

APPROVED BY
JINR Vice Director

“ ____ ” _____ 2019

SCIENTIFIC AND TECHNICAL JUSTIFICATION FOR EXTENDING A THEME
to be included in the
TOPICAL PLAN FOR JINR RESEARCH FOR 2020–2023

Theme code 05-6-1119-2014/2023

Laboratory LIT
Department

Research area: Networking, Computing, Computational Physics (05)

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

Theme leaders: Gheorghe Adam, Petr V. Zrelov

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Abstract

Carrying out paramount advanced research in computational mathematics and physics, directed to the creation of new mathematical methods, algorithms, and software for the numerical or symbolic-numerical solution of topics arising in experimental and theoretical physics studies. This subject area includes a wide spectrum of investigations approved for completion in JINR within the seven year period 2017–2023 in high energy physics, nuclear physics, physics of condensed matter and of nanostructures, biophysics, information technologies, the solution of which is inseparable from the use of computing. Such subject matters of the outmost importance in JINR are the NICA project, the neutrino program, the superheavy and exotic nuclei physics, the neutron based investigations. The needed numerical or symbolic-numerical computing will be done on the Multifunctional Information and Computing Complex (MICC), primarily the HybriLIT heterogeneous computing platform which involves the training and test cluster HybriLIT and the “GOVORUN” supercomputer and the emerging Big Data distributed infrastructure. The research teams include both experienced scientists with outstanding scientific achievements and enthusiastic young scientists and engineers. The requested financing will cover salaries, participations in scientific conferences, scientific visits and the acquisition of a minimal number of personal computers and licenses, within the approved resources for LIT-JINR. A distinctive feature of this research is the close cooperation of the Laboratory of Information Technologies (LIT) with research groups from all JINR laboratories and Member State institutions.

List of activities

(1) Mathematical and computation methods for simulation of complex physical systems.

Leaders: Gh. Adam, J. Buša, I.V. Puzynin

(2) Software complexes and mathematical methods for processing and analysis of experimental data.

Leaders: P.V. Zrelov, V.V. Ivanov

(3) Numerical methods, algorithms and software for multicore and hybrid architectures and Big Data analytics.

Leaders: Gh. Adam, O. Chuluunbaatar, O.I. Streltsova, V.V. Korenkov, P.V. Zrelov

(4) Methods, algorithms and software of computer algebra and quantum computing.

Leader: V.P. Gerdt

(1) Mathematical and computation methods for simulation of complex physical systems

This activity comprises the development and use of mathematical and computing methods for modeling new experimental facilities, accelerating complexes and their elements, nuclear-physical processes, complex physical systems. New mathematical methods will be developed and, where suitable, existing ones will be extended with the aim to take into account the main features of the physical processes and mathematical models: non-linearity, multi-parametric behavior, the existence of critical modes and phase transitions. The model refinement, the investigation of the possibilities of their use and comparison with experimental data will be mainly done by means of the development of parallel algorithms and their implementation in software packages tuned for the present day hardware architectures, primarily the HybriLIT heterogeneous computing platform.

- Calculations of magnetic fields for different facilities:

- Three-dimensional computer simulation of magnetic systems in the framework of the NICA (JINR) and FAIR (GSI) projects. Calculation of the required characteristics of the magnetic field in the working areas of the magnets.

- Developing fast FEM algorithms for 3D simulation of the magnetic field distributions in COMSOL Multiphysics software.

- Development of methods and algorithms for efficient highly accurate three-dimensional modeling of magnets and computations targeted to the creation of superconducting cyclotrons for proton therapy, in collaboration with DLNP.

- Optimization of beam dynamics programs in cyclotrons aimed at increasing speed, efficiency, and accuracy of calculations.

