## THEME PROPOSAL FORM

**Opening/renewal of a theme/large research infrastructure project within the Topical plan of JINR**

## 1. General information on the theme

### 1.1. Theme code
05-6-1119-2014/…

### 1.2. Laboratory
Meshcheryakov Laboratory of Information Technologies

### 1.3. Scientific field
Networking, computing, computational physics

### 1.4. The title of the Theme
Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data

### 1.5. Theme Leaders
S.V. Shmatov,
O. Chuluunbatar.

### 1.6. Theme Deputy Leaders
N.N. Voytishin,
P.V. Zrelov

## 2. Scientific case and theme organization

### 2.1. Annotation

The theme is aimed at organizing and providing computational, algorithmic and software support for the preparation and implementation of experimental and theoretical studies conducted with the participation of JINR, the ellaboration, development and use of computational methods for modeling complex physical systems studied within the framework of JINR Topical Plan projects. Within the framework of the topic, mathematical methods and software will be developed, including those based on machine and deep learning algorithms using recurrent and convolutional neural networks, for modeling physical processes and experimental facilities, processing and analyzing experimental data in the field of elementary particle physics, nuclear physics, neutrino physics, radiobiology, etc. Particular attention will be paid to the creation of systems for distributed processing and analysis of experimental data and information and computing platforms to support research conducted at JINR and other research centers.

The main areas of work are mathematical and computational physics to support major JINR infrastructure projects, primarily the JINR flagship project NICA in the fixed target mode (BM@N) and

in the collider mode for relativistic heavy ion collisions (MPD) and polarized beams (SPD), Baikal-GVD neutrino telescope. Cooperation will also be continued with experiments at the world's accelerator centers (CERN, BNL, etc.), experiments in the field of neutrino physics and astrophysical experiments, and radiobiological research programs. The possibility of using the developed methods and algorithms in the framework of other projects is being considered.

The main direction in modeling complex physical systems, including the states of dense nuclear matter and quantum systems, will be the development of methods, software packages and numerical research based on the solution of the corresponding systems of nonlinear, spatially multidimensional integral, integro-differential or differential equations in partial derivatives with large number of parameters characterized by the presence of critical modes, bifurcations and phase transitions with the complex application of methods of computational physics, quantum information theory and hybrid quantum-classical programming methods.

Also, within the framework of the topic, it is planned to develop works on quantum intelligent control of technological processes and physical installations at JINR and quantum computing in quantum chemistry and physics.

In addition, the training of specialists in the field of computational physics and information technology within the framework of the IT school will be continued.

## 2.2. Projects in the Theme / LRIP subprojects

Project "Mathematical methods, algorithms and software for modeling physical processes and experimental facilities, processing and analyzing experimental data"
Leader: S.V. Shmatov
Deputy Leaders: A.S. Ayriyan, N.N. Voytishin

Project "Methods of computational physics for the study of complex systems"
Leaders: O.Chuluunbaatar, E.V.Zemlyanaya
Deputy Leaders: Yu.L.Kalinovsky, A.Khvedelidze

Activity "Intelligent control of technological processes and physical equipment's in JINR and quantum computing in quantum chemistry and physics"
Leaders: S.V. Ulyanov, P.V. Zrelov

Activity "Training of specialists in the field of computational physics and information technology"
Scientific Leader: V.V. Korenkov
Leaders: A.V. Nechaevsky, D.I. Pryahina, O.I. Streltsova

## 2.3. Scientific case

In accordance with the Seven-Year Plan for the Development of JINR for 2024−2030 and the JINR Long-Term Development Strategy up to 2030 and beyond, an important area of activity of the Meshcheryakov Laboratory of Information Technologies is to provide mathematical, algorithmic and software support for experimental and theoretical research conducted at JINR. The goals are to model physical processes, create algorithms and software systems for processing and analyzing experimental data, develop algorithms in the field of machine and deep learning, artificial intelligence and cognitive intelligent robotics, quantum intelligent control systems, development of computer algebra and quantum computing methods.

