Proposal for Theme 1119 Extension during 2017-2019

1. **Title of the theme.** 05-6-1119-2014/2019, "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data"
   Priority: 1   Status: Extended
   Leaders: Gheorghe Adam, Petr V. Zrelov
   Theme beginning: 2014
   Participating JINR Laboratories: LIT, VBLHEP, BLTP, FLNR, FLNP, DLNP, LRB, UC
   Participating Countries, Institutes and International Organizations:
   Armenia, Australia, Azerbaijan, Belarus, Belgium, Brazil, Bulgaria, Canada, CERN, China, Czech Republic, France, Georgia, Germany, Greece, India, Italy, Japan, Kazakhstan, Moldova, Mongolia, Poland, Portugal, Romania, Russia, Slovakia, South Africa, Switzerland, Taiwan, Tajikistan, USA, Vietnam.

2. **Abstract of the theme.**
Carrying out paramount advanced research in the field of computational mathematics and computational 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 studies, by using the newest computational tools, primarily the heterogeneous cluster HybriLIT. This subject area includes a wide spectrum of investigations underway at JINR in high energy physics, nuclear physics, condensed matter physics and nanotechnologies, biophysics, information technologies, etc., which demand the development of new mathematical methods and approaches for modeling physical processes, processing and analysis of experimental data, including the use of these studies in the NICA project, the neutrino programme and other JINR strategic goals. A distinctive feature of these investigations is the close cooperation of the Laboratory of Information Technologies (LIT) with research groups from all the JINR laboratories and from Member State institutions.

3. **Introduction.**
   The overwhelming part of the scientific projects approved to be carried on during the next seven year period 2017-2023 in the Joint Institute for Nuclear Research (JINR) asks for the solution of a broad spectrum of computing intensive tasks of ever increasing complexity. The LIT proposals aimed at coping with the information technologies and computational needs of a large and diverse scientific community were approved by all the JINR Programme Advisory Committees (PACs), in particular by the 42-nd CMP-PAC of 22-23 June 2015 [Recommendations – page 11; details at http://indico.jinr.ru/conferenceDisplay.py?confId=1309 (Programme-Points 05.6.Adam, 5.6., 13.)]. These proposals foresee two basic directions of the research done in LIT, which are intimately related with each other and with the research underway in the JINR.

   The first direction involves the design, implementation, and maintenance of a top level dedicated information-computing infrastructure the evolution of which will grow up during the next years into a Multifunctional Information and Computing Complex (MICC) [http://indico.jinr.ru/conferenceDisplay.py?confId=1589 (Programme-Point 11.2) http://indico.jinr.ru/materialDisplay.py?contribId=28&materialId=1&confId=1589 (45_PAC_PP_Recommendations_eng.doc Recommendations-Chapter V)], and the related research theme 1118 [Theme 05-6-1118-2014/2019, "Information-Computing Infrastructure of JINR"].

   The second direction is the present theme 1119, the detailed description of which follows.

   The basic feature of the Theme 1119 can be simply characterized as *unity in diversity*. The latter characteristic is best illustrated by the involvement of the LIT scientists in the solution of computing tasks raised by over 40 JINR scientific projects.

   Unity through *unifying principles* comes from the existence of a *common mathematical background* of all these projects. The strongest requirement following from this common background is to get *reliable* solutions within a *rapidly evolving hardware – software environment*.

While the numerical and symbolic-numerical algorithms developed for the solution of the physical models rest on the *discretization* of their definition domains, the enforcement of the *reliability* of the numerical solutions asks for supplementary demands, apart from the classical *stability* requirement:

(i1) The discrete scheme is to *inherit all the algebraic properties* of the continuous mathematical model. Our straightforward experience has shown that this inheritance property is of crucial importance in the solution of *strongly non-linear* models.

(i2) The discrete scheme is to show *insensitiveness* with respect to the approximation of the infinite set of the real numbers by the finite set of the machine floating point numbers. More often than not, the implementation of this feature may ask for the use of *scale-adapted algorithms*. The specificity of the multi-scaling approach heavily depends on the nature of the problem described by the mathematical model.

(i3) The *computational complexity* of the derived numerical solutions is to be as low as possible. To get low complexity algorithms characterized by increased accuracy and quality, it is often necessary to develop *new principles of approximation*. The derivation of new methods based on such principles needs deep culture, talent, inspiration, innovative thinking.

(i4) The *rapidly changing hardware environment*, characterized with surprising accuracy by the famous *Moore's law* for more than half a century, raises enormous difficulties in the implementation of *long lasting* numerical software. The last hardware revolution, starting about a decade ago, provided a radical solution to the thermal wall threshold problem preventing further increase of the processor clock frequency: the *single-processor chips* were fully replaced by a variety of *multi-core processor* dies, *manycore processor* dies, GPU *accelerators* in conjunction with multi-core processors, etc. In connection with this radical change of the hardware, the renowned *Gartner Institute* (GI) – specialized in long term predictions in the information technology (IT), has estimated that the design and implementation of *effective software*, able to fully exploit the newly launched hardware architectures, is one of the seven global challenges to be faced by the IT during the next quarter of century. The huge variety of reports along this direction confirms, without exception, the veracity of the GI prediction.

