeling complex processes in dense nuclear matter based on the equation of state.

V. Modeling of quantum systems using methods of quantum information theory and hybrid quantum-classical programming methods.

As a result of studies carried out using the developed methods and software packages, new fundamental information about the objects under study will be got, with impact on the further development of mathematical models for theoretical and experimental investigations in JINR.

2.2 Scientific case (aim, relevance and scientific novelty, methods and approaches, techniques, expected results, risks)

Aim

Development and software implementation of computational approaches for the study by methods of mathematical modeling of physical phenomena that are the focus of the Institute's research in accordance with the JINR Seven-Year Research Plan for 2024–2030; on this basis, obtaining new knowledge necessary for understanding the physical processes under study, further theoretical research and planning of experimental projects that are relevant from the point of view of practical applications.

Main areas of research

The project research is closely related to a wide range of scientific areas within the framework of the JINR Topical Plan and is aimed at creating new mathematical methods, algorithms and programs for successfully solving urgent problems that arise in the course of implementing scientific programs at JINR. Research in the framework of the project covers the following range of tasks.

I. Development of methods, algorithms and software packages for carrying out numerical studies of interactions of various types in complex systems of nuclear physics and quantum mechanics, including:

- investigation of physical characteristics of sub-barrier fusion/fission reactions of heavy nuclei based on the development of the strong coupling channel method, potential models of atomic nuclei and the application of the finite element method for high-precision discrete approximation of the corresponding systems of equations;
- study of the processes of scattering of heavy ions and particles on nuclei and the interaction of heavy ions in the medium energy range based on microscopic optical potential models and within the transport-statistical approach;
- modeling chemical bonds and reactions involving heavy and superheavy elements with the aim to interpret the results of thermochromatographic experiments at FLNR;
- development of methods and research into the dynamics of spin ensembles and cold atoms in traps within quantum mechanical models.

II. Studies of intricate processes in materials and condensed media under external influences, including:

- simulation of physical–chemical and structural changes in materials under the action of irradiation with charged (nano)particles and laser radiation; development of methods for calculating the characteristics of energy losses by heavy ions in an irradiated material in a wide range of the charge number of incident particles and their relative velocities;
- simulation of superconducting processes in Josephson structures of various types; simulation of the dynamics of spin systems in nanomaterials aimed at providing inferences to the prospects for creating memory elements and information transfer;
- study of the structure and properties of polydisperse phospholipid vesicular systems of various types, including nanodrugs, based on molecular dynamics approaches and within the framework of the separated form factors method;
- development of methods and modeling of complex processes in dissipative condensed matter under external influences, described by nonlinear field theory equations.

III. Solutions of modeling problems in the design of experimental facilities and optimization of their operating modes, including:

- development of methods for the numerical solution of systems of equations arising in the simulation of physical fields;
- development and software implementation of algorithms aimed at improving the efficiency and optimization of numerical simulation of complex magnetic systems of accelerators;
- Simulation of magnetic systems for experimental facilities, including numerical simulation of physical processes during the formation of the magnetic field of the MSC230 cyclotron (DLNP).

IV. Modeling complex processes in dense nuclear matter based on the equation of state, including:

- simulation of complex processes in hot and dense matter during heavy ion collisions in the NICA energy range, phase transitions with the formation of quark-gluon plasma;
- modeling of complex processes in astrophysical systems.

V. Development of new methods of the computational physics based on hybrid quantum-classical programming of computer mathematics and their application to the study the information characteristics of quantum states in elementary particle and nuclear physics, quantum chemistry and biophysics.

Despite the wide diversity of the above tasks, the process of developing methods and conducting mathematical modeling is generally carried out according to a pattern, which covers the following stages:

- Formulation of the mathematical statement of the problem that correctly reflects the main features of the topic under study and the purpose of the investigation;
- Development of a computational approach to the solution based on finely tuned methods of computational mathematics, symbolic-numerical and numerical-analytical algorithms, neural network and molecular dynamics methods, methods of quantum computing and computer algebra, parallel computing algorithms;
- Software implementation of the developed computational scheme using high and ultra-highlevel programming tools, techniques for organizing parallel and hybrid computations on modern high-performance computing systems, using existing libraries of computer programs and problem-oriented software packages, using specialized tools to create a comfortable environment for programming and calculations;
- Validation of the correctness of the developed methods and programs and verification of models based on test calculations with variable computational parameters, comparison of numerical results with available theoretical estimates and experimental data;
- Carrying out mathematical modeling and derivation of new information about the simulated physical systems during the analysis of numerical results, which can serve as a basis for refining and further development of the theoretical approaches and experiment planning.

The research within the project assumes the creation of new methods or improvement of the existing ones, by the project participants, at each of the listed stages. Thereby, during the implementation of the project, new methods will be developed that are necessary for the successful conduct of fundamental prospective and advanced research of complex physical phenomena described by nonlinear multidimensional multiparameter systems of equations.

There will be two kinds of results of the project:

(1) original developments in the field of methods of computational mathematics, high-performance computing and mathematical modeling;

(2) new physically significant results obtained on this basis.

I. Investigation of complex processes in nuclear physics and quantum mechanics

This section combines a number of tasks related to the numerical study of the characteristics of nuclear-physical processes necessary for understanding the mechanisms of nuclear interactions

and the structure of nuclei involved in reactions, testing existing theoretical hypotheses, interpreting the experimental data obtained, including ongoing and planned experiments on the synthesis of superheavy elements and on reactions involving light exotic nuclei. The formulations of the problems are mostly based on the principles of quantum mechanics and require high accuracy calculations of solutions of multidimensional Schrödinger-type equations and of corresponding eigenvalue problems, the solution of nonlinear integral equations for calculating nuclear potentials, the solution of nonlinear dynamics equations within the transport-statistical approach, the solution of algebraic high order systems. The research will be carried out in cooperation with BLTP and FLNR.

