Annex 3.

Form of renewal for Project
06-6-1119-2-2024/2026

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SCIENTIFIC AND TECHNICAL REASONING FOR THE RENEWAL
OF THE PROJECT IN RESEARCH AREA
WITHIN THE TOPICAL PLAN FOR JINR RESEARCH

1. General information on the project
1.1 Theme code
06-6-1119-2014

1.2 Project of a MIP code (for renewed projects)
06-6-1119-2-2024/2026

1.3 Laboratory
MLIT

1.4 Scientific field
06 – Information technologies

1.5 The name of the Project
Methods of computational physics for the study of complex systems

1.6 Project Leaders
E.V. Zemlyanaya, O. Chuluunbaatar

1.7 Project Deputy Leaders
Yu.L. Kalinovsky, A. Khvedelidze

1.8. Scientific supervisor of the project

2. Scientific rationale and organisational structure
2.1. Annotation
The project aims at the development and use of mathematical and computational methods for modeling complex physical systems studied within the JINR Topical Plan and described by systems of dynamic nonlinear, spatially multidimensional integral, integro-differential or differential equations driven by the parameters of the models. The evolution of the solutions of such systems may be characterized by the occurrence of critical regimes, bifurcations and phase transitions. Mathematical modeling is an indelible part of the modern scientific research. It needs adequate mathematical formulations of the problems within 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 elaboration of algorithms and software packages for high-performance simulation on modern computer systems, primarily the MICC MLIT resources. During 2027–2031, the research 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, atomic physics, molecular 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 of complex processes in dense nuclear matter, including astrophysical models and processes in experimental facilities.

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

As a result of the studies conducted by means of the developed methods and software packages, new fundamental information about the investigated physical systems will be obtained, enabling further development of mathematical models for theoretical and experimental investigations at JINR.

2.2. Scientific justification (purpose, relevance and scientific novelty, methods and approaches, methodologies, expected results, risks)

Purpose

Development and software implementation of computational approaches for the study, by means of mathematical modeling methods, of physical phenomena that are the focus of the Institute's research set by the Seven-Year Plan for the Development of JINR for 2024–2030. Derivation, on this basis, of the new knowledge asked by the understanding of the involved physical processes, accomplishment of further theoretical research and inference of experimental projects that are relevant from the point of view of practical applications.

Relevance and novelty

The proposed project tasks bear relevance to a wide range of scientific areas within the JINR Topical Plan and are aimed at creating new mathematical methods, algorithms and programs for successfully solving urgent problems that arise during the implementation of the scientific programs set up in JINR. Based on the solutions of the tasks formulated within the proposed project extension, new methods, algorithms and software packages will be developed and implemented that are fundamental for the accomplishment of cutting-edge research into complex physical phenomena described by nonlinear, multidimensional, multiparameter systems of equations.

The accomplishment of the proposed project tasks will result in:

(1) new original developments in the fields of the computational mathematics methods, high-performance computing, and mathematical modeling;
(2) the numerical research results obtained on this basis will be highly relevant for the understanding of the physical problems under study.

Main areas of research

The research within the project involves the development of new methods and the improvement of existing ones, including those created by the project team, in each of the areas listed below. It 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, atomic physics, molecular 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 the high-precision discrete approximation of the corresponding systems of equations;
- study of processes of scattering of heavy ions and particles on nuclei and the interaction of heavy ions at ranges of intermediate energies within either microscopic optical potential models or the transport-statistical approach;
- modeling chemical bonds and reactions involving heavy and superheavy elements with the aim to grasp the meanings of the thermochromatographic experiments done at FLNR;
- development of methods and conducting research into the dynamics of spin aggregates and cold atoms in traps within quantum mechanical models.

II. Studies of intricate processes in materials and condensed media subject to external impacts, including:

- simulation of physical–chemical and structural changes in materials under the action of irradiation with charged particles, nanoclusters and laser radiation; development of methods for calculating the characteristics of energy losses of heavy ions in irradiated materials under wide ranges of the charge numbers of the 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 reliable inferences to the perspectives for creating memory elements and information transfer;
- study of the structure and properties of polydisperse phospholipid vesicular systems of various types, nanodrugs included, based on molecular dynamics approaches and within 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 the numerical simulation of complex magnetic systems of actual accelerators;
- modeling of magnetic systems for experimental setups, including numerical modeling of physical processes during the formation of the magnetic field of the MSC230 cyclotron (DLNP).

IV. Equation of state based modeling of complex processes in dense nuclear matter, 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 computational physics based on hybrid quantum-classical programming, computer mathematics, and their application to study the information characteristics of quantum states in elementary particle and nuclear physics, quantum chemistry and biophysics.

Methods and approaches, techniques

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 that, covers the following stages:

- *Formulation of the mathematical statement of the problem* that properly 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 concerning: symbolic-numerical and numerical-analytical algorithms, neural network and molecular dynamics methods, methods of quantum computing and computer algebra, parallel computing algorithms, artificial intelligence-based technologies;
- *Software implementation* of the developed computational scheme using high and ultra-high level programming tools, techniques for organizing parallel and hybrid computations on modern high-performance computing systems, existing libraries of computer programs and problem-oriented software packages, specialized tools to create a suitable 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 deriving new information* about the simulated physical systems during the analysis of numerical results, which can serve as a basis for the refinement and further development of the theoretical approaches and experiment planning.

