Referee report
on the proposal for theme 1119 extension during 2020-2023

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0. Title of the theme "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data"
Leaders: Gheorghe Adam, Petr V. Zrelov
Deputies: Ján Buša, Ochbadrakh Chuluunbaatar
Status: Proposed for extension till the end of 2023, the concluding year of the present JINR Seven Year Plan 2017-2023

1. Scientific merits, elements of novelty, timely nature of the research

The proposal combines two opportunities at the Laboratory of Information Technology (LIT) of the JINR:
(i) the existence of top computing tools enabling large scale and new approaches to computing: the heterogeneous HybriLIT computing platform (which involves a training and testing polygon and the "GOVORUN" supercomputer) and an emerging Big Data distributed infrastructure;
(ii) the unique experience and know-how for symbolic or symbolic-numerical solution of applied and fundamental scientific problems.

A distinctive feature of the proposal under review, visible throughout the presentation, is the corroboration of the research done in the LIT, based on the existing local expertise, with the global research effort of the Joint Institute for Nuclear Research (JINR) as a whole. This is part of the conception of the current seven year plan of development of JINR for 2017-2023, aimed at giving top priority to the most important milestones of the research done in JINR.

The proposal strongly illustrates the fact that the methods of the applied mathematics and computational simulation combined with sophisticated data treatment are an indelible part of successful fundamental science and applied research. The problematic of the effective utilization of powerful computing infrastructures like the "GOVORUN" supercomputer is emphasized and timely instances of actual scientific problems solved with modern mathematical algorithms are provided. The overwhelming part of these problems stems from the requirement to provide computer support to the development and exploitation of installations and facilities (detectors) under evolving conditions characterized by features such as incomplete observation, incomplete statistics, tiny signals immersed in huge backgrounds, etc. In this context it is to be noted the development of new solving approaches like neural networks based on machine learning and deep learning, Big Data analytics, quantum computing.

The extension of the Theme 1119 proposed for the four-years 2020–2023 is primarily motivated by the continuation of the demands coming from the most important JINR projects under development during 2017–2023 (NICA, Baikal GVD, superheavy nuclei production).

The characterization of the activity done within the Theme 1119 as unity in diversity is preserved. The active participation of LIT scientists in over 40 JINR scientific projects points to the diversity and variety of the solved tasks. 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.

The formation of efficient top working groups within theme 1119 asks for four complementary features: (a) Computer scientist thinking, based on expert knowledge of several modern programming techniques; (b) Deep mathematical expertise, for correct model formulation, irrespective of their origin, in experimental or theoretical physics, the right definition of their features; (c) High education level in numerical analysis for correct computational complexity tackling, avoidance of the pitfalls coming from the operation with machine numbers instead of the real/complex numbers underlying the continuous mathematical models; (d) Profound understanding of the physics side of the problems, for correct inferences on the hierarchical importance of the different quantities entering the investigated phenomena.

The four chapter structure of activities proposed for the 2014-2019 period is preserved, with updates concerning chapters 3 and 4. Within each chapter, new tasks are formulated which add weight to the importance of the research done in the LIT for the solution of the computing intensive tasks asked by the research done in other JINR laboratories.

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

Of primary importance will be the calculations of magnetic fields for different facilities (3D modeling of magnetic fields for NICA-JINR, FAIR-GSI, SPD-NICA, cyclotrons for proton therapy, etc.). LIT information-computing support will be continued for the improvement of the working regimes of several experimental facilities like YuMO and HRFD setups at IBR-2M, BAIKAL GVD, processing and analysis of the neutron noise of the IBR-2M reactor. 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 investigation of mathematical models of complex physical processes will be pursued in the frame of quantum-field and molecular-dynamics approaches. 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 primarily for the HybriLIT heterogeneous computing platform.

(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 (ATLAS, CMS), NICA (BM@N, MPD), FAIR (CBM) 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. Further development of Geant4 modules will be continued. The development of deep learning neural network algorithms will become a significant part of this activity.

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

This central chapter of the proposal foresees two top lines of investigations.

A. Developments for Multicore and Hybrid Architectures

The mainstream of this activity is aimed at the development of numerical methods, algorithms and software packages on the basis of parallel programming techniques OpenMP, MPI, CUDA/OpenCL, machine learning methods and deep learning (ML/DL), intended to the effective use of multicore and hybrid architectures for significant speed up of the solution of a wide range of massively parallel, resource-intensive problems of theoretical and experimental physics 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 will be actively pursued within the heterogeneous platform HybriLIT.

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, SPD 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).

(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.

To conclude this section of the review, there are lots of elements of novelty going either along the general IT worldwide trends or uniquely in-house devised. The orientation of the research toward the solution of computing intensive tasks of broader interest to the JINR research points to the timely nature of the proposed undertakings.

2. Expertise of the group and technical feasibility of the project within the proposed timescale

The adequate expertise of the basic staff of theme 1119 is probed by the existing high level of qualification (1 Academician, 23 DSc, 47 PhD – figures in continuous evolution), the developed highly efficient parallel packages for solving special tasks, new methods for the analysis of data characterized by incomplete observation and incomplete statistics, the solution of reputedly hard problems, such as the algorithmic linearizability of a general non-linear ordinary differential equation, the accurate numerical solution of few-body problems by new algorithms, new discretization approaches to the algorithm derivation involving new principles of approximation, multiscaling, new search methods of extrema of discontinuous functions, new progress in the algorithmic description of quantum computations.

To alleviate the abrupt learning curve of arid computer mathematics and programming topics by young scientists, a variety of instruction and educational methods and forms are used: regular scientific seminars, intensive courses, lectures, tutorials, consultations with leading specialists, etc. Considerable progress was achieved in grasping subtleties of the programming on a supercomputer.

Many tasks foreseen inside the theme proposal are characterized by input and feedback from the collaborating groups. Without exception, these are scientific tasks the expected solutions of which are heavily based on the existing LIT expertise. This topic corroboration considerably increases the chances to in-time develop and implement algorithms and software.

3. Compliance of the requested financial resources with the objectives of the project/theme

The requested financial resources fully comply with the objectives of theme 1119.

4. Availability of human resources at JINR and in the collaborating institutions

The existing human resources are of good quality, the LIT is an attractor for young talents, both from Russian institutions and from JINR Member State institutions.

5. Conclusions

The proposal for the extension of theme 1119 for 2020-2023, the last four years of the current seven year plan of development of the JINR, articulates the important directions of the future activity in the LIT in the field of mathematical modeling and computational physics in accordance with the most stringent JINR tasks.

The successful development of software on the heterogeneous HybriLIT computing platform as the fundamental high performance computing resource of JINR is of the maximal importance for the Institute and should be supported. At the same time, the completely new approaches involving Big Data analytics and quantum computing offer possible breakthroughs in the solution of the most stringent tasks of the JINR research in the relativistic nuclear physics (NICA) and neutrino physics (BAIKAL GVD). Last but not least, the solution of scientific topics which stay at the basis of the success of specialized JINR projects is a further factor which brings strong motivation to the approval of the theme 1119 for the next four year period.

In conclusion, I propose the approval of the extension of theme 1119 during 2020-2023 with the first priority.

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