One of the tasks of the project is the study of the physical characteristics of deep sub-barrier fusion/fission reactions of heavy nuclei. In this approach, the original multichannel scattering problem in the oscillator representation, which takes into account vibrational and rotational oscillations of the surfaces of a pair of ions, is reduced to a system of second-order ordinary differential equations with asymptotic boundary conditions for large and small values of the radial variable of the relative motion of colliding ions. Within the channel coupling method, a program package will be developed that implements, under strong coupling conditions, the calculation of matrix elements and the numerical solution of the corresponding system of Schrödinger equations with off-diagonal boundary conditions, as well as the calculation of the cross sections for the fusion and fission reactions of heavy nuclei at energies significantly below the Coulomb barrier. The cornerstone of the solution will be the KANTBP 3.1 [1], package developed by the authors of the project, which implements stable computational schemes of high order of accuracy based on the finite element method. This program has been successfully used to calculate the fusion cross sections for heavy ions $^{12}C+^{12}C$, $^{64}Ni+^{64}Ni$, $^{64}Ni+^{100}Mo$, $^{28}Si+^{64}Ni$, $^{36}S+^{48}Ca$ [2].

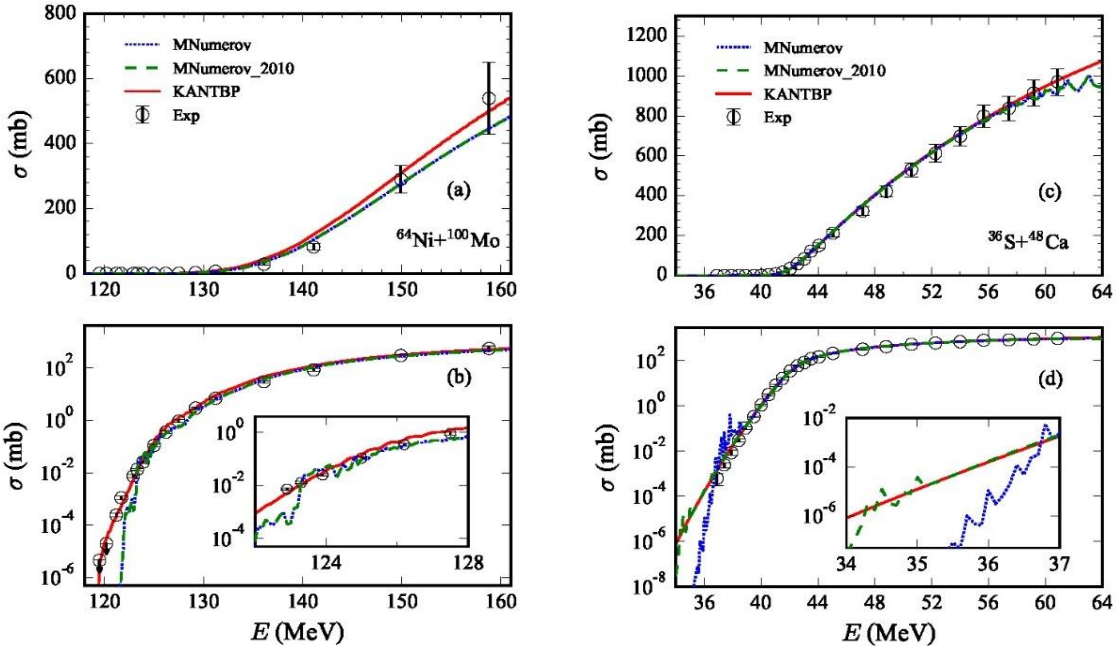

Fig. 1. The fusion cross sections of $^{64}Ni+^{100}Mo$ and $^{36}S+^{48}Ca$ (a,c) on a linear scale and (b,d) on a logarithmic scale in comparison with the experimental data, calculated using the modified Numerov method implemented in the CCFULL program [K. Hagino, et al, CPC 123 (1999) 143] (dotted blue line) and its updated version in 2010 (dashed green line), as well as based on the KANTBP package (solid red line).

[1] O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky, A.G. Abrashkevich, P.W. Wen, C.J. Lin, Comput. Phys. Commun. 278, 108397–1–14 (2022).

[2] P.W. Wen, O. Chuluunbaatar, A.A. Gusev, R.G. Nazmitdinov, A.K. Nasirov, S.I. Vinitsky, C.J. Lin, H.M. Jia, Phys. Rev. C **101**, 014618–1–10 (2020); P.W. Wen, C.J. Lin, R.G. Nazmitdinov, S.I. Vinitsky, O. Chuluunbaatar, A.A. Gusev, A.K. Nasirov, H.M. Jia, A. Góźdź, Phys. Rev. C **103**, 054601–1–6 (2021).

The Figure 1 shows some of the results from this paper, confirming the higher accuracy and the better agreement with the experimental data in comparison with other methods. The possibility to understand the processes of formation of superheavy elements by means of the proposed approach was noted, in particular, in the review [3].

Another project task related to the study of superheavy elements is the development and computer implementation of a stochastic model of chemical reactions involving heavy and superheavy elements for the interpretation of data from FLNR experiments on thermochromatography. Based on the application of methods of the electron density functional theory using various exchange-correlation potentials and methods of statistical physics and chemical kinetics, the model is described by numerically solvable systems of differential equations in partial derivatives under various initial and boundary conditions. On this basis, it is planned to obtain refined and new information on the characteristics of nuclei participating in the planned experiments on the synthesis of superheavy elements, on the electronic structure and chemical bonds in superheavy atoms, on the influence of relativistic effects on these characteristics by mathematical modeling methods.

