# Report from the Executive Committee

# Paul Mackenzie mackenzie@fnal.gov

- USQCD All Hands' Meeting
- Brookhaven
- April 30-May 1, 2016

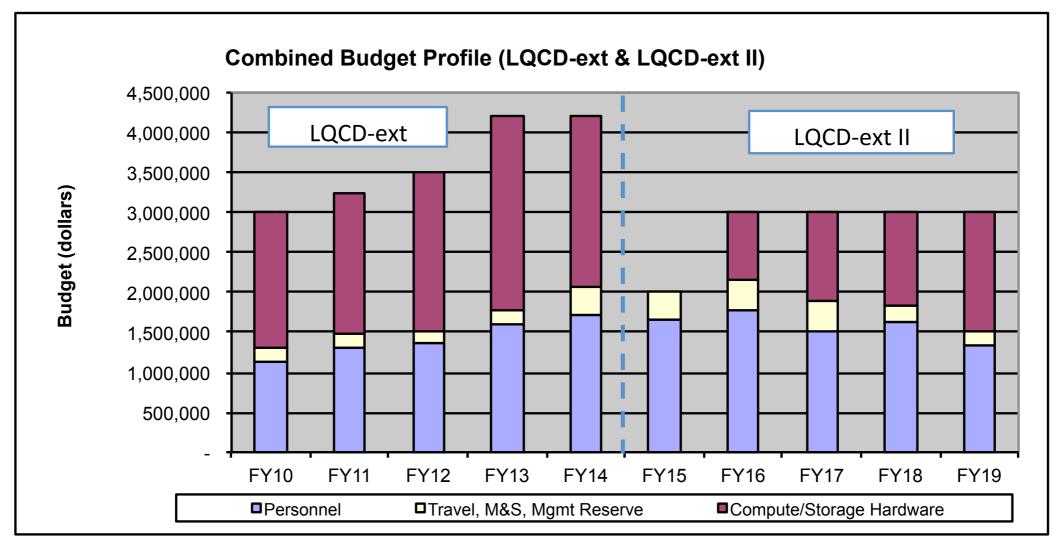


# New activities and issues this year

- Late penalties for late use of USQCD hardware
- The Exascale Applications Program
- INCITE proposal strategies
- Elections

# The LQCD-ext II Project

- \$14.0 M over five years, 2015-19.
  - Reduced from over \$4 M/year at the end of LQCD-ext.



A large amount of hardware was installed in FY13 and 14, so in the first year of the current project, there was only enough funding to operate the existing hardware, and not enought to make a significant new purchase.

# **Budget scenarios**



- Most likely, there will be negligible expansion of USQCD hardware in 2015-16.
  - How should this affect our program.
- In these days of desperate shortage of funds, it's essential to keep utilization at 100%.
  - If we don't, we look unserious to the people of whom we are asking more money.
  - We make our best friends in Germantown who are asking for more money for us look foolish.

# **Budget scenarios**



- Most likely, there will be negligible expansion of USQCD hardware in 2015-16.
  - How should this affect our program.
- In these days of desperate shortage of funds, it's essential to keep utilization at 100%.
  - If we don't, we look unserious to the people of whom we are asking more money.
  - We make our best friends in Germantown who are asking for more money for us look foolish.

We totally flopped on this in the 2015/16 allocation year.

# Late penalties

- The majority of allocated projects were unprepared to start when the allocation year began on July 1.
  - ~20% of available resources went unused.
  - Another 20% went to unallocated projects who volunteered to use time.
- To discourage this problem, we are instituting late penalties like the ones at NERSC.
  - If you don't use a certain fraction of your allocation each quarter, you are dinged an increasingly draconian amount each time.
  - See <a href="http://www.nersc.gov/users/accounts/allocations/allocation-reductions/">http://www.nersc.gov/users/accounts/allocations/allocation-reductions/</a> for details.

