Overview of the Progress in the LIT Theme 1119 during 2019-2020

(Extended Annotation)

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• **Title of the theme:** 05-6-1119-2014/2023, "*Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data"*
Priority: 1
Leaders: Gheorghe Adam, Petr V. Zrelov
Deputies: Ján Buša, Ochbadrakh Chuluunbaatar
Participating JINR Laboratories: LIT, VBLHEP, BLTP, FLNR, FLNP, DLNP, LRB
Participating Countries and International Organizations:
Armenia, Australia, Azerbaijan, Belarus, Belgium, Brazil, Bulgaria, Canada, CERN, China, Czech Republic, France, Georgia, Germany, Italy, Japan, Kazakhstan, Moldova, Mongolia, Poland, Portugal, Romania, Russia, Slovakia, South Africa, Switzerland, Tajikistan, USA, Vietnam.

• *Characteristics which single out the theme 1119 in the JINR Topical Plan of Research*

The *overwhelming feature* of the research done within the theme 1119 during the present Seven Year Plan for JINR Development is the *work done in close cooperation* with research groups from all JINR Laboratories and Member State institutions. This assumes the use of the existent expertise of the LIT staff for the solution of challenging problems, in over 40 JINR projects, which ask for advanced research in computational mathematics and physics, directed to the creation of new mathematical methods and algorithms for the numerical or symbolic-numerical solution of topics arising in experimental and theoretical physics studies, their implementation into software packages. 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 IBR-2 neutron based investigations.

The large scale computing is done on the Multifunctional Information and Computing Complex (MICC), primarily on the HybriLIT heterogeneous computing platform (which involves the training and test cluster HybriLIT and the "Govorun" supercomputer) and on the emerging Big Data distributed infrastructure.

The scientific environment in LIT encourages a *deep and extensive professional expertise* along four critical directions: thinking as computer scientist with several computing paradigms; expert knowledge of the mathematical problems backing the topic of the collaboration; in depth grasp of the numerical analysis topics enabling the achievement of both reduced complexity and full reliability of the developed algorithms; deep knowledge of the physics side of the problem at hand as a precondition of performing significant mathematical modeling undertakings. The leadership of the theme 1119 has put great efforts to back the agreed cooperation in the large scale projects by working groups the complementarity of the knowledge of the members of which secure the coverage of all the four mentioned critical directions. Inside the JINR ecosystem we heavily rely on the decisions of the JINR Directorate and the Program Advisory Committees.

The Covid-19 pandemic forced us to change substantially, for a while, the form (place and style) of the scientific work. While over 90 percent of the LIT staff involved in the solution of the theme 1119 tasks were passed at work at the distance, the pace of the scientific effort remained at a high level. New forms of communication, like the scientific webinars, came to the first plan. Striking examples are the webinar held on 21-st April 2020 by Prof. V. V. Korenkov, leader of the Big Data analytics within this theme and the 5-th Collaboration Meeting of the BM@N Experiments at the NICA Facility with significant participation from theme 1119 (seven reports).

• ***Five directions of achievements got within the theme 1119***

The analysis of the progress got by the research done within the theme 1119 will cover five directions of the obtained achievements, each of which bringing specific contributions to:
(1) *The advancement of the JINR research as a whole;*
(2) *Advances to the solution of tasks within special research projects;*
(3) *Creation of specialized computing tools at the disposal of JINR scientific teams;*
(4) *Contributions to the JINR excellence in the worldwide research landscape;*
(5) *Grow up of the scientific competence in using the JINR computer tools.*

(1) *Contributions to the advancement of the JINR research as a whole*

The staff involved in the theme 1119 brings its specific contribution along this direction in close cooperation with the staff engaged in the LIT theme 1118 (on JINR computing infrastructure) and its MICC (Multifunctional Information and Computing Complex) project. Our activity is focused along two main directions of software developments. The first concerns the heterogeneous computing platform which involves the HybriLIT cluster (now learning and testing polygon) and the "Govorun" supercomputer. The second concerns the emerging field of the Big Data Analytics.

We solve specific tasks concerning the creation of ***basic software enhancing the availability and capabilities of the high performance computing* (HPC) *facilities, primarily the "Govorun" supercomputer, cornerstone of the JINR scientific computing.*** Through the three main components of the "Govorun" heterogeneous structure, applications are developed for HPC with distributed memory (in the CPU Intel Gold component), HPC with shared memory (in the CPU Intel Phi component), HPC and, especially, neural network methods based on machine learning and deep learning (in the GPU NVIDIA accelerator component). Computer programs using MPI, OpenMP, CUDA, OpenCL parallelization techniques are currently developed on the "Govorun". Therefrom, the essential task resolved within theme 1119 concerns the *design, development, implementation, and maintenance on "Govorun" of a user friendly environment*. An ecosystem was created and is extended for the solution of ML/DL (Machine Learning / Deep Learning) tasks (see https://jhub2.jinr.ru for the computation component and https://jhub.jinr.ru for the development component). An HPC environment was also created for the development of parallel algorithms and applications.