A brief description of the main objectives of the project, together with some results already obtained, which serve as a basis for further research within the project, are given below.

The first area of the project encompasses a range of tasks related to **the numerical study of the characteristics of complex processes described by models of atomic, molecular, nuclear physics, semiconductor physics, and quantum mechanics.** Such tasks are necessary for understanding the mechanisms of nuclear interactions and the structure of nuclei involved in reactions, testing existing theoretical hypotheses, and interpreting the obtained experimental data, including ongoing and planned experiments on the synthesis of superheavy elements and 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.

Research into the physical characteristics of sub-barrier fusion reactions of heavy nuclei will be continued[1] within the channel coupling method. To this purpose, a set of computer codes for the numerical solution of scattering problems and problems on metastable states of the corresponding system of Schrödinger equations with a large number of coupled channels will be improved. To calculate the spectral characteristics of atomic nuclei in modern collective models, computational schemes, algorithms and programs based on the finite element method will be adapted for solving multidimensional (up to 6-dimensional) elliptic boundary value problems[2].

Research into the physical characteristics of nucleus-nucleus interactions, including reactions involving light and heavy nuclei with a neutron halo, will be continued with the aim at obtaining new information on the structure of such nuclei based on the corroboration of numerical and experimental results. In 2004–2005, in collaboration with BLTP, based on the analysis, within the microscopic model of optical potential, of proton-nucleus scattering data in a wide energy range, estimates of the influence of the nuclear medium on the scattering amplitude depending on the

[1] P.W. Wen, O. Chuluunbaatar, P. Descouvemont, et al., Phys. Lett. B 863, 139383 (2025).
[2] O.O. Kovalev, B. Batgerel, A.A. Gusev, et al., Lect. Notes Comput. Sci. 16235, 210–222 (2026).

energy of the incident proton were obtained[3]. The scattering reaction of $^{7}Li+^{10}B$ and the transfer neutron reaction $^{7}Li+^{10}B \rightarrow ^{6}Li+^{11}B$ at the laboratory beam energy 58 MeV were studied. The results of the microscopic analysis of data obtained at the U-400 cyclotron at FLNR indicate the presence of a proton-neutron halo in the structure of the excited state $^{6}Li_{0+}$ (3.56 MeV)[4]. A modernization of the microscopic approach is planned, with the aim at expanding the spectrum of energies and the reaction types. This will serve to the study of the characteristics of nuclear interactions over a wide range of energies and atomic numbers of the colliding nuclei.

To get accuracy enhancement and computing time decrease, methods and programs implementing the transport-statistical model for calculating the physical characteristics of heavy ion interactions at medium energies will be modernized. A number of computational and physical parameters of the model were refined based on comparisons of theoretical estimates with available experimental data. The modification of the procedure for modeling fragmentation reactions in the BNV-SMM model resulted in the computing time decrease and the improvement of the agreement with experimental data on fragmentation reactions in comparison with other known approaches[5]. It is expected that this approach will be further enhanced and that calculations will be carried out for an extended range of physical characteristics.

The simulation of the dynamics of spin aggregates and cold atoms in traps is 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. Based on the developed approaches[6] it is expected that new results on modeling the dynamics of systems, that are relevant from the perspective of technological applications, will be obtained.

A further objective of the project is to construct a stochastic model of chemical reactions involving heavy and superheavy elements. As part of this effort, the functionality of the TANGELO software package for simulating quantum computations has been expanded to include relativistic corrections to Coulomb interactions when calculating chemical compounds involving superheavy elements[7]. It is expected to obtain, by means of mathematical modeling methods, updated and new information on the characteristics of nuclei participating in planned experiments on the synthesis of superheavy elements, on the electronic structure and chemical bonds in heavy atoms, as well as on the influence of relativistic effects on these characteristics.

The studies of intricate processes in condensed matter and materials under external actions require, as a rule, taking into account such features as the significant dependence of the modeled processes on the model parameters, phase transitions, multiple solutions, possible bifurcations and critical modes.

One of the important tasks in this direction is the study, by means of mathematical modeling methods, of complex processes in materials under the irradiation with high energy charged particles. The relevance of such studies is determined by the perspectives for the development of methods for targeted modification of the properties of materials, as well as the need to study the resistance of materials to various types of irradiation.

During the first two years of the project's implementation, the dynamics of laser ablation of materials under the action of ultrashort laser pulses was studied using the non-stationary heat conduction equation in a coordinate system associated with a moving evaporation front, as well as within a two-temperature thermal peak model[8]. The further development and use of hybrid

[3] I. Abdul-Magead, V.K. Lukyanov, E.V. Zemlyanaya, K.V. Lukyanov, Intern. J. Modern Phys. E 33, 2441012 (2024).
[4] E.V. Zemlyanaya, K.V. Lukyanov, V.K. Lukyanov, et al., Bulletin Rus. Acad. Sci.: Phys. 89, 1236–1240 (2025).
[5] T.I. Mikhailova, B. Erdemchimeg, Yu.M. Sereda, Bulletin Rus. Acad. Sci.: Phys. 89, 1216–1222 (2025).
[6] V.I. Yukalov, E.P. Yukalova, Ann. Phys. 467, 169716 (2024).
[7] V.Yu. Yushankhai, L.A. Siurakshina, Phys. Part. Nucl. 56, 1004–1008 (2025).
[8] I.V. Amirkhanov, I. Sarkhadov, Z.K. Tukhliev, et al., J. Surf. Investig.: X-ray, Synchrotron Neutron Tech. 18, 348–353 (2024).

computational schemes, combining the advantages of models based on continuum equations with models described by systems of particle motion equations, are planned.

