Lattice QCD Computing Projects
LQCD-ext and LQCD-ARRA

Response to Recommendations from the 2012 DOE Annual Progress Review of the LQCD-ext/ARRA Computing Projects

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LQCD-ext/ARRA 2012 Annual Progress Review

Response to Review Recommendations

INTRODUCTION

On May 16-17, 2012, the U.S. Department of Energy (DOE) Office of High Energy Physics and the Office of Nuclear Physics conducted an Annual Progress Review of the LQCD-ext (LQCD Extension) and LQCD-ARRA (American Recover and Reinvestment Act) projects. The review was held at Brookhaven National Laboratory and resulted in a written report that contained four suggestions and four recommendations to help improve project effectiveness and impact. This document summarizes the project response to the recommendations, along with subsequent actions taken.

RESPONSE TO RECOMMENDATIONS

Suggestion #1: USQCD, the governing collaboration of the LQCD-ext/ARRA project, presented demographic statistics that showed that the field attracts students and post-docs, but universities rarely hire them into junior faculty positions. It would benefit LQCD-ext/ARRA if USQCD could develop strategies to address this shortcoming.

This is a critical issue that is central to the health of NP and, especially, HEP theory. It is certainly not an easy problem to solve and some of us have devoted substantial energy to both creating academic positions and promoting strong lattice physics candidates. We will continue to look for new ways to increase the number of jobs in the field. One action that we think will help with this is the creation of a speakers committee to support young people for talks, as described in the response to Suggestion #3 below. We have discussed with DOE and with NSF the possibility of funding additional bridge positions in lattice gauge theory. Simona Rolli of DOE/HEP and George Fai of DOE/NP both told us that such positions can be very useful and that they supported them in principle. However, in the current state of budget reduction and uncertainty, they saw it as very unlikely to be possible for them to support in the next year or two. Keith Dienes of the NSF told us that influencing the direction of university faculty hiring is not normal operating procedure for the NSF, so that the creation of bridge positions with the NSF is very unlikely. We believe that our main activity, the deployment of the hardware and software infrastructure required for research in our field, plays two important roles in addressing this problem. First, young people use this infrastructure for physics projects that they develop themselves, which is critical for enabling their careers to blossom and making them strong candidates for junior faculty positions. Second, the infrastructure has made possible major progress in lattice gauge theory, which is crucial for convincing departments that investments in faculty positions for the field are warranted.

Suggestion #2: The review panel felt that the Scientific Program Committee, which oversees resource allocations for USQCD, would be more effective if it includes representative of the relevant experimental communities.

Ensuring that the USQCD program is maximally useful to the experimental programs of the Offices of High Energy and Nuclear Physics is one of USQCD's highest priorities, and we agree that we need to leave no stone unturned in our efforts to coordinate our programs with the experimental programs. The current operating practices of the Scientific Program Committee would not allow a straightforward implementation of this suggestion. The seven members of the SPC currently spend dozens of hours each year studying the details of 35-40 proposals to arrive at a recommended program, examining carefully the importance and feasibility of the proposed program. It does not seem reasonable to expect that level of commitment or expertise from experimental members. However, we do see ways of increasing the level of formal input from experimenters and phenomenologists into our program.

We have always solicited a lot of advice informally from our colleagues in experiment and phenomenology. We plan to formalize this input by naming a Science Advisory Board, composed of a roughly even mix of experimenters, theorists, and representatives of the SPC. (A group of experimenters and phenomenologists is already advising us in the preparation of the white papers referred to in the response to recommendation #1, below. We imagine the members of the SAB as the same type of people.) The SAB will be charged with advising the SPC and the Executive Committee on the evolution of our priorities before each allocation season, before major proposals, and when writing new white papers. It will also be invited to look at each year's physics proposals and comment as appropriate. Its members will be invited to each year's All Hands' Meetings, and to make comments there if they wish.

In fact, we have begun to change the format of the USQCD annual All Hands Meeting to make it more effective at stimulating and guiding future proposals. In the most recent meeting, members of the SPC summarized the priorities and opportunities in each of the four general areas in which USQCD supports major programs. We plan to strengthen this planning function in future meetings, encouraging presentations of future physics directions and new numerical methods from USQCD members. This portion of the meeting should provide an ideal opportunity for advice and dialogue with interested members of the SAB, who will be encouraged to attend.