These hardware driven exceptional circumstances promote the *parallel computing* as the most necessary future development in LIT-JINR, under various programming paradigms grasped by the LIT staff. In this respect, the heterogeneous computing cluster HybriLIT (http://hybrilit.jinr.ru/), under development in LIT-JINR as an indelible part of the MICC, is the main resource for high performance computing (HPC) in JINR.

4. State-of-the-art of the research field within the theme 1119.

The basic motivation of the need for the extension of the theme 1119 during the next three years, 2017-2019, comes from the existing JINR culture characterized by symbiotic synergy between different research groups from all the JINR Laboratories and research groups in LIT. The first ones ask for the solution of specific mathematical topics raised by and needed for the fulfillment of their research projects. The LIT groups contribute to the development of mathematical methods, design of algorithms, and their implementation into software directed to the solution of the defined mathematical topics. Instances of such collaboration are spread throughout the proposal.

Here there are two striking examples. First, a continuously upgraded complex of four program packages allows unique analysis of the widest possible classes of spectrometric data (including peaks of arbitrary shapes, 3D data). It enables reliable and unrivalled processing of Fourier diffractometer data. It is widely used in JINR (FLNP, DLNP), PNPI-Gatchina, MSU (Chemistry Faculty, INP-MSU), etc.

Second, this is the modeling of thermal regimes of work of devices generating multiply charged molecules for ion sources needed by various technical installations (collaboration with VBLHEP).

The viability of such an interaction scheme heavily depends on the good relationships of the group coordinators of the two sides and, last but not least, on the decisions of the JINR and JINR Laboratories management leaderships. From the perspective of all interested parties, these relationships can be characterized as excellent, with the highest chances of enhancement and fruitful continuation in the future.

One of the high advantages of this scheme is its *versatility*: the existing mathematical computing expertise in LIT frequently accommodates *several* concurrent needs coming from different JINR teams, hence overall harmonization of a broad range of scientific interests thus avoiding waste coming from unrelated developments of a same scientific expertise.

An inspection of the JINRLIB software library, maintained both in English and Russian provides many relevant illustrations to this statement. Thus, a same LIT author (A.G. Soloviev) has contributed to the creation of 13 different program packages used in three JINR Laboratories (FLNP, FLNR, VBLHEP). Among them, the repeatedly upgraded programs SAS (version 5.0.16, 23/02/2016) and FITTER (version 3.0.2, 04/04/2015) provide the online respectively offline information-computing environment for data processing and analysis of the most demanded IBR-2 detector, YUMO. The YUMO upgrade with position sensitive detectors will radically change the design and implementation of these packages.

Another, not less important, advantage is the possibility to *generalize* the derived specific solutions based on the already existing general expertise and the specific newly accumulated expertise in LIT during the current work. In this way, extensions of the limits of applicability of the mathematical methods are often obtained which prove useful in the solution of other, broader in scope, problems. The final output is the derivation of original methods and approaches without analogy in the scientific literature worldwide.

For example, successive developments combining together the Kantorovich method, the finite element method, and asymptotic methods resulted in a complex algorithm implemented in a series of symbolic-numerical and numerical packages for the investigation and simulation of few-body quantum systems with application to nuclear and atomic physics. The designed algorithms and created programs allow solving, with high accuracy, the boundary-valued problems for the multidimensional Schrödinger equation and for certain systems of second-order ordinary differential equations, to compute the related eigenvalues and eigenfunctions, to compute metastable and resonance states, to solve scattering problems and problems of tunneling through repulsive barriers. These program packages, which are quite useful for a wide range of users, were published in the CPC Program Library and in JINRLIB. Further continuations are devised.

The singular role of the heterogeneous HybriLIT cluster in this research effort deserves separate consideration. The HybriLIT cluster has had a short but rapid evolution driven by the supervision and the key decisions of the LIT management concerning its design and implementation:

(i) *Modular development* based on the most successful new hardware offers on the market. This decision mainly followed from the study of the trends in the buildup of the largest HPC facilities worldwide. Periodic scrutiny of the biannual TOP 500 lists has shown a gradual shift of these facilities from the very expensive traditional ones to cheaper modular heterogeneous HPC cluster structures.

(ii) *Minimization of the acquisition costs* by maximal use of the in-house engineering background.

(iii) *Gradual acquisition of new cluster modules*, aimed both at minimizing the strain on the JINR budget and at getting significant increase over time of the performance-to-cost ratio due to the rapid pace of the new developments on the hardware market.

The accommodation of a large variety of a variable number of hardware modules within the same cluster raised important compatibility and consistency problems, needing the development of an original conception and new approaches to the efficient system administration matching the requirements of *scalability* and *high fault tolerance*.

(iv) *Customization (optimization) of the parameters of the acquired hardware modules* asked for extensive benchmark studies which enabled tailoring the blade parameters at specifications different from those of the standard vendor offers and resulted in significant performance increase at the expense of a marginal cost increase.

(v) *Buildup from scratch of the information-computing environment* of HybriLIT was the toughest and most ambitious decision. Its solution, based on the available mature open source primary software, on the invaluable expertise gained during the development of primary software for the LIT-JINR grid sites, and on in-house research provides full support to all the user needs and requests formulated so far.