The simulation of superconducting processes in Josephson and spin nanostructures, in terms of the configuration of the systems under study and the nature of the 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 due to the foreseen perspectives for creating memory 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. The numerical investigations involve the development and comparative testing of computational schemes in order to select appropriate numerical approaches, as well as the parallel implementation for high-performance computer simulation in a wide range of model parameters to study the influence of various factors on the dynamics of superconducting processes. The results in this area were included in the successfully defended in 2025 Ph.D. thesis of the project participant and MLIT employee M.V. Bashashin. To improve the efficiency of computer program creation and calculations, an ecosystem for modeling Josephson structures is currently developed on the basis of the Jupyter Book platform. The ecosystem was supplemented in 2024 with software modules for studying the dynamics of a superconducting quantum interferometer with two or more Josephson junctions (SQUID). A parallel implementation using the Numba library provided a significant acceleration of the computations[9] in the developed numerical scheme for constructing the current-voltage characteristic of a SQUID subject to a magnetic field. The computer simulation of a controlled magnetization flip in a chain of ϕ_0 junctions was conducted[10].

Modeling complex processes in condensed matter described by nonlinear field theory equations requires the use of parameter continuation methods with identification of bifurcations and access to new branches of solutions. Such procedures result in the increase of the accuracy of the discrete approximations of the computational schemes ensuring the reliability of the obtained numerical results. The parallelism implementation speeds up the mass calculations in a wide range of model parameters. Methods will be developed and nonlinear processes of localized structure formation in condensed matter under external influences, described by various types of field theory equations, will be studied. In particular, to account for the influence of Coulomb forces on the self-localization of a solvated electron, the method and software package implementing the numerical solution of the corresponding system of nonlinear equations were modified in 2024 to improve the agreement of the numerical results with the available experimental data. Another important area is the study of oscillons in the φ^4 model – long-lived spatially localized structures oscillating in time, which have a number of relevant applications in cosmology and high-energy physics. In collaboration with the University of Cape Town, a numerical study to examine the role of frequency and radius parameters on the structure and properties of standing waves in a ball of finite radius, approximating three-dimensional φ^4 oscillons, was conducted. Coexisting types of standing waves were found, and their interrelationships, as well as the dependence of the energy and stability intervals of the waves on radius and frequency, were investigated[11].

There is a twofold importance of the study of the structure and dynamics of the evolution of phospholipid membranes in vesicular and bicellar systems: for understanding fundamental biochemical processes in living organisms and for obtaining information needed 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. Such calculations are planned to be implemented on graphics accelerators to simulate the longest possible system evolution time. The results of

[9] A. Rahmonova, I. Rahmonov, O. Streltsova, M. Zuev, Phys. Part. Nucl. 55, 528–531 (2024).
[10] A. Rahmonova, O. Streltsova, I. Rahmonov, M. Zuev, Phys. Part. Nucl. 56, 1592–1598 (2025).
[11] E. Zemlyanaya, A. Bogolubskaya, M. Bashashin, et al., Discrete Contin. Models Appl. Comput. Sci. 32, 106–111 (2024).

studies already conducted jointly with colleagues from FLNP and LRB on the reorganization of lipid membranes induced by the Aβ (25–35) peptide under conditions simulating the preclinical stage of Alzheimer's disease were published in 2024[12]. Research on vesicular systems of various types depending on the temperature and chemical composition of the medium using the separated form factor method and various models of the phospholipid bilayer is also underway. A web interface for the online analysis of experimental small-angle scattering data was implemented on the JINR cloud infrastructure, utilizing ROOT package tools for parallelism[13]. In collaboration with FLNP and the Institute of Biomedical Chemistry of the Russian Academy of Sciences, a study on the structure of vesicles of a phospholipid transport nanosystem and drugs based on it was conducted using small-angle neutron scattering data obtained on the "Yellow Submarine" small-angle spectrometer (Budapest). Significant influences of several factors, including the presence of impurities and the concentration of the solution, on the size of the vesicles and their structure were demonstrated[14].

The solutions of the problems arising in the development and optimization of operating modes of experimental facilities ask for the facility-adapted discretizations of the mathematical equations and the buildup of effective numerical solutions of the emerging nonlinear equations. The reliable calculations of the many magnetic fields characteristics required for 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. Among the project participants' achievements is the computer modeling of magnetic systems, including dipole and quadrupole superconducting magnets for the collider and booster of the JINR NICA project[15].

To obtain reliable results, it is often necessary to reduce the sizes of the grid cell discretizations. This process results in very large dimensions of the systems of nonlinear equations asking for solutions and, consequently, to a significant increase in the computing time. In this respect, it is necessary to optimize the computing schemes and to develop parallel algorithms for the efficient use of high-performance computing resources, the MICC ones included. The project embraces the development, optimization for high-performance calculations, and testing of methods for numerically solving magnetostatic problems in various mathematical settings.