Before each allocation season, the Science Advisory Board will be asked to advise the SPC and the Executive Committee on pieces of our program that may be missing, underemphasized, or proceeding too slowly. Informed by this advice, the Executive Committee may give additional political or strategic advice to the SPC. The annual Call for Proposals may incorporate new advice on priorities (for example, by stating that it would particularly welcome new proposals in a particular area). The SPC will then make its allocations consistent with these inputs.

Suggestion #3: USQCD could publicize the achievements of LQCD-ext/ARRA more effectively if it formed a speakers' bureau modeled after successful HEP/NP experimental collaborations' bureaus.

This is a good suggestion and we intend to follow it. Note that the individuals and collaborations that make up USQCD actually perform and publish the research. They presently take responsibility for publicizing their work, especially presenting it at major conferences. We believe that the review committee is correct in stating that we could publicize the achievements of USQCD more effectively by creating a central structure that would organize and oversee this important aspect of our research, and we intend to do so.

Since the people we most want to promote are people in tenure-track positions or who deserve tenure track-positions, we see this committee as being composed of people with tenure. They should be people with good connections to experiment as well. We believe that the most important targets for talks are plenary ones at the major US meetings, such as APS, DPF, and DNP. We will ask the committee to target any additional venues that it sees as appropriate. We will create a web page on our web site advertising particularly good talks we have available, with links to the talks.

Suggestion #4: USQCD would be a more potent governing body if it drafted a constitution that codifies a periodic rotation of all its leadership and executive positions based on a democratic process.

The USQCD Executive Committee was formed in 1999 at the suggestion of officials in the DOE Office of High Energy Physics. The purpose of the Executive Committee from its inception has been to lead the development of the computational infrastructure needed for the study of lattice gauge theory. Peter Rosen, then head of the Office of High Energy Physics, made it clear that if the DOE was to fund this infrastructure, it must supply the computing needs of all lattice gauge theorists in the US. Therefore, any lattice theorist in the US is eligible to be a member of USQCD, and to submit proposals for use of USQCD computational resources. Similarly, all software produced by USQCD under its SciDAC grants is publicly available. We do not negotiate with new members as to what their contribution to the collaboration will be, as is common in experimental collaborations. The full membership of USQCD does not sign the resulting physics papers, only those who have actually done the calculations. In these ways, USQCD resembles an accelerator facility like Fermilab, more than an experimental collaboration like CDF or D0. In the LQCD-ext/ARRA hardware project, members of the USQCD Executive Committee serve as advisors to the Contract Project Manager regarding the hardware needs of the US lattice gauge theory community, and oversee the allocation of the resources produced by the project. Members of the EC also serve as the Principal Investigators of USQCD's SciDAC software grants and of USQCD's INCITE grants. At present, members of the Executive Committee rotate approximately every ten years, while members of the Scientific Program Committee rotate every four years. The chairs of the Executive Committee, the Scientific Program Committee, and the

Software Committee, as well as new members of these committees, are selected by the Executive Committee.

We think that this organizational structure is very appropriate for us, and has been very successful. Lattice gauge theory calculations are typically performed by groups of five to fifteen people. Sometimes these groups work together on calculations of mutual interest. In other cases, groups have quite different ideas about the best approaches, and compete vigorously in their science, even though we all work together to create the computational infrastructure we need. We think that this competition, where it exists, has been very healthy for the US, and do not see an advantage in asking all lattice gauge theorists in the United States to agree on a single physics program. Another advantage to the current organizational structure is that sufficiently talented young people can formulate their own physics programs and apply for time on USQCD computers. The work can be conceived and carried out by a small group of post-docs independent of senior members of the field, with the resulting publications signed only be them, and not all of the members of USQCD. They can thereby establish their own physics records in a way that is not available in a very large collaboration.

The review panel suggested, "that the possibility of younger physicists obtaining permanent jobs is enhanced if they show leadership potential. The best way to show ability in leadership is to give physicists the opportunities to lead and to give them career development paths within the collaboration that increase their opportunities... The tool for doing this is a set of bylaws or a constitution. The review panel, therefore, suggested that the USQCD collaboration draft a constitution that codifies a periodic rotation (every 2 or 3 years) of all its leadership and executive positions based on a democratic process."