- The investigation of mathematical models of complex physical processes will be pursued in the frame of quantum-field and molecular-dynamics approaches:

- Development of effective QCD-motivated models for describing properties of nuclear matter at NICA energies:

- (a) Generalization of the model Nambu – Jona-Lasinio with Polyakov loop and numerical analysis of the behavior of the masses and coupling constants of the quarks, diquarks, mesons and nucleons at finite temperature and density;

- (b) Completion of the construction of a model for the numerical solution of hydrodynamic equations using new state equations and its combination with the kinetic description of the initial state and the state after freezeout;

- (c) Simulation of specific properties of equations of state, in particular, the dependence of physical quantities on the magnetic field strength at low temperatures and large values of the chemical potential;

- (d) Based on the hybrid model and using the developed codes combining the properties of the kinetic and hydrodynamic approaches, analysis of the available experimental data on the collision of heavy ions in the energy region of the future NICA accelerator.

- Development of new molecular dynamics algorithms aimed at increasing accuracy and significantly reducing the computing time.

- Development of models of interaction of ion beams with targets in order to explain various effects: long-range and description of structural changes of materials under heavy ion and nanocluster irradiation, finding threshold values of energy loss in irradiated materials, leading to structural changes and through tracks in thin targets.

- Development of mathematical models, algorithms and programs for the study of processes of local nonequilibrium created by the impact of ultrashort laser pulses on materials. Formulation and solution of systems of the heat conduction equations for the study of laser ablation, carrying out numerical experiments in the framework of molecular dynamics. Validation of theoretical models by comparing the obtained numerical results with experimental data.

- New mathematical methods will be developed and, where suitable, existing ones will be extended with the aim to take into account specific features of the physical processes:

- Development of numerical methods for describing equilibrium and nonequilibrium properties of mesoscopic systems of trapped atoms.

- Numerical investigation of optical and self-assembled atomic lattices, with emphasis on the control of their properties by external fields. The extension of optimized perturbation theory and self-similar approximation theory for these systems.

- Investigation of nonlinear multiparameter processes in complex physical systems under external fields, including models of superconducting structures, localized states in condensed media, simulation of gas-hydrodynamic processes in porous media.

- Numerical investigation of nuclear-physical processes based on a hybrid model of microscopic potential, including reactions with light exotic nuclei.

- Development of methods for modeling the reflection of neutrons from layered nanostructures. Studies of magnetic films as structures consisting of vector micro-objects.

- Studies of black hole and wormhole models, both in astrophysics and in cosmology, are aimed at understanding the results of new experiments.

- The continuous LIT information-computing support is instrumental for the improvement of the working regimes of several experimental facilities:

- Group of small-angle neutron scattering, FLNP (YuMO spectrometer at the IBR-2 reactor):

- (a) Maintenance of the SAS primary processing program for the YuMO spectrometer;

- (b) Development of a program for working with position sensitive detectors for isotropic and anisotropic scattering samples and for ring detectors;

- (c) Development and maintenance of a parallel version of the Fitter program.

- For the BAIKAL project, DLNP: step-by-step creation of an alert system.

- Modeling of electromagnetic cascade showers in the field of ultrahigh energies and numerical study of their characteristics in experimental data obtained in such astrophysical projects as IceCube, Antares, Baikal.

- Development of reliable scale-adapted algorithms of reduced computational complexity:

- Development of an extrapolation method of the sixth order with the aim at improving the algorithm efficiency for the numerical solution of a wide range of tasks.

- Development of methods and algorithms for processing and analysis of the neutron noise of the IBR-2M reactor.

- Multistage multiscale approach to the Bayesian automatic adaptive quadrature.

- Development of algorithms for the numerical simulation of the evolution of a liquid crystal in a pulsed electric field, as well as under the influence of an orienting structured surface.

- Simulation of peculiarities of the absorption-emission and photon density of states of a cholesterol liquid crystal with isotropic defect inside.

- Quantum-chemical cluster approach to electronic systems with strong spin-orbit interactions.

- Carrying out calculations of electromagnetic and thermal quantities characterizing physical processes in MgB₂ superconductors.

(2) Software complexes and mathematical methods for processing and analysis of experimental data

This activity is directed at the solution of the following main tasks: derivation of new mathematical methods for the extraction of the useful information from the raw data obtained in experiments done in JINR or with the JINR participation; development of algorithms and implementation of program packages for the solution of problems arising in the high energy physics – including the data got at the accelerator facilities LHC, NICA, FAIR as well as at the experimental facilities of the JINR neutrino program, the nuclear physics, the condensed matter physics and the physics of radiation biology. The development of deep learning neural network algorithms will become a significant part of this activity.