(2) *Advances to the solution of tasks within special research projects*

This concerns the bulk of the activity done in cooperation for the solution of computing tasks raised by different research projects.

- Intense current research involves three-dimensional computer simulation of magnetic systems in the framework of NICA (JINR) and FAIR (GSI) projects for the validation of the magnetic field uniformity in the working areas of the new physical magnets; case studies for the design of the magnet prototype of the future SPD setup at NICA; modeling the CBM 3D shielding dipole magnet at GSI to accommodate the modifications proposed in the conception of the CBM experiment in two possible options (MUCH and RICH); design of new medical purpose cyclotrons.

- 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, SPD and BM@N experiments at the NICA accelerator and within the JINR neutrino program.

- The design, development, implementation, and maintenance of object oriented scientific library modules solve scientific problems in support of experimental facilities. Instances:

• Upgrade of the GEANT4 package with new modules (FTF modeling of nucleon coalescence, FTF and QGS modeling of hard QCD processes), Monte Carlo HIJING generator developments.

• Software support of large scale experiments {at LHC: CMS (**CMSSW** – CMS SoftWare package – modules CSCSegAlgoRU, CSCHitFromStripOnly, CSCRecHitDBuilder) and ATLAS (EI3 – EventIndex for LHC Run 3, TDAQ – Controls and Configuration Software, monitoring improvement, NETIS for network traffic monitoring, Condition DB Athena implemented in December 2019)}; {at

FAIR: CBM (**CBMROOT** – first version of Geometry Database), PANDA (UrQMD + SMM modeling)}; {at JINR-NICA: BM@N [**BMNROOT** – First stage of development of Event Tag Geometry Database module; specific modules for each of the four detectors entering the setup: ***DCH*** (***Drift Chamber***) ***detector*** (ROOT geometry, BmnDchTrackFinder, BmnDchHitProducer, BmnDchHitProducerData); ***GEM*** (***Gas Electron Multiplier***) ***detector, Silicon detector*** and ***CSC*** (***Cathode Strip Chamber***) ***detector*** (ROOT geometries, Hit-reconstructions); ***STS*** (***Silicon Tracking System***) ***detector*** (ROOT geometry).]}

- For each detector of the BM@N setup, specific computing intensive Monte Carlo simulations and realistic simulations have been done.

- Design and extensive testing of the new Monte-Carlo Generator of Heavy Ion Collisions **DCM-SMM** for simulation and analysis of the collisions of particles and nuclei in the new experimental setups BM@N and MPD on the accelerator complex NICA.

- Development and maintenance of software for high resolution detectors in IBR-2 experiments (YuMO, HRFD) for in-house projects in condensed matter physics investigations.

- Development and maintenance of software for the BAIKAL GVD experimental facility of the JINR neutrino program.

- Software development for the analysis of data acquired at ACULINA-2 facility.

- Further development of statistical methods for the analysis of experimental data under small statistics and incomplete observation of the studied processes, in direct connection with the creation of new superheavy nuclei.

- Development of highly performant analysis frameworks based on deep learning neural network algorithms: (a) successful implementation of a Data Management System for the study of air-pollution within the UNECE ICP Vegetation project, in collaboration with FLNP; (b) deep Siamese neural network implementation with 99% recognition accuracy in a multifunctional platform for plant disease detection; (c) use of deep neural tracking to face the tracking crisis challenge in detector environments, such as HL-LHC Run-4 and MPD-NICA.

(3) ***Creation of specialized computing tools at the disposal of JINR scientific teams***

- Implementation in the JINRLIB of the most important developed HPC parallel packages:

• **EORP 2020** – software package for computing closed equilibrium orbits in magnetic fields of an isochronous cyclotron http://wwwinfo.jinr.ru/programs/jinrlib/eorp/index.html (in Russian) http://wwwinfo.jinr.ru/programs/jinrlib/eorp/indexe.html (in English)

• **Split** (2020) – parallel MPI implementation of numerical solution of three diagonal systems of algebraic equations http://wwwinfo.jinr.ru/programs/jinrlib/split/index.html (in Russian) http://wwwinfo.jinr.ru/programs/jinrlib/split/indexe.html (in English)