Two kinds of results reported during 2024–2025 in this area are worth mentioning. First, a proposed combined procedure[16], implementing a finite element method for a magnetic vector potential, allows for the reduction of the computational cost without loss of accuracy when solving 3D magnetostatic problems with complex geometry. Second, the implementation of computer vision and artificial intelligence capabilities for optimizing the beam motion within the CORD (Closed ORbit Dynamics) program, highly enhanced the quality of the predictions concerning the influence of betatron oscillations and phase motion of beam particles on the magnetic field of the MSC230 cyclotron[17]. The results achieved during the first two years of the project's implementation open up new ways for further research both in the field of developing new computational methods for modeling physical fields under various conditions, and in the field of computer modeling and various operating modes of large-scale experimental facilities at JINR with the aim of achieving their optimizations.

Progress in **the study of the fundamental properties of 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

[12] S. Kurakin, D. Badreeva, E. Dushanov, et al., Biochim. Biophys. Acta Biomembr. 1866, 184237 (2024).
[13] K. Lukyanov, A. Soloviev, T. Solovjeva, E. Zemlyanaya, Phys. Part. Nucl. 56, 1509–1513 (2025).
[14] E. Zemlyanaya, M. Kiselev, V. Chausova, et al., Int. J. Mod. Phys. E, 2025, https://doi.org/10.1142/S021830132641003X
[15] H.G. Khodzhibagiyan, P.G. Akishin, A.V. Butenko, et al., Nat. Sci. Rev. 1, article number 6 (2024).
[16] A.M. Chervyakov, Phys. Part. Nucl. Lett. 21, 1074–1083 (2024).
[17] O.V. Karamyshev, I.D. Lyapin, T.V. Karamysheva, et al., Phys. Part. Nucl. Lett. 22, 690–698 (2025).

super dense nuclear matter, which is expected to occur during heavy ion collisions in the NICA energy range. A topical task that is closely connected with the planned experiments at the NICA facility is the study of the properties of the bound states in dense and hot nuclear media. To conduct the numerical modeling of physical phenomena based on the equation of state of the dense nuclear matter, mathematical formulations of problems for nonlinear differential equations, formulated by project participants will be used. These equations describe complex processes both in astrophysical systems and in heavy-ion collisions under experimental conditions. They take into account such features of the simulated systems as the possibility of phase changes in nuclear matter, the short duration of the processes being studied, and the need to account for temperature effects. Specifically, the project participants have developed a quantitative model with nonlocal interactions[18], within which a system of equations was formulated for the description of the vector meson spectrum. This allows for the calculation of the mass spectrum, interaction constants, normalizations, and selection of suitable form factors. The phenomenological choice of the vector meson vertex used in this nonlocal model will be sufficient to describe the properties of heavy J/ψ(Y) quarkonia: the processes of quarkonia production and dissociation at heavy-ion collision energies at the NICA experiment.

Numerical modeling in this area requires the use of both traditional iterative and grid methods for solving nonlinear differential and integral equations, as well as the development of neural network algorithms for solving differential equations and calculating multidimensional integrals arising in the description of particle scattering and production processes in dense and hot nuclear matter. It is planned to develop procedures for verifying the results of computer modeling based on the use of observational data on compact stars and experimental data on heavy ion collisions, using Bayesian methods for estimating free parameters of the modeled processes and models of the equation of state of superdense matter. Methods and programs for modeling processes in strongly interacting hot and dense nuclear matter arising in heavy-ion collisions at NICA energies, including particle scattering and production processes and the formation of quark-gluon plasma, will be developed. Numerical results obtained using the developed methods and programs will make a significant contribution to understanding the fundamental processes in the simulated systems. A model verification method based on the equation of state of ultradense nuclear matter using 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 various models, including interactive calculations of neutron star characteristics based on the equation of state of cold and dense matter.

A key focus of the project is **the development of quantum system modeling methods using quantum information theory and hybrid quantum-classical programming algorithms.** Modern advances in quantum technologies, driven by the synthesis of knowledge of the fundamental laws of the microworld and the solution of nontrivial engineering problems, have served as a powerful motivation for the creation of a new field of science — quantum information science. The achievements of quantum information science, in turn, are related to the development of new areas of computational physics and computer mathematics, which are based on the fundamental principles of quantum theory. A multifactorial description of the quantum systems within the quantum information science implies, along with a standard set of physical characteristics, the use of statistical and informational quantities. To solve quantum modeling problems, the project utilizes computer algebra methods and symbolic-numerical algorithms in combination with the formalism developed at MLIT for describing quantum systems in phase space in terms of quasi-probability distributions. When solving evolutionary problems in quantum systems, it is proposed to apply the theory of Lie algebras and groups in synthesis with known quantum-classical algorithms for quantum computing.

The research planned for 2027–2031 will include investigations of the computational resources of composite quantum systems, enabling the development of efficient computational schemes

[18] A. Friesen, Yu. Kalinovsky, A. Khmelev, Eur. Phys. J. A 62. article number 6 (2026).

based on quantum algorithms and computer algebra methods. The developed methods and algorithms will be applied to calculating physical characteristics in various quantum-field and finite-dimensional quantum systems. This will be used to develop new methods for the quantum modeling of information storage and transmission processes in open and closed quantum systems, taking into account their information resources.