In the framework of the project, the characteristics of nucleus-nucleus interactions will be studied, including reactions that involve light with light and heavy nuclei with a neutron halo, which, based on a joint analysis of numerical and experimental results, will allow the derivation of new information about the structure of such nuclei. In these studies, a parallel software implementation of the method for calculating the microscopic optical potential in the framework of the double folding model [4] (the program was deposited to the JINRLIB library) will be used. The microscopic potential model will be significantly upgraded to expand the range of energies and types of reactions. On this basis, it is planned to study the characteristics of nucleus-nucleus interactions in a wide range of energies and atomic numbers of colliding nuclei. Also, the approach developed on the basis of the microscopic model of the optical potential for studying the characteristics of pion-nucleus scattering [5] will be adapted to the analysis of the effect of the nuclear matter on the amplitude of proton-nucleon scattering.

In order to increase the accuracy and reduce the calculation time, the methods and programs that implement the transport-statistical model for calculating the physical characteristics of heavy ion interactions at medium energies [6] will be significantly modernized. Refinement of computational and physical parameters will be carried out on the basis of comparison with available experimental data and theoretical estimates. The study will be carried out in collaboration with colleagues from FLNR. Using the developed approaches, a realistic description of the isotope and velocity distributions in heavy ion fragmentation reactions at medium energies will be obtained.

The simulation of the dynamics of spin ensembles and cold atoms in traps will be based on the numerical solution of the formulated nonlinear integro-differential equations and the use of the method of self-consistent self-similar approximations, optimized for solving nonlinear equations that do not contain small parameters [7]. The developed methods and programs will provide new numerical results on modeling the dynamics of spin systems and cold atoms in traps, which are relevant from the point of view of technological applications.

II. Studies of intricate processes condensed matter and materials under external actions

The numerical study of the intricate processes in condensed matter under external actions, assumes, as a rule, mass calculations of numerical solutions of systems of nonlinear equations of

[3] C.L. Jiang et al, Eur. Phys. J. A **57**, 235–1–47 (2021).

[4] M. Bashashin, E. Zemlyanaya, K. Lukyanov, European Phys. J. Web of Conf. **226,** 02002 (2020).

[5] V.K. Lukyanov, E.V.Zemlyanaya, K.V. Lukyanov, I. Abdul-Magead, Nucl. Phys. A **1010**, 122190 (2021).

[6] T.I. Mikhailova, B. Erdemchimeg, A.G. Artukh, M. Di Toro, H.H. Wolter, Acta Phys. Polon. Supp. **12**, 3, 619–628 (2019).

[7] V.I. Yukalov, E.P. Yukalova, Intern. J. Mod. Phys. **B 34** 2050208-13 (2020).

various types in a wide range of model parameters. At the level of the mathematical formulation of the problem, it is required to take into account such features of the simulated processes as phase transitions, multiplicity of solutions, possible bifurcations and critical regimes. To solve the tasks set, the existing ones will be significantly modernized and new computational schemes will be developed for mathematical modeling based on the combined use of various numerical methods, a combination of analytical and numerical methods, and the widespread use of parallel computing.

One of the main tasks of the project in this direction is the study, by means of mathematical modeling methods, of complex processes in materials under the bombardment with highly energetic charged (nano)particles. The relevance of such studies is due to the prospects for the development of methods for purposefully changing the properties of materials, as well as the need to study the resistance of materials to various types of irradiation. An example of modeling the dynamics of changes in a material under the action of irradiation based on the approaches [8] developed by the project participants is shown in fig. 2.

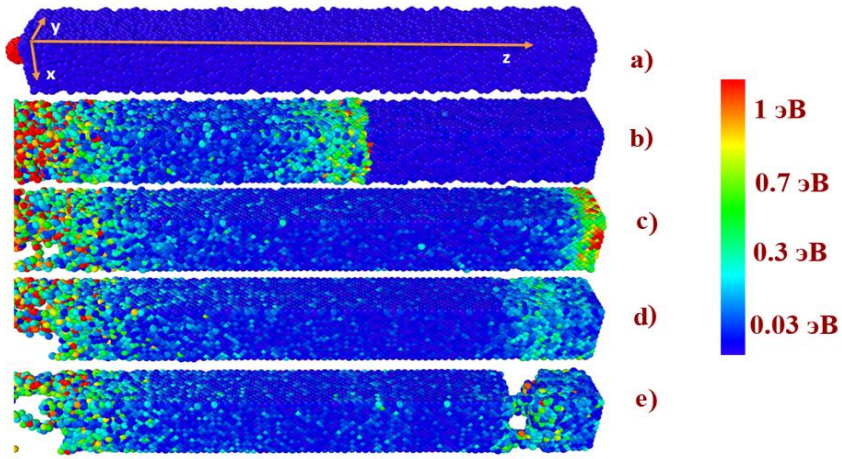

Fig. 2. Dynamics of the shock wave at the depth of the target upon irradiation with one nanocluster of energy 100 eV/atom at instants of time 1 ps (a), 4 ps (b), 7 ps (c), 10 ps (d) and 15 ps (e). Figure from Bulletin of the Russian Academy of Sciences: Physics. Vol. 83, № 10, P.1306-1310, 2019.

To carry out mathematical modeling, it is planned to develop and use computational schemes based on a mixed continuum-atomistic approach that combines the advantages of models based on continuum equations with models described by systems of equations of motion of particles [9]. Computational schemes and a set of programs for the numerical solution of the corresponding systems of equations will be created. Using mathematical modeling methods, new results will be obtained on the study of the dynamics of defective structures in metal targets under the influence of irradiation at different energies of the irradiating beam. In particular, threshold values of the irradiation energy leading to changes in the defective structures of the target will be found, methods for calculating the average distributions of energy losses by heavy ions in irradiated materials will be developed, taking into account Mott corrections, ensuring that the calculated characteristics agree with the available experimental data.

