Evaluation of a Project Proposal in the frame of the Theme 1119 for 2024–2026

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Proposal details

Theme 1119: "Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data"

Project Proposal: Methods of computational physics for the study of complex systems

Proposed by: M.G. Meshcheryakov Laboratory of Information Technologies (MLIT)

Leaders: O. Chuluunbaatar, E.V. Zemlyanaya

Deputies: Yu.L. Kalinovsky, A. Khvedelidze

Status: Project proposal, within the Theme 1119, for 2024–2026, to be analyzed and decided at the 57-th Meeting of the Program Advisory Committee for Condensed Matter Physics (CMP-PAC)

Project evaluation

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

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

- The submitted project proposal formulates ambitious interdisciplinary computing based tasks the solution of which is intended to contribute to the progress of the JINR research as a whole during the next Seven-Year Plan for the Development of JINR for 2024–2030.
- This undertaking rests on the combination of two basic opportunities at the MLIT: (i) the existence of top computing infrastructure (comprising the heterogeneous HybriLIT computing platform which involves a training and testing polygon and the "Govorun" supercomputer) enabling large scale and new approaches to highly performant computing) and (ii) a highly qualified research team possessing a unique experience and know-how for numerical, 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 MLIT, based on the existing local expertise, with complementary research effort done by groups from all the other JINR Laboratories. This is a part of the conception of the next Seven-Year Plan on 2024–2030 of giving top priority to the most important milestones of the research done in the JINR.
- The proposal strongly illustrates the continuation of the red thread characterizing the Theme 1119 during the last years, that a successful computational simulation of very

different classes of physical phenomena is made possible by two pillars: solid specific mathematical ground, together with skillful identification and exploitation of the available hardware features in terms of which a substantial acceleration of the algorithmic inner information transfer is possible. 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. In this context, it is to be noted the attempt at developing such a new solving approach like the quantum computing.

- Having in mind the main directions of the JINR research program, the specific tasks of the project are grouped into five subject areas, each of which shows distinctive features concerning original development regarding, on the one side, methods of computational mathematics, high-performance computing and mathematical modeling and, on the other side, new physically significant results obtained on this basis:

  (1) Investigation of complex processes in nuclear physics and quantum mechanics;

  (2) Studies of intricate processes in condensed matter and materials under external actions;

  (3) Solution of problems arising in the development and optimization of operating modes of experimental facilities;

  (4) Modeling physical phenomena in dense nuclear matter, based on the equation of state;

  (5) Modeling of quantum systems using methods of quantum information theory and hybrid quantum-classical programming methods.

- To summarize the above discussion, this is a comprehensive well written research project proposal directed to the study of complex physical processes asking for numerical solutions of difficult mathematical and computational physics problems for wide ranges of values of the parameters of the models.

- Such processes are described, as a rule, by systems of dynamic nonlinear, spatially multidimensional, integral, integro-differential, or differential equations. The processes can be characterized by the occurrence of critical regimes, bifurcations and phase transitions.

- These features make vitally important the development of numerical approaches, which should be finely tuned to characteristic special features of the problems asking for solutions. The coverage umbrella of the project problems stems from research projects defined in the Seven-Year Plan 2024–2030 to be of the first importance for the JINR.

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

- The adequate expertise of the basic staff of the proposed project is probed by the existing high level of qualification (1 Academician, 12 DSc, 30 PhD – figures in continuous evolution). Besides the experienced scientists, the research team includes enthusiastic young scientists and engineers.

- The publication, during the last three years, of more than 150 scientific papers in peer-reviewed scientific journals, of 16 monographs or contributions to monographs, the presentation of 30 plenary or invited lectures at international conferences, in the area

covered by the project, the defense of three PhD theses on the subject of the project completes the statistics of the contribution to the JINR excellence trough publications. The development and implementation of eight high-performance software packages in the Program Library JINRLIB and of three packages in the international library of computer programs of the Computer Physics Communications journal are additional proofs of a lasting prestigious output simultaneously based on in-depth grasp of right computing paradigms and the formulation of breakthrough ideas.

- The project proposal assumes the promotion and support of a scientific environment in MLIT, which encourages and rewards 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 reduced computational complexity, robustness and reliability of the developed algorithms; deep knowledge of the physics side of the problem at hand as a precondition of significant mathematical modeling undertakings. The leadership of the project will put efforts to back the agreed cooperation with 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, the decisions will heavily rely on those of the JINR Directorate and of the Program Advisory Committees, the CMP-PAC in the first instance.

Criterion 3: *Compliance of the requested financial resources with the objectives of the project*

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

Criterion 4: *Availability of human resources at JINR and in the collaborating institutions*

- The existing human resources are of good quality, the MLIT 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 present project proposal for 2024–2026 with the first priority.

Date   Signature

30.05.2023   Acad. Prof. Deleg Sangaa