The theme combines JINR projects and activities in the field of computational physics aimed at the development and use of methods of mathematical physics, the development of algorithms based on them and the creation of appropriate software for research carried out within the framework of the JINR Topical Plan in the field of elementary particle physics, nuclear physics, neutrino physics, condensed matter physics, radiobiology and applied research. The main priorities of JINR research in the

"Networking, Computing, Computational Physics" direction include the provision of mathematical, algorithmic and software support for experimental and theoretical studies conducted at JINR, and, in particular:

- development of algorithms based on recurrent and convolutional neural networks for the tasks of machine and deep learning, designed primarily for solving various tasks in particle physics experiments, including the NICA megaproject and neutrino experiments;
- creation of modern research tools for international collaborations (NICA, the JINR neutrino program, LHC experiments);
- elaboration of scalable algorithms and software for processing multi-parameter, multidimensional, hierarchical data sets of exabyte magnitude;
- development of information and computing systems for experimental data analysis and processing in the field of radiobiology;
- developments of new numerical and computational models including quantum computing for theoretical studies carried out at JINR;
- development of algorithms for intelligent control of technological processes and physical equipment's in JINR using quantum approach.

## I. Mathematical methods, algorithms and software for modeling physical processes and experimental facilities, processing and analyzing experimental data

The main goal of this part of the theme is to do research and development works in the field of mathematical and computational physics for experiments in elementary particle physics, physics of the atomic nucleus, condensed matter physics, radiobiology and applied research within the JINR Topical Plan. The project provides for the creation and development of mathematical methods and proper software, research tools for international collaborations (NICA, the JINR neutrino program, LHC experiments, etc) and the implementation of these methods and algorithms for applied research. The main areas of work are:

- development and application of modern methods and algorithms for modeling physical processes and experimental facilities;
- development and application of modern methods and algorithms for physical object reconstruction, event visualization and data analysis;
- development of a program, together with the staff of JINR and other Russian and world centers, for experiments aimed to study the fundamental properties of matter, their preparation and implementation;
- creation and development of information and computing systems for experimental data processing and analysis, participation in the organization and processing of experimental data and analysis of physics information, including Open Data of world experiments, using GRID technologies and computer centers of distributed computing, in particular, the JINR MICC, including the "Govorun" supercomputer;
- creation of modern research tools for international collaborations (NICA, the JINR neutrino program, LHC experiments), including software for the control of data quality, characteristics and calibration of experimental facilities within the JINR Topical Plan;
- creation and development of information and computing systems for radiation research in life sciences;
- application of the developed methods and algorithms for applied purposes.

The main strategy is to use common solutions and methods for different experiments to develop software for physics simulation, data processing and analysis, as well as computing systems. All developments are aiming at realizing the actual research tasks of the JINR experimental programs,

analytical or numerical calculations will be carried out within the framework of physical scenarios that can be proved experimentally.

Project structure includes the following directions:

- Simulation of physical processes and experimental facilities:
    - analytical and numerical calculations of physical processes, software optimization, including tuning and adaptation of physics event generators;
    - mass modeling and creation of event databases;
    - participation in the creation of computer models of experimental facilities and simulation of elementary particles passing through them based on GEANT4 (and others) and fast simulation of the response of the detectors.

- Reconstruction of physical objects and analysis of experimental data:
    - development of algorithms, including those based on recurrent and convolutional neural networks for machine and deep learning tasks, and creation of corresponding software for the reconstruction of physical objects (tracks, particles, clusters, etc.) and physical processes;
    - development of methods and algorithms for data analysis, including statistical analysis;
    - adaptation of existing software for specific experiments, reconstruction and analysis of experimental data;
    - analysis of Open Data of experiments, in particular, experiments at the LHC;
    - conducting a global analysis of data from various experiments (in particular, a combined analysis of data from accelerator and astrophysical experiments in search for candidates for the role of dark matter).

- Support and development of the software environment for experiments
    - optimization of the data structure, development of methods for collecting, processing and storing data for the experiments at NICA;
    - support and development of databases;
    - creation of software for event visualization (simulation and experimental data).

## II.   Methods of computational physics for the study of complex systems

This part of the theme 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:

- development of methods, program packages and numerical studies of various interactions in complex systems of nuclear physics and quantum mechanics;
- studies of intricate processes in condensed matter and materials under external actions;
- solutions of modeling problems in the design of experimental facilities and optimization of their operating modes;
- modeling complex processes in dense nuclear matter based on the equation of state;

− 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.

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:

- Development of methods, program packages and numerical studies of complex nuclear-physical and quantum-mechanical processes, 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.

- 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.

- Solving problems arising in the development and optimization of operating modes of experimental facilities, 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).

- Modeling of physical phenomena based on the equation of state of 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.