The simulation of superconducting processes in Josephson and spin nanostructures, depending on the configuration of the systems under study and the nature of external influences, has a solid background at MLIT, the studies are carried out in collaboration with colleagues from BLTP. The active interest of researchers in this topic is associated with the prospects for creating memory

[8] I.V. Puzynin, T.P. Puzynina, I.G. Hristov, R.D. Hristova, Z.K. Tukhliev, Z.A. Sharipov, Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques **14**, 1342–1345 (2020); Z.A. Sharipov, B. Batgerel, I.V. Puzynin, T.P. Puzynina, I.G. Hristov, R.D. Hristova, Z.K. Tukhliev, Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques, **16**, 4, 576–580 (2022).

elements and information transfer on this basis. The corresponding mathematical models are described by initial-boundary value problems for systems of nonlinear partial differential equations with a large number of parameters [10]. The numerical investigations involve the development and comparative testing of computational schemes in order to select numerical approaches that are stable to the round off error accumulations [11], as well as the parallel implementation for high-performance computer simulation in a wide range of model parameters in order to study the influence of various factors on the dynamics of the superconducting processes.

In these studies, in order to increase the efficiency of the work on creating computer programs and performing calculations, it is planned to develop and use the HybriLIT information-computing environment based on JupyterHub, which provides ample opportunities for organizing calculations with visualization of all stages of modeling during the task solving [12]. An information-computing environment will be created, including the developed algorithms and software modules adapted to the numerical simulation of complex processes in superconducting systems with a magnet, which will allow efficient research of superconducting elements in nanoscale structures. New results, relevant for understanding the mechanisms of physical processes in the simulated nanostructures will be obtained on this basis.

The study of the structure and dynamics of the evolution of phospholipid membranes in vesicular and bicellar systems is important for understanding the fundamental biochemical processes in living organisms, as well as for obtaining information that is important for the practical development and improvement of the effectiveness of the drugs. Research in this direction will be carried out on the basis of molecular dynamics approaches using the GROMACS package on the HybriLIT heterogeneous computing platform. These approaches have already been used for research carried out in collaboration with the FLNP[13].

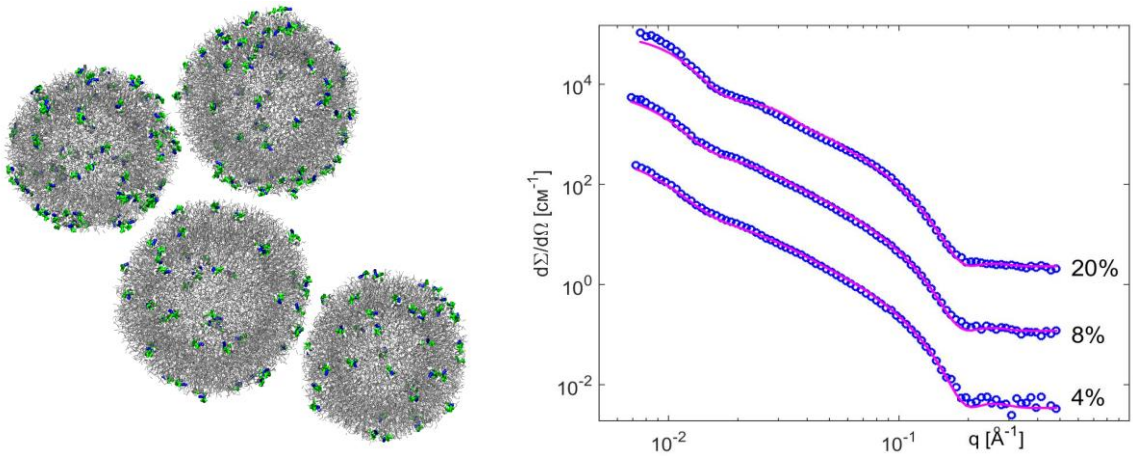

Fig. 3. Left: calculation based on the molecular dynamics approach – the result of self-assembly of DPPC vesicles from randomly distributed DPPC lipids and beta-amyloid peptides at a temperature above the main phase transition temperature of the DPPC lipid. Right: cross sections of small-angle neutron scattering on the vesicular system of the drug "Indolip" calculated within the framework of the separated form factors model in comparison with the experimental data obtained at the FLNP YuMO small-angle spectrometer.

Fig. 3 on the left shows the result of the formation of vesicles consisting of DPPC and amyloid beta peptides, obtained by the molecular dynamics method. In the future, it is planned to implement

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[10] I.R. Rahmonov, Y.M. Shukrinov, E.V. Zemlyanaya, M.V. Bashashin, P.K. Atanasova, Journal of Experimental and Theoretical Physics **124**, 1, 131-138, (2017); P. Kh Atanasova, S.A. Panayotova, I.R. Rahmonov, Yu.M. Shukrinov, E.V. Zemlyanaya, M.V. Bashashin, JETP Letters volume **110**, 11, 722–726 (2019).

[11] M.I. Zuev, S.I. Serdyukova, Computational Mathematica and Mathematical Physics **62**, 1, 1-9 (2022).

[12] Yu. A. Butenko , D. M. Marov, A. V. Nechaevskiy, O. I. Streltsova, I. R. Rahmonova, M. V. Bashashin, Modern Information Technologies and IT-Education 16, 3, 633–642 (2020).

[13] O. Ivankov, T.N. Murugova, E.V. Ermakova, T. Kondela, D.R. Badreeva et al. Scientific Reports **11**, 21990 (2021).

such calculations on graphics accelerators in order to simulate the longest possible time of the system evolution in a reasonable computing time. Moreover, studies of vesicular systems of various types depending on the temperature and chemical composition of the environment will be carried out using the separated form factors method [14] under different approaches for modeling the phospholipid bilayer. Experimental data on small-angle scattering of neutrons and X-rays will be used as a criterion for verifying models and choosing parameters.

The simulation of complex processes in condensed systems, described by nonlinear equations of field theory, requires the use of methods of numerical continuation in parameters with the identification of bifurcations and access to new branches of solutions, increasing the accuracy of discrete approximation in computational schemes to ensure the reliability of the obtained numerical results, the use of parallelism to speed up mass calculations in a wide range of model parameters. Methods will be developed and research will be carried out on nonlinear processes of formation of localized structures in damped-driven condensed systems, described by various types of field theory equations. In particular, studies of the hydration processes of electron will be continued in the framework of the dynamic polaron model. The results of a numerical study of this model are presented in the review [15] and in the PhD Thesis of A.V. Volokhova, successfully defended at MLIT in 2022. As part of the project, a significant modernization of this model is planned, which will require a new mathematical formulation of the problem, the development of a new computational scheme and computer programs to study the influence of various factors on the electron hydration process and on the behavior of respective observables.

