# Lattice QCD Extension II Computing Project (LQCD-ext III)

# Response to Comments and Recommendations from the 2019 LQCD-ext III Science Review

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# LQCD-ext III 2019 Science Review Response to Review Recommendations

# INTRODUCTION

On July 9-10, 2019, the U.S. Department of Energy (DOE) Office of High Energy Physics conducted a review of a proposal to extend the LQCD research program to the next five-year period (FY20-24). The review was held at the Cambria Hotel in Rockville, MD, and resulted in one comment warranting a response, in addition to eight recommendations.

- Three of the recommendations are directed to DOE. They are acknowledged in this document two are addressed to share our perspective.
- One of the recommendations is directed to the two laboratories providing institutional computing resources. A response is provided based on interactions between LQCD and the two laboratories.
- One of the recommendations is directed to all stakeholders (DOE, BNL, Fermilab, LQCD management, the USQCD collaboration), and we share our perspective.
- Responses to the comment and three recommendations directed to LQCD & USQCD are presented below, along with subsequent actions planned or taken.

### **RESPONSE TO COMMENTS**

<u>Comment #1:</u> The integration of the cluster resource management into the IC resources has started. Overall, the collaboration seems satisfied with how this new arrangement is working. Further monitoring and reporting about how this new arrangement work compared to dedicated resources would be very valuable, also for other communities who might want to make a case for resources within the ICs at Fermilab and BNL.

Report Section: Charge 4, p. 11.

<u>Response</u>: LQCD project management will monitor the effectiveness and efficiency of the institutional cluster model and prepare two reports comparing the performance of the new IC arrangement to the dedicated resource model. The first report will be issued in June 2020 and will summarize performance during the first half of FY2020. The second report will be issued in October 2020 and will summarize performance over the entire fiscal year.

### **RESPONSE TO RECOMMENDATIONS**

<u>Recommendation #1:</u> The mid-scale computing clusters should continue to compose a significant portion of the resources available for USQCD research.

Report Section: Charge 3, p. 11.

<u>Response</u>: We read this recommendation as being directed at DOE-HEP, BNL, and FNAL, in addition to the USQCD collaboration and LQCD-ext III program management. As the review committee describes in its

report, mid-scale computing clusters are essential for a variety of tasks that are cumbersome or essentially impossible at leadership-class facilities. These include smaller-scale simulations to test and flush out innovative ideas, carry out statistical and systematic error analyses (which are high throughput rather than high capability), and fostering careers of junior scientists. These elements are key to near-term success, such as on the muon anomalous magnetic moment, as well as for the longer term, for example for mature calculations pertaining to neutrino-nucleus scattering. BNL and FNAL have committed to providing midscale computing resources into the foreseeable future. By approving funding for an additional five years, the DOE Office of High Energy Physics (DOE-HEP) has ensured that the mid-scale computing resources provided by BNL and FNAL will remain a significant portion of the computing resource portfolio enabling USQCD research.

<u>Recommendation #2:</u> The current project execution plan should be reviewed and revised after more experience is gained with the design, procurement, and operations phases of running on the institutional clusters.

Report Section: Charge 4, p. 12.

<u>Response</u>: The Project Execution Plan (PEP) presented at the review was in draft state. The PEP will be updated and prepared for signature approvals, which will provide an opportunity to revise the PEP to reflect early experience gained from running on institutional clusters. Going forward, the PEP will be reviewed and updated on an annual basis. These reviews will provide additional opportunities to revise the PEP based on additional experience gained through interactions with the host laboratories and the use of institutional clusters.

<u>Recommendation #3:</u> The USQCD collaboration should review its additional storage needs and strategy and propose a specific plan at a future annual review.

# Report Section: Charge 4

<u>Response</u>: Prompted by review committee suggestions, USQCD studied additional storage needs shortly after the July review. The initial focus was on archival storage needs and the economics of storing vs. recomputing specific data sets. Eigenvectors, for example, were determined to be cost-effective to store as this type of data is useful for many QCD science projects. Likewise, it is economical to archive commonly used propagators (e.g., all-to-all propagators). This analysis determined that ~10 PB of tape storage would provide adequate space for existing data sets. On the advice of the DOE LQCD-ext III Federal Program Director, the Field Work Proposal (FWP) was revised to include funding of ~\$200,000 per year through the duration of the approved program. Over the coming years, USQCD will continue to review its storage needs and data management strategy and, as recommended, develop a proposal for addressing new data storage requirements.

