Review of the Proposal to Extend the Theme 1119 during 2020-2023

The theme **05-6-1119-2014/2023**, "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data" is implemented under the direction "Networking, Computing, Computational Physics" of the "Topical Plan for JINR Research and International Cooperation" and aims to provide mathematical and computational support for a wide range of research done at JINR according to the 7-year JINR development plan for 2017-2023. The fulfillment of works in frame of the theme assumes conducting of fundamental advanced research in computational mathematics and computational physics aimed at the creation of new mathematical methods, algorithms and software for the solution of actual problems arising in experimental and theoretical studies by means of the newest computational hardware resources available in LIT. It includes the new HybriLIT Platform (involving the training and testing cluster HybriLIT) and the "GOVORUN" supercomputer – a joint project of the Bogolubov Laboratory of Theoretical Physics and the Laboratory of Information Technologies as part of the Multifunctional Information and Computing Complex project at LIT and the emerging Big Data distributed infrastructure. These objectives are related to the strategic lines of the JINR research, such as the NICA project, the neutrino program, the physics of superheavy and exotic nuclei, the neutron based investigations, and directed for the development of new mathematical methods and approaches for accurate modeling of the physical processes, the processing and analysis of experimental data.

The research within the theme 1119 is divided into four basic directions:

1. **Mathematical and computation methods for simulation of complex physical systems**: development and use of mathematical and computetional methods for modeling new experimental facilities, accelerating complexes and their elements, nuclear-physics processes, and complex physical systems. 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 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 available and developing in LIT, primarily the HybriLIT heterogeneous computing platform.
2. **Software complexes and mathematical methods for processing and analysis of experimental data**: 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 from the accelerator facilities NICA, LHC, FAIR as well as from the experimental facilities of the JINR for the programs of the neutrino physics, the nuclear physics, the condensed matter physics and the radiation biology. 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** will follow two mainstreams.
   A. *Developments for Multicore and Hybrid Architectures*: numerical methods, algorithms and software packages developed on the basis of parallel programming techniques using OpenMP, MPI, CUDA/OpenCL, machine learning methods and deep learning (ML/DL), intended to the effective use of multicore and hybrid architectures for the solution of massively parallel, resource-intensive problems of theoretical and experimental physics. To this aim, an ecosystem for data analysis and ML/DL tasks was set up and is under active development within the heterogeneous computing platform HybriLIT.

B. *Big Data Analytics*: explores new concepts and methods for modeling, reconstruction and processing of experimental data (installations at the NICA accelerator complex, JINR neutrino program experiments, LHC experiments) and their step-by-step implementation within the Big Data approach.

4. **Methods, algorithms and software of computer algebra and quantum computing**: 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.

The outcome of the theme will be the creation of mathematical and computational tools for modeling physical systems, the mathematical processing and analysis of experimental data subject to the newest developments of the computational architectures that will allow the Institute to carry out its tasks at the high level. s combining fourfold skills: thinking as computer scientists – with expert knowledge of several

I should like to mention that the LIT staff has developed and maintains a fruitful friendly collaboration with all the other JINR Laboratories. The workforce contributing to the implementation of the tasks of the topic consists both of experienced scientists (23 DrSc and 47 PhD) and young scientists and engineers. A variety of means is used for the increase of the level of education of all the staff, such as to have working groupmodern programming techniques; deep mathematical expertise – to secure correct formulation of the mathematical methods; high education level in numerical analysis – to assess the computational complexity of the problems to be solved; profound understanding of the physics side of the problems.

The proposal to extend the theme 1119 for the 2020-2023 is well prepared. It covers the mathematical support for all the key activities of JINR and takes into account the modern tendencies of the development of top methods of the mathematical modeling as well as approaches to the solution of theoretical and experimental topics of the highest interest to the JINR. This support will allow the JINR to solve its tasks at the high level.

The expenses asked for the fulfillment of the tasks foreseen for the LIT topic 1119 for the four year period 2020-2023 are within the previsions of the JINR Seven Year Plan 2017-2023.

I consider that the extension of the topic "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data" deserves full approval and support with the first priority.

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