The coprocessor adapted installed software enables computations under the use of a variety of parallel programming techniques asked by the cluster users: CUDA – for computations on GPU compute nodes; MPI and OpenMPI – for computations on multicore and many-core components; OpenMP – for computation on the compute nodes with Intel Xeon Phi coprocessors; OpenCL – grasping both coprocessor kinds; combined techniques MPI+CUDA, MPI+OpenMP+CUDA, etc.

A set of on-line installed and continuously supported services help the users to optimize their work and to have quick access to useful information while working on the cluster. Instances:

• HybriLIT *web-page* (http://hybrilit.jinr.ru) contains detailed information about the resources provided to the users of the cluster. Particular emphasis is put on hardware that contains cluster specifications and software installed on the cluster. The registration procedure is very important. Therefore, its detailed description is provided at the web-page.

• Indico system (http://indico-hybrilit.jinr.ru) is used by the HybriLIT team for the organization of conferences, seminars and training sessions dedicated to parallel programming techniques. Free download of all the posted materials is possible.

Instances of services aimed at close interaction between users and the HybriLIT team:

• HybriLIT User Support is a project developed in the Project Management Service system (http://pm.jinr.ru). It allows answering user questions, uploading useful materials, publishing news, etc., it secures quick and efficient interaction between the cluster users and developers.

• GitLab (http://gitlab-hybrilit.jinr.ru) is a service aimed at mutual parallel development of applications. This is a control system version which allows following the changes in the code of projects. The HybriLIT team has developed several projects within this system, e.g., a project on writing documentation, the development of a monitoring system, etc.

Bilingual support in Russian and English of all web resources meets the needs of scientist and specialist users from different countries.

The nowadays HybriLIT can be characterized as a scalable top level HPC facility which adequately covers the needs of a wide variety of users from the JINR and JINR Member States within a threefold way: (a) design and implementation of parallel software for computing intensive research by means of several supported programming paradigms; (b) porting to the cluster open software packages, numerical libraries, and parallel codes which are already tuned for hybrid architectures; (c) development of new mathematical methods and parallel algorithms adapted to heterogeneous architectures.

5. Description of the proposed research.

The research done within theme 1119 can be conveniently divided into four kinds of activities. Besides the two theme leaders, the coordinators of these activities are reputed LIT scientists, energetic and with proved leadership qualities.

(1) Mathematical and computation methods for simulation of complex physical systems. Leaders: Gh. Adam, 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 computationally adapted to multicore and hybrid architectures. Leaders: Gh. Adam, P.V. Zrelov, O.I. Streltsova

(4) Methods, algorithms and software of computer algebra. Leader: V.P.Gerdt

There is an intimate twofold relationship between MICC and the theme 1119. First, the MICC traditionally provides computing power to the run of both sequential codes and classical parallel codes. Second, the information-computing environment of the HybriLIT cluster, the tutorials enabling the alleviation of the sharp HybriLIT learning curve are tailored by a young enthusiastic team from within theme 1119.

While the activity (3) deals particularly with the development and maintenance of the underlying HybriLIT information-computing environment, the use of the HybriLIT HPC resources may be accessed by any other activity within this theme or from other JINR themes and/or projects. Therefore, the reference to HybriLIT in this sense is legitimate and highly desirable.

The output of the LIT scientists' activity within theme 1119 is twofold. One consists in the *creation of computational tools*, the other one in the *publication* of scientific papers.

The computational tools encompass three broad destinations, each of which asking for specific abilities and expertise.

(a) The straight solution of tasks emerging from projects conducted in JINR or done with JINR participation refers, as a rule, to the information-computing support of various experiments.

Since the *online data collection* is tuned to the detector details, the created software support necessarily depends on the details of the detector. Every modification of the detector design obligatorily asks for new contributions from the personnel securing the software support. As a consequence, *the software support lasts over the whole lifetime of the experiment*. A detail of practical importance is that the software support provision is a *discontinuous* process which liberates in the meantime the energies of the software specialists for other endeavors.

This pattern of interaction is of general validity, irrespective of the fact that the above mentioned YUMO detector is involved or large scale experiments (like ATLAS and CMS at LHC or CBM at FAIR) are under scrutiny.

An interesting example concerns the development of software support for the microstrip GEM chambers of the BM@N experiment of the NICA project and the cathode strip chambers (CSC) of the CMS setup. The expertise got by the LIT group led by V.V. Palichik in the development of software for the CSC trek-segment builder and spatial resolution greatly helped in solving the BM@N tasks. At the same time, the work done on the upgrade of the CSC software under their substantial modification together with the whole CMS setup during the LHC first long shutdown between RUN1 and RUN2 resulted in a substantially modified approach with significant improvement of the muon reconstruction. The long certification procedure of this software upgrade approaches an end, such that it will soon become part of the fundamental CMS data processing software. Since the future high luminosity LHC (HL-LHC) will ask for further substantial modifications of the CMS setup, the CSC segment included, further research on the future upgrades of this software support will be demanded.

(b) The software developed for offline data processing and analysis is under two strong pressure factors imposing new developments.