III. Solving problems arising in the development and optimization of operating modes of experimental facilities

The design and operation of the experimental facilities ask for the derivation of reliable numerical solutions of a great many problems. Among them, the numerical simulation of the complex magnetic systems of the accelerators is of fundamental importance[16]. Reliable calculation of the large number of characteristics of the magnetic fields required in the preparation of new configurations of experimental facilities places high demands on the correctness of the mathematical formulations of the problems, the robustness of the numerical approaches used, the high accuracy and performance of the calculations.

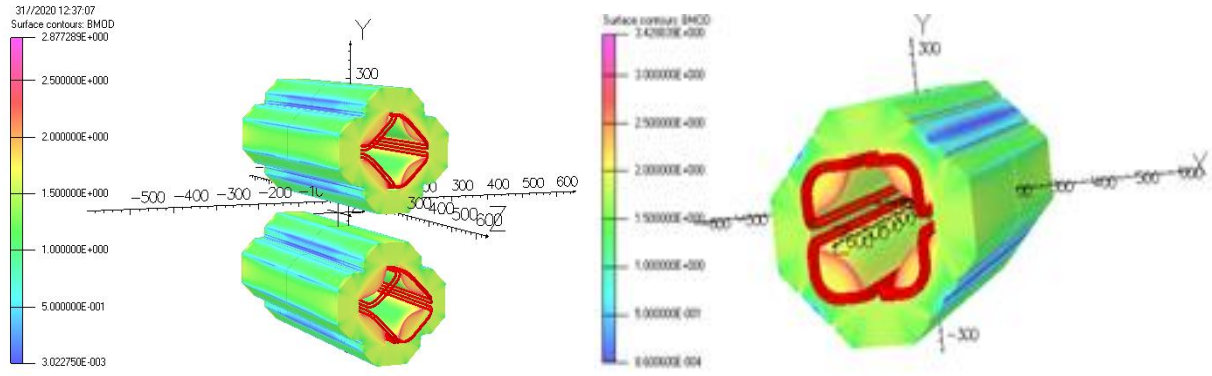

Fig. 4. Calculations of the magnetic field distributions in the NICA collider systems for a quadrupole magnet (left) and a final focus lens (right).

This direction has a long tradition among the DCP MLIT scientists. An enumeration of the achievements of the project participants includes the computer simulation of magnetic systems,

[14] M.A. Kiselev, E.V. Zemlyanaya, E.I. Zhabitskaya, M.V. Bashashin, O.I. Ivankov, Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques **17**, 1, 1–6 (2023);
[15] V.D. Lakhno, I.V. Amirkhanov, A.V. Volokhova, E.V. Zemlyanaya, I.V. Puzynin, T.P. Puzynina, V.S. Richvitsky, M.V. Bashashin, Physics of elementary particles and atomic nucleus, 2023, accepted for publication.
[16] P.G. Akishin, V.P. Ladygin, Particles and Nuclei Letters **19**, 6, 785–788 (2022).

such as dipole and quadrupole superconducting magnets of the collider and booster of the NICA JINR project, dipole and quadrupole superconducting magnets of the SIS100 FAIR accelerator, the magnetic system of the CBM FAIR experiment (GSI, Darmstadt), the magnetic system of the MSC230 cyclotron (DLNP) and others. Examples of calculations of the magnetic field of the quadrupole magnet and the lens of the final focus of the NICA collider are shown in Fig. 4. Note that in 2020, A.S. Ayriyan and A.A. Sapozhnikov defended successfully their PhD These in the dissertation council of MLIT. Subjects of their dissertations were related to the modeling of complex processes in large experimental facilities.

When solving problems that arise during the development and optimization of operating modes of experimental facilities, it is necessary to ensure facility adapted discretization of the mathematical equations, effective numerical solutions of the emerging nonlinear equations. To get reliable results, it is necessary to reduce the size of the discrete grid cells. This results in very large dimensions of the systems of nonlinear equations being solved and, as a result, to a significant increase in the computing time. In this regard, it is necessary to optimize all stages of computing and to develop parallel algorithms for the efficient use of the high-performance MICC computing resources.

Within this project, mixed formulations of the magnetostatics problems, based on magnetic vector and full scalar potentials, will be developed and tested, and the combined finite and boundary element method will be adapted and tested for 3D modeling of magnetic systems characterized by complex geometry and nonlinear variation of the magnetization. Numerical methods for modeling magnetic systems will be developed within the integral formulation of volumetric integral equations with piecewise polynomial approximations of the magnetization within the finite elements.

Methods will be developed with the aim at improving the efficiency and optimization of the numerical simulation of the complex magnetic systems of accelerators. Finite and boundary element methods, including the development of scalable algorithms with a high potential for parallelism, will stay at the basis of the new discrete algorithms. It is planned to adapt the developed algorithms within the COMSOL Multiphysics® package on the resources of the MICC computing complex.

The CORD (Closed ORbit Dynamics) [17] program will be refined and optimized, and with its help, in collaboration with colleagues from the DLNP, the analysis of the frequencies of betatron oscillations and the phase motion of particles in various versions of computer models and in the formation of the magnetic field of the MSC230 cyclotron (DLNP) will be carried out. It is planned to prepare the CORD program and its description for inclusion in the JINRLIB library.

IV. Modeling physical phenomena in dense nuclear matter, based on the equation of state

Progress in the study of the fundamental properties of the nuclear matter at extreme densities requires the creation of reliable computational methods that implement new theoretical and phenomenological approaches to the simulation of complex processes and phase transitions in the super dense nuclear matter, which is expected to occur during heavy ion collisions in the NICA energy range.

