

Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data

Theme leaders: S.V. Shmatov
O. Chuluunbaatar

Deputies: N.N. Voytishin
P.V. Zrellov

Participating countries and international organizations:

Armenia, Belarus, Bulgaria, CERN, China, Egypt, France, Georgia, Italy, Kazakhstan, Mexico, Mongolia, Russia, Serbia, Slovakia, South Africa, United Kingdom, USA, Uzbekistan.

The problem under study and the main purpose of the research:

The theme is aimed at organizing and providing computational, algorithmic and software support for the preparation and implementation of experimental and theoretical research conducted with JINR's participation, at elaborating, developing and using computational methods for modelling complex physical systems studied within the projects of the JINR Topical Plan. Within the theme, mathematical methods and software, including those based on machine and deep learning algorithms using recurrent and convolutional neural networks, will be developed for modelling physical processes and experimental facilities, processing and analysing 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 the distributed processing and analysis of experimental data, as well as information and computing platforms to support research conducted at JINR and other research centres.

The main directions of work are mathematical and computational physics to support JINR's large research infrastructure projects, primarily, the NICA flagship project in the fixed target mode (BM@N) and in the collider mode for relativistic heavy ion collisions (MPD) and polarized beams (SPD), the Baikal-GVD neutrino telescope. Cooperation with experiments at the world's accelerator centres (CERN, BNL, etc.), experiments in the field of neutrino physics and astrophysics, radiobiological research programmes will also be continued. The possibility of using the developed methods and algorithms within other projects is being considered.

The major direction in modelling 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 a 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.

Within the theme, it is also planned to develop work on the quantum intelligent control of technological processes and physical facilities at JINR, as well as quantum computing in quantum chemistry and physics.

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

Projects in the theme:

| Name of the project | Project Leaders | Project code |
|--|---|-----------------------|
| 1. Mathematical methods, algorithms and software for modeling physical processes and experimental facilities, processing and analyzing experimental data | S.V. Shmatov <i>Deputies:</i> A.S. Ayriyan N.N. Voytishin | 06-6-1119-1-2024/2026 |
| 2. Methods of computational physics for the study of complex systems | E.V. Zemlyanaya O. Chuluunbaatar <i>Deputies:</i> Yu.L. Kalinovsky A. Khvedelidze | 06-6-1119-2-2024/2026 |

Projects:

| | Name of the project | Project Leaders | Status |
|--------|--|---|-------------|
| 1. | Mathematical methods, algorithms and software for modeling physical processes and experimental facilities, processing and analyzing experimental data | S.V. Shmatov <i>Deputies:</i> A.S. Ayriyan N.N. Voytishin | Realization |
| MLIT | P.G. Akishin, E.P. Akishina, A.I. Anikina, E.I. Alexandrov, I.N. Alexandrov, D.A. Baranov, T.Zh. Bezhanian, J. Busa, K.A. Chizhov, S. Hnatch, H. Grigorian, O.Yu. Derenovskaya, A.V. Didorenko, N.D. Dikumar, V.V. Ivanov, I.S. Kadochnikov, A.A. Kazakov, O.L. Kodolova, Yu. V. Korsakov, B.F. Kostenko, Z.K. Khabaev, M.A. Mineev, Zh.Zh. Musulmanbekov, A.V. Nechaevsky, A.N. Nikitenko, E.G. Nikonov, D.A. Oleynik, G.A. Ososkov, V.V. Palichik, V.V. Papoyan, I.S. Pelevanyuk, A.Sh. Petrosyan, D.V. Podgainy, D.I. Pryahina, N. Saktaganov, I. Satyshev, K.V. Slizhevsky, A.G. Soloviev, T.M. Solovjeva, O.I. Streltsova, Z.K. Tuhliev, S.A. Shadmehri, Z.A. Sharipov, S.K. Slepnev, A.V. Uzhinsky, V.V. Uzhinsky, A.V. Yakovlev, V.B. Zlokazov, M.I. Zuev | | |
| VBLHEP | V. Yu. Aleksakhin, A.A. Aparin, Yu.V. Bepalov, 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, A.V. Lanev, V.V. Lenivenko, S.P. Lobastov, S.P. Merts, A.A. Moshkin, Yu.A. Murin, D.N. Nikiforov, M. Patsyuk, O.V. Rogachevsky, V.G. Riabov, V.V. Shalaev, S.G. Shulga, A.V. Taranenko, I.A. Zhizhin, V. Zhezher, A.I. Zinchenko, D.A. Zinchenko | | |
| BLTP | D.I. Kazakov, M.V. Savina, O.V. Teryaev, V.D. Toneev, V.A. Zygunov | | |
| FLNP | M. Balasoiu, M.V. Frontasyeva, A.I. Ivankov, A.H. Islamov, Yu.S. Kovalev, A.I. Kuklin, Yu.N. Pepelishv, Yu.L. Ryzhikov, A.V. Rogachev, V.V. Skoy, K.N. Vergel | | |
| DLNP | V.A. Bednyakov, I.A. Belolaptikov, I.V. Borina, A.N. Borodin, V. Dik, I.I. Denisenko, T.V. Elzhov, A.A. Grinyuk, A.V. Guskov, E.V. Khramov, V.A. Krylov, V.S. Kurbatov, D.V. Naumov, A.E. Pan, A.E. Sirenko, M.N. Sorokovikov, L.G. Tkachev, B.A. Shaibonov, E. Sholtan, A.C. Zhemchugov, D.Yu. Zvezdov | | |
| LRB | I.A. Kolesnikova, Yu.S. Severyukhin, D.M. Utina | | |
| UC | D.V. Kamanin, A.Yu. Verkheev, B.S. Yuldashev | | |