Our experience in university departments suggests that scientific leadership is more important in faculty hiring than bureaucratic service to a collaboration. Our current system allows young people to formulate and lead their own projects as soon as they are capable, and then to publish the results under their own names. This is an opportunity that is not found with the normal experimental collaboration organization. Further, the suggestion that all leadership positions be rotated every two or three years seems problematical to us in other ways, as well. For a group with a four to five year grant cycle, a rotation of the entire leadership every two or three years seems unwise. New members of the Executive Committee are chosen so as to maintain a careful balance between nuclear and high energy physics, between the areas of physics interest, and between labs and universities. We don't see a simple way of maintaining that in an electoral process.

We have discussed collaboration governance with several experimenters. We have examined the governance documents of UNEDF, as well as the D0, g-2, and Belle experiments, and have talked to members of CMS and CDF. We have not found any that are governed as suggested by the review panel. A model that would be closest to ours could be based on elements from D0 and g-2 governance, in which a spokesperson is elected periodically based on one or more nominations. The spokesperson then appoints the rest of the leadership positions. However, we do not see a particular advantage in reorganizing in this way, and we are hesitant to institute a *significant change to a structure that has worked well for over thirteen years in response to a suggestion that seems inappropriate given the structure and goals of USQCD.*

CONTINUED SIGNIFICANCE AND RELEVANCE

<u>Recommendation #1:</u> Each subfield within the LQCD program (precision calculations of parameters for the Standard Model, Relativistic Heavy Ion Collisions, etc.) should be tasked with providing a small number of high impact results deliverable prior to the 2014 funding renewal. The SPC should give priority in its allocation decisions to those proposals that will most likely further the program of high impact results.

We agree that the USQCD Collaboration should carefully set scientific directions and priorities for the use of LQCD-ext/ARRA resources and for the use of the allocations we receive on leadership class computers. Our process for doing so is to periodically draw up white papers describing scientific opportunities and priorities in each of the major areas in which lattice gauge theory can have a major impact in the near future. At present these areas are 1) high precision determination of parameters of the standard model, 2) high temperature QCD, 3) the structure and interaction of hadrons, and 4) theories for physics beyond the standard model. The most recent set of white papers was prepared in 2007, and is available on the Collaboration's website http://www.usqcd.org. These white papers have been prepared in advance of major requests for funding for US lattice resources, and planning for the next set of white papers has begun with the goal of completing them by the next LQCD-ext/ARRA review. The purposes of the white papers are to guide the Scientific Program Committee (SPC) in its allocation of computing resources, to guide the Executive Committee in writing proposals on behalf of USQCD and in making presentations to the DOE and its Review Committees, and to publicize the achievements and prospects of the USQCD Collaboration, as well as the field of lattice gauge theory as a whole, to the broader physics community. Other inputs into the setting of USQCD's scientific priorities come from the regular ``Lattice meets experiment'' workshops, the USQCD All-Hands meetings, and Nuclear Physics Milestones established by NSAC. The Executive Committee organizes the preparation of the white papers. It obtains input from the SPC and from experimentalists regarding scientific directions and priorities. Up to now, the input from experimentalists has been obtained informally, but starting with the coming set of white papers, we are developing a formal procedure for obtaining experimental input. The Executive Committee appoints a writing committee for each white paper, which may include both members of the Executive Committee and other experts from inside USQCD.

