Review on the proposal to extend the scientific project "Methods of computational physics for the study of complex systems":

SCIENTIFIC AND TECHNICAL REASONING FOR THE RENEWAL OF THE PROJECT IN RESEARCH AREA WITHIN THE TOPICAL PLAN FOR JINR RESEARCH

The project under consideration presents a plan of scientific research in the field of computational physics and information technology for the period 2027–2031. The project is fully consistent with the section "Information Technologies & High-Performance Computing", of "JINR Long-Term Development Strategy up to 2030 and beyond"[1], and, indirectly, with all other sections.

As follows from the presentation of the project, its purpose is twofold. *On the one hand*, the project provides computational support for the ambitious theoretical projects, current and newest experimental programs, both technologically and with respect to modelling and optimizing the operating modes of experimental facilities. Moreover, this block includes, in particular, the development of new mathematical methods, algorithms and software packages for numerical studying various types of complex systems with interactions on scales from nuclear to molecular. *On the other hand*, the authors have planned general-purpose research in the field of computational mathematics, high-performance computing, and neural network algorithms targeted for mathematical modeling of fundamental processes. The results of this universal research are expected to be effective in a wide range of scientific fields: astrophysics, nuclear physics, condensed matter physics, biology, biochemistry, etc. An important part of this research area is the development of new computational methods and mathematical modeling methods in the field of quantum information science and quantum technologies.

First of all, since the proposal under consideration is a continuation of the project[2] started in 2024, it makes sense, as far as possible, to evaluate the results obtained at the 2024-2026 stage. The results of implementing the previous stage of the project are quite impressive. They are reflected in more than 120 publications including scientific journals having high impact factor and in 3 monographs. Among everything in this collection of publications, there should be mentioned specifically a scientific review, published in Natural Science Review, and two monographs devoted to modified iterative schemes for the Continuous Analogue of Newton's method. These algorithms have a high degree of universality and play a key role in solving systems of nonlinear equations that arise in computational physics. The third monograph is devoted to the development of iterative methods and algorithms for solving systems of equations of various types using the finite difference method and the high-order finite element method. In addition, it is important that two textbooks, based on the results of research, have been prepared and published.

The proposals for extending of the project for 2027–2031 contain mainly the same directions of research, but the range of problems to be solved and areas of their application have been significantly expanded. In particular, the following areas of investigations have been expanded: numerical simulation and mathematical modeling of physicochemical and structural changes in materials under irradiation with charged particles, nanoclusters and laser radiation; complex

[1] https://www60.jinr.ru/posts/jinr-long-term-development-strategy-up-to-2030-and-beyond/

[2] https://lit.jinr.ru/en/Science/ResearchAreas/2026/ComputationalPhysicsMethods

processes in dissipative condensed matter under external influences, described by nonlinear field theory equations; investigations of interactions in hot and dense matter in the NICA energy range during heavy ion collisions that are accompanied by phase transitions and the formation of quark-gluon plasma; superconducting processes and Josephson junctions in spin nanosructures; some problems of modeling complex processes in astrophysical systems. Relatively new directions of research include quantum computing (modeling of quantum systems using methods of quantum information theory, hybrid quantum-classical programming, classical simulation of quantum computations) and quantum technologies (modeling the dynamics of spin ensembles and cold atoms in traps).

Summarizing the above overview of the project, it can be argued that the project covers a significant variety of topics, united by the same set of numerical methods and similar approaches to the construction of mathematical models. It is important to note that the second stage of the project (*the renewal of the project*) has been planned by the same research team. I think that announced goals of the project are quite adequate, correspond to the present level of investigations, and can be implemented. I believe that the implementation of this project will be an important step in the development of applied mathematical models of complex systems in various fields of physics and biology.

Based on the above, I strongly recommend to support the extending of the project.

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