There are four classes of JINR undertakings covered with LIT participation.

- Development of mathematical methods, algorithms and software for reliable simulation and interpretation of the experimental data:

- Within the Geant4 package: simulation of the generation of charmed particles and their transport in matter; improvement of the algorithm for calculation of excitation energies of nuclear residuals and improvement of the description of nuclear fragment formation; improvement of FTF and QGSM models and their application for modeling the conditions of various experiments (PANDA, NICA/MPD, NICA/SPD).

- Development of software support, processing and analysis of data collected at the NUCLEON and COMBAS experiments.

- Investigation of the structure and properties of vesicular systems of phospholipids and medical drugs based on the phospholipid transport nanosystem by means of analysis of the neutron and X-ray small-angle scattering data, depending on external factors and chemical composition.

- Development of deep learning neural network algorithms:

- Development of a framework for the analysis and management of biological monitoring data for controlling and forecasting the status of the environment.

- Development of mathematical methods for the determination of fine structures in the distribution of nuclear reaction products by mass and energy.

- Development of software for the reconstruction of elementary particle tracks based on deep learning methods in the processing of experimental information from modern high-energy physics track detectors.

- Software-information support of JINR projects:

- Improvement of information systems for online and offline data processing of experimental facilities of the NICA complex: Database developments for the tasks of experiments BM@N and MPD.

- Software support for the BM@N experiment: Development and implementation of algorithms for modeling, processing and analysis of data for the BM@N track system consisting of gas and semiconductor detectors with microstrip information acquisition (GEM, SILICON, CSC) and their subsequent integration into the BmnRoot.

- Development and refinement of the DQGSM model by comparison with experimental data of the BM@N.

- The BM@N experiment:

- (a) trajectory reconstruction of charged particles in outer tracking detectors: MWPC, Si, CSC, DCH, GEM;

- (b) Particle identification in the TOF700 time-of-flight detector;

- (c) Search for strange hyperons on data from the Nuclotron.

- The MPD experiment: Participation in the realization of a laser calibration system for detector alignment, monitoring drift velocity and for taking electric field distortion into account inside the Time-Projection Chamber (TPC) of the MPD central barrel.

- Further development of statistical methods for the analysis of experimental data under small statistics and incomplete observation of the studied processes: testing the likelihood of hypotheses, estimates of the half-life

of the nucleus and of the reaction cross section and of their accuracy, noise filtering and buildup of the optimal experimental design.

- Development of batch processing of neutron diffraction spectra measured in real-time in situ mode (HRFD at IBR-2, FLNP).

- Software information support of large scale outer experiments done with JINR participation:

- Software support of ATLAS experiment: (a) Development and maintenance of configuration and management of ATLAS TDAQ; (b) Development and support of modules of the EventIndex project; (c) Development of modules of Project ATLAS Condition DB (in preparation for RUN3).

- Software support of CMS experiment:

- (a) Development, testing and implementation into the official CMS release of algorithms for the separation of overlapping signals and for building track segments in cathode strip chambers (CSC);

- (b) Evaluation of the CSC spatial resolution and effectiveness on experimental data with LHC;

- (c) Study of the effects of CSC ageing on muon beam tests with radiation source (CERN Gamma Irradiation Facility (GIF++));

- (d) Background rates estimation in CSCs with LHC data.

- Software support of CBM experiment:

- (a) Development of methods for the selection of rare processes: models, methods, algorithms and software;

- (b) Development and maintenance of the complex of databases.

(3) Numerical methods, algorithms and software for multicore and hybrid architectures and Big Data analytics

A. Developments for Multicore and Hybrid Architectures

The mainstream of this activity is aimed at the development of numerical methods, algorithms and software packages developed on the basis of parallel programming techniques using OpenMP, MPI, CUDA/OpenCL, machine learning methods and deep learning (ML/DL), intended to the effective use of multicore and hybrid architectures for the solution of massively parallel, resource-intensive problems of theoretical and experimental physics. The worked out methods and algorithms will take into account the trends in the development of the computational architectures and of the IT-technologies allowing implementing the necessary functionality for different high-performance computing tools and to significantly speed up the solution of a wide range of tasks facing JINR.