Brief annotation and scientific rationale:

The project is aimed at organizing and providing computational support for physics research programmes implemented with JINR's participation, at developing mathematical methods and software for modelling physical processes and experimental facilities, processing and analysing experimental data in the field of elementary particle physics, nuclear physics, neutrino physics, condensed matter, radiobiology, etc. The particular attention will be paid to the creation of systems for the distributed processing and analysis of experimental data, as well as information and computing platforms to support research at JINR and other world centres.

The main areas of work are mathematical and computational physics to support JINR's large research infrastructure projects, first of all, the experiments at the NICA accelerator complex and the Baikal-GVD neutrino telescope. Further cooperation with experiments at the largest world accelerator centres (CERN, BNL, etc.), experiments in the field of neutrino physics and astrophysics, radiobiological research programmes will also be continued. The possibility of using the developed methods and algorithms within other megascience projects is being considered.

Expected results upon completion of the project:

Revision of interaction generators and their development for modelling the processes of interactions of light and heavy nuclei, including those at NICA energies (FTF, QGSM, DCM-QGSM-SMM, etc.), and processes beyond the Standard Model, such as the production of candidate particles for the role of dark matter, additional Higgs bosons and processes that violate the lepton number, etc. (QBH, Pythia, MadGraph, etc.) for LHC conditions at a nominal energy and a total integrated luminosity up to 450 fb⁻¹.

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, the study of the physical and technical characteristics of detector systems.

Development of scalable algorithms and software for processing multi-parameter, multi-dimensional, hierarchical data sets of exabyte volume, including those based on recurrent and convolutional neural networks, for machine and deep learning tasks, designed primarily for solving various problems in particle physics experiments, including for the NICA megaproject and neutrino experiments.

Creation and development of data processing and analysis systems and modern research tools for international collaborations (NICA, JINR neutrino programme, experiments at the LHC).

Development of algorithms and software for JINR's research projects in the field of neutron physics.

Development of algorithms, software and computing platforms for radiobiological research, applied research in the field of proton therapy and ecology.

Expected results of the project current year:

Completion of the revision of the Geant4 FTF model, more accurate specification of the functions of fragmentation of quarks and diquarks into strange particles in the Geant4 QGS model, conducting numerical experiments on the production of hypernuclei.

Physics analysis of data obtained in the NICA MPD, NICA BM@N and NA61/SHINE experiments within the Geant4 FTF model.

