

LQCD Response to 2023 DOE Annual Review

This document contains the responses of the LQCD-ext III/NP LQCD Initiative to the comments and recommendations in the 2023 annual review. It is organized by the items contained in the review charge. Each section contains a summary of the comments and recommendations, if any, for the given charge item, followed by the Initiative's response.

1. The Program's Continued Significance and Relevance

Reviewer Comments:

One hundred and seventy people are involved in the entire USQCD collaboration. Communication between them, their elected management, the DOE site offices, and the DOE is working very well and has resulted in a very successful enterprise sustained over 15+ years. Everyone involved is to be commended.

Since lattice QCD simulations have been possible at physical quark masses, LQCD is in an era where its results are directly impacting particle and hadron phenomenology; see for instance the Flavor Lattice Averaging Group (FLAG) review. USQCD is strongly represented overall in that review, and sometimes dominant. Machine-learning based methods already have interesting applications in computing observables or in the data analysis stage for QCD. There is potential for interdisciplinary exchanges of methods and ideas with other areas of science.

Recommendations:

None

Response:

We thank the reviewers for recognizing the hard work of the collaboration and associated personnel.

2. The Progress toward Scientific and Technical Milestones

Reviewer Comments:

The collaboration is to be commended for the clarity and organization of the presentations, and the comprehensive answers to the reviewer's questions. A number of top highlights were shown and an impressive set of activities at the forefront of research in lattice field theory were described. The impact in the heavy-quark sector, in the muon $g-2$, in the spectroscopy of exotics and in some aspects of nucleon structure is particularly high. The breadth of the program is very impressive.

BSM represents about 10 percent of the USQCD program but trains a disproportionate number of young scientists. If/when BSM physics is discovered, this workforce will be extremely useful. There is a positive synergy between BSM studies and the core work on LQCD, with studies of the former introducing new methods to apply to the latter.

In the nucleon sector, there will likely be a "consolidation period", where the same PDFs are recomputed with higher statistics, smaller lattice spacings, better control of excited-state effects, etc. In that period, the quoted errors might not shrink much, but instead become more robust.

Neutrino physics is a relatively new application of LQCD, and the first encouraging results have been obtained spearheaded by early career researchers. This is commendable. It is important going forward to ensure that this effort is broadly supported within the collaboration. Nuclear response and matrix elements of large nuclei is a very difficult problem and thus, the goal must be to create a community of researchers both within LQCD and the community at large which can bring together the necessary expertise to eventually provide experimentally relevant predictions. Within NP, topical collaborations have proven to be an invaluable framework allowing for the collaboration of experts across disciplines, e.g., in the case of matrix elements for neutrino-less double beta decay. It, therefore, seems plausible that topical collaborations also can play a useful and essential role for neutrino nucleus scattering. Without a supporting community the efforts by LQCD will remain insular and will not have the desired impact on the experimental program.

There is always a balance to strike between having a broad program and focusing on a smaller number of physics projects. Given the bottom-up approach of USQCD in allocating computing time, its tendency is naturally to err on the side of having lots of projects. In some cases, it might be worth enforcing stronger focus "from above", e.g., allocating resources only to the part anticipated to be the most impactful within an application. Given the oversubscription of USQCD-managed resources, this must be happening already to some extent.

Recommendations:

DOE HEP and LQCD-ext III should seriously consider taking the lead in the creation of one or several topical collaborations focused on neutrino nucleus interactions with the goal to provide experimentally relevant predictions. The NP Topical Collaborations could serve as a model here.

Response:

The Executive Committee, in consultation with USQCD members, has begun discussions regarding the formation of new Topical Collaborations along the recommended lines. The Committee expects to provide a proposal to DOE in the fall of CY23.

3. The Status of the Technical Design and Proposed Technical Scope for FY2023-2024

Reviewer Comments:

The technical designs are being done in close coordination with other common resources at the labs (networks, storage, cooling) even though the model is shifting towards dedicated compute resources. This is a good and necessary method of planning, and we encourage this to continue to ensure optimal designs for LQCD-specific resources going forward.