- 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 types 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.

## III.  Intelligent control of technological processes and physical equipment's in JINR and quantum computing in quantum chemistry and physics

Within a separate Activity the development of embedded quantum self-organized regulators for intelligent control systems of technological processes, JINR devices and equipment, and intellectual cognitive robotics tasks is planned. The software product creation for computing the electronic and magnetic structures of molecular complexes and crystal fragments of new functional materials applying quantum simulators on computers with classical architectures is envisaged.

The main studied problem of this Activity is the effective application of computational intelligence technologies in robust control tasks in order to increase the reliability of the functioning of physical equipment. The solution of the problems is based on the possibility of increasing the robustness of existing control systems due to embedded knowledge bases and switching to appropriate intelligent

control systems, which are designed and supported by software tools developed in the project based on a platform combining soft computing and quantum computing knowledge base optimizers.

The investigation of the effectiveness of quantum algorithms in solving problems of quantum chemistry and physics of new functional materials. The application of well-known quantum algorithms and their development will be carried out on simulators with classical computing architecture.

The main tasks comprise the following:

- development of embedded self-organized controllers for intelligent control systems of technological processes, devices and equipment in JINR (including for cases of unforeseen and unpredictable situations) based on the application of different types of robotic systems.

- development of the upper (intelligent) level of control of cryogenic systems of superconducting magnets of the NICA accelerator complex.

- development of an artificial intelligence platform based on quantum genetic algorithms, quantum deep learning and quantum optimization for intelligent control tasks.

- development and modification of algorithms and quantum circuits with implementation applying software simulators on computers of classical architecture for tasks of cognitive robotics and intelligent control.

- selection and modification of quantum algorithms taking into account the specifics of computational tasks in the study of electronic and magnetic structures of molecular complexes and crystal fragments of new functional materials with strong electronic correlations. Performing calculations for physics-chemical systems using quantum simulators.

## IV.     Training of specialists in the field of computational physics and information technology

As part of a separate Activity, it is planned to conduct training and retraining of specialists in the field of computational physics and information technology on the basis of the MICC JINR and its educational components in order to achieve:

- advanced level of training of JINR staff aimed at the development of scientific projects, including the megascience class, implemented at JINR or with its participation, as well as for the creation and support of the JINR digital ecosystem;

- dissemination of competencies in the field of computational physics and information technologies to the regions of Russia and the JINR Member States to increase the personnel potential of JINR and organizations cooperating with the Institute.

**Expected results upon completion of the theme (for 2026)**

- Completion of the revision of the interaction generators and their development for modeling the processes of interactions of light and heavy nuclei, including at NICA energies
  - revision of the FTF and QGSM models and inclusion of the developed software modules for modeling nuclear interactions of unstable, long-lived particles, namely, charmed hadrons, bothonium, light hyper-nuclei and anti-hyper-nuclei, after comprehensive verification and testing in the Geant4 package;
  - development of the DCM-QGSM-SMM generator: taking into account the dependence of the lifetime of resonances on the density of the nuclear medium, suppression of the cross section of the production of pseudoscalar mesons in a dense nuclear medium, enhancement of the production of hyperons in a dense nuclear medium; enhancement of the dilepton yield, replacement of the Woods-Saxon model of colliding nuclei with a lattice one, which will allow including the deformation of nuclei;