# Two new LQCD Project resources

#### Two new resources

- BNL Institutional cluster
  - Use of about 40 (out of 200) dual K80 GPUs.
  - Part of a move by BNL into the type of clusters that we use.
- New JLab purchase.
  - Could be KNLs, GPUs, conventional, a mixture.
  - SPC has helped poll projects on readiness.
  - Committee to help evaluate options: Rob Kennedy (chair), Amitoj G Singh, Balint Joo, Carleton E. Detar, Don Holmgren, Gerard Bernabeu Altayo, James Osborn, Robert D. Mawhinney, Shigeki Misawa, Steve Gottlieb.

# Storage

- We are spending a growing fraction of our hardware budget on storage.
  - Disk was a few % of our budget, then 5%, in FY14 8% and growing.
  - 2015: growth slowed. Good.
  - Eigenvector methods, for example, are very demanding.
- The projects have historically done a very poor job of estimating their needs.
- We should be aware that we have already sacrificed nearly 10% of our new incremental capacity in flops for storage, and should be asking whether this is what we want to be doing.
  - Are we storing propagators that could just as easily be regenerated?
  - Are we forgetting to delete data that's needed only for a short time?
  - Are we storing more multiple ensembles than necessary? (Gauge fixed...)
  - Should we be pushing the supercomputing centers to have better storage?

# Oak Ridge, Argonne, and NCSA

- USQCD also receives allocations at DoE's Leadership Class Facilities and at NSF's Blue Waters.
  - Argonne LCF: 180 M core-hours.
  - Oak Ridge LCF: 100 M core-hours.
  - Blue Waters: 30 M node-hours.
- New LCF machines expected:
  - OLCF: Summit NVIDIA GPU based. 2017?
  - ALCF: Aurora Intel MIC based. 2019
    - A smaller, Knight's Landing-based precursor, Theta, is due this year.

# LCF proposals

- Ten years ago, LCF type computers were used mainly to generate gauge configurations. Proposals were planned by the Executive Committee.
  - Propagators and physics analysis were done on commodity hardware and allocated by the Scientific Program Committee.
- With improvements in gauge algorithms and the push to physical quark masses, the most demanding analysis must now also be done at LCFs.
  - Broader input is needed to plan proposals beyond the EC.
  - This year the LCF programs in our four main subject areas will be planned by subcommittees consisting of the EC and SPC members in each subject area plus any additional people needed.

# One INCITE proposal or several?

- A single unified proposal has the advantage that we can allocate according to our own scientific judgment rather than having a committee of non-experts decide the value of different parts of our program.
  - On the other hand, a unified proposal gives us very little space explain the various sub-fields, and
  - we've had the feeling that we may be suffering from a "unitarity bound", with the LCFs limiting the size of any single proposal no matter how broad it is.
- We tried four proposals for Blue Waters last year.
  - Result: Cold QCD, thermodynamics, and BSM got zero. HEP QCD went from 30 M hours  $\rightarrow$  17.424 M hours.
- A new three-year INCITE proposal is due the end of June.
  - What's the right strategy?



# NERSC, ALCF, and OLCF application readiness and early science programs

- Leading HPC chip designers Intel and NVIDIA are moving to more and more complicated chips to push performance.
  - More cores, more complicated memory hierarchies, etc.
- Early science programs ⇒ Early access to hardware, industry, and computer lab experts.
  - → Optimized codes for inverters, configuration generation ready as soon as new machines are available.
- Adds to already close relationship we have with Intel and NVIDIA, with lattice gauge theory experts inside both companies.

- At NERSC, Cori coming this year.
  - Based on Intel Knight's Landing chips.
  - MILC, RBC, and JLab all have "NESAPs" to get ready.
- At Argonne, we have a second tier Early Science award.
  - We're getting early access to hardware and experts for "Theta", the KNLbased precursor to Aurora, but not time for actual Early Science running as we've sometimes gotten previously.
- At Oak Ridge, our Early Science proposal wasn't successful.
  - One explanation we heard was that we were so successful at the LCFs that we didn't need Early Science help.