The SPC is charged with using the allocation process to develop a scientific program that is in accordance with the priorities set out in the most recent USQCD white papers and proposals. We think that it is crucial that resources be allocated in line with the Collaboration's priorities and goals. However, we also think that focusing solely on a small number of high priority projects would not lead to the best use of resources, and could damage the long-term physics prospects for lattice QCD in the US, for example by discouraging the development of untried methods or by impeding the ability of young people to formulate their own projects. Our present high *priority projects result from a confluence of high energy and nuclear physics (often experimental) interest, and the capability of lattice techniques to deliver a result of sufficient accuracy, with controlled errors. This latter capability is usually developed over five and sometimes ten years of research. This research often requires large-scale computer resources and is to a degree speculative - not every idea for a potentially important lattice calculation turns out to be successful. These new, and often adventurous, ideas are frequently explored by the junior physicists in the field, whose career prospects depend critically on the resources of USQCD. Clearly the SPC must balance carrying out mature calculations which immediately lead to important results and the initiation/exploration of new directions, some of which will form the basis of important calculations for future years. While the program of calculations crafted by the SPC could seem like a complex mixture of many unrelated topics, on closer examination, we believe it reflects a thoughtful balance between the substantial demands of current high-profile calculations, attempts to expand the physics reach of lattice methods and the development of new numerical strategies. These are all essential ingredients for a vibrant program in HEP and NP research using lattice methods*.

PROGRESS TOWARDS SCIENTIFIC AND TECHNICAL MILESTONES

Recommendation #2: The clusters should implement prioritized batch queues to place lower priority jobs on slower processors and to more rapidly execute the high priority calculations.

This recommendation follows from a prior comment in the review report, "[o]ne panelist had a minor criticism which was that only one of the clusters (TJNAF) used prioritized batch queues." This misunderstanding of the configuration of the Fermilab clusters resulted from a response to oral questions during the review that was not sufficiently clear.

Fermilab has operated prioritized batch queues since the beginning of the LQCD-ext project (and since the beginning of the prior LQCD project). An explanation of our job scheduling policies and batch queue descriptions follows:

Fermilab uses the Torque and Maui batch queue management software. Torque, AKA PBS (Portable Batch System), is the batch queue system which accepts, authenticates and submits jobs to the various queues setup on the Fermilab LQCD clusters. The Maui scheduler works in concert with Torque to schedule the running of jobs in queue.

At Fermilab there are a total of four LQCD clusters each differentiated by the hardware type of the cluster worker nodes. Within a cluster all the worker nodes are homogeneous and managed by a single distinct Torque and Maui installation. There is no inter-cluster routing of jobs between the different Torque installations. In principal this could be done, however, there are significant architectural differences between the various clusters, such as different core counts per node and different amounts of system memory per core, which would require users to modify significantly their run scripts so that jobs would be portable across the different clusters.

Job Scheduling Policy

The Fermilab Torque batch queue system uses the FIFO (First In First Out) policy to schedule "eligible" jobs that are in queue. An "eligible" job is one that does not violate any node limits. Per-project node limits restrict the number of nodes per cluster consumed by each project. With node limits enforced, once a project reaches its node limit, any additional jobs past the node limit submitted by the project will be considered ineligible and will not accumulate any priority while waiting in queue. Node limits avoid a situation where a project submits hundreds of jobs in queue and essentially consumes or blocks all available resources on the cluster. When free nodes are available, Maui chooses the job with the highest accumulated priority. The rate at which each job accumulates priority while waiting in the queue can be adjusted by user and by project. Within a group of jobs of equivalent accumulated priority, a first-in first-out algorithm selects the order of execution.

Job Queues

We operate four types of queues per cluster as follows:

1. *Normal: Normal queues are used for all standard running. Jobs in these queues run at normal priority.*

2. *Background: The background queues are used for background jobs that will be run when unused nodes are available. Such jobs will be scheduled at the lowest priority and will run only when there are no other jobs in the corresponding queue.*

3. *Test: The test queues are used for high priority, short jobs that require modest resources. Test queue jobs have the highest priority and will run as soon as nodes are available. A maximum of 2 test queue jobs may execute at a time, but only two per user per cluster. All test queue jobs have a maximum walltime limit of 1 hour, and a limit of 64 cores on the Infiniband clusters (i.e., 2 nodes on Ds, 8 nodes on Jpsi and 16 nodes on Kaon). On the accelerated cluster (Dsg), the limit is 2 nodes. Most benchmark or code development jobs are run under this queue.*

4. *High Priority: For high priority projects, or for a sequence of high priority jobs, we routinely set aside dedicated nodes that a particular project or user can access via a high priority queue. Users or projects using these queues are instructed to keep the nodes associated with these queues busy, and these queues are automatically monitored for any idle time. Users or projects can request such queues anytime during the allocation year, subject to the approval of the scientific liaison (currently Paul Mackenzie).*

Through the combination of node limits, user and project priority rate adjustments, and queue types, we believe we have sufficient controls to properly assign a range of priority levels to the various allocated projects. These controls can be adjusted dynamically, and in fact Fermilab staff adjust the scheduling system throughout the year.