Releasing a fair and open Request for Proposal for computer procurements is a desirable aim to ensure the advantages obtained from competition. LQCD should carefully examine the computing landscape at any given time in the “ping-pong” model of procurement to evaluate the feasibility of fielding an appropriate amount of resources of any given type given price constraints. Specifically, this information should inform the effort expended on benchmarking against various designs where the likelihood exists that those platforms will prove to be prohibitively expensive.

Recommendations:

None

Response:

We thank the reviewers for their endorsement of the current resource planning methods. LQCD agrees that it is important to continually monitor the computing landscape and plans to continue doing so to ensure that resource remain adequate while still within budget constraints.

4. The Merits of Including the Construction and Operation of Dedicated Hardware

Reviewer Comments:

Collaboration with industry partners for the development of future improved hardware should be strongly encouraged.

The required change of policy to buy dedicated hardware at BNL seems sensible and does not, in practice, lead to substantial changes. We encourage this change.

Recommendations:

We recommend allowing the flexibility to buy dedicated hardware in appropriate circumstances. This mitigates the risk associated with IC updates.

Response:

Going forward, LQCD plans to continue to consider buying dedicated hardware if and when circumstances are such that dedicated hardware is the best and most cost-effective choice.

5. The Feasibility and Completeness of the Proposed Budget and Schedule

Reviewer Comments:

The purchase model has worked effectively. The choice of whether to purchase computer processing unit-based or GPU-based machines is based on demand as gauged by the proposals.

The proposed use of funds for the remainder of the present proposals is reasonable and efficient.

We support the aims of the preliminary 5-year plan for NP-LQCD, since LQCD will play an ever-increasing role in NP, particularly with the upcoming Electron-Ion Collider.

Recommendations:

None

Response:

Both HEP and NP plan to spend down the remainder of the current proposals as described.

6. The Effectiveness of the Proposed Management Structure, and Responsiveness to Recommendations

Reviewer Comments:

The detailed timeline for results is an excellent addition to the documentation.

While, to date, the system set up by the CDEI to deal with complaints or issues has not been tested, several issues will need to be addressed when it is, and it would be good to prepare for this by further consultations with DE&I officers at the labs. One tricky issue in this regard is whether and how to notify home institutions in the case of sanctions. Another issue is the extent to which any sanctions are made known to the entire collaboration, i.e., the transparency of procedures.

The successful proposal for a training program is to be commended. We look forward to hearing more about the details of this program next year.

Recommendations:

None

Response:

Current plans include continuing with the proposed training program, and with gathering user feedback on a regular basis.

7. The Effectiveness of USQCD

Reviewer Comments:

The procedures for the allocation process are clear and communicated to all proposers.

The yearly allocation cycle seems appropriate to ensure that the scientific aims of the collaboration are pursued, and the resulting scientific impact is maximized.

The reliance on leadership computing facilities as a primary source of gauge generation is recognized as a source of possible risk. Estimates for available time based on historical allocations on Leadership Class Facilities (LCF) resources are used for planning but are not assumed. Planning includes LCF allocation fractions for LQCD as low as 4 percent of the total available hours per year. This is likely a reasonable lower limit.

Despite this reasonableness, LQCD might consider adding the possibility of a marked reduction in LCF allocations in any given allocation year to the formal risk register.

The smooth running of operations of USQCD is a very nice example of NP and HEP physicists sharing resources. It is very appropriate for things to continue to be run in this fashion given the many overlapping physics goals and common computational techniques.

The early career allocation program track evaluates proposals from early career researchers along with all other proposals, providing context and allowing scientific priorities to be considered straightforwardly. This is likely a best practice for these kinds of programs, and matches what is done, e.g., in the INCITE program.

As for the response rate to surveys, perhaps it would help to point out to USQCD members (raise awareness) that responding strengthens the case made to DOE for continued funding as part of this and future reviews.

Recommendations:

None

Response:

We thank the reviewers for their constructive and supportive comments. We will incorporate the suggested point about the importance of responding to the user surveys into our future survey solicitations.