The first factor, already mentioned at the end of the section 3., comes from the multi-core, manycore, and GPU compute elements asking for *parallelization* as a means to increase the efficiency of the computations.

The second factor comes from the changes, by many orders of magnitude, of the parameters at which the new experiments are done. Heuristic assumptions holding at lower energies, which entered software designed decades ago and becoming a common place by repetition, were shown in LIT scrutiny to be unreliable under the parameters of the new high energy physics experiments. As a result, bugs in the widely used Higgins Monte Carlo generator were removed. Vital modules of the Geant4 package were included in the new 2010-2015 Geant4 releases. The present status of Geant4 was defined with the important co-authorship of V.V. Uzhinsky (LIT). Further LIT contributions to the development of Geant4 and Monte Carlo simulations will follow.

(c) Finally, we have to add to this incomplete enumeration the solution of *difficult mathematical problems* resisting so far to the previous attempts to get guaranteed output under controlled accuracy.

The quality of such results, obtained within select international collaborations, is best illustrated by the *four JINR Prizes* awarded during 2014-2016 (for the previous calendar year) to teams including LIT staff, in tough competitions which involved all the JINR Laboratories:

- Gh. Adam and S. Adam (LIT) [plus four other authors] First prize (2013) for the theory of spin fluctuations and high temperature superconductivity in cuprates;

- I. Amirkhanov (LIT) [plus seven other authors] Second prize (2013) for the implementation of the operation mode of the AIC-144 cyclotron (Poland) for the proton therapy of eye melanoma;

- O. Chuluunbaatar, A. Gusev, V. Gerdt, V. Rostovtsev (LIT) [plus six other authors] Second prize (2015) for the problem-oriented complex of programs for solving boundary value problems in the dynamics of few-body quantum systems;

- I.L. Bogolubsky (LIT) [plus five other authors] Second prize (2015) for the Lattice studies of Landau gauge gluon and ghost propagators in Quantum Chromodynamics.

Yu. Kalinovsky and O. Grigorian (LIT) [plus other seven authors] have received two 2014 awards for outstanding results in the investigation of the QCD-phase diagram and means of diagnosing the onset of the deconfinement from hadron structure and their reactions: *Small Prize of the International Academic Publishing Company Nauka/Interperiodika* and *Best Publication in PEPAN Letters*.

Two LIT young laureates of the Moscow region Governor's Prize for science and innovation achievements of young scientists are A. Ayriyan (2014) and O. Derenovskaya (2015).

The Dubna University conferred the title of Honorary Professor to our venerable colleague G.A. Ososkov (LIT) in 2014.

A summary of the *scientific publications* coming from activity within theme 1119 of the LIT personnel during the last three years points to 339 co-authorships within the CMS project and other 284 articles published in refereed journals; 66 publications in periodical volumes; 33 invited lectures and 91 oral presentations at international conferences; 58 electronic publications. A list of selected papers of the staff of the LIT Department of Computational Physics (NOVF), which provides the bulk of these publications, is given in the Appendix.

(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. 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 cluster.

- The buildup of 3D computing models of the dipolar and quadrupole superconducting magnets entering the NICA (JINR) and SIS100 (GSI) facilities, the computation of the distributions of the magnetic fields within the working regions of the magnets are intrinsic parts of the certification process of the newly constructed magnet modules in VBLHEP.

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

- Of the outmost importance is the development of effective QCD-motivated models for describing properties of nuclear matter at NICA energies, computer simulations of the behavior of the nuclear matter near the critical points at the QCD phase diagram.

- Studies will be done concerning the applicability of fractal analysis methods for processing and systematization of the results of molecular dynamics simulations of the interaction of nanocluster beams with thin metal films.

- Development of models for dimesoatom formation in processes of multiple particle production at high energies including coherent production of long lived *nP* states of $\pi^+\pi^-$ atoms.

- 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.

- Numerical analysis of properties of Bose condensates with nonlocal interaction potentials.

- Development of methods for numerical investigations of structures and bifurcation regimes in non-linear models of condensed matter physics.

- Numerical solution of boundary value problems for the nonlinear Boltzmann-Poisson equations describing the interaction of protein macromolecules with the solvent.

- Study within the microscopic optical potential model of the mechanisms of various nuclear processes, including pre-equilibrium processes in the reactions (p, alpha) ^{59}Co at energies from 65 to 160 MeV, disintegration processes in the interactions of boron isotopes and other exotic nuclei with protons and nuclei, the inelastic interaction of pions with nuclei at (33)-resonance energies.

- Study of astrophysics models aimed at accommodating the results of new experiments.

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

- The primary data processing at the YuMO spectrometer at IBR-2 was developed and is maintained through the SAS package developed in LIT. This will ask for substantial future reworking and development determined by the addition of the position sensitive detectors.

- The future development of superconducting multipurpose isochronous cyclotrons will need development of mathematical modeling of beam dynamics and implementation of fast packages enabling numerical experiments asked by the design of such facilities.

• Generalization of previous methods to scale-adapted algorithms of reduced computational complexity.

- Generalization of the three-fixed-point basic element method (BEM) of high polynomial degree for function interpolation and data smoothing to multi-dimensional problems by means of parametric functional representations.