- obtaining unambiguous information about the admixture of quark states at NICA energies in the weakly excited and ground states of the deuteron.
- Completion of the revision of the interaction generators and their development for simulation of the processes of production of the candidates for non-baryonic dark matter, extra Higgs bosons and processes that violate the lepton number for the LHC conditions
  - revision of the space of model parameters of a number of dark matter scenarios available for study at the LHC at a nominal energy and total integrated luminosity up to 350 fb$^{-1}$, full modeling of the processes of formation of dark matter particles within simplified and extended Higgs models;
  - full modeling of processes that occur with the violation of the lepton number, using the QBH, Pythia, MadGraph generators, etc.
- Development of algorithms for the reconstruction of charged particle tracks for experimental facilities, including those at NICA and the LHC, creation of appropriate software and its application for data processing and analysis, study of the physical and technical characteristics of detector systems
  - universal algorithm based on wavelet analysis for the recognition of overlapping signals in tracking detectors of HEP experiments with the amplitude representation of the signal;
  - assessment of background particle rates and the effect of aging in the CSC detectors of the CMS experiment on various types of data and under various data collection conditions;
  - optimization of the tracking algorithm in the DCH detectors of the BM@N experiment for the data set from the interaction of heavy ions with the target. Automation of obtaining the transfer function for the DCH detectors of the BM@N experiment. Improvement of charged particle trajectory reconstruction in the CSC detectors of the BM@N experiment;
  - elaboration and implementation of modeling and data processing methods, as well as their development and adaptation for current configurations of a number of tracking detectors (Forward Silicon, GEM, small CSC, large CSC, Silicon Beam Tracker, Silicon Profilometer.) of the BM@N experiment tracking system;
  - development of a methodology and software implementation of the system for the global alignment of detectors in the BM@N experiment;
  - technique for identifying charged particles, in particular, in the MPD detector, based on machine learning methods, software implementation of the developed approaches in the mpdroot experiment processing and analysis software environment, integration of modern machine and deep learning libraries into the mpdroot software environment.
- Creation and development of a data processing and analysis system for the experiments at the JINR NICA accelerator complex
  - formation of a version of the mpdroot package that works with clear support rules for the entire duration of the MPD experiment, with regular updates of the entire working environment (in terms of software) and software adaptation to current project requirements;
  - realization, methodological confirmation and implementation of data processing algorithms using artificial intelligence elements into the application software of the experiment;
  - implementation and commissioning of a set of systems and services that provide data processing for the SPD experiment in a distributed heterogeneous computing environment, with support for predictable loads for timely data processing at the first stage of the experiment;
  - creation of auxiliary information services for the experiments of the NICA megaproject: logbook, e-log, a single graphical interface for managing the experiment, information service, implementation of interfaces for data conversion in the subsystems of the experiment, creation of specialized databases, monitoring systems, other services requiring general IT support.
- Support and development of the software environment for experiments at the LHC

- development of a prototype of the CREST project as part of the ATLAS experiment for Run 4 of the LHC, support of the operation of the Pickup Service and monitoring of the EventIndex project of the ATLAS experiment.

- Development of the data processing and analysis system for the reconstruction of experimental events within the JINR program in the field of neutrino physics
  - debugging the data processing system on a large amount of experimental data and achieving its performance at the level of the main processing system in the BAIKAL-GVD project;
  - development of software for the reconstruction of cosmic rays and high-energy gamma quanta based on data from the TAIGA-HiSCORE and TAIGA-IACT detectors.

- Development of algorithms and software for JINR research projects in the field of neutron physics
  - development of a software package for the primary processing of small-angle experimental data from the YuMO spectrometer for a multi-detector system with a position-sensitive detector with distributed capabilities for a combination of processing types, including normalization to fluxes, adaptation to a possible change in the pulse frequency of the IBR-2 reactor, methods for accounting for background conditions and adaptation to changes in the multi-detector system of the YuMO spectrometer;

- Development of algorithms, software and computing platforms for radiobiological research, applied research in the field of proton therapy and ecology
  - creation of software for track reconstruction in the digital calorimeter prototype for proton therapy;
  - creation of an information and computing system that provides a convenient environment for storing experimental data, analyzing the results of laboratory radiobiological studies, creating data sets, developing and applying algorithms based on methods and approaches of machine and deep learning;
  - building a hierarchical data storage and processing system for the created information and computing system for laboratory radiobiological studies based on the multi-layer storage system created on the HybriLIT platform, operating on the principle from "hot" to "cold" layers; filling the algorithmic block of the information and computing system for laboratory radiobiological studies with three main modules: a module for studying the behavioral patterns of small laboratory animals exposed to physical or chemical influences, a module for histological studies and a module for the statistical complex analysis of biological data;
  - implementation of the intelligent platform for determining the condition of agricultural and decorative plants, which presents a significant number of detectable diseases, provides detailed treatment plans and uses advanced artificial intelligence technologies;
  - platform for monitoring and predicting the state of the environment, combining advanced data management technologies and artificial intelligence to solve environmental monitoring tasks.

- Development of methods, software and carrying out numerical study of complex processes in nuclear physics and quantum mechanics:
  - 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 framework of 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 within the framework of a quantum mechanical model based on the solution of a system of nonlinear equations using an optimized method of self-similar approximations.