Using hybrid quantum-classical programming schemes, it is planned to optimize existing classical simulators and develop new ones, reducing the required computing power by developing new efficient methods and programs oriented toward the HybriLIT heterogeneous platform. In 2024–2025, the implementation of project objectives in this area covered the simulation of the quantum approximation algorithm for optimization problem (QAOA). The simulation was carried out on the Cirq quantum computing simulator of the HybriLIT quantum polygon at JINR in relation to the problem of finding the state with the lowest energy for the Ising model with a longitudinal magnetic field[19].

Expected results in the first year of implementation of the project

1. Development of finite-element methods for solving boundary-value problems for a system of a large number of ODEs to calculate above- and below-barrier fusion reactions of heavy and superheavy nuclei; development of finite-element methods for solving multidimensional (up to 6-dimensional) elliptic boundary-value problems aimed at analyzing collective models of the atomic nucleus; methods for calculating the characteristics of the ionization of atoms from inner shells by fast electrons in electron momentum kinematics, taking into account the distortion of electron plane waves.

2. Numerical study of the observed physical characteristics of nucleus-nucleus interactions and particle-nucleus interactions over a wide energy range based on microscopic models of the optical potential and transport-statistical models, including nucleon transfer processes and nuclear fragmentation during heavy-ion interactions.

3. Further development and optimization of the self-similar approximation method for solving nonlinear equations that do not contain small parameters and its application for the analysis of quantum-mechanical systems, including spin ensembles and cold atoms in traps.

4. Development of tensor network methods and their application to describing the nonequilibrium dynamics of low-dimensional multiparticle quantum systems, including modeling the dynamics of the C_{13} nuclear spin system in a diamond lattice.

5. Further study of oscillons within the one- and three-dimensional φ^4 model based on the combined application of the variational approach and approximation of oscillons by standing waves in a ball of finite radius, with the goal of gaining new insights into the dynamics of oscillons in the high- and low-frequency ranges, their stability, bifurcations, resonance phenomena, and new solution branches.

6. Further development of a potential quarkonium model with a nonlocal interaction core, and calculation of the mass spectrum, interaction constants, and normalizations with an appropriate choice of form factors and wave functions for heavy quarkonia.

7. Development of methods and software for calculating collective pion states in dense nuclear matter based on the Migdal and Lindhard functions. Development of algorithms for the analysis of the pion excitation spectrum, pion gaps, and critical parameters for a pion condensate formation over a wide range of densities at zero temperature. Analysis of the accuracy of computational schemes based on the Migdal and Lindhard functions in comparison with other approximations widely used in neutron star cooling models.

8. Development of a software package for simulating neutron star cooling within various models based on the equation of state of dense nuclear matter, allowing for the existence of several stable configurations of compact stars of equal mass. Numerical modeling of the thermal evolution

[19] Yu. Palii, D. Belyakov, A. Bogolubskaya, et al., Phys. Part. Nucl. 56, 1661–1669 (2025)

of neutron stars for cases where the same gravitational mass corresponds to different internal structures of matter. Analysis of the influence of phase transitions in dense matter on the thermal evolution of compact stars.

9. Development of finite element analysis methods and their application to modeling and predicting the electromagnetic, mechanical, and thermal properties of the new superconductor MgB_2 taking into account the available experimental data, with the aim of assessing its potential use in accelerator magnetic systems.

10. Study and classification of various sources of adaptivity in the numerical solution of Riemann integrals using artificial intelligence; development of methods for increasing the accuracy of Riemann integral calculations.

11. Numerical simulation of the interaction of various types of low- and intermediate-energy ions and tungsten targets based on the continuum-atomistic model.

12. Optimization of a program for simulating beam motion in cyclotrons, including the development of a code for the numerical solution of the corresponding equations of motion using the Boris–Vay method, and a comparative analysis of the accuracy of the fourth-order Runge–Kutta and Boris–Vay methods for the acceleration times of charged particles characteristic of cyclotrons.

13. Investigation of the dependence of the Shapiro step width on the amplitude of external radiation in the ϕ_0 junction on the surface of a topological insulator. Investigation of the possibilities of controlling the magnetization state in a SQUID based on the ϕ_0 junction on the surface of a topological insulator.

14. Numerical study of the influence of aperiodic ordering, geometric frustration, and topology on the local superconducting properties of quasicrystalline lattices, including the conditions for the nucleation, suppression, and spatial redistribution of the superconducting order parameter.

15. Computer modeling of magnetic systems with the aim of finding ways of their optimization, in collaboration with VBLHEP and DLNP, within experiments conducted at JINR.

16. Detailed review and classification of existing approaches to the decomposition of finite-dimensional quantum systems, constructing a representation of the Weyl–Heisenberg groups and shift operators in a basis adapted to the tensor product structure.

17. Calculation of quantitative characteristics of the quantum Bernstein effect.

18. Formulation an efficient scheme for preparing the initial state, trotterization of the evolution operator for the Lindblad equation, and implementation of the corresponding quantum scheme on the NVIDIA cuQuantum quantum simulator.