<u>Recommendation #4:</u> The LQCD-ext III risk register should add the risk that IC technical solutions supported by FNAL or BNL become, in the future, not optimal in performance per unit cost for LQCD computing needs.

# Report Section: Charge 4

<u>Response</u>: This risk was added to the risk register and will be reviewed and updated on an annual basis, and sooner if warranted by changing conditions. In accordance with the LQCD Risk Management Plan, a risk rating score was determined based on an analysis of probability and impact, and an appropriate risk

mitigation strategy was developed based on the rating score. The risk rating and mitigation strategy were subsequently reviewed and approved by the LQCD-ext III DOE Federal Program Director.

<u>Recommendation #5:</u> For DOE: We urge DOE to continue monitoring the usage and availability of the ICs at BNL and Fermilab to ensure that the USQCD collaboration obtains the full support and resources they need from the ICs.

## Report Section: Charge 4

<u>Response</u>: Monitoring the usage and availability of the ICs at BNL and FNAL occurs during the monthly progress call between the LQCD Computing Program and DOE Federal Project Director. On a monthly basis, the Associate Contractor Program Manager (ACPM) collects data on system availability, system usage by scientific project, and system utilization from the BNL and FNAL Site Managers. Data is collected for each IC system used by USQCD. The ACPM uses the data to create charts and graphs showing actual usage and utilization against annual plans and presents these to the DOE Federal Project Director for review and discussion. Also discussed are operational issues associated with the ICs that are relevant to USQCD usage. The Chair of the USQCD Executive Committee is also a regular participant on these monthly calls, which provides a regular and direct channel of communication between the LQCD Computing Program, USQCD, and DOE regarding usage and sufficiency of the IC resources.

<u>Recommendation #6:</u> For Fermilab/BNL: We urge both laboratories to keep ensuring that USQCD has sufficient input into the design decisions for the systems so that they will continue to provide the best possible computing environment for their projects.

### Report Section: Charge 4

<u>Response</u>: Immediately after receiving the Review Report, LQCD program management set up two meetings, one with BNL's Director of Computational Science Initiative and the other with the Fermilab CIO to discuss this issue. They assured us once again that the needs of the USQCD community will be valued in design decisions for future computing systems. Expectations regarding USQCD input into system designs will be documented in the Memoranda of Understanding (MOUs) developed between LQCD and each laboratory providing computing resources. Participation in the design process will be a continuation of current practice. Subject matter experts (SMEs) representing USQCD computing needs were directly involved in the design and planning of the most recent institutional cluster procurements at each laboratory. Specifically, these were the FY17 Skylake cluster procurement at BNL (BNL-SL) and the FY19 Cascade Lake cluster procurement at FNAL (FNAL-LQ1). Both laboratories have stated the importance of the LQCD program to their respective science programs and emphasized their commitment and support for the USQCD science program. The LQCD program management will maintain a 5-year Computing Hardware Portfolio Roadmap that communicates each laboratory's plans for future hardware deployments and documents the alignment of those plans with the USQCD science project needs.

<u>Recommendation #7:</u> For DOE: We recommend funding at the requested level for the proposed duration of the project.

### Report Section: Charge 4

<u>Response</u>: In August 2019, the DOE Office of High Energy Physics (HEP) informed the LQCD-ext III Program Manager that the proposed program of work was approved at a funding level of \$2.5 million per year for five years. This is an increase of ~\$500K above the original request. The approved budget includes \$2.3 million per year for the purchase and management of computing and data storage resources for the study

of lattice QCD (an increase of \$300K over the initial request). It also includes \$200K per year for additional data storage to provide space to archive commonly used and shared data, such as propagators (e.g., low-precision, wall-source, point-source, and random-source generators) and eigenvectors (for use in deflated solves in a number of lattice computing projects).

<u>Recommendation #8:</u> Given the exploratory nature of some of the presented activities (a promising example is PDF calculations), and the fact that theory can be fast evolving in unexpected directions over a span of several years, the DOE should consider the possibility of increasing the USQCD budget for specific new research efforts during this grant period.

## Report Section: Charge 4

<u>Response</u>: On behalf of the national USQCD community, the USQCD Executive Committee will remain cognizant of the potential for additional funding to support specific new research efforts. When a promising new research effort with potentially significant impact is identified, it will be presented to the LQCD-ext III Federal Program Director for consideration. The Federal Program Director will provide direction on how to proceed.