- In the field of studies of intricate processes condensed matter and materials under external actions:

  - Development of computational schemes and software packages that implement the solution of systems of equations within the framework of 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 media, described by various types of nonlinear field theory equations. Simulation of electron hydration within the dynamic polaron model modified to study the influence of various factors on this process.

- For solving problems arising in the development and optimization of operating modes of experimental facilities, including:

  - 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 on MICC resources to implement these methods.

  - 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. Including 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.

- In the field of modeling of physical phenomena based on the equation of state of dense nuclear matter, including:

  - 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.

- Obtaining numerical results relevant for understanding fundamental processes in considering physical systems.

- 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:

  - 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 for the study of quantum systems based on the integration 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.

  - Studies 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.

- Development of embedded quantum self-organized regulators for intelligent control systems of technological processes, JINR devices and equipment:

  - development of a prototype of a quantum fuzzy PID controller and a demonstration sample of a robot with a built-in prototype of the intelligent quantum controller.

  - development of a prototype of an intelligent control system for cryogenic systems for superconducting magnets of the NICA accelerator complex based on a quantum fuzzy PID controller. Preparation of the patent.

  - design methodology and structure of the intelligent control system of the HF (high frequency) station.

- Usage of quantum algorithms for solving problems of quantum chemistry and physics:

  - Verification of the effectiveness of variational-type quantum algorithms implemented on quantum simulators of classical architecture by applying them to the quantitative description of the dissociation of simple molecules, as well as the electron and spin structure of the ground state of typical lattice models of quantum theory.

- Training of specialists in the field of computational physics and information technology

**Risks (SWOT Analysis)**

|  | Positive | Negative |
|---|---|---|
| **Internal** | **Strengths**<br>– wide approbation of research (at meetings of the governing bodies of JINR and a large number of international conferences);<br>– theme participants are recognized experts in various research fields (information technology, mathematical physics, theoretical and experimental physics of elementary particles and atomic nucleus, radiobiology);<br>– experience in the field of modeling physical processes, processing and analyzing experimental data, creating information and computing systems and software libraries in the world largest research centers (JINR, CERN, Fermilab, etc.);<br>– experience of participation in major international collaborations (WLCG, JINR, CERN, DESY, Fermilab, etc.);<br>– balanced composition of researchers group: 20 doctors and 45 candidates of sciences. | **Weaknesses**<br>– restrictions for participants from the Russian Federation to visit a number of scientific centers and international conferences;<br>– possible partial revision of theme priorities;<br>– partial shortage of personnel in a number of areas of the theme |
| **External** | **Opportunities**<br>– development of new methods of modeling, data processing and analysis (deep and machine learning, etc.);<br>– emergence of new experimental data that gives a boost to the development of theoretical and computational methods for describing and calculating physical processes;<br>– development of the JINR MICC and other world data processing centers;<br>– increase in the availability of quantum computers | **Threats**<br>– possible changes in the timing of the implementation of research projects at JINR and other centers;<br>– uncertain situation with the extension of the agreement on scientific cooperation between JINR and CERN, possibility of suspending scientific cooperation with other world centers |

Most of the research programm is related to the basic facilities of JINR, in the event of termination of the agreement on scientific cooperation between JINR and CERN, research related to data processing and analysis will be partially continued using the open data of collaborations (LHC Open Data).

## 2.4. Participating JINR laboratories

**MLIT** (V. Abgaryan, I.V. Amirkhanov, A.S. Ayriyan, E.A. Ayrjan, Akishina, A.I., P.G. Akishin, E.I. Alexandrov, I.N. Alexandrov, E.P. Anikina, D.R. Badreeva, D.A. Baranov, I.V. Barashenkov, M.V. Bashashin, T.Zh. Bazhenyan, A.A. Bogolubskaya, M. Bures, Yu.A. Butenko, J. Busa, J. Busa Jr., A.M. Chervyakov, G. Chuluunbaatar, Kh. Chuluunbaatar, O. Chuluunbaatar, O.Yu. Derenovskaya, N.D. Dikusar, P.I. Gluhovtzev, S. Gnatich, D. Goderidze, P.V. Goncharov, O.A. Grygoryan, A.A. Gusev, V.V. Ivanov, O.V. Ivantsova, I.S. Kadochnikov, Yu.L. Kalinovsky, T.V. Karamysheva, M.S. Katulin, A.A. Kazakov, A.I. Kazimov, A.M. Khvedelidze, V.V. Kornyak, Yu. V. Korsakov, B.F.