19. Investigation of the analytical properties of multiple hypergeometric series arising from the functional reduction of Feynman integrals. Derivation of systems of differential equations for integrals depending on a minimal number of variables.

20. Enhancement of the robustness of SU(2) quantum gates with respect to external noise by factorizing them into elementary components.

21. Conducting initial methodological research on the problems of embedding QUBO graphs into the topology of quantum annealers (D-Wave Zephyr). Development and testing of a software prototype of embedding algorithms using the D-Wave Ocean SDK libraries.

Expected results upon completion of the project

1. Development of new computational schemes, algorithms, and software packages for solving initial-boundary value and boundary value problems for systems of multidimensional equations to study the collective models of the atomic nucleus and nuclear fusion reactions.

2. Development of methods and software for studying nucleus-nucleus interactions and particle-nucleus interactions at intermediate energies based on microscopic models of the optical potential and transport-statistical models. This will yield new information on the mechanisms of such reactions under the influence of the energy of incident particles and other factors.

3. Development and computer implementation of optimal methods for describing complex statistical and quantum systems using new characteristics of order, correlation, and complexity.

This will be used to study the functioning of probabilistic dynamic networks, with the possibility of controlling them using machine learning.

4. Study of the nonequilibrium dynamics of low-dimensional multiparticle quantum systems using tensor network methods, including the quench protocol calculation of the spectral functions of one-dimensional Hubbard and Ising models in a transverse field.

5. Development of methods and software for the numerical study of the formation processes and properties of localized structures in nonlinear media described by various types of nonlinear field theory equations and having relevant applications within multifactor models of complex physical systems. Study of nonlinear PT-symmetric systems and systems with PT-symmetry breaking, describing finite-dimensional models of condensed matter theory.

6. Development of new algorithms for analytical and numerical calculations of $J/\psi(Y)$ production diagrams in $gg\psi \rightarrow gJ/\psi$ reactions, study of helical amplitudes in such reactions, dependences of heavy quarkonia production cross sections on the transferred momentum, generalization to the case of finite temperatures and densities.

7. Development of a software package for the numerical modeling of microphysical and thermal processes in neutron stars. Computer simulations of neutron star cooling over a wide range of equation-of-state parameters and nucleonic matter superconductivity models. Comparison of the numerical modeling results with observational data on the temperature evolution of neutron stars. Adaptation of the developed methods and programs for calculations on high-performance computing systems.

9. Development of methods for improving calculation efficiency and reducing computational costs when solving magnetostatic problems in mixed mathematical formulations and systems of equations describing the distribution of physical fields in 2D and 3D regions of various configurations.

10. Optimization of methods and software for simulating beam motion in cyclotrons; development of a software module for simulating the backward motion of a particle beam, taking into account losses in structural elements.

11. Elaboration of methods for modeling the interaction of various types of particles with metallic and composite targets based on a continuous-atomistic model to predict structural changes in materials under irradiation.

12. Developing methods and conducting numerical studies of complex processes in superconducting structures, including various configurations of Josephson junction systems and intertype superconductors.

13. Developing methods and conducting, in collaboration with VBLHEP and DLNP, computer modeling of magnetic systems at the JINR experimental facilities with the aim of their optimization.

14. Development of a decomposition theory for the fundamental constructs of N-dimensional quantum mechanics of composite systems (Weyl–Heisenberg groups, displacement operators, Wigner functions) using various factorizations of N and the Chinese remainder theorem. Creation and testing of a prototype software package that implements the corresponding algorithms and enables the calculation of entanglement effects in the quantum states of composite systems.

15. Analysis of multiparticle quantum correlations in multi-qubit systems, including systems of identical particles, within the phase space formalism of finite-dimensional quantum systems.

16. Simulation of quantum bits based on quantum dots with nonresonant laser control.

17. Simulation, on a quantum computing simulator, of a nonrelativistic open quantum field system with the SU(2) gauge group and dynamical fermions in the Hamiltonian formalism in the Markov limit described by the Lindblad equation.

18. Creation of a database of analytical results for one-loop Feynman integrals. Calculation of corrections $\varepsilon = (4-d)/2$ for one-loop Feynman integrals arising in processes studied at the LHC using the functional reduction method.

19. Development of quantum algorithms and circuits for the dynamic description of topological phase transitions and creation of software tools for studying the critical behavior of open quantum systems.

20. Development of methods for increasing the robustness of quantum gates to external noise using differential-geometric structures of the unitary group.

21. Elaboration and implementation of a software framework for the implementation (minor embedding) of quadratic binary optimization (QUBO) problems arising in track reconstruction problems into the architecture of quantum annealers (D-Wave, Zephyr topology).

22. Implementation and testing of embedding algorithms using the D-Wave Ocean SDK libraries (dwave-neal, qbsolv) and other optimizers (CPLEX, Gurobi) for the comparative analysis of hybrid computing schemes.

23. Research and development of methods for mapping problem graphs onto the physical connectivity of quantum hardware qubits, taking into account the geometric and modular properties of detector topologies.