<u>Recommendation #3:</u> In the past, the project has relied on a few simple kernels to measure system performance. The project has now modified that approach to account for overheads when using accelerators like GPUs. The project has established a GPU effective performance (GPUEP) metric for its procurements. The project should adopt this approach for tracking progress toward its technical milestones. This will allow the project to more accurately measure the improvements from new architectures such as GPU or Intel MIC. However, this requires developing a conversion that is defensible.

The simple kernels used to measure system performance on non-accelerated computing systems, and to set and measure progress against major milestones, are the conjugate gradient inverters for the asqtad and DWF actions. These kernels capture the effects on performance of memory bandwidth, floating point capability, and network bandwidth and latency. They have proven to be predictive of performance on such hardware for other actions and important parts of LQCD algorithms other than the inverter. They are not appropriate, however, for GPU-accelerated clusters or for any other heterogeneous system that is subject to Amdahl's Law effects.

After three years of observing production on the JLab ARRA GPU clusters and for the past year on the Fermilab LQCD-ext GPU cluster, it is clear that a wider range of full application timing should be used in order to capture the full range of performance. This performance range will likely vary by as much as an order of magnitude across the applications, in contrast with the maximum 30% variation observed over the years between the DWF and asqtad inverters on conventional hardware.

We propose using the following applications, all of which we believe will be available in stable form shortly:

1. *Anisotropic clover propagator production.*
2. *Anisotropic or isotropic clover gauge configuration generation.*
3. *HISQ (highly improved staggered quark) propagator production.*
4. *HISQ gauge configuration generation.*

Each of these applications would be configured to use at least 16 GPUs across at least 2 host machines. The problem size will be fixed, and the number of GPUs used on a given cluster would depend on the particular model used (e.g., 16 "Fermi" GPUs with 3 GB of memory each, or 8 K20 "Kepler" GPUs with larger memory per GPU). We will consult with experts in each area to determine lattice sizes that will fit on 16 "Fermi" GPUs and will be representative of physics production during at least the next five years. With each application we will measure the wall clock time for a standard unit of work. For propagator production this will consist of the calculation and storage of a single quark propagator, including the time to read in the necessary gauge configuration. For gauge configuration generation this will consist of the calculation of one time step, the time to read out and store the resulting configuration, and the time to read in *the necessary initial gauge configuration. In all cases the flop count necessary to do the same units of work will be determined using a conventional cluster, and from the wall clock times and flop counts effective performance in Flops/second will be calculated.*

Parallel DWF action codes are not currently available but are under development. Once these become available, DWF propagator production and gauge configuration generation will be added to these four benchmark applications.

Once codes and run scripts are available, performance measurements using these benchmarks will be performed on the existing USQCD GPU-accelerated cluster resources (9g, 10g, Dsg, 12k). Based on the observed range of performance, the project will determine the averaging type (arithmetic or geometric) and any per benchmark weighting, with the goal of determining a stable, representative performance metric. Future revisions to LQCD-ext milestones and determination of any follow-on project milestones will be based on this metric. Because GPU and many-core technologies may advance in unforeseen directions, this benchmark set may require modification at the beginning of any follow-on project to LQCD-ext.

TECHNICAL DESIGN AND SCOPE FOR FY2012-13

<u>Recommendation #4:</u> The project should evaluate establishing a method for appropriately scaling the IO subsystem (both capacity and bandwidth). This should be coupled to application needs and should reflect any expected changes in behavior. This could be based on a system characteristic like total system memory or specific applications that are particularly IO demanding.