Kostenko, D.S. Kulyabov, E.A. Kuznetsova, K.V. Lukyanov, N.V. Makhaldiani, S.D. Mavlonberdieva, T.I. Mikhailova, M.A. Mineev, Zh.Zh. Musulmanbekov, A.V. Nechaesky, E.G. Nikonov, D.A. Oleynik, G.A. Ososkov, V.V. Palichik, Yu. Palii, G.V. Papoyan, V.V. Papoyan, I.S. Pelevanyuk, A.Sh. Petrosyan, D.V. Podgainy, R.V. Polyakova, D.I. Pryahina, I.V. Puzynin, T.P. Puzynina, A.R. Rakhmonova, A.M. Raportirenko, A.G. Reshetnikov, V.S. Rikhvitsky, I.A. Rogojin, A.R. Ryabov, N.V. Ryabov, B. Saha, I. Sarkhadov, I. Satyshev, S.I. Serdyukova, Z.A.Sharipov, N.Yu. Shirikova, S.K. Slepnev, K.V. Slizhevsky, S.V. Shmatov, A.G. Solovyev, T.M. Solovyeva, O.I. Streltsova, L.A. Syurakshina, O.V. Tarasov, A.G. Torosyan, Z.K. Tuhliev, S.V. Ulyanov, A.V. Uzhinsky, V.V. Uzhinsky, A.V. Volokhova, A.S. Vorontsov, O.O.Voskresenskaya, E.N. Voytishina, N.N. Voytishin, E.V. Zemlyanaya, V.B. Zlokazov, P.V. Zrelov, D.P. Zrelova, M.I. Zuev, A.V. Yakovlev, R.M. Yamaleev, D.A. Yanovich, E.P. Yukalova, O.I. Yuldashev, M.B. Yuldasheva)

**VBLHEP** (V. Yu. Aleksakhin, A.A. Aparin, Yu.V. Bespalov, O.I. Brovko, D.V. Budkovski, A.V. Bychkov, I.R. Gabdrakhmanov, A.S. Galoyan, K.V. Gertsenberger, V.M. Golovatyuk, D.K. Dryablov, M.N. Kapishin, V.Yu. Karzhavin, A.A. Korobitsyn, A.V. Krylov, V.V. Lenivenko, S.P. Lobastov, S.P. Merts, A.A. Moshkin, A.A. Mudrokh, D.N. Nikiforov, M. Patsyuk, G.P. Reshetnikov, O.V. Rogachevsky, V.G. Ryabov, V.V. Shalaev, S.G. Shulga, I.A. Zhizhin, V. Zhezher, A.I. Zinchenko)

**BLTP** (M. Hnatic, A.A. Donkov, V.K. Lukyanov, A.V. Friesen, D.I. Kazakov, P.A. Maksimov, R.G. Nazmitdinov, M.V. Savina, Yu.M. Shukrinov, O.V. Teryaev, V.D. Toneev, I.R. Rahmonov, S.I. Vinitsky, V.I. Yukalov, V.Yu.Yushankhai)

**FLNP** (N. Kucerka, M.A. Kiselev, E.E. Perepelkin, E.P. Popov)

**FLNR** (M. Balasoiu, M.-O. Dima, M.-T. Dima, A.I. Ivankov, A.H. Islamov, Yu.S. Kovalev, A.I Kuklin, Yu.N. Pepelishev, Yu.L. Ryzhikov, A.V. Rogachev, V.V. Skoy, M.V. Frontasyeva)

**DLNP** (V.A. Bednyakov, A.P. Belova, I.A. Belolaptikov, I.V. Borina, A.N. Borodin, V. Dik, I.I. Denisenko, T.V. Elzhov, A.A. Grinyuk, A.V. Guskov, O.V. Karamyshev, G.A. Karamysheva, E.V. Khramov, I.N. Kiyan, V.A. Krylov, V.S. Kurbatov, D.V. Naumov, A.E. Pan, D. Seitova, A.E. Sirenko, M.N. Sorokovikov, L.G. Tkachev, B.A. Shaibonov, E. Sholtan, A.C. Zhemchugov, D.Yu. Zvezdov)