Considering various effects of the DCM-QGSM-SMM generator: dependence of the lifetime of resonances on the density of the nuclear medium, suppression of the production cross section of pseudoscalar mesons, enhancement of the production of hyperons in a dense nuclear medium, nucleus deformations. Elaboration of a lattice model of the nucleus and a percolation model of multifragmentation.

Mathematical modeling of the production and identification of non-resonant dibaryons at the NICA SPD facility.

Mathematical modeling of the events of knocking out pairs of high-momentum nucleons from atomic nuclei by accelerated particles. Elaboration of a draft of an experimental proposal for the NICA facility.

Evaluation of the cross sections of the processes of production of dark matter particles and new scalars within the extended two-doublet Higgs model (2HDM+a/S, MadGraph generator) in the channel of production of a muon/b-quark pair and the missing energy, performing corresponding modeling and data analysis under LHC RUN2/3 conditions.

Evaluation of the cross sections of the processes of production of dark matter particles and new scalars within the Inert Doublet Model in the final state with two muons and the missing energy, performing corresponding modeling and data analysis under LHC RUN2/3 conditions.

Debugging of the procedure for testing sensitive elements of the high-granularity calorimeter of the CMS experiment, including track reconstruction and the evaluation of the efficiency of each detector cell.

Development and adjustment of algorithms and methods for reconstructing muon trajectories in the Cathode-Strip Chambers (CSCs) of the muon system of the CMS experiment for the comparison of the continuous and discrete approaches of wavelet analysis for separating overlapping signals; estimation of the CSC spatial resolution and the aging effect on data obtained in 2025 at the GIF++ facility at CERN and in proton-proton beam collisions at the LHC.

Development of machine learning models and approaches for their application to particle identification within the BM@N experiment on the basis of a sample balanced by the types of classified particles.

Finding correction parameters in coordinate and angular space for the geometry of the STS and GEM detectors of the BM@N experiment, elaboration and software implementation of modeling and data processing methods, as well as their development and adaptation for the current configurations of a number of GEM and Silicon Profilometer tracking detectors in 2024-2025.

Introduction of alignment corrections to the geometric models of the microstrip tracking detectors (FSD, GEM and CSC) of the BM@N experiment obtained as a result of analysis of the reconstructed trajectories of charged particles on the basis of the first physical run data. Elaboration and software implementation of modeling and data processing methods for the vertex silicon detector plane (VSP) for upcoming experimental runs.

Transition from the global classifier that identifies particles within the MPD experiment in a full momentum range to local classifiers based on gradient boosting and operating in a given momentum range in order to enhance the efficiency of particle detection.

Modernization of the MPD experiment software package to enhance the accuracy and speed of event reconstruction by implementing the ACTS tracker into the MPDroot software shell. Integration of the latest versions of external dependencies into the MPDRoot shell (ACTS, FairRoot, GEANT4, ROOT). Transition of the build system to Alma Linux 9.5.

Optimization of the codes of charged particle trajectory reconstruction programs in the track system of the SPD experiment to speed up the offline event processing procedure.

Application of graph neural networks to detect charged particle trajectories in the MPD experiment.

Investigation of the properties of hadron jet/cluster reconstruction algorithms under SPD conditions. Evaluation of the cross sections of the process of direct photon production in quark-gluon scattering.

Implementation of a model for processing and storing simulated data from the SPD experiment, relevant for 2025-2026, on the basis of the previously created prototype of a distributed mass data processing system and new application software created on the Gaudi software platform.

Functional testing and debugging of components and interfaces between the components of the system that provides multi-stage data processing on the real-time event filtering cluster (SPD OnLine Filter).

Provision of the required level of functioning that meets the needs for the mass modeling of physics processes of the SPD experiment in a distributed computing environment based on the PanDA load management system and a data management system on top of the RUCIO DDM package. Development of processing management systems.

Adaptation of the program code for high-energy cascade reconstruction to the fast Baikal-GVD data processing system.

Elaboration of data processing programs for a complex of scattering detectors, including a position-sensitive detector and a direct beam detector.

Modernization of the ATLAS CREST system to a new architecture with Dto classes, development of the EventIndexPicking service for performing R2R4 Milestone tests, modification of the TDAQ resource manager for use in Run4. Development and support for the operation of information systems for the BM@N and MPD experiments to describe the facility geometry, detector configurations and management process. Participation in the development of the DAQ MDT online system.