To provide opportunities for the development of mathematical models and algorithms as well as for resource-intensive calculations, including graphics accelerators which significantly reduce the computing time, an ecosystem for data analysis and ML/DL tasks was set up and is under active development within the heterogeneous computing platform HybriLIT. The created ecosystem includes two components: the first one is designed for resource-intensive, massively parallel learning tasks of neural networks using NVIDIA graphics accelerators; the second is devoted to the design and implementation of models and algorithms based on JupyterHub – a multi-user platform for working with Jupyter Notebook.

- The emerging ecosystem is expected to serve to the development of ML/DL based algorithms:

- using recurrent and convolutional neural networks with deep learning for solving problems of fast recognition of multiple tracks in particle physics experiments, including the NICA megaproject and the neutrino program;

- using the neural network approach for tasks of analyzing and classifying medical and biological data.

- Large scale numerical experiments will be done, within the recently signed Memorandum of Scientific Collaboration (MoSC), for the project ELI-NP, specifically by the implementation and refinement of the PIconGPU code for the laser acceleration of elementary particles.

- Support will be extended to the solution of applied engineering and physics problems on the HybriLIT platform using software packages adapted for parallel computations, e.g., selected COMSOL Multiphysics modules, LAMMPS, GAMESS, etc.

- New parallel implementations of software packages will be developed for solving a number of current and new specific tasks, namely:
 - parallelization of the most time-expensive functions using tools such as OpenMP, MPI, CUDA/OpenCL, in the event modeling and reconstruction in NICA experiments;
 - calculations on heterogeneous computing platforms for the study of long Josephson junctions;
 - the numerical study of multidimensional models based on evolutionary equations;
 - solving equations of motion of the molecular dynamics and equations of continuous media;
 - calculations of multiple integrals arising from theoretical studies related to the NICA megaproject and entering the study of various physical processes;
 - solution of multi-physical problems in accelerator design, dosimetry and radiation safety;
 - study of the possibility of increasing the performance of data analysis in ROOT through the use of graphics processors, the comparative analysis of parallelization using PROOF and OpenCL (for the application of the obtained results in the work on the NICA project);
 - diagonalization of large matrices in the theory of random matrices for the description of the decay properties of giant multipole resonances of heavy and medium nuclei;
 - computations of non-standard problems of the magnetostatics;
 - solving optimization problems aimed at getting the best parameters of superdense nuclear matter models in the simulation of heavy ion collisions and in astrophysical applications;
 - development of LDPC-like efficient decoding algorithms based on a genetic approach;
 - development of finite element method based computational schemes for the description of the quadrupole oscillations of the collective model of the nucleus;
 - development of computational schemes for the triangular three-center Coulomb problem and application to the H_3^+ molecule ion and H_2O molecule;
 - modeling processes of single and multiple ionization/photoionization of biomolecules by the method of separable potentials;
 - study of single ionization of atoms and molecules by fast proton impact in different kinematic regimes.

B. Big Data Analytics

- Development of the concept and step-by-step implementation within the Big Data approach of a scalable software-analytical platform for the collection, storage, processing, analysis, retrieval of relevant information and visualization of results for the MPD and BM@N experiments at the NICA accelerator complex and for experiments within the JINR neutrino program.
- Development of methods and software for effective use of Big Data analytics for resource-intensive computations on coprocessors and graphics processors for modeling, reconstruction and processing of experimental data (installations at the NICA accelerator complex, JINR neutrino program experiments, LHC experiments).
- Development of techniques for event reconstruction and intellectual monitoring of detectors using methods and technologies of Big Data and machine learning. The use of powerful high-level Big Data libraries, including the Spark MLlib machine learning library, the GraphX operations library for performing graphs and parallel operations with them, the Spark Streaming library for processing real-time streaming data, and the SparkSQL library. Use of new mathematical methods such as DQC (Dynamic Quantum Clustering), Complex Networks, etc.
- Development of time series analysis methods using Big Data technologies for intelligent monitoring of distributed computing systems. Application of machine learning and artificial intelligence to the optimization of the functionality of the distributed computing for physical experiments.

