Report from the Executive Committee

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- USQCD All Hands' Meeting

- Jefferson Lab

- April 28-29, 2017

Activities and issues this year

- ## Hardware

  - Clusters: LQCD-ext II 2015-2019. Post-2019?

  - LCFs: INCITE (Argonne and Oak Ridge), Blue Waters. How should we apply?

- ## Software

  - Exascale Computing Project.

  - SciDAC 3 ends in FY2017. NP and HEP SciDAC 4 proposals submitted.

- ## USQCD organization:

  - New SPC and EC members

HARDWARE

USQCD's portfolio of hardware

|				Total M core-hours. (Unnormalized hours.)	Grand total
LQCD Project		**clusters**	DOE/HEP&NP	263	
		GPUs	"	688	
		BNL BGQ	"	116	
		Jlab KNL	"	250	
Leadership Class		**LCF INCITE**	DOE/ASCR	494	
		LCF zero priority	"		
		Blue Waters	NSF	272	
		LCF ALCC	DOE/ASCR	598	
General purpose		**NERSC**	DOE/ASCR		
				158	
					2839

The LQCD Project, INCITE, and Blue Waters were applied for by USQCD as a whole.
The physics collaborations making up USQCD also apply for time at NERSC, NSF XSEDE, ALCC ..., independently of USQCD.

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.

Combined Budget Profile (LQCD-ext & LQCD-ext II)
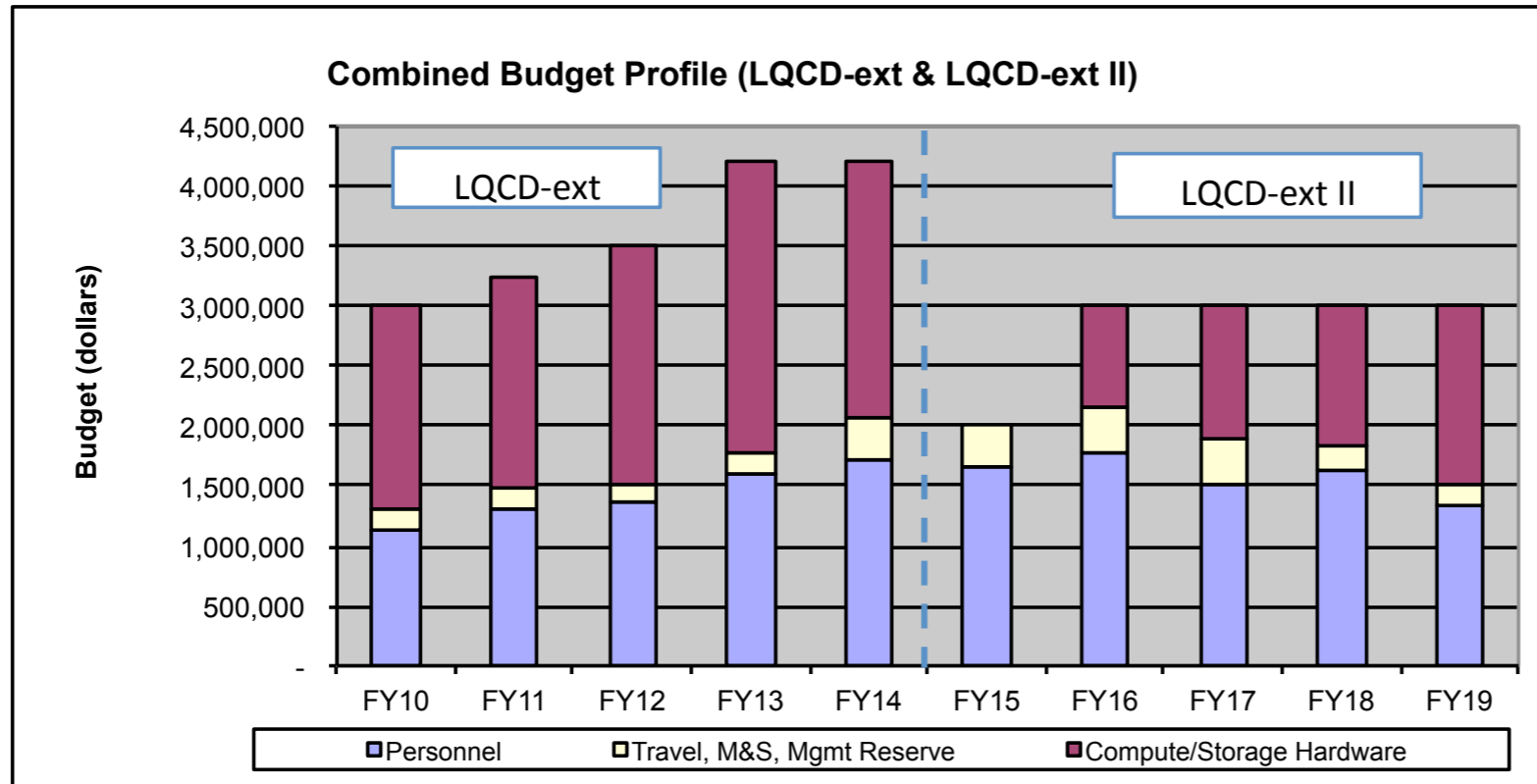
- ## Difficult budget climate is expected post-2019,