Construction of a machine learning model for the hadron and gamma quantum classification task in the TAIGA experiment.

Modeling of the OLVE-HERO detector resolution for a simplified model of various sizes.

Development of mathematical methods and algorithms for trajectory reconstruction in the proton digital calorimeter simulation task.

Application of high-order BEM polynomials to enhance the methodology of processing reactor data and neutron noise from the IBR-2M reactor.

Elaboration of a web service to automate the analysis of data obtained using the Morris Water Maze test system in experiments aimed at studying the behavioral reactions of laboratory animals exposed to various factors.

Research in the field of enhancing the accuracy of models for classifying plant diseases by photos. Assessment of the impact of various data augmentation policies and attention mechanisms on the model performance.

Investigations in the field of predicting soil pollution using remote sensing data and various machine learning methods. Enhancement of the existing functionality and provision of new capabilities for monitoring and predicting the state of the environment.

Elaboration of an algorithm for neutron energy spectrum reconstruction based on the results of measurements with the Bonner spectrometer.

2. Methods of computational physics for the study of complex systems

E.V. Zemlyanaya
O. Chuluunbaatar
Deputies:
Yu.L. Kalinovsky
A. Khvedelidze

| |
|-------------|
| Realization |
|-------------|

| | |
|--------|--|
| MLIT | V. Abgaryan, G. Adam, S. Adam, P.G. Akishin, A.S. Ayriyan, E.A. Ayrjan, D.R. Badreeva, I.V. Barashenkov, M.V. Bashashin, A.A. Bogolubskaya, L. Bordag, A.D. Burakova, M. Bures, 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. Korniyak, O.O. Kovalev, D.S. Kulyabov, K.V. Lukyanov, N.V. Makhaldiani, S.D. Mavlonberdieva, T.I. Mikhailova, A.V. Nechaevsky, 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, S.I. Serdyukova, Z.A. Sharipov, O.I. Streltsova, L.A. Syurakshina, 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. Hnatic, K.V. Kulikov, V.K. Lukyanov, R.G. Nazmitdinov, I.R. Rahmonov, Yu.M. Shukrinov, S.I. Vinitzky, D.N. Voskresensky, V.I. Yukalov, V.Yu. Yushankhai |
| FLNR | E. Batchuluun, A.V. Karpov, M.N. Mirzayev, V.V. Samarin, Yu.M. Sereda |
| FLNP | M.A. Kiselev, N. Kucerka, E.E. Perepelkin |
| DLNP | O.V. Karamyshev, G.A. Karamysheva, I.N. Kiyani, E.P. Popov |
| VBLHEP | A.V. Bychkov, H.G. Khodzhigaiyan |
| LRB | A.N. Bugay, A.V. Chizhov |

Brief annotation and scientific rationale:

The project is aimed at the development and application of mathematical and computational methods for modelling complex physical systems studied within the JINR Topical Plan and described by systems of dynamic nonlinear, spatially multidimensional integral, integro-differential or differential equations that depend on the parameters of models. The evolution of solutions to such systems can be characterized by the occurrence of critical modes, bifurcations and phase transitions. Mathematical modelling is an inseparable part of modern scientific research. It entails an adequate mathematical formulation of problems within the models under study, the adaptation of known numerical approaches or elaboration 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 resources of the JINR Multifunctional Information and Computing Complex.

Expected results upon completion of the project:

Development of methods, algorithms and software packages for conducting the numerical research of interactions of various types in complex systems of nuclear physics and quantum mechanics.

Methods for modelling multifactorial processes in materials and condensed matter under external actions.

Methods for solving simulation tasks in the design of experimental facilities and the optimization of their operating modes.

Methods for modelling complex processes in dense nuclear matter based on the equation of state.

Methods for modelling quantum systems using quantum information theory methods and hybrid quantum-classical programming methods.

Expected results of the project current year:

Numerical study of deep subbarrier fusion and quasi-elastic scattering reactions of heavy nuclei within the coupled channel method with optical potentials. Development of algorithms and programs for calculating the characteristics of heavy nuclei, including the uranium-238 nucleus with a two-well potential, within geometric collective models.