**LRB** (A.N. Bugay, A.V. Czhizhov I.A. Kolesnikova, Yu.S. Severyukhin, D.M. Utina)

**UC** (A.Yu. Verkheev, B.S. Yuldashev)

## 2.5. Participating countries, scientific and educational organisations:

| Organisation | Country | City | Participants | Type of agreement |
|---|---|---|---|---|
| Foundation ANSL | Armenia | Yerevan | A. Tumasyan<br>A. Ayrapetyan<br>A. Gevorkyan<br>N. Ananikian<br>A. Piloyan | Collaboration |
| BrSU | Belarus | Brest | B.P. Katz | Collaborations |
| IM NASB | Belarus | Minsk | A.D. Egorov<br>V.B. Malyutin | Agreement |
| GSU | Belarus | Gomel | V.V. Andreev<br>N.V. Maximenko | Collaboration |
| INP BSU | Belarus | Minsk | D.V. Ermak | Collaboration |

| | | | V.V. Makarenko V.A. Mosolov | |
|---|---|---|---|---|
| SU | Bulgaria | Sofia | I.G. Hristov R.D. Hristova D. Mladenov | Collaborations |
| CIAE | China | Beijing | Chengjian Lin, Peiwei Wen | Collaborations |
| CU | Egypt | Giza | I.M. Abdul-Magead | Collaborations |
| TSU | Georgia | Tbilisi | A. Elashvili G. Giorgadze | Collaborations |
| UG | Georgia | Tbilisi | Gogilidze S. | Collaborations |
| Univ. | Great Britain | Oxford | E. Gallas | Collaboration |
| INFN | Italy | Genova | D. Barberis | Collaboration |
| UNAM | Mexico | Mexico | Peter O. Hess | Collaborations |
| IMDT MAS | Mongolia | Ulan-Bator | B. Batgerel | Collaborations |
| NOSU | Russia | Vladikavkaz | A.K. Gutnova | Collaboration |
| NRC KI PNPI | Russia | Gatchina | B.T. Kim A.K. Kiryanov | Collaboration |
| BM@N Collaboration | Russia | Dubna | M.N. Kapishin | Collaboration |
| MPD Collaboration | Russia | Dubna | V.G. Ryabov | Collaboration |
| SPD Collaboration | Russia | Dubna | A.V. Guskov | Collaboration |
| ITEP | Russia | Moscow | A.N. Nikitenko | Collaboration |
| SINP MSU | Russia | Moscow | E.E. Boos L.V. Dudko I.P. Lohtin O.L. Kodolova S.V. Petrushanko | Collaboration |
| NNRU "MEPhI" | Russia | Moscow | M.V. Danilov | Collaboration |
| LPI RAS | Russia | Moscow | I.M. Dremin | Collaboration |
| RSTSREC | Russia | Moscow | A.A. Egorov | Collaborations |
| PFUR | Russia | Moscow | L.A. Sevastyanov K.A. Bronnikov Yu.P. Rybakov | Collaborations |
| IMPB RAS | Russia | Pushchino | V.D. Lakhno | Collaborations |
| SSU | Russia | Saratov | V.L. Derbov | Collaborations |
| IHEP | Russia | Protvino | A.V. Petrova | Collaboration |
| SSU | Russia | Samara | A.V. Baskakov V.A. Saleev | Collaboration |
| SPbSU | Russia | St. Petersburg | A.V. Bogdanov A.B. Degtyarev A.K. Zarochentsev | Collaboration |
| INR RAS | Russia | Moscow, Troitsk | S.N. Gninenko | Collaboration |
| UTA | USA | Arlington | N. Ozturk | Collaboration |
| INP AS RUz | Uzbekistan | Tashkent | B.S. Yuldashev | Collaboration |
| CEA | France | Saclay | A.Formika | Collaboration |

| | | | | |
|---|---|---|---|---|
| UCT | South Africa | Cape Town | N. Alexeeva | Collaboration, JINR-NRF grant |
| CERN | Switzerland | Geneva | G. Avolio<br>Sh. Roe<br>A. Ribon | Collaboration |
| ALICE Collaboration | Switzerland | Geneva | M. van Leeuwen | Collaboration |
| ATLAS Collaboration | Switzerland | Geneva | A.Hoecker | Collaboration |
| CMS Collaboration | Switzerland | Geneva | P. Mc Bride | Collaboration |

**2.6. Key partners** *(those collaborators whose financial, infrastructural participation is substantial for the implementation of the research program on the theme. Example – JINR participation in the LHC experiments at CERN).*