The numerical simulation of the physical phenomena based on the equation of state of the dense nuclear matter, will need new mathematical formulations in terms of nonlinear differential equations that describe complex processes in astrophysical systems [18] and in heavy ion collisions

[17] O. Karamyshev, T. Karamysheva, I. Lyapin, V. Malinin, D. Popov, Physics of Particles and Nuclei Letters **18**, 4, 481–487 (2021).

[18] M. Shahrbaf, S. Antić, A. Ayriyan, D. Blaschke, A.G. Grunfeld, Phys. Rev. D **107,** 054011 (2023); A. Ayriyan, D. Blaschke, A.G. Grunfeld, D. Alvarez-Castillo, H. Grigorian, V. Abgaryan, Eur. Phys. J. A **57**, 318 (2021).

in experimental facilities [19], considering the possibility of phase transition in nuclear matter, the short duration of the processes, temperature effects etc.

Numerical modeling will be based on the use of the traditional iterative and grid methods for solving nonlinear differential and integral equations, as well as new developments based on neural network algorithms concerning both the solution of differential equations and the computation of multidimensional integrals that arise in the description of the processes of scattering and of particle yield in dense and hot nuclear matter. This undertaking will also involve the development of methods devoted to the validation of the results of computer simulations based on the comparison with observational data for compact stars and with experimental data on heavy ion collisions. These methods will make heavy use of Bayesian inference to estimate the free parameters of the simulated processes and to model the equation of state of superdense matter. Instances of computations along this direction based on approaches developed by the project participants are shown in Fig. 5.

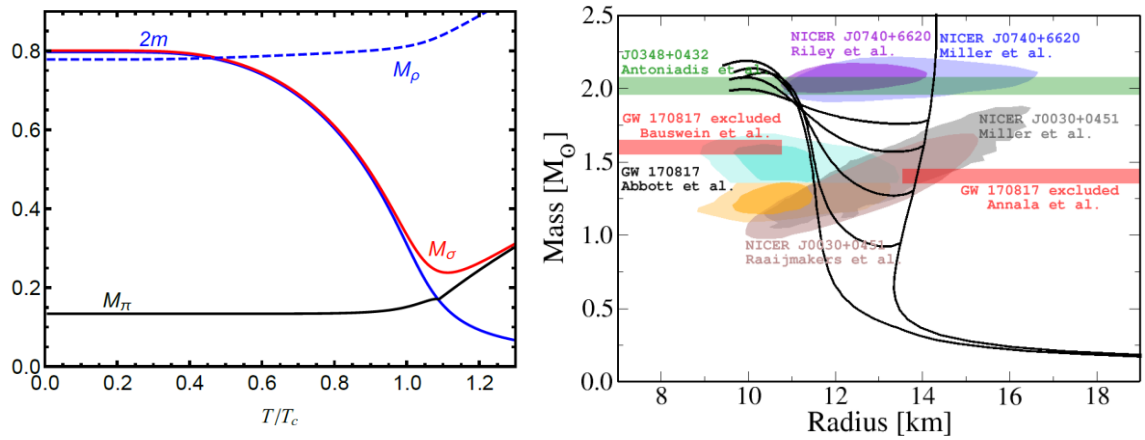

Fig. 5. Left: temperature dependence $M_i(T)$ of the meson mass spectrum (i=π,σ,ρ) and double quark mass $m(T)$ in dense nuclear matter (the picture is taken from [19]). Right: a diagram of neutron star mass-radius relationships for various models of the equation of state for superdense nuclear matter compared to multichannel astronomy data, including gravitational wave signals from neutron star mergers.

Methods, algorithms and software packages will be developed for modeling processes, in strongly interacting hot and dense nuclear matter, arising in heavy ion collisions at NICA energies, including the processes of particle scattering and production and the formation of quark-gluon plasma. Numerical results obtained on the basis of the developed methods and programs will bring significant contributions to the understanding of the fundamental features of the processes occurring in the simulated systems. A method enabling the validation of the models devoted to the description of the equation of state of superdense nuclear matter based on multichannel astronomy data will be developed and implemented. The developed and existing software will be integrated into a single information and computing system for unified work with different models of the equation of state, including interactive calculations of the mechanical characteristics of neutron stars based on the equation of state of cold and dense matter.

V. Modeling of quantum systems using methods of quantum information theory and hybrid quantum-classical programming methods

The modern progress of quantum technologies, rooted in the synthesis of the knowledge of the fundamental laws of the microworld and the solution of non-trivial engineering and technical problems, served as the strongest motivation for the creation of a new branch of science - quantum informatics. In turn, the achievements of the latter stem from the emergence of new areas of

[19] D. Goderidze, A. Friesen, Yu. Kalinovsky, Intern. J. Modern Physics A **37**, 22, 2250135 (2022); A. Friesen, D. Goderidze, Yu. Kalinovsky, Physics of Particles and Nuclei Letters, **19** (2022) 337; D. Blaschke, A. Friesen, Yu. Kalinovsky, Symmetry **15**, 117 (2023).

computational physics and computer mathematics, which are spanned by the basic principles of the quantum theory. A multilateral description of the quantum systems in the framework of the quantum informatics implies, along with a standard set of physical characteristics, the use of statistical and informational quantities (entropies, indicators of correlation and entanglement of quantum states, etc.) [20]. This is necessary for the effective development of quantum information technologies [21]. To solve quantum modeling problems, computer algebra methods, symbolic-numerical algorithms will be used in combination with the formalism developed in MLIT for describing quantum systems in phase space in terms of quasi-probability distributions [22]. Moreover, the solution of evolutionary problems in quantum systems, the use of the theory of algebras and Lie groups in connection with known quantum-classical algorithms for quantum computing are necessary. New methods for quantum modeling of the processes of storage and transmission of information in open and closed quantum systems will be created, taking into account their information resource. Based on the use of hybrid quantum-classical programming schemes, it is planned to optimize existing classical simulators and to create new ones, enabling the decrease of the needed computing power by means of the design and implementation of new efficient methods and programs focused on the heterogeneous HybriLIT platform.