Development of methods for modeling chemical bonds and reactions involving heavy and superheavy elements for the interpretation of FLNR thermochromatographic experimental data.

Investigation of the equilibrium properties and nonequilibrium dynamics of complex statistical systems, including trapped atoms and heterogeneous neural networks, within optimized perturbation theory.

Modification of the method and computer codes for modeling nuclear reactions within the transport-statistical approach. Calculation of the physical characteristics of transfer and fragmentation processes in heavy ion collisions.

Study of the nuclear matter influence on the processes of elastic and inelastic interaction of protons with nuclei in a wide range of energies. Analysis of observables in reactions of various types involving light exotic nuclei.

Computer simulation of complex processes in materials under the irradiation of heavy ion beams based on the combined application of molecular dynamics and continuum mechanics methods. Development of methods for assessing the distribution of energy losses by irradiating particles in such processes.

Simulation of complex processes in superconducting structures. Development of methods for the high-performance computing of physical observables in a wide range of parameters of Josephson junction models. Development and software implementation of a computational scheme for modeling the dynamics of a ring system of parallel j_0 -junctions. Study of intervortex interaction in intertype superconductors with impurities.

Development of a software module for analytical calculations using Python libraries, allowing one to automate the representation of equations for the numerical modeling of a chain of nanomagnets associated with a Josephson junction, taking into account various types of interactions between the elements.

Modeling of complex processes in physical and chemical systems of various types. Development of methods for the high-performance numerical investigation of the structure and properties of vesicular systems of various types. Computer simulation, by molecular dynamics methods, of the interaction of beta-amyloid peptides with phospholipid membranes in vesicular, bicelle-like and bilayer structures in order to study the influence of the peptide and lipid charge, as well as the composition of the lipids on this interaction in various thermodynamic phases of the lipid. Obtaining on this basis new information about the structural and dynamic properties of phospholipid membranes.

Numerical study of localized structures in systems described by nonlinear dynamic equations, including periodic solutions (oscillons) in one- and three-dimensional field theory models.

Development of methods and computer programs for modeling the formation of magnetic fields of isochronous cyclotrons under various operating modes. Development of finite and boundary element methods in the COMSOL environment to optimize the calculations of electromagnetic and thermal processes of complex physical systems.

Development of methods for modeling matrix elements of volumetric integral equations of magnetostatics. Calculation of the optimized characteristics of superconducting magnets based on three-dimensional computer modeling.

Development of effective methods for solving equations that describe the models of physical fields and the operating modes of experimental facilities. Development of high-performance methods for the numerical solution of elliptic problems. Development and study of the properties of a computational scheme based on Appelrot quadratization and the Kagan difference scheme for the numerical integration of dynamic systems with a polynomial right-hand side.

Study of the Einstein-Maxwell-Dirac system within the astrophysical and cosmological gravitational field. Investigation of the superconducting properties of strongly interacting nuclear matter in the depths of neutron stars on the basis of the automated selection of cooling models for these stars. The introduction of a criterion for assessing the adequacy of the models based on the observational data of the surface temperature and star age.

Development of models of pseudoscalar and vector mesons with nonlocal interaction; calculation of the mass spectrum, interaction constants and other characteristics on this basis. Description of the processes of production and dissociation of heavy quarkoniums.

Development and enhancement of an algorithm for modeling particle tracking within processes that are planned to be studied at the NICA facility (SPD). Study of the applicability of the Bjorken model to the survival of J/ψ particles in a medium formed by the collision of heavy ions under NICA conditions.

Development of constructive methods for describing composite finite-dimensional quantum systems within the Weyl-Schwinger formalism using computer algebra and computational group theory.

Derivation and application of functional relations for the reduction of multi-loop Feynman integrals.

Development and implementation, on the MICC quantum polygon, of a quantum circuit of the QAOA algorithm for finding the ground state of the Schwinger model with a topological term.

Solution to the problem of optimizing the operation of single-qubit gates under the influence of a control radio frequency field.

Comparative analysis of quasiprobability distributions in elementary and composite finite-dimensional quantum systems.