- Development of BEM-based algorithms and software for predictive analysis and forecasting parameters of the IBR-2M reactor (fluctuations of the pulse energies, the flow of liquid sodium through the core, etc.)

- Bayesian automatic adaptive quadrature, with scale dependent quadrature sums, resulting in output insensitiveness to the finite significand length.

(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.

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

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

- Development and support of Glauber Monte Carlo program as well as adaptation of Geant4 FTF model for NICA/MPD and CBM experiments.

- Development of neural network applications for performing nonlinear principal components analysis and for image clustering using neural networks with deep learning.

- Processing and analysis of data collected at the NUCLEON and COMBAS experiments.

- Development of methods for automatic analysis of gamma spectra and software for automatic calibration of low statistics gamma spectra.

- Development and adaptation of methods of data analysis to the conditions of small statistics and incomplete observations (estimated half-lives).

- Development of methods based on the generalized separate form factor model, for the analysis of experimental data of small angle neutron and synchrotron radiation on vesicular polydisperse nanosystems.

- Development of methods and algorithms for massive calculations of electrostatic potentials of molecules of DNA, RNA and protein factors, as well as maps of the surface of these biopolymers. Calculation at the HybriLIT cluster of electrostatic potentials and surface maps of biopolymer molecules enabling solutions of biomolecular recognition problems

- Generation of random rough surfaces to simulate features of diffraction patterns at neutron reflection from the surface of nanostructured objects.

• Software-information support of JINR projects

- Development of the dataflow control system in the experiments of the NICA project

- Software development for the GEM tracking detector entering the detector complex of the BM@N experiment (development of algorithms and software for the simulation and data handling with the microstrip GEM chamber; development and software implementation of algorithms for the reconstruction of the spatial coordinates of the points of interaction of charged particles with the registering elements of the GEM detector; software implementation of GEM detector models for the foreseen configurations planned in the upcoming sessions of the BM@N experiment).

- BM@N: Event reconstruction with 2016-2019 Nuclotron data; development of algorithms and programs for the particle trajectories recognition in the MPD setup

- Development of VMRIA package for the automatic analysis of large spectra collected in experiments carried out on HRFD at IBR-2

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

- Software support of ATLAS experiment (maintenance of the TDAQ components previously developed in LIT; new developments: network monitoring dashboard, online TDAQ Log Manager)

- Software support of CMS experiment: improvement of the Cathode Strip Chamber (CSC) local reconstruction for high luminosity LHC data

- Software support of CBM experiment: development of various algorithms (including vectorization and parallelization) on recognition and track reconstruction for various detectors of the CBM setup (MVD, STS, MUCH, RICH); development of selection criteria and algorithms for recognition and reconstruction of rare decays; development, optimization and testing of algorithms for the processing system FLES; development of a complex of database systems for the CBM experiment.

(3) Numerical methods, algorithms and software computationally adapted to multicore and hybrid architectures

This activity is directed along two main lines. The first consists in the development of numerical methods, algorithms, and program packages optimized for manycore and hybrid architectures with the aim at providing efficient numerical solutions to large scale problems of the theoretical and experimental physics of the highest interest in JINR. The second concerns the development and maintenance of the information-computing environment of the heterogeneous cluster HybriLIT.

• This part of the research done inside the theme 1119 emphasizes the special role of our team in the grasp of the possibilities offered by the heterogeneous computing, in making it available to the scientific community of the JINR and JINR Member States, in understanding and tailoring the future development of the HybriLIT cluster, such as to maximize its role in the whole HPC based JINR research.

• To enable the solution of practical engineering-physical problems in JINR Laboratories and JINR Member States (e. g., the ELI project), the computing environment is to be created at HybriLIT for the testing, validation, and adaptation of modules of large packages (COMSOL Multiphysics, CATIA-GDML geometry builder, EPOCH). The acquisition of a top graphical station and its customization is a must.

• The development of new algorithms, either by creating them from scratch or parallelizing existing ones, concern:

- Development of parallel algorithms for numerical investigation of multi-dimensional models of evolutionary equations modeling physical processes in different materials under irradiation with heavy ions and pulsed beams, Josephson barriers in high-temperature superconductors.

- Development of efficient algorithms for the solution of molecular dynamics equations on hybrid computing infrastructures.

- Development of methods and MPI packages for the computation of multiple integrals for the study of processes of ionization and photoionization of the He atom, polyatomic molecules, and their ions.

- Development and implementation of new parallel algorithms into the MCTDHB software complex and their adaptation to the new KNL architecture of the Intel Xeon Phi.

- Development and maintenance of a parallel version of the Fitter program for offline processing and analysis of data collected at the YUMO spectrometer at IBR-2.

- HybriLIT devoted optimization of selected programs of the ROOT software package, in particular, improvement, using technologies of parallel computing, of the software implementation of the filling algorithms of the special data structure Tree.

- Elaboration of effective algorithms for solving elliptic nonlinear hp-adapted finite-element systems of equations and their program implementation on heterogeneous architectures.

- Adaptation of the multibranch solutions of the Tolman-Oppenheimer-Volkov system of equations to hybrid computing architectures.

- Creation of parallel versions of sequential programs of JINRLIB library of the highest interest for the JINR computing community.