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 28 candidates and 14 doctors of sciences among the project participants. Thanks to meetings, schools, workshops, and seminars regularly held at MLIT, young specialists have the opportunity to improve their scientific level and IT qualifications necessary to successfully solve the project's tasks. In 2024–2025, the staff of the MLIT Scientific Department of Computational Physics, in cooperation with colleagues from the other Laboratories and foreign research centers, prepared more than 120 scientific papers in the area covered by the project. Three monographs and two textbooks on the project's topic were published, and two new software packages implementing methods for high-performance modeling of physical characteristics in Josephson structures were transferred to the Program Library JINRLIB. The leaders of the project prepared a review paper[20] in Natural Science Review on the development and use of iterative schemes based on the Continuous Analogue of Newton's Method, an important tool for solving a number of the project's tasks. In 2025, a series of works within the project entitled "Numerical Methods and Problem-Oriented Program Complexes for Solving Some Partial Differential Equations of Physical Processes and Systems" was awarded the 3rd JINR Prize for Methodology, Research and Technology Papers of 2024. The project's team increased on the account of hiring graduate students and young specialists to MLIT. Several master's projects by students from the Dubna branch of the Computational Mathematics and Cybernetics Institute of Moscow State University are directly related to the project's objectives. Thus, taking into account the scientific background available to the team of project participants and the results already achieved in the first two years of the project's implementation, there is reason to believe that the goals of the project will be successfully attained.

We note the following risk factors.

- Since the research within the project is closely linked with research conducted at other JINR Laboratories, a significant change in the research plans of the collaborating JINR subdivisions may lead to partial 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 the project's objectives.

[20] E.V. Zemlyanaya, O. Chuluunbaatar, Natural Science Review 3, 200605 (2026)

- 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's tasks.

2.3. Estimated completion date

2027–2031

2.4. Participating JINR laboratories

MLIT V. Abgaryan, Gh. Adam, S. Adam, P.G. Akishin, A.I.Anikina, A.S. Ayriyan, E.A. Ayrjan, D.R. Badreeva, I.V. Barashenkov, M.V. Bashashin, A.A. Bogolubskaya, L. Bordag, M. Bureš, J. Buša Jr., J. Buša, A.M. Chervyakov, G. Chuluunbaatar, Kh. Chuluunbaatar, D. Goderidze, H. Grigorian, A.A. Gusev, T.V. Karamysheva, A.V. Khmelev, V.V. Kornyak, O.O. Kovalev, D.S. Kulyabov, K.V. Lukyanov, N.V. Makhaldiani, M.D. Malykh, S.D. Mavlonberdieva, T.I. Mikhailova, E.G. Nikonov, Yu. Palii, V.V. Papoyan, D.V. Podgainy, R.V. Polyakova, A.R. Rakhmonova, V.S. Rikhvitsky, I.A. Rogojin, B. Saha, I. Sarkhadov, Z.A. Sharipov, O.I. Streltsova, L.A. Syurakshina, Yu.N. Talochka, O.V. Tarasov, A.G. Torosyan, Z.K. Tukhliev, K.D. Verkhovtseva, A.V. Volokhova, O.O. Voskresenskaya, R.M. Yamaleev, E.P. Yukalova, O.I. Yuldashev, M.B. Yuldasheva, M.I. Zuev

BLTP M.A. Abdelghani, A.A. Donkov, A.V. Friesen, M. Hnatič, K.V. Kulikov, V.K. Lukyanov, E.V. Mardyban, R.G. Nazmitdinov, Yu.V. Popov, I.R. Rahmonov, Yu.M. Shukrinov, S.I. Vinitsky, D.N. Voskresensky, V.I. Yukalov, V.Yu. Yushankhai

FLNR E. Batchuluun

FLNP M.A. Kiselev, N. Kučerka, E.E. Perepelkin

DLNP O.V. Karamyshev, G.A. Karamysheva, G.K. Lavrov, I.D. Lyapin, E.P. Popov

VBLHEP O.V. Belov, A.V. Bychkov, D.N. Nikiforov

LRB A.N. Bugay, A.V. Chizhov

2.4.1. MICC resource requirements

Computing resources	**Distribution by year**				
	1st year	2nd year	3rd year	4th year	5th year
Data storage (TB) - EOS - Tapes					
Tier 1 (core-hour)					
Tier 2 (core-hour)					
SC Govorun (core-hour) - CPU - GPU	 300000 10000	 300000 10000	 300000 10000	 300000 10000	 300000 10000

Clouds (CPU cores)					

