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## Evaluation of the Proposal for Theme 1119 Extension during 2020-2023

### Proposal details

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

Proposed by: Laboratory of Information Technology

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Status: Suggested for extension till the end of 2023

### Introduction

The proposal combines the unique infrastructure at the Laboratory of Information Technology (LIT) – the HybrLIT computation cluster and the “GOVORUN” supercomputer with the cumulated experience and know-how for solving applied and fundamental scientific problems. The subject of the proposal is very general and it has an impact over a large number of scientific units like instrumental groups, large scale facilities, institutes and even international communities overcoming the borders of a local institutional project.

Nowadays the role of the applied mathematics and computational simulations combined with sophisticated data treatment is a key factor for successful fundamental science and applied research. The continuous improvement of the computation power of the available hardware and the optimization of the existing algorithms allow for processing of data

volumes unimaginable few years ago. The proposal emphasizes the problematic of effective utilization of powerful computation infrastructures like HybriLIT and the “GOVORUN” supercomputer with the cumulated experience and know-how for solving applied and fundamental scientific and provides good examples for actual scientific problems solved with modern mathematical algorithms for example the presented development of methods and algorithms for processing and analysis of the neutron noise of the IBR-2M reactor. From the other side the experimental facilities produce complex data sets which require dedicated expertise and computation resources for successful data treatment without loses of sampled resolution like the mentioned development of batch processing of neutron diffraction spectra measured in real-time in situ mode (HRFD at IBR-2, FLNP).

The main impression from the proposal is that it closely follows the criteria of evaluation as discussed below.

**Criteria 1: *Scientific merits, elements of novelty, timely nature of the research***

- The theme 1119 aims at 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 and the “GOVORUN” supercomputer.
- By its very nature, the theme 1119 is multidisciplinary. Its 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., asking for the development of new mathematical methods and approaches for modeling physical processes, processing and analysis of experimental data.
- The unifying features of all studies come from their common mathematical background asking for the existing LIT expertise for obtaining reliable symbolic-numerical or numerical solutions from computer software implementation of the derived algorithms. It is important to mention the development of deep learning neural network algorithms which are allowing new level of data processing and analysis in the scientific infrastructure.
- The definition of the problem-oriented topics was done in agreement with the leaders of research groups in the collaborating JINR Laboratories, both as it concerns the in-house research and the participation in outer large scale experiments.

- Striking examples concerning condensed matter physics are the new computer developments for the YuMO setup, the HRFD, the assessment of IBR-2M status from experimental measurements, the automatic calibration of gaseous spectrometers.
- The outstanding participation in the development of computer software for large scale experiments (BM@N and MPD at NICA, CMS and ATLAS at LHC, CBM at FAIR, the general Geant4 package) is documented by inclusion of the LIT-developed modules into the dedicated software packages of these experiments.
- Of special concern within the theme 1119 will be the creation of efficient computing tools for solving the ever increasing number of computing intensive tasks in the JINR research, with the aim of overcoming the notorious inefficiency of the existing computer codes on the multi-core, manycore, and GPU accelerator processors which constitute the today exclusive deliveries on the hardware market. To this aim, the information-computing environment of the heterogeneous computing cluster will be improved, new efficient parallel algorithms and codes will be derived for the solution of the new tasks arising in the JINR research.
- Another timely subject of research is the data analysis based on the design of deep neural networks which were recently successfully started in LIT-JINR. The availability of sufficient resources for the deep learning starting period will result in unsurpassed performance of such algorithms at the predictive stage.
- The Big Data analytics, raised by the very large scale experiments will be a new direction of investigation which asks for the grasp of new ways of thinking, e.g. the implementation of the PIconGPU package on the "GOVORUN" supercomputer will help to characterize the laser based acceleration of elementary particles, which promises to result in revolutionary changes of the principles guiding the buildup of the future new accelerators.

**Criteria 2:** *Expertise of the group and technical feasibility of the project within the proposed timescale*

- The existence of adequate expertise of the basic staff of theme 1119 is probed by the existing high level of qualification (23 DSc, 47 PhD – figures in continuous evolution), the developed new discretization approaches to the algorithm derivation involving, among them, inheritance of the basic algebraic properties of the initial mathematical models, new principles of approximation, multiscaling, new search

methods of extrema of discontinuous functions, new canonic basis expansions in computer algebra.

- To alleviate the abrupt learning curve of arid computer mathematics topics and programming 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. Online modern methods (like the pm, the Gitlab, both for HybriLIT) are used.

**Criteria 3:** *Compliance of the requested financial resources with the objectives of the project/theme*

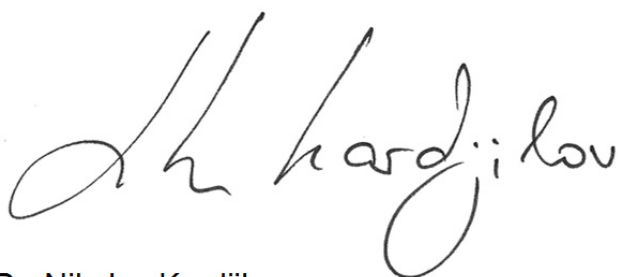
- The requested financial resources fully comply with the objectives of theme 1119.

**Criteria 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.

**Conclusions**

- In conclusion, I estimate that the proposed tasks are well formulated, are ambitious, they are directed to the solution of top difficult topics of the JINR research, they are feasible.
- I propose the CMP-PAC to approve the support of the theme 1119 extension on 2020-2023 with the first priority.



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