(4) Methods, algorithms and software of computer algebra

This activity foresees the development of methods of computer algebra for numerical solution of differential equations and for simulation of quantum information processes; creation of algorithms and program packages for symbolic-numerical solution of problems arising in experimental and theoretical studies, using the latest computational hardware resources, mostly the heterogeneous cluster HybriLIT.

• Advances in computer algebra methods for modeling quantum systems and quantum information processes

- Development and investigation of a new model of quantum networks with memory function

- Description of separable and entangled X-states of two-qubit systems.

- Calculation of relativistic corrections in the description of dynamics of spin particles in strong laser fields (for project ELI-NP, Romania).

- Derivation, based on unitary representations of finite groups, of combinatorial algorithms and algorithms of statistical modelling of quantum systems.

• Development of computer algebra methods with application to symbolic-numerical solution of differential equations

- Creation of a symbolic-numerical package implementing the finite element method with associated Hermite polynomials for the solution of equations describing the dynamics of low-dimensional few-particle quantum systems. Adaptation of the developed algorithms and codes to hybrid architectures

- Algorithmic construction of difference schemes inheriting the basic algebraic properties of the initial differential equations

• Development of algorithms requested by special topics

- Computation of the renormalization constants for the two-loop propagator of quark mixtures.

- Developing recursive methods for calculating Feynman integrals and their application for calculating one- and two-loop radiative corrections.

- Development of different methods of derivation of functional equations for Feynman integrals and their use for analytic continuation of Feynman integrals as function kinematic arguments.

- Design and implementation of algorithms for computation of rotational-vibrational basis functions in the space of parameters describing quadrupole and octupole deformation of spherical nuclei

• Development and implementation of special computational tools

- Implementation in Lucid Common Lisp of the computer algebra systems Reduce, Axiom, Maxima with convenient user interfaces toward libraries of numerical programs

6. Personnel (**limited to 1 page**).

As compared to the previous theme 1119 proposal for 2014-2016, a significant step forward of the present theme extension proposal is the explicit nomination of the main co-workers (group leaders) from other JINR Laboratories, the role of whom is seminal in the formulation of the specific problem to be solved as well as in the interpretation of the obtained results. The strong interaction with the MICC team is emphasized at activity number 3.

	Activity or experiment Laboratory or other Division of JINR	**Leaders** Main researchers
1.	**Mathematical and computation methods for simulation of complex physical systems**	**Gh. Adam** **I.V. Puzynin**
	LIT	S. Adam, P.G. Akishin, I.V. Amirkhanov, E.A. Ayrjan, A.S. Ayriyan, I.V. Barashenkov, M.V. Bashashin, I.L. Bogolubsky, N.D. Dikusar, H. Grigorian, Yu.L. Kalinovsky, T.V. Karamysheva, D.S. Kulyabov, K.V. Lukyanov, D.V.A. Luu, A. Machavariani, N.V. Makhaldiani, T.I. Mikhailova, G.J. Musulmanbekov, E.G. Nikonov, G.A. Ososkov, D.I. Podgainy, R.V. Polyakova, T.P. Puzynina, V.N. Robuk, B. Saha, N.Yu. Shirikova, A.G. Soloviev, T.M. Solovieva, Yu.B. Starchenko, O.I. Streltsova, A.V. Volokhova, O.O. Voskresenskaya, A. Wojczechowski, R.M. Yamaleev, E.P. Yukalova, E.V. Zemlyanaya
	VBLHEP	E.E. Donets, S. Gevorkyan, M.N. Kapishin, A.O. Kechechyan, H.G. Khodzhibagiyan, V.A. Nikitin, O.V. Rogachevski, W. Scheinast
	BLTP	A.V. Friesen, M. Hnatic, E.-M. Ilgenfritz, R.V. Jolos, V.K. Lukyanov, V.D. Toneev, S.N. Vinitsky, V.V.Voronov, V.I. Yukalov
	FLNR	A.G. Artukh, Yu.K. Kochnev, S.M. Lukyanov, Yu.E. Penionzhkevich, R.A. Rymzhanov, Yu.M. Sereda, V.A. Skuratov
	FLNP	A.V. Belushkin, N. Korepenova, S.A. Manoshin, A.I. Kuklin, A.I. Ivankov, Yu.N. Pepelyshev, D.V. Soloviev
	DLNP	L.G. Afanasiev, G.A. Karamysheva, I.N. Kiyan
2.	**Software complexes and mathematical methods for processing and analysis of experimental data**	**P.V. Zrelov** **V.V. Ivanov**
	LIT	T.O. Ablyazimov, E.P. Akishina, V.P. Akishina, E.I. Aleksandrov, I.N. Aleksandrov, D.A. Baranov, S. Belogurov, O.Yu. Derenovskaya, A.A. Kazakov, A.I. Kazymov, P.I. Kisel, B.F. Kostenko, G.E. Kozlov, L.Yu.