C. Scientific library developments

- The development of the JINRLIB library is foreseen in three directions:

- (a) Transition to modern software development tools (Intel Parallel Studio), including freely distributed ones (GNU Compiler Collection).
- (b) Creation of interfaces to modern high-level languages (Python, C++) and Fortran enabling the use of libraries written in Fortran (CERNLIB, JINRLIB).
- (c) Development and support of parallel programs of the JINRLIB library.

(4) Methods, algorithms and software of computer algebra and quantum computing

This activity foresees the development of methods of computer algebra and quantum computing for simulation of quantum information processes; creation of algorithms and programs for symbolic-numerical solution of problems arising in experimental and theoretical studies, using the latest computational hardware resources, including the heterogeneous platform HybriLIT.

- Advances in computer algebra methods for modeling quantum systems and quantum information processes:
 - Development of methods of quantum information processing by means of dipolar and spinor atomic systems, derivation of optimal methods for spintronics.
 - Modeling of intelligent networks performing operations based on quantum decision theory. Numerical analysis of artificial intelligence models.
 - Investigation of methods and algorithms for quantum computing and quantum informatics focused on machine learning (quantum machine learning) in order to adapt them to the task of track reconstruction and data processing for the NICA collider.
 - Comparison and analysis of the computational efficiency of the adiabatic and "universal" quantum computing on real equipment available through the cloud.
 - Development of constructive algorithmic methods based on the computational theory of finite groups for studying the entanglement of many-particle quantum systems.
 - Development of quantum algorithms for the study of phase transitions in lattice QCD models at finite density in the framework of tensor network methods.
- Development of computer algebra methods with application to symbolic-numerical solution of differential equations
 - Improvement of algorithms and programs for the study and solution of systems of nonlinear algebraic and differential equations arising in the simulation of quantum computing and other physical processes, based on the capabilities of the heterogeneous HybriLIT cluster and the "GOVORUN" supercomputer.
- Development of algorithms requested by special topics
 - Development of a new computational scheme for constructing a quasi-probability Wigner distribution for composite systems.
 - Development of a relativistic version of the Lindblad equation for open systems based on the Bogolyubov equations for the state vector in relativistic quantum field theory.
 - Application of the proposed versions of the quasi-probabilistic Wigner distributions and the relativistic Lindblad equations to the study of composite systems interacting with an intense laser field.
 - Development of algebraic methods for the computation of radiation corrections, depending on many kinematic variables and masses, based on functional equations and recurrence relations.
- Development and implementation of special computational tools
 - Embedding into the system of computer algebra of the Axiom module of field-theoretical calculations in high-energy physics, which is part of the FORM system – the most efficient among the computer algebra systems in terms of the speed of calculations of this type.

Results expected upon completion of the theme

1. Mathematical and numerical methods for modeling complex physical systems: development and use of mathematical and computer methods for modeling new experimental facilities, accelerator complexes

and their elements, nuclear physics processes, complex physical systems. Agreed construction of 3D computer models of dipole and quadrupole magnets for NICA (JINR) and SIS100 (GSI) and for other installations; calculation of magnetic field distributions in the working areas of the magnets. Study of mathematical models of complex physical processes in the framework of quantum field and molecular dynamics approaches; development of new and of existing numerical methods for effective account of the basic features of the physical processes and their mathematical models: nonlinearity, multiparameter, existence of critical regimes, phase transitions. Refinement of models, study of the possibilities of their use and comparison with experimental data will be carried out mainly through the development of parallel algorithms and their implementation in software packages configured for modern hardware architectures, primarily the heterogeneous computing platform HybriLIT (training and testing cluster and supercomputer “GOVORUN”).