## Software: SciDAC-3

- NP SciDAC-3 five-year grant ends in 2017.
  - ~\$1.0 M/year
- HEP SciDAC-3 three-year grant ended in 2015.
  - Two year extension approved to bring in sync with rest of SciDAC.
    - \$0.55 M/year.
- This software and algorithmic work is critical in an era when
  - Industry is moving to more and more complicated nodes,
  - Increase of hardware resources is slowing way down.

# New software program: the Exascale Applications Program

- Presidential Executive Order -- "Creating a National Strategic Computing Initiative"
  - July 29, 2015.
  - Large number of agencies involved.
- DoE Office of Advance Scientific Computing Research (ASCR) is receiving ~ \$158 M in 2016 for its part in this.
  - Many components: working with Intel and NVIDIA on hardware, system software, application co-design, and of interest to us, the Exascale Application Program.
- Exascale means, roughly, computers arriving ten years from now, 100x Mira and Titan.

# Exascale Applications Program

- Seven or eight projects funded at ~ \$2.5 M/year for four years, renewable.
- About 60 white papers (expressions of interest) were submitted.
  - Winnowed to ~ 25 projects being asked to submit full proposals.
  - Due May 20.

### USQCD Exascale team

- Proposal is being planned by a sub-committee: Rob Kennedy (chair), Paul Mackenzie, Norman Christ, Peter Boyle, Carleton Detar, Steve Gottlieb, Robert Edwards and Balint Joo.
- We're getting important assistance and participation from well-known computer scientists:
  - Bill Gropp, Chief Scientist at NCSA, Seibel chair of Computer Science at U of I, Urbana.
  - Barbara Chapman, chair of BNL computer science department, professor at SUNY Stony Brook, member or ASCAC

# Organizational odds and ends

### Users survey.

- DoE mandates that the project team take a user survey every year.
  - Only way for DoE to judge if users are happy with project management.
- Logging in to a USQCD computer during the year constitutes an agreement to complete the survey.
  - Can be done rapidly.

#### Travel funds

The SciDAC grants contain a small amount of funds for travel. This is mainly for sending software workers on software business, occasionally have a little extra available for worthy projects, such as sending young people without travel funds on physics trips to report on the USQCD physics program.

# USQCD facebook page



- Send physics results, highlights,
  - graphics and short text
  - to Martin Savage.

- Related Meetings
  - highlights, etc.
  - photos.

### Committees and election

- Current Executive Committee is Paul Mackenzie (chair), Rich Brower, Norman Christ, Robert Edwards, Frithjof Karsch, Julius Kuti, Kostas Orginos, Martin Savage, and Bob Sugar.
  - This year, David Richards -> Robert Edwards.
  - Bob is due to be replaced by Carleton later this year.
  - The Executive Committee has been rotating at the rate of about one turnover/year for the last few years. We expect to more or less continue that rate.
- Current Scientific Program Committee is Anna Hasenfratz (chair), Tom Blum, Will Detmold, Aida El-Khadra, Steve Gottlieb, Swagato Mukherjee, Kostas **Orginos** 
  - This year, Ruth Van der Water and Peter Petreczky -> Aida El-Khadra and Swagato Mukherjee.
  - Rotates at a rate of about two /year.

# **Executive Committee composition**

- A large part of USQCD's activities as a group involve developing and deploying hardware and software community infrastructure for lattice calculations.
- Executive Committee membership is weighted toward labs and large collaborations with strong expertise in delivering on these things.
- Typically, we've also had one or two members not associated with these efforts who play the role of representatives of the community at large.

- This year we have decided to choose one of this last type of member by election.
  - Terms will be two years.
  - Goals include to providing window into the Executive Committee for younger people, providing the Executive Committee with improved input from the community, and providing management experience for younger members of USQCD.
- The Executive Committee left the detailed rules of the process in the hands of the SPC.
  - Anna asked Aida El-Khadra to take charge on behalf of the SPC.
- Rob Kennedy handled the mechanics of the process using the Surveymonkey technology that the LQCD project uses for the annual user survey.