• PROGRAM LIBRARY JINRLIB **SAS** - package for small-angle neutron scattering data treatment, (Upgrade SAS 5.2.0 December 2019 https://gitlab-hybrilit.jinr.ru/yumo-updates/sas) https://wwwinfo.jinr.ru/programs/jinrlib/sas/indexe.html

• PROGRAM LIBRARY JINRLIB **DFM-POTM** - parallel calculation of the double folding nucleus-nucleus potential (Upgrade 04.09.2019) https://wwwinfo.jinr.ru/programs/jinrlib/dfm-potm/indexe.html

- Package publications in CPC Program Library:

• Comp. Phys. Comm., CPC Program Title: **PBCAVE**; Published: 28 Nov 2019; Version 1; Program Files doi: http://dx.doi.org/10.17632/d77n7yskmc.1

• "The MAPLE package **TDDS** for computing Thomas decompositions of systems of nonlinear PDEs", Mendeley Data, v1 http://dx.doi.org/10.17632/twk8zjxgbz.1 . Published under GNU LGPL license, *this code has become part of the annual releases of the* MAPLE OS *in* 2019 *and* 2020.

- Software implemented in the operation systems developed for the online and offline data processing of various detector setups, such as YuMO, HRFD, ACULINA-2, COMBAS, TAIGA, etc.

(4) *Contributions to the JINR excellence in the worldwide research landscape*

An overall statistics of the scientific output of the theme 1119 staff for the period under consideration points to the publication of 206 articles in refereed journals (among them, 35 in highly ranked journals such as Nature Physics, Phys. Rev. Lett, Phys. Rev. A, B, C, Phys. Rev. Res., Comp. Phys. Comm., Chem. Phys. Lett., Eur. Phys. J. A, D, Physica D, J. Phys. G, ZhVM & MF (Rus.), Mat. Mod. (Rus.), TMF (Rus.), ZhETF and Pis'ma v ZhETF (Rus.)); five monographs; five papers in scientific collections; 18 electronic publications; four JINR preprints; one textbook on MPI parallel programming. An additional number of 150 papers were published in the frame of the CMS collaboration.

The subject matters of these publications cover almost all the topics foreseen in the research plan of the theme 1119. *A selective enumeration of the most important results is given below*.

- Mathematical modeling and derivation of algorithms for numerical solution of a wide range of problems: QCD-motivated models for describing properties of nuclear matter at NICA energies; near-barrier heavy-ion fusion; new molecular dynamics algorithms aimed at explaining long-range structural changes of materials under heavy ion and nanocluster irradiation; numerical methods for describing equilibrium and nonequilibrium properties of mesoscopic systems of trapped atoms; numerical investigation of nonlinear multiparameter processes in complex physical systems under external fields, including optical and self-assembled atomic lattices, models of superconducting structures, localized states in condensed media, simulation of gas-hydrodynamic processes in porous media, stable solitons in a nearly PT-symmetric ferromagnet with spin-transfer torque; new method for solving the Gross-Pitaevskii equation with a PT-symmetric complex potential; modeling the reflection of neutrons from layered nanostructures, studies of magnetic films as structures consisting of vector micro-objects; nuclear-physical processes based on a hybrid model of microscopic potential, including reactions with light exotic nuclei.

- Mathematical modeling, derivation of algorithms, and rigorous solution of numerical analysis topics the state-of-the-art solution of which is unsatisfactory for resolving current theoretical and experimental problems investigated in the JINR and partner institutions: digital processing of plane curves (with application to fast neutron noise analysis of the IBR-2M reactor), two-rule quadrature for the computation of observables, new symbolic-numerical schemes using finite element method, non-canonical Bargmann–Moshinsky basis; interpolation Hermite polynomials in d-dimensional hypercube; compact three center wave function constructed by use of irreducible representations of the D_{3h} point group for solving the ground and five excited states of the equilateral triangular H_3^+ molecule; Compton ionization of hydrogen atom near threshold by photons; kinematically complete experimental study of Compton scattering at helium atoms near the threshold.

- Solution of massively parallel, resource-intensive problems raised by the theoretical and experimental physics: discontinuous hp-adaptive schemes for finding optimal configuration of a magnetic device with highly-uniform magnetic fields for experiments with neutrons (collab. FLNP); derivation of constraints for the dense matter equation of state to explain observations of the binary neutron star merger GW170817; Landau mass parameters of the extended σ-ω model for neutron star matter (collab. LIT, BLTP, Wigner Institute – Hungary), interactions in model membranes mimicking preclinical conformational diseases (collab. LIT, FLNP, LRB – journal cover 2020); model description of the interaction of atomic and molecular hydrogen, hydrogen anion and water molecule with an external ultrashort laser pulse; MPI implementation of the method of separated form factors for data analysis in polydispersed vesicular systems (collab. FLNP); HPC of physical observables in spintronics; HPC for design optimization of a pulsed cryogenic cell; single ionization of helium by fast proton impact, etc.