Expected results at the end of 2024

On the Section I.

Development of a mathematical formulation of the problem within the strong coupling channels method with the Woods–Saxon optical potential and regular boundary conditions for modeling sub-barrier heavy ion fusion and fission reactions.

Development of methods and calculation of the energy of adsorption on the Au layer of heavy and superheavy atoms; preparation of publication.

Development and optimization of the method of self-similar approximations for solving nonlinear equations that do not contain small parameters and describe quantum mechanical systems, including spin ensembles and cold atoms in traps. Preparation of publications on this matter.

Development of a method and program that initiates, in the framework of the transport-statistical approach, the initial state of colliding nuclei with nuclear potentials, which are used to further calculations in the collision dynamics.

Modeling the proton-nucleus interactions, based on a microscopic model of the optical potential, over a wide range of energies and for a large variety of atomic numbers of the target nuclei with the aim at assessing the influence of the nuclear medium on the processes of proton scattering by intranuclear nucleons; preparation of a publication.

On the Section II.

Investigation of the dynamics of a shock wave in an irradiated material based on a model described by the combination of molecular dynamic equations, thermal conductivity equations and wave equations. Determination of the parameters of the wave equation based on the results of the numerical solution of molecular dynamics equations. Development and software implementation of methods for estimating the spread of energy losses of heavy charged particles in materials due to large momentum transfers. Investigation and classification of changes in defective structures within a molecular dynamics approach under the influence of various types of irradiation and over a large energy range.

Simulations of the interaction of amyloid beta and antimicrobial peptides with phospholipid membranes in vesicular and bicellar structures in the coarse-grained model; study of the dynamic properties of this interaction based on the calculation of the phonon spectra of systems;

[20] V. Abgaryan, A. Khvedelidze, A. Torosyan, Physics Letters A **412**, 7, 127591 (2021)

[21] V.V. Kornyak. Programming and Computer Software **47**, 2, 124–132 (2021); O.V. Tarasov, J. High Energy Phys. **6**, 155–205 (2022).

[22] V. Abgaryan, A. Khvedelidze, Symmetry **13** ,6, 1013 (2021).

construction of the free energy profile of the process of pulling the peptide out of the membrane depending on the distance between the centers of mass and conformation of the peptide (replica exchange umbrella sampling).

Study of localized structures in systems described by nonlinear damped-driven equations. Investigation of the formation of a hydrated electron based on a modified polaron model that takes into account the Coulomb interaction, calculation of the observed characteristics of this process.

On the Section III.

Adaptation of the COMSOL Multiphysics® package to the heterogeneous HybriLIT platform in order to increase the efficiency of the computations and to reduce the computational time through the use of a mixed vector-scalar formulation of magnetostatics and a hybrid finite and boundary element method. Development and software implementation of difference schemes for solving a boundary value problem for a 4th order equation describing the distribution of physical fields in 2D and 3D regions of various configurations.

Development of methods and study of the formation of magnetic fields of isochronous cyclotrons under various operating modes. Preparation of instructions and registration of the CORD (Closed ORbit Dynamics) program in the JINRLIB library. CORD implements calculations to study the effect of betatron oscillations and phase motion of beam particles on the magnetic field of the MSC230 cyclotron.

On the Section IV.

Adaptation of the neural network approach to the approximate calculation of multiple integrals arising in the study of pion survival in heavy ion collisions; ellaboration of methods aimed at extending to finite temperatures the previously developed model of the quark-hadron phase transition in cold nuclear matter.

Modeling and calculation of cosmological redshift values based on the equation of state; investigation of the possibility of reconstructing the mass spectrum of an isolated neutron star from the data on the age and surface temperature of pulsars, based on simulations of their temperature evolution; simulation of processes of scattering and creation of particles in dense and hot nuclear matter; preparation of publications.

On the Section V.

Development of an evolution operator trotterization algorithm for the von Neumann and Lindblad equations and implementation of the corresponding quantum circuit on a quantum simulator in the QISKit environment. Improving the performance of the quantum circuit simulator by increasing the simulation speed using multiprocessing.

Creation of a package of modules designed to decompose a quantum system into subsystems based on the use of tensor products of representations of wreath products of finite cyclic groups.

Determination of the relationship between the characteristics of entanglement of composite quantum systems and the negativity of the Wigner quasiprobability distributions. Development of a functional reduction method for two-loop Feynman integrals and its application to the calculation of integrals corresponding to diagrams with four and five external lines.

Expected results in 2024-2026

On the Section I.

Development of a method, a program package and the calculation with their help of cross sections for deep sub-barrier heavy nuclei fusion/fission reactions under conditions of strong coupling channel based on the numerical solution of the corresponding system of Schrödinger equations with asymptotic boundary conditions.

Investigation of the structure of light and heavy nuclei with a neutron halo based on the calculation of the characteristics of the nucleus-nucleus and proton-nucleus interactions in the framework of a modified model of the microscopic optical potential.

Creation of a software package for a realistic description of isotope and velocity distributions of heavy ion fragmentation reactions at medium energies within the transport-statistical approach.

Construction and software implementation of a stochastic model that provides a quantitative description of chemical reactions involving heavy and superheavy elements in FLNR chromatographic experiments.

Numerical study of the dynamics of spin systems and cold atoms in traps in the frame of a quantum mechanical model based on the solution of a system of nonlinear equations using an optimized method of self-similar approximations.

On the Section II.

Development of computational schemes and software packages that implement the solution of systems of equations in continuum-atomistic models of interaction of an irradiating beam of charged particles with a target material. Obtaining new information about the dynamics of the formation of defective structures under the influence of irradiation by mathematical modeling methods.