2. Software complexes and mathematical methods for the analysis of experimental data: development of new mathematical methods for extracting meaningful information from data obtained in experiments conducted at JINR or with the JINR participation; algorithms and software packages for solving agreed problems in high energy physics, nuclear physics, condensed matter physics, radiation biology physics, in particular in experiments conducted at the accelerator facilities NICA (BM@N, MPD), LHC (ATLAS, CMS), FAIR (CBM), as well as at experimental facilities of the JINR neutrino program.
3. Development of numerical methods, algorithms and software packages using new computational techniques for multi-core and hybrid architectures in order to solve computationally intensive problems of theoretical and experimental physics; conducting large-scale numerical experiments on the “GOVORUN” supercomputer; development and support of the ecosystem for data analysis and also for machine learning and deep learning (ML/DL) tasks. Developments in the framework of the Big Data approach: the concept and gradual implementation of scalable software and analytical platform for the collection, storage, processing, analysis, search of relevant information and visualization of results for the MPD and BM@N experiments at the NICA accelerator complex and for JINR experiments within the neutrino program; methods and software for the effective use of Big Data analytics for resource-intensive calculations on coprocessors and graphics processors for modeling, reconstruction and processing of experimental data; methods for event reconstruction and intelligent monitoring of detectors and of distributed computing systems.
4. Development of methods of computer algebra and quantum computing for simulation of quantum information processes; creation of algorithms and program packages for symbolic-numerical solution of differential equations and of problems arising in experimental and theoretical studies, by means of the latest computational hardware resources, including the heterogeneous platform HybriLIT; development and implementation of special topmost efficient computational tools.

Participants from JINR

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**4. Methods, algorithms and software of V.P. Gerdt
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	Gatchina	PSNRU
	Perm	IHEP
	Protvino	IMPB RAS
	Puschino	ITEB RAS
		IPR RAS
	Saratov	SSU
	St. Petersburg	SPbSU
		NIEFA

	Tomsk	TSU
	Tver	TvSU
Slovakia	Kosice	IEP SAS
		TUKE
		PJSU
	Presov	PU
	Banska Bistrica	UMB
South Africa	Cape Town	UCT
	Stellenbosch	SU
Switzerland	Zurich	ETH
Tajikistan	Dushanbe	TNU
		PHTI ASRT
	Khujent	KSU
USA	Cambridge, MA	MIT
	Davis, CA	UCDavis
	Los Angeles, CA	UCLA
	Madison, WI	UW-Madison
	San Diego, CA	UCSD
Vietnam	Hanoi	VNU

Time frame of the theme: 2020–2023

Total estimated cost of the theme

k\$

	Chapters of the JINR budget	Previsions 2020–2023	Yearly distribution			
			2020	2021	2022	2023
1	2	3	4	5		6
1	Salaries	8761.8	1887.9	2076.7	2284.4	2512.8
2	Unified social tax	2646.1	570.1	627.2	689.9	758.9
3	Social national fund	569.5	122.7	135.0	148.5	163.3
4	International cooperation expenses	238.8	59.7	59.7	59.7	59.7
	a) business trips to Member States	60.8	15.2	15.2	15.2	15.2
	b) business trips to Non-Member States	72.0	18.0	18.0	18.0	18.0
	c) business trips in Russia	28.0	7.0	7.0	7.0	7.0
	d) arrivals to JINR	50.0	12.5	12.5	12.5	12.5
	e) Conferences, protocol expenses	28.0	7.0	7.0	7.0	7.0
5	Materials	104.0	20.0	24.0	28.0	32.0
6	Equipment	365.0	80.0	90.0	95.0	100.0
7	Electro energy costs					
8	Heating and water supply costs					

9	Payment of commissioning and adjustment works					
10	Service payments to scientific-research organizations					
11	Scientific and information support					
15	Payment of communication services					
	TOTALS	12685.2	2740.4	3012.6	3305.5	3626.7

Other financing sources --

Cost estimates for the theme

№.№ of items	Budget items	Total 2020-202	Including 2020
	Total		

AGREED:

JINR Chief Scientific Secretary

_____/_____
" " _____ 2019

Head of Planning and Finance Department

_____/_____
" " _____ 2019

Head of Science Organization Department

_____/_____
" " _____ 2019

Laboratory Director

С.А. Колесников В.В.
" 25 " _____ 2019

Laboratory Scientific Secretary

В.В. Степанов
" 25 " _____ 2019

Laboratory Economist

Л.А. Дуванкина О.И.
" 25 " _____ 2019

Theme leader

И.В. Степанов 13.09.2019
" 25 " _____ 2019