	Kruglova, I.N. Kukhtina, A.A. Lebedev, T.I. Mikhailova, M.A. Mineev, G.A. Ososkov, E.V. Ovcharenko, V.V. Palichik, V.S. Rikhvitsky, V.N. Shigaev, L.A. Siurakshina, S.K.Slepnyov, A.N. Sosnin, V.A. Stepanenko, V.V. Uzhinsky, N.N. Voitishin, A.V. Yakovlev, E.V. Zemlyanaya, E.I. Zhabitskaya, V.B. Zlokazov
VBLHEP	A.S. Galoyan, K.V. Gertsenberger, M.N. Kapishin, V.P. Ladygin, V. Lenivenko, A.I. Malakhov, S.A. Movchan, O.V. Rogachevsky, M.G. Sapozhnikov, N.D. Topilin
FLNR	A.G. Artukh, A.S. Fomichev, Yu.E. Penionzhkevich, Yu.M. Sereda, Yu.G. Sobolev, Yu.S. Tsyganov, V.K. Utenkov
FLNP	A.M. Balagurov, I.A. Bobrikov, M.A. Kiselev, D.P. Kozlenko, M.V. Frontasyeva
DLNP	G.D. Alekseev, I.V. Bednyakov, V.A. Bednyakov, A.G. Olshevsky, D.B. Pontecorvo, A.S. Zhemchugov
UC	S. Pakuliak

3. Numerical methods, algorithms and software computationally adapted to multicore and hybrid architectures — **Gh. Adam, P.V. Zrelov, O.I. Streltsova**

LIT	E.I. Aleksandrov, I.V. Amirkhanov, A.S. Ayriyan, E.A. Ayrjan, M.V. Bashashin, D.V. Belyakov, A.M. Chervyakov, O. Chuluunbaatar, M. Kirakosyan, M.A. Matveev, E.V. Ovcharenko, D.V. Podgainy, T.P. Puzynina, A.A. Sapozhnikov, T.F. Sapozhnikova, N.R. Sarkar, I. Sarkhadov, S.I. Serdyukova, Z.A. Sharipov, A.G. Soloviev, T.M. Solovieva, Sh. Torosyan, Z.K. Tukhliev, A.V. Volokhova, O.I. Yuldashev, M.B. Yuldasheva, E.V. Zemlyanaya, E.I. Zhabitskaya, M.I. Zuev
LIT-MICC	V.V. Korenkov, V.V. Mitsyn, T.A. Strizh
FLNR	P.Yu. Apel, V.A. Skuratov
BLTP	D.B. Blashke, A.A. Bulychev, Yu.V. Popov, Yu.M. Shukrinov

4. Methods, algorithms and software of computer algebra — **V.P. Gerdt**

LIT	V. Abgaryan, A.A. Bogolubskaya, O. Chuluunbaatar, S.A. Evlakhov, A.A. Gusev, A.M. Khvedelidze, V.V. Kornyak, A.M. Raportirenko, I.A. Rogozhin, O.V. Tarasov, A.G. Torosyan, D.A. Yanovich, E.P. Yukalova
BLTP	A.V. Czhizhov, P. Fiziev, A.I. Titov, S.I. Vinitsky, V.I. Yukalov
FLNR	B.N. Gikal

7. Budget estimation (limited to 1 page).

The core of the LIT investments is related to the MICC project and theme 1118. The theme 1119 secures a convenient superstructure with expenses summarized in the following table.

k$

	Chapters of the JINR budget	Previsions 2017-2019	Yearly distribution		
			2017	2018	2019
1	2	3	4	5	6
1	Salaries	4073.8	1279.6	1356.4	1437.8
2	Unified social tax	1230.2	386.4	409.6	434.2
3	Social national fund	264.8	83.2	88.2	93.4
4	International cooperation expenses	179.1	59.7	59.7	59.7
	a) business trips to Member States	60.3	20.1	20.1	20.1
	b) business trips to Non-Member States	53.4	17.8	17.8	17.8
	c) business trips in Russia	20.4	6.8	6.8	6.8
	d) arrivals to JINR	25.5	8.5	8.5	8.5
	e) Conferences, protocol expenses	19.5	6.5	6.5	6.5
5	Materials	36.0	10.0	12.0	14.0
6	Equipment	282.7	92.7	94.0	96.0
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	**6066.6**	**1911.6**	**2019.9**	**2135.1**

8. Concise SWOT analysis. Each of the items 3–7 should clearly indicate the major strengths and weaknesses of the project/theme for each specific issue.

• ***Strong sides of theme* 1119**

- With 24 DSc (3 defenses in 2010-2013) and 47PhD (11 defenses in 2010-2016), the theme 1119 staff represents a force of very highly qualified scientific level.

- The interest to get PhD or DSc titles is high. The existing LIT Dissertation Council (DC) D720 001.004 (with 11 LIT members out of a total of 20) has defined and maintains the quality target at the highest possible level (with 100% validation of its previous proposals). It is the undisputable merit of the DC members, primarily of its chair, V.V. Ivanov, that the acquirement of a scientific title at this DC is a real school of mastering the competences requested for skillful scientific thinking and for expressing the scientific thoughts in clear professional language.

- The elder staff possesses highest class scientific knowledge acquired by hard work.

- The honest presentation of the opinions is a plus.

- A variety of means is supported for the increase of the level education of all the staff, especially young (training courses, tutorials, dedicated conferences and workshops for young scientists and specialists, group and individual consultations, scientific seminars, etc.)

- Of special importance for the theme 1119 community are the periodic LIT *conferences and workshops*.