Calculations of the entanglement – positivity correlation of the Wigner function for qudits.

Activities:

| Name of the activity | Leaders | Implementation period Status |
|--|--|---------------------------------|
| Laboratory Responsible from laboratories | | |
| 1. Intelligent control of technological processes and physical equipment's in JINR and quantum computing in quantum chemistry and physics | P.V. Zrelov S.V. Ulyanov | 2024-2026 Realization |
| MLIT | D.A. Baranov, O.V. Ivantsova, M.S. Katulin, E.A. Kuznetsov, A.G. Reshetnikov, A.R. Ryabov, N.V. Ryabov, L.A. Syurakshina, D.P. Zrelova | |
| VBLHEP | Yu.G. Bespalov, O.I. Brovko, D.N. Nikiforov, G.P. Reshetnikov | |
| BLTP | V.Yu. Yushankhai | |

Brief annotation and scientific rationale:

The main addressed issues of the activity are the development and effective application of intelligent computing technologies and the quantum self-organization of inaccurate knowledge in robust control tasks in order to enhance the reliability of the functioning of physical facilities. The solution of the tasks is based on the possibility of increasing the robustness of existing control systems through embedded knowledge bases. Self-organized control systems are designed and supported by software tools developed in the project on the basis of a platform that combines soft computing and quantum knowledge base optimizers. Embedded self-organized controllers will be developed for systems of the intelligent control of JINR's technological processes, devices and facilities (including for cases of unforeseen and unpredictable situations) and intelligent cognitive robotics tasks.

The investigation of the effectiveness of quantum algorithms is aimed at solving the tasks 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 of classical computing architecture. It is planned to create a software product for calculating the electronic and magnetic structures of molecular complexes and crystal fragments of new functional materials using quantum simulators on classical computing architectures.

Expected results upon completion of the activity:

Creation of a prototype of a quantum fuzzy PID controller and of a demonstration robot with a built-in controller prototype.

Creation of a prototype of an intelligent control system for cryogenic systems of superconducting magnets of the NICA accelerator complex on the basis of the quantum fuzzy PID controller. Preparing a patent.

Methodology of building and structure of an intelligent control system for a high-frequency station.

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

Expected results of the activity in the current year:

Elaboration of a platform-independent software library of a quantum simulator for executing a quantum fuzzy inference algorithm in real time on a computer with a classical architecture in relation to the task of constructing a control system for the nitrogen cooling of the booster arm of the NICA accelerator complex.

Development of a reinforcement learning algorithm for a quantum fuzzy neural network with demonstration on an autonomous robot on a robotics polygon.

Elaboration of route formation and obstacle avoidance algorithms based on quantum machine learning for a mobile robotic platform.

Within the task of multi-loop system control, a method of quantum intelligent coordination control on top of quantum fuzzy inference in a control system for superconducting magnet cooling will be developed.

Within the investigation of multi-qubit hidden correlations in self-organizing control systems, the structure of a knowledge base simulator of a quantum coordination regulator in a control system for the nitrogen cooling of a superconducting magnet on a classical computer for 30 input qubits will be elaborated.

Within the construction of a methodology for remote configuration and knowledge exchange for an intelligent control system, protocols for the exchange of knowledge bases and remote configuration of regulators in the TANGO Control environment of a control system for the nitrogen cooling of the booster of the NICA accelerator complex will be developed.

Automation of the preparation of a universal computing environment for quantum computing on various architectures.

Study of the potential of quantum generative adversarial networks (QGANs) using the example of the task of generating synthesized RGB images.

In the context of materials science, a computational description of chemical reactions on crystal surfaces is planned. For this purpose, the process of modeling the adsorption and reaction of molecules on surfaces will be implemented using quantum computing algorithms.

