

Referee report

on the proposal for the theme 1119 extension during 2017-2019

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

Time schedule of the first part of the theme: 2014-2016

Period of the theme extension: 2017-2019

Following the **criteria of evaluation** included in the Guidelines for evaluation of the proposals for the opening or extension of a project or a theme, the present referee report on the proposal for the extension of theme 1119 for 2017-2019 is divided into four main parts and ends with a concluding section.

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

A distinctive feature of the proposal under review, visible throughout the presentation, is the corroboration of the research done in the Laboratory of Information Technology (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 new seven year plan of development of JINR for 2017-2023, aimed at defining the most important milestones of the future research to be done in JINR. The present proposal for the three-year extension of the theme 1119 at the 45-th Meeting of the CMP-PAC goes along the LIT contribution to the JINR Seven year plan, discussed and approved at the 42-nd CMP-PAC of 22-23 June 2015, at the 45-th PP-PAC meeting of June 2016, and at the 44-th NP-PAC meeting of June 2016.

The four chapter structure of activities proposed for the 2014-2016 period is maintained:

- (1) Mathematical and computation methods for simulation of complex physical systems.
- (2) Software complexes and mathematical methods for processing and analysis of experimental data.
- (3) Numerical methods, algorithms and software computationally adapted to multicore and hybrid architectures.
- (4) Methods, algorithms and software of computer algebra.

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.

Starting from the fundamental premise of the information technology (IT) development that the existing hardware-software background plays the decisive role in the solution of the computing intensive large scale tasks in all the JINR fields of activity, the energetic development of the software-information environment of the heterogeneous computer cluster HybriLIT, as an indelible part of the Multifunctional Information and Computing Centre (MICC) project, will be the task of general interest within the theme 1119. In this way, the premises for safe and reliable design and implementation of parallel software as a means to increase the efficiency of the large scale computations in JINR will be consolidated.

A second broad direction of research is the information-computing support of the JINR experiments. Since the support of a specific experiment lasts over the whole lifetime of the experiment itself, the started efforts are to be continued, both at the in-house JINR experiments or setups (like the YUMO and HRFD at IBR-2, the super heavy element search and the exotic nuclei investigation at FLNR, the neutrino experiments in DLNP, or, last but not least, the BM@N and MPD setups of the NICA project) and the outer large scale experiments done with JINR participation (like CMS and ATLAS at LHC, CBM at FAIR).

A third direction of research of primary importance is the development of computational tools for the off-line data analysis (like the general purpose Geant4 package) and the computational support of practical engineering-physical problems in JINR Laboratories and JINR Member States.

Finally, a fourth direction of research is the symbolic-numerical or numerical solution of difficult mathematical problems. To this aim, purpose adapted methods are developed like the enforcement of discretization schemes which inherit all the algebraic properties of the original continuous mathematical models, development of scale-adapted algorithms, development of new principles of approximation resulting in drastic reduction of the computational complexity, result validation by Bayesian analysis, etc.

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 proposal for theme extension on 2017-2019 and the report on the activity done during 2014-2016 are rich in evidence substantiating the existence of a high rank scientific qualification, a high level scientific expertise, plenty of skills developed and maintained through hard work.

Several JINR prizes were awarded, within tough competitions, to LIT scientists during 2014-2016 for top level scientific publications. Other prizes rewarding scientific publications and recognizance of the value of the scientific results by Russian Federation forums complete this enumeration.

A separate category of outstanding outputs of the research done within the theme 1119 is the creation of computation tools for the benefit of the scientific research both in JINR and in outer large scale projects developed in partnership with JINR.

Of the widest interest and utmost importance is the development of the modular hybrid computing cluster HybriLIT as the main resource for the high performance computing (HPC) in JINR and JINR Member States. Since the acquisition of the first HybriLIT modules during the first half of 2014, a home-made devised conception of the software-information environment of the HybriLIT cluster was developed. Its implementation secures system scalability, efficient use of the computing resources, high fault tolerance. The proposed future HybriLIT enhancements and developments are based on a valuable accumulated expertise which is a strong argument in favor of their successful fulfillment.

The many other particular tasks foreseen inside the theme proposal are explicitly 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 improved formulation of the theme proposal constitutes a substantial progress as compared to the previous ones. In this way, considerable increase is get of 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 explicitly requested financial resources for the accomplishment of the theme proposal will basically cover the cost of the workforce (91% of the foreseen expenses), equipment (4.7%), and international cooperation (3%).

The fact that the research done in frame of the theme 1119 does not need substantial investments follows from the general structure of the LIT expenses. Since the MICC is developed as a single project defining all the aspects concerning the JINR basic facilities for information and computing, the investments for the HybriLIT hardware development are included there. Moreover, the primary software needs for the development of the HybriLIT cluster are confined to the realm of the freely available mature open software. This is a wise decision since it enables the implementation of a flexible software-information structure which can be quickly reshaped according to the user feedback concerning the actual needs of the JINR computing community.

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

The proposal for theme 1119 extension during 2017-2019 does a careful analysis of the strong and the weak sides of the existing human workforce.

The drawn frame points to a dynamic evolution within which the aspiration to reporting highest class scientific outputs (either as new computational tools or as scientific publications) is doubled by the wish to get formal certification of the acquired scientific expertise through a doctoral title (with 24 DSc and 47 PhD, figures which are continuously evolving, the qualification inside theme 1119 is very high indeed).

The promotion of organized frames of scientific education (with the best available lecturers, through specialized courses, tutorials, seminars, etc., which address both the JINR scientific community and the scientific community of the JINR Member States at large), is an all Laboratory feature. A weakness, discussed at large in the proposal, is the misfit between the areas of expertise of the mature scientists and the younger ones. Since expertise cannot be gained overnight, ways of striving to get it in the shortest time are stressed.

An insufficiency of highly qualified scientists necessary for solving tasks of special importance for the JINR, in particular the flagman JINR project NICA is underlined and the newly proposed ways of overcoming it through special lecture courses on the occasion of the traditional MMCP (Mathematical Modeling and Computational Physics) July 2017 Conference are welcome.

To end this section, the supervision and encouragement of prospective young people for their solid professional growth and their desire to wish to develop scientific careers precisely in LIT deserves full PAC support.

5. Conclusions

The proposal for the extension of theme 1119 for the next three year period, 2017-2019, is made in full agreement with the stipulations of the new seven year plan of development of the JINR. It articulates the important directions of future activity for the next three years in the LIT in the field of mathematical modeling and computational physics in accordance with the most stringent JINR tasks.

The successful development of the heterogeneous computing cluster HybriLIT as the fundamental HPC resource of JINR is of the maximal importance for the Institute and should be supported.

At the same time, the solution of scientific topics which stay at the basis of the success of specialized JINR projects is the second factor which brings strong motivation to the approval of the theme 1119 for the next three year period.

In conclusion, I propose the CMP-PAC to support the extension of theme 1119 during 2017-2019 with the first priority.

Prof Valeriu Kantser,
Institute of Electronic Engineering
and Nanotechnologies of The
Academy of Sciences of Moldova,
Chisinau, Academiei str3/3,
R.Moldova
Chairmen of the PAC on Condensed Matter Physics