The International MMCP Conferences (Mathematical Modeling and Computational Physics), organized once every two years, have got a solid international reputation, with the publication of the MMCP Conference Proceedings under a severe refereeing process (Editors Gh. Adam, J. Buša, M. Hnatič), MMCP 2011 – at Springer (vol. LNCS 7125) in 2012 (a real bestseller according to the Springer marketing reports) and MMCP 2015 – at EPJ Web of Conferences (vol. 108, 2016).

The next MMCP 2017 Conference, which will be organized during July 3-7, 2017 at LIT-JINR, is planned to bring some interesting innovations: a significant expansion of the section on mathematical modeling in biology; organization of two parallel schools for young people on the mathematical modeling on NICA physics and on the broader range of the high energy physics (with the aim to contribute to the completion of the gap concerning the involvement of skillful specialists in the numerical investigation of NICA problems). The already traditional tutorial on parallel and heterogeneous computing will contribute to the shortage of lack of skills in the work at the HybriLIT cluster.

• ***Weak sides of theme*** **1119**

- The *professional mobility* of the mature scientists is, as a rule, reduced as compared to the outer expectations.

The major factor to be blamed is the too rapid pace of expansion of the hardware-software environment. The occurrence of several major changes of the computing paradigms during the last three decades was hard to digest.

The senior scientists did not migrate to the basic today object-oriented programming paradigm. This hinders their work with the latest packages and creates difficulties in the supervision of the work of the young scientists.

This is, however, only one facet of the medal.

- The depth of the *initial mathematical training* of the young scientists is relatively low. Often, the present day graduates miss solid knowledge of many chapters of applied mathematics and numerical analysis, together with a basic grasp of the physical phenomena and models. This initial drawback can be gradually overcome through hard work on specific problems. All the means discussed above at the "Strong side" bring their contribution to the stimulation of this process.

There is, however, an empirical fact which deserves consideration.

- The high *rate of failure* of the attempts of young people to develop a successful carrier in computer mathematics and computational physics. Only the strong pass the endurance test required by the grasp of the mastership in this field.

Often, this difficulty is associated with the salary gap: people working in IT business get significantly higher salaries under an intellectual effort which fits their education level.

However, the remainder of this churning process is hard characters who like their work and want to become more and more skillful in its exercise.

Collaboration

Country or International Organization	City	Institute or Laboratory
Armenia	Yerevan	YSU
		IIAP NAS RA
		RAU
		Foundation ANSL
Australia	Sydney	Univ.
Azerbaijan	Baku	IP ANAS
Belarus	Minsk	IM NASB
	Gomel	GSTU
Belgium	Brussels	ULB

	Liege	ULg
Brazil	Sao Carlos, SP	IFSC USP
Bulgaria	Sofia	IMI BAS
		INRNE BAS
		SU
	Plovdiv	PU
Canada	Edmonton	U of A
	Toronto	IBM Lab
CERN	Geneva	CERN
China	Hangzhou	ZJU
Czech Republic	Prague	CTU
France	Nancy	UL
	Nantes	SUBATECH
Georgia	Tbilisi	UG
		TSU
		GTU
Germany	Bonn	UniBonn
	Darmstadt	GSI
	Dresden	IFW
	Frankfurt/Main	Univ.
	Giessen	JLU
	Hamburg	Univ.
	Heidelberg	Univ.
	Jena	Univ.
	Wuppertal	UW
	Freiberg	TUBAF
	Kassel	Uni Kassel
	Marburg	Univ.
	Munich	LMU
Greece	Thessaloniki	AUTH
India	Calcutta	JU
Italy	Turin	INFN
	Bari	UniBa
Japan	Osaka	Kansai Univ.
Kazakhstan	Almaty	INP
Moldova	Chisinau	IAP ASM
Mongolia	Ulaanbaatar	NUM
		MUST
Poland	Krakow	NINP PAS
	Lublin	UMCS
	Otwock-Swierk	NCBJ

	Warsaw	WUT
	Wroclaw	UW
Portugal	Lisbon	UL
Romania	Bucharest	IFA
		IFIN-HH
		ISS
		UB
	Cluj-Napoca	INCDTIM
Russia	Moscow	IPMech RAS
		ITEP
		NNRU "MEPhI"
		KIAM RAS
		MSU
		PFUR
		SINP MSU
		RCC MSU
		GPI RAS
		NRC KI
		ICS RAS
	Dubna	Dubna Univ.
	Gatchina	PNPI
	Protvino	IHEP
	Puschino	IMPB RAS
		ITEB RAS
		IPR RAS
	Saratov	SSU
	St. Petersburg	FIP
		NIIEFA
	Tomsk	TSU
Slovakia	Kosice	IEP SAS
		TUKE
		PJSU
	Presov	PU
	Banska Bistrica	UMB
South Africa	Cape Town	UCT
	Pretoria	UP
	Stellenbosch	SU
Switzerland	Zurich	ETH
Taiwan	Taipei	AS
Tajikistan	Dushanbe	TNU
		PHTI ASRT

	Khujent	KSU
USA	Argonne, IL	ANL
	Stanford, CA	SU
Vietnam	Hanoi	VNU