This response also addresses these two related comments in the review report:

> *"Some sites (TJNAF) are charging for storage usage using a conversion factor to translate storage into core hours. This is useful since it creates an incentive for users to monitor and control storage usage. This should be adopted at the other sites, if feasible."*
>
> *"It may become necessary to upgrade servers at each site to provide full 10 Gb access to storage resources associated with the project. This includes both archival storage and file system storage. Some of the storage resources are already accessible at 10 Gb, but other end-points need to be upgraded so that scientists can take full advantage of the available bandwidth."*

The USQCD-ext/ARRA projects attempt to balance the funding going into the three major expense categories to yield the greatest scientific output. These categories are (1) computing capacity, (2) disk and tape resources, and (3) staff. Since the computational needs are great, computing capacity is the largest expense. Keeping the machines running at a reasonable level is also a major expense, and we do make trade-offs between up-time and total capacity so as to yield highest throughput. Thus, we typically accept 95% up-time, since achieving 99% up-time *would require additional staff and therefore less computing capacity and lower science production.*

For disk capacity and bandwidth, we make the same careful trade-offs. We procure less expensive hardware with fewer capabilities (that we don't need) and lower fault tolerance (for example, without redundant fiber-channel or Infiniband connectivity). This saves up to a factor of two in cost and results in minimal impact on computing, and provides sufficient capacity and bandwidth.

Historically, we have spent 5% to 10% of the hardware (non-staff) budget on disk servers and tape. Clearly, paying twice as much for servers to gain high fault tolerance would not be a good trade off. However, we must buy enough capacity and bandwidth to keep from idling our much more expensive compute resources. For two years the project attempted to squeeze the fraction going to disk systems to 5%, and that proved to be insufficient to meet needs. The balance is examined annually (as the detailed budget is prepared for the coming year), and the fraction has been increased to 8%, which we believe to be adequate for the current demand.

Each project allocated time on USQCD facilities must include in their annual proposal their requested quantities of disk and tape resources. The Scientific Program Committee allocates both computing time and storage based on available resources. Historically storage requests have not been reduced in allocations. The increase in the last two cycles in storage requests resulted in the increase in storage budget fraction to 8%. All allocations regardless of site are charged periodically for disk and tape utilization. The conversion between TBytes of disk and tape to core hours is modified approximately every two years to reflect relative prices of the different types of hardware. This policy encourages users to make wise use of storage resources and to plan for and communicate storage requirements.

Fermilab and Jefferson Lab host the largest fraction of the computing capacity, and both have adopted a scale-out approach for disk systems, using the open source Lustre filesystem to achieve that capability in a seamless fashion. Early on, the dominant factor was enough disk capacity to keep users productive (i.e. to not require tightly managed staging to and from tape).

More recently, I/O bandwidth has become a factor, as users have changed the mix of jobs to be more dependent upon fast I/O. In fact, some job classes require a significant amount of fast I/O and if a large number of these jobs run concurrently, the aggregate I/O bandwidth of the disk servers does not always keep up. We only detect this as it happens, as our users are more focused upon expressing the computational requirements and to some extent their disk cache requirements, and not as much their bandwidth I/O requirements. Both Fermilab and Jefferson Lab have active monitoring of Lustre activity to help detect and diagnose I/O bottlenecks.

We are doing two things to address I/O bandwidth. First, we will include I/O bandwidth as a procurement factor of higher weight (e.g. pay 5% more for 20% more bandwidth but the same storage capacity). Second, we will buy additional Lustre storage nodes, scaling out to deliver more bandwidth. Our current systems actually do have bandwidth per terabyte comparable to *much higher end systems, and so scaling out is one way to address this need. If 8% is not sufficient to yield a balanced system, we will consider increasing the storage budget fraction to 10%, and perhaps with careful tuning of system designs achieve a 50% gain in bandwidth.*

Even with these measures, the cost of acquiring sufficient bandwidth to meet possible peak requirements is not reasonable, and at times we adjust the queuing system to limit the number of extremely I/O intensive jobs that can run (or start) at the same time.

The Lustre filesystems at Fermilab and Jefferson Lab are connected to the computing clusters with DDR and QDR Infiniband. Since the review, Fermilab has upgraded the connectivity between their interactive nodes, which have DDR or QDR access to the Lustre filesystem, and the site mass storage system to 10G Ethernet, as recommended in the comments. The tape library at Jefferson Lab is connected to their LQCD clusters with DDR Infiniband.