- Solutions of difficult problems of computer algebra: constructive models for the description of finite quantum systems; functional equation methods for reduction of Feynman integrals; table-based representation of polynomials in the computations of involutive and Gröbner bases; parametric occurrence of multiple steady states in biological networks.

- Creation of algorithms and programs possessing strong consistency property, for symbolic-numerical solution of systems of nonlinear PDEs; algorithmic linearizability for nonlinear ODEs.

- Solutions of problems related to quantum computing: entanglement production by statistical operators; mid-range order in trapped quasi-condensates of bosonic atoms; classicality indicator of an arbitrary N-level quantum system; quantum teleportation of two-qubit Bell states; entanglement sudden death and birth effects in two qubit maximally entangled mixed states under quantum channels; robustness of entanglement under quantum decoherence channels.

(5) ***Grow up of the scientific competence in using the JINR computer tools***

Only educated users can grasp the complex JINR hardware infrastructure. Therefrom, an essential task resolved within theme 1119 concerns the implementation and promotion, in cooperation with theme 1118, of *an articulated and permanent educational system* with the aim to surpass the huge difficulties associated with the learning curves of the modern computing. The HybriLIT polygon has become the practical center for the education and growth of young specialists both from JINR and JINR Member States. Prominent specialists from JINR and from partner institutions in Russia and abroad are frequently giving lectures and tutorials at HybriLIT. Within the collaboration with Dubna University, the students are using HybriLIT for the completion of twofold purpose works: solving tasks within JINR projects and preparation of bachelor's and master's theses; the Summer Computer School "Big Data Analytics Dubna-2019" was organized. The periodical international conferences have become opportunities for intensive tutorials in high demand at associated satellite IT International Students' Schools. In 2019, the associated event to the "Mathematical Modeling and Computational Physics 2019" Conference (MMCP 2019) was the International IT-School "Machine Learning, Parallel and Hybrid Computations & Big Data Analytics" using the ML/DL ecosystem of the HybriLIT polygon (attendance 26 students). At the "27th International Symposium on Nuclear Electronics and Computing, 2019" (NEC 2019) organized by LIT-JINR and CERN, in Budva, Montenegro, the associated second "Big Data Analytics" IT School was attended by 32 students. A third IT-school "Distributed Computing and Big Data", planned on April 2020 at Budva, Montenegro as well was postponed to the autumn 2020, due to the Covid-19 pandemic.

- ***Organization of the International Conference MMCP 2019. Participation in other Scientific Conferences***

The Mathematical Modeling and Computational Physics (MMCP 2019) International Conference was held during July 1–5, 2019 at the Congress Center Academia of Slovak Academy of Sciences (SAS) in Stará Lesná, High Tatra Mountains, Slovakia. Together with the permanent organizer of the MMCP conferences, the Laboratory of Information Technologies (LIT) of the JINR, the co-organizers of the tenth MMCP edition have been the Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH), Bucharest, Romania, and four Institutions from Košice, Slovakia (the Institute of Experimental Physics (IEP) SAS, the Slovak Physical Society (SPS), the Technical University (TU), and the Pavol Jozef Šafárik University (PJŠU)). In the tradition of the previous MMCP conferences, it was an open forum to exchange ideas, strengthen personal relations, find incentives for future cooperation, learn and communicate within a wide range of topics. A satellite event of the MMCP 2019 was the abovementioned HybriLIT based International IT-School. The MMCP 2019 was attended by 104 participants from 12 countries. A number of 18 invited and plenary lectures and 74 oral communications (3+23 from theme 1119) were delivered. The Proceedings (revised selected papers) published in EPJ Web of Conferences, Vol. 226 (2020), (Editors Gh. Adam, J. Buša. M. Hnatič), present the 48 contributions which passed all the steps of a high standard reviewing process (19 papers with authors from theme 1119).

A total of 22 invited lectures and 34 oral contributions have been delivered by authors working in theme 1119 at other International Conferences. From them, 10 presentations have been given at the NEC 2019 Symposium (Budva, Montenegro). Other Conferences with participation from theme 1119: the 21-st International Workshop on Computer Algebra (23-24 May 2019) was organized and held in LIT-JINR, ICASC 2019 (Sinaia, Romania), Conf. Series "Mathematics. Computer. Education" (XXVI-2019, Pushchino, RAS; XXVII-2020, DSU), Supervychisleniya & Mat. Modelirovanie (Sarov), POMI Seminars (St. Petersburg), ITTMM 2019 (ИПМиТ), etc.