## 3. Manpower
### 3.1. Manpower needs in the first year of implementation

| No. | Personnel category | JINR staff, FTE amount | JINR associated personnel, FTE amount |
|---|---|---|---|
| 1. | research scientists | 74 | 5 |
| 2. | engineers | 6,8 | 1 |
| 3. | specialists | 9,1 | |
| 4. | managment | 2,1 | |
| | **Total:** | **92** | **6** |

### 3.2. Available manpower
**3.2.1. JINR staff** (total number of participants)

| No. | Personnel category | Division | Position | Amount FTE |
|---|---|---|---|---|
| 1. | research scientists | LIT | − laboratory director, deputy directors of the laboratory, scientific secretary, director-adviser, heads of departments, heads of sectors | 7,9 |
| | | | − chief researchers | 4 |
| | | | − lead researchers | 13,8 |
| | | | − senior researchers | 24,55 |
| | | | − researchers | 8,2 |
| | | | − junior researchers | 4,5 |

| No. | | | | |
|---|---|---|---|---|
| | | | − intern-researchers | 6,4 |
| | | | **Total research scientists** | **69,35** |
| 2. | engineers | LIT | − software engineers | 3,3 |
| | | | − software engineers of I category | 1,0 |
| | | | − software engineers of II category | 2,5 |
| | | | **Total engineers** | **6,8** |
| 3. | specialists | LIT | − lead programmers | 6,5 |
| | | | − segnior laboratory assistants | 1 |
| | | | − laboratory assistants | 1,5 |
| | | | − translators | 0,1 |
| | | | **Total specialists** | **9,1** |
| 4. | management | LIT | − assistant director | 0,8 |
| | | | − deputy head of division | 0,8 |
| | | | − head of group | 0,5 |
| | | | **Total management** | **2,1** |
| | **Total:** | | | **87,35** |

### 3.2.2. JINR associated personnel

| No. | Personnel category | Partner organization | Amount of FTE |
|---|---|---|---|
| 1. | research scientists | | |
| 2. | engineers | | |
| | **Total:** | | |

## 4. Financing

### 4.1. Total estimated cost of the theme

| No. | Items of expenditure | Cost | Expenditure per year (thousands of the US dollars) | | |
|---|---|---|---|---|---|
| | | | 1st year | 2nd year | 3rd year... |
| 1. | International cooperation | **450** | 150 | 150 | 150 |
| 2. | Materials | | | | |
| 3. | Equipment, Third-party company services | **338,3** | 110 | 112,8 | 115,5 |
| 4. | Commissioning | | | | |
| 5. | R&D contracts with other research organizations | | | | |
| 6. | Software purchasing | **255** | 75 | 85 | 95 |
| 7. | Design/construction | | | | |
| 8. | Service costs (*planned in case of direct affiliation*) | | | | |
| **TOTAL:** | | **1043,3** | 335 | 347,8 | 360,5 |

### 4.2. Extra funding sources
Expected extra funding from partners/customers (total for all projects).

**AGREED:**

| | |
|---|---|
| **Chief Scientific Secretary** | **Laboratory Director** |
| _____/_____/ | _____/_____/ |
| "_____" _____ 202_. | "_____" _____202_. |
| | |
| **Head of BEPD** | **Scientific Secretary of the Laboratory** |
| _____/_____/ | _____/_____/ |
| "_____" _____202_. | "_____" _____ 202_. |
| | |
| **Head of DSOA** | **Laboratory Economist** |
| _____/_____/ | _____/_____/ |
| "_____" _____ 202_ . | "_____" _____202_. |
| | |
| **Head of HRRMD** | **Theme leader** |
| _____/_____/ | _____/_____/ |
| "_____" _____ 202_. | "_____" _____ 202_. |
| | |
| | **Theme leader** |
| | _____/_____/ |
| | "_____" _____ 202_. |
| | |
| | **Theme deputy leader** |
| | _____/_____/ |
| | "_____" _____ 202_. |
| | |
| | **Theme deputy leader** |
| | _____/_____/ |
| | "_____" _____ 202_. |
| | |
| | **Project leader (project code) /** |
| | _____/_____/ |
| | "_____ " _____202_. |
| | |
| | **Project leader (project code) /** |
| | _____/_____/ |
| | "_____ " _____202_. |
| | |
| | **Project leader (project code) /** |
| | _____/_____/ |
| | "_____ " _____202_. |