2.5. Participating countries, scientific and educational organisations

Organisation	Country	City	Participants	Type of agreement
AANL	Armenia	Yerevan	Ananikyan N. Piloyan A.	Collaborations
IP	Azerbaijan	Baku	Mirzaev M.N.	Collaborations
IM NASB	Belarus	Minsk	Egorov A.D. Malyutin V. B.	Agreement
SU	Bulgaria	Sofia	Hristov I.G. Hristova R.D. Mladenov D.M.	Collaborations
HCMUE	Vietnam	Ho Chi Minh City	Luongh L.H.	Collaborations
GTU	Georgia	Tbilisi	Giorgadze G.	Collaborations
TSU	Georgia	Tbilisi	Elashvili A. Giorgadze G.	Collaborations
UG	Georgia	Tbilisi	Gogilidze S.	Collaborations
CU	Egypt	Giza	Abdul-Magead I.	Collaborations
CIAE	China	Beijing	Lin C.J. Wen P.W.	Collaborations
IMNU	China	Hohhot	Saheya B.	Collaborations
IMDT MAS	Mongolia	Ulaanbaatar	Batgerel B.	Collaborations
MUST	Mongolia	Ulaanbaatar	Ulziibayar V.	Collaborations
Collaboration BM@N	Russia	Dubna	Kapishin M.N.	Collaborations
Collaboration MPD	Russia	Dubna	Ryabov V.G.	Collaborations
MSU	Russia	Moscow	Kouzakov K.A.	Collaborations
PFUR	Russia	Moscow	Bronnikov K.A. Sevastianov L.A. Rybakov Yu.P.	Collaborations
IMPB RAS	Russia	Pushchino	Lakhno V.D.	Collaborations
SSU	Russia	Saratov	Derbov V.L.	Collaborations
LTPC	France	Metz	Joulakian B.B.	Collaborations
KSU	Tajikistan	Khujand	Khamdamov Sh.D.	Collaborations
UCT	South Africa	Cape Town	Alexeeva N.V Dika A.	Collaborations, grant JINR-NRF

2.6. Co-executing organisations *(those collaborating organisations/partners without whose financial, infrastructural participation the implementation of the research programme is impossible. An example is JINR's participation in the LHC experiments at CERN).*

3. Staffing

3.1. Staffing needs in the first year of implementation (total number of participants)

№№ n/a	Category employee	Core staff Amount of FTE	Associated Personnel Amount of FTE
1.	Scientific staff	44.8	
2.	engineers	5.4	

3.	leaders	0.8	
Total:		**51.0**	

3.2. Human resources available

3.2.1. JINR core staff (total number of participants)

№№ п/а	Category of employees	Division	Position	Amount of FTE
1.	scientific staff	MLIT	Dep. Dir. – 2 Head of Dept. – 1 Dep. Head of Dept. – 1 Head of Sector – 5 Chief researcher – 3 Leading researcher – 8 Senior researcher – 20 Researcher – 4 Young researcher – 4 Trainee researcher – 2 Fellowship holder – 1	40.8
2.	engineers	MLIT	Lead programmer – 1 Engineer-programmer – 4 Assistant – 3	5.4
3.	leaders	MLIT	Assistant Dir. – 1	0.8
Total:				**47.0**

3.2.2. JINR associated personnel (total number of participants)

№№ п/а	Category of employees	Partner organisation	Amount of FTE
1.	Scientific staff		
2.	engineers		
Total:			

4. Financial support

4.1. Total estimated cost of the project / subproject – $ 950 000

Forecast of the total estimated cost (specify cumulatively for the whole period, excluding FPC). The details are given in a separate form.

4.2. Extrabudgetary funding sources

Estimated funding from co-executors/customers - total.

Project Leaders _____/_____/

_____/_____/

Date of submission of the project to DSOA: _____

Date of decision of the laboratory's STC: _____ document number: _____

Year of the project opening

(for renewable projects) – Project start year: **2024**

Schedule proposal and resources required for the implementation of the Project

Names of costs, resources, sources of funding			Cost (thousands of dollars) resource requirements	Cost, distribution by year				
				1st year	2nd year	3rd year	4th year	5th year
		International cooperation (IC)	450	90	90	90	90	90
		Materials						
		Equipment and third-party services (commissioning)	180	36	36	36	36	36
		Commissioning work						
		Services of research organisations						
		Acquisition of software	320	64	64	64	64	64
		Design/construction						
		Service costs (*planned in case of direct project affiliation)*						
Resources required	**Normo-hours**	Resources						
		– the amount of FTE,						
		– accelerator/installation,						
		– reactor,….						
Sources of funding	**Budgetary resources**	JINR budget *(budget items)*						
	Extrabudgetary (supplemen	Contributions by co-contractors Funds under contracts with customers Other sources of funding						

Project Leaders _____/_____/

_____/_____/

Laboratory Economist _____/_____

APPROVAL SHEET FOR PROJECT

TITLE OF THE PROJECT

Methods of computational physics for the study of complex systems

SHORT DESIGNATION OF THE PROJECT

PROJECT CODE 06-6-1119-2-2024/2026

THEME CODE 06-1119-2014/…

NAME OF THE PROJECT LEADERS E.V. Zemlyanaya, O. Chuluunbaatar

AGREED

JINR VICE-DIRECTOR	SIGNATURE	NAME	DATE
CHIEF SCIENTIFIC SECRETARY	SIGNATURE	NAME	DATE
CHIEF ENGINEER	SIGNATURE	NAME	DATE
LABORATORY DIRECTOR	SIGNATURE	NAME	DATE
LABORATORY CHIEF ENGINEER	SIGNATURE	NAME	DATE
LABORATORY SCIENTIFIC SECRETARY	SIGNATURE	NAME	DATE
THEME LEADERS	SIGNATURE	NAME	DATE
	SIGNATURE	NAME	DATE
PROJECT LEADERS	SIGNATURE	NAME	DATE
	SIGNATURE	NAME	DATE

- to sign in frame after PAC

APPROVED BY THE PAC	SIGNATURE	NAME	DATE