Obtaining new information about the formation process, structure and properties of phospholipid objects of various types (vesicles, bicelles) by methods of classical and quantum molecular dynamics and based on the method of separated form factors, including simulations of the interaction of amyloid beta and antimicrobial peptides with the system of phospholipid membranes.

Investigation of complex processes in Josephson and spin nanostructures depending on the configuration of the systems under study and the nature of external influences in order to assess the influence of various factors on the physical characteristics and dynamics of superconducting processes.

Development and use of an information-computing environment based on JupyterHub for comfortable and unified work with models of superconducting structures.

Development of methods and study of the formation process and properties of localized structures in condensed matter, described by various types of nonlinear field theory equations. Simulation of the electron hydration within a modified dynamic polaron model devoted to the study of the influence of various factors on this process.

On the Section III.

Development, software implementation, and testing of mixed formulations of magnetostatics problems based on magnetic vector and total scalar potentials, as well as on the basis of volumetric integral equations with piecewise polynomial approximation of magnetization within a finite element.

Adaptation and testing of the combined finite and boundary element method for 3D modeling of magnetic systems with complex geometry and nonlinear magnetization. Adaptation of the COMSOL Multiphysics® package to the MICC resources.

Development of methods for increasing the efficiency and optimization of numerical simulation of complex magnetic systems of accelerators, including the development of scalable algorithms with a high potential for parallelism.

Carrying out calculations aimed at studying the influence of various factors and optimizing the operating mode of the MSC230 cyclotron. Implementation of the analysis of the frequencies of

betatron oscillations and the phase motion of particles in various versions of computer models and during the formation of the magnetic field of the MSC230 cyclotron.

On the Section IV.

Methods for verifying the results of computer simulation of complex processes in dense nuclear matter based on observations of compact stars and experimental data on heavy ion collisions, implementing Bayesian approaches for estimating the free parameters of simulated processes.

Methods and programs for modeling processes in strongly interacting hot and dense nuclear matter arising in heavy ion collisions at NICA energies, including the processes of particle scattering and production and the formation of quark-gluon plasma.

Development of an information and computing environment for unified work with different models of the equation of state, including interactive calculations of the mechanical characteristics of neutron stars based on the equation of state of cold and dense matter.

Derivation of numerical results relevant to the understanding of fundamental processes in the modelled physical systems.

On the Section V.

Development of methods combining problem-oriented quantum programming and computational mathematics methods to obtain new information about quantum systems of various nature.

Development of new and adaptation of existing quantum simulators for high-performance computing on hybrid architecture computers; application of quantum programming for modeling quantum computing and for solving a number of problems in condensed matter physics, high energy physics, quantum chemistry, artificial intelligence, etc.

Development of new approaches to the study of quantum systems based on combination of methods of computational physics, methods of quantum information theory, hybrid methods of quantum-classical programming of computer mathematics and symbolic-numerical algorithms. Investigation on this basis of information characteristics and description of the dynamics of quantum states in elementary particle and nuclear physics, quantum chemistry, biophysics, etc.

Study and classification of informational characteristics of the states of finite-dimensional quantum systems in the phase-space representation of quantum theory to determine the most important characteristics necessary for modeling quantum systems of various classes and to improve the efficiency of quantum computing.

Scientific background and risks

The project participants are highly qualified in the field of computational physics and modern information technologies, have significant experience in developing methods and programs for studying complex physical systems, as well as in successfully conducting high-performance computer simulations. The research team includes enthusiastic young scientists and engineers, as well as experienced scientists known for their achievements in the development of computational methods and mathematical modeling. There are 30 candidates and 13 doctors of sciences among the project participants. Thanks to meetings, schools, workshops, and seminars regularly held at LIT JINR, young specialists have the opportunity to improve their scientific level and IT qualifications necessary to successfully solve the project's tasks. In 2020–2022 The staff of the MLIT Scientific Department of Computational Physics, in cooperation with colleagues from other laboratories and foreign research centers, prepared more than 150 scientific papers in peer-reviewed scientific journals in the area covered by the project. Three PhD theses of MLIT staff on the subject of the project were successfully defended in the MLIT Dissertation Council. During 2020–2022, the project participants implemented eight high-performance software packages in the Program Library JINRLIB while three packages have been included in the international library of computer programs of the Computer Physics Communications journal. Thus, taking into account

the scientific background available to the team of project participants, there is reason to believe that the tasks of the project will be successfully completed.

We note the following risk factors.

- Since research within the framework of the project is closely linked with research conducted in other JINR laboratories, a significant change in research plans in other JINR subdivisions might lead to incomplete fulfillment of the objectives of this project.
- Access restrictions to licensed software and high-performance computing resources may have a negative impact on the successful implementation of project objectives.
- Force majeure circumstances, including those related to possible complications of the geopolitical situation and restrictive measures during epidemics may also hinder the full completion of the project tasks.

2.3. Estimated completion date

2024-2026

2.5. Participating countries, scientific and educational organizations

Organisation	Country	City	Type of agreement
Foundation ANSL	Armenia	Yerevan	Collaborations
BrSU	Belarus	Brest	Collaborations
IM NASB	Belarus	Minsk	Agreement
SU	Bulgaria	Sofia	Collaborations
CIAE	China	Beijing	Collaborations
TSU	Georgia	Tbilisi	Collaborations
UG	Georgia	Tbilisi	Collaborations
CU	Egypt	Giza	Collaborations
UNAM	Mexico	Mexico	Collaborations
IMDT MAS	Mongolia	Ulan-Bator	Collaborations
BM@N Collaboration	Russia	Dubna	Collaborations
MPD Collaboration	Russia	Dubna	Collaborations
RSTSREC	Russia	Moscow	Collaborations
PFUR	Russia	Moscow	Collaborations
IMPB RAS	Russia	Pushchino	Collaborations
SSU	Russia	Saratov	Collaborations
UCT	South Africa	Cape Town	Collaboration, JINR-NRF grant