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

**V.V. Korenkov
A.V. Nechaevsky
D.I. Pryahina
O.I. Streltsov**

2024-2026

Realization

MLIT T.Zh. Bezhanyan, O.Yu. Derenovskaya, E.Mazhitova, I.S. Pelevanyuk, A.S. Vorontsov, E.N. Voytishina, M.I. Zuev

UC D.V. Kamanin, A.Yu. Verkheev

Brief annotation and scientific rationale:

The training and retraining of specialists in computational physics and information technology on the basis of the Multifunctional Information and Computing Complex (MICC) of the Joint Institute for Nuclear Research (JINR) and its educational components are performed for:

- upskilling JINR staff members in order to develop scientific projects, including megascience ones, which are implemented at JINR or with its participation, as well as to create and support the JINR Digital EcoSystem (DES);
- disseminating competencies in computational physics and information technology to the regions of Russia and the JINR Member States to enhance the personnel potential of JINR and organizations cooperating with the Institute;
- the main prerequisite for the creation of the activity is the necessity to form a research environment in order to ensure the professional growth of IT specialists, the creation and development of scientific groups, and the engagement of new specialists in JINR projects. The additional training of the personnel, mainly on request of the JINR Laboratories, should be aimed at developing special competencies, in-depth knowledge and practical skills in computational physics and information technology.

Expected results upon completion of the activity:

Holding events for JINR staff members to study state-of-the-art information technologies and opportunities to work on the MICC components and in the DES.

Forming a set of JINR projects in which students can participate.

Forming a list of competencies and required courses for the implementation of projects.

Elaboration of training courses and educational programmes that will provide personnel training for solving a variety of tasks within projects.

Creation of an ecosystem for the implementation of educational programmes on the basis of the JINR MICC, including the cloud infrastructure, the HybriLIT heterogeneous computing platform, which comprises the education and testing polygon and the "Govorun" supercomputer.

Creation of a software and information environment and a platform for organizing and holding events, lectures, workshops, hackathons, etc.

Involvement of specialists from JINR and JINR Information Centres, researchers from the JINR Member States' organizations, lecturers from leading educational organizations that cooperate with JINR in order to hold educational and scientific events.

Forming event programmes and organizing interaction with universities and JINR Information Centres.

Expected results of the activity in the current year:

Holding scientific seminars on information technologies, including for JINR MICC and DES users.

Elaboration and implementation of educational programs, training courses on information technologies.

Information support of the activity: creation and development of a website containing educational materials, results of work on projects of participants of Schools of Information Technologies.

Development of the ecosystem components for the implementation of educational programs.

Holding Schools of Information Technologies, educational practices for students of universities of the Russian Federation and the JINR Member States.

Collaboration

| Country or International Organization | City | Institute or laboratory |
|--|--------------------------|---|
| Armenia | Yerevan | Foundation ANSL YSU |
| Belarus | Gomel Minsk | GSU IM NASB INP BSU IP NASB |
| Bulgaria | Sofia | SU |
| CERN | Geneva | CERN |
| China | Beijing | CIAE |
| Egypt | Cairo | ASRT |
| | Giza | CU |
| France | Saclay | IRFU |
| Georgia | Tbilisi | GTU TSU UG |
| Italy | Genoa | INFN |
| Kazakhstan | Almaty | IETP KazNU INP ENU |
| | Astana | ENU |
| Mexico | Mexico City | UNAM |
| Mongolia | Ulaanbaatar | IMDT MAS MUST |
| Russia | Arkhangelsk | NArFU |
| | Chelyabinsk | SUSU |
| | Dubna | Dubna State Univ. MSU Branch |
| | Gatchina | NRC KI PNPI |
| | Irkutsk | ISU |
| | Moscow | ITEP LPI RAS MSU NNRU "MEPhI" NRU HSE PFUR RCC MSU RSTSREC SINP MSU |
| | Moscow, Troitsk | INR RAS |
| | Petropavlovsk-Kamchatsky | KSU |
| | Protvino | IHEP |
| | Puschino | IMPB RAS |

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| | Saint Petersburg | SPbSU |
| | Samara | SSU |
| | Saratov | SSU |
| | Sarov | MSU Branch |
| | Tomsk | TPU |
| | | TSU |
| | Tula | TSU |
| | Tver | TvSU |
| | Vladikavkaz | NOSU |
| | Vladivostok | FEFU |
| | Voronezh | VSU |
| | Belgrade | Univ. |
| | Kosice | UPJS |
| | Cape Town | UCT |
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