- ## Plus, current events have been happening recently.

  - ### May affect DoE budgets.

New LQCD Project resources

- JLab KNL cluster

- 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 BNL purchase.

  - Could be KNLs, GPUs, conventional, a mixture.

  - SPC has helped poll projects on readiness.

  - Acquisition Review Committee to help evaluate options: Rob Kennedy (chair), Amitoj G Singh, Balint Joo, Carleton E. Detar, Don Holmgren, Chulwoo Jung, Gerard Bernabeu Altayo, James Osborn, Robert D. Mawhinney, Shigeki Misawa, Steve Gottlieb, Chip Watson, Frank Winter, Alex Zaytsev.

- Bob Mawhinney's talk on Saturday.

LQCD post-2019

- LQCD-ext II is funded FY 2015-2019.

  - DoE has started asking for our ideas.

- DoE is interested in whether more of USQCD's program could be run at the LCFs using the software used by the LHC experiments to farm out large numbers of small simulation jobs.

  - Some thermodynamics one-node GPU jobs could probably use this.

- They're also interested in our opinion about "institutional clusters" at labs like the one at BNL.

- Time scales:

  - We'll start to discuss at the review in May.

  - New white papers and a proposal over the next year.

  - Around the end of FY 18, the review process begins with a science need review

Late penalties

- The majority of allocated projects were unprepared to start when the allocation year began in 2015.

  - ~20% of available resources went unused.

  - Another 20% went to unallocated projects who volunteered to use time.

- To discourage this problem, we have instituted 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.

  - Designed to get people's attention by making life unpleasant.

  - See   http://www.usqcd.org/reductions.html for details.

  - PIs who have gotten dinged have told us that this policy is very unpleasant, compounding the difficulty of using their allocation rapidly at the end of the year when everyone else is trying to run

Storage

- We are spending a growing fraction of our hardware budget on storage.

  - In 2016, the SPC passed on to Fermilab tape storage requests of 4X Fermilab capacity.

- We've historically done a very poor job of estimating needs.

- A tech fix is harder for tape than for disk.

- 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.

Oak Ridge, Argonne, and NCSA

- USQCD also receives allocations at DoE's Leadership Class Facilities and at NSF's Blue Waters.

  - Argonne LCF: 240 M core-hours.

  - Oak Ridge LCF: 108 M core-hours.

  - Blue Waters: 17 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 now at Argonne.

- "Exascale" machines expected

  - 2021, an initial system "based on **advanced architecture**".

  - 2023, a "**capable exascale** systems, based on ECP R&D".

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 ➜ 17.424 M hours.

- We received three-year INCITE last year.

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.

- Discussion of this topic at round table tomorrow.

- At NERSC, Cori.

  - 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 KNL-based 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

The Exascale Computing Project

- ~$160 M/year for 7 years - a billion dollar project in total.

- Nearly $2.5 M/year for us. More than SciDAC at its peak.

  - But some strings attached.

- Being managed like a construction project by the facilities part of ASCR (not the CS research part).

  - *Lots* of bureaucracy, milestones, reports, figures of merit, …

- Aimed at long-term software development.

Applications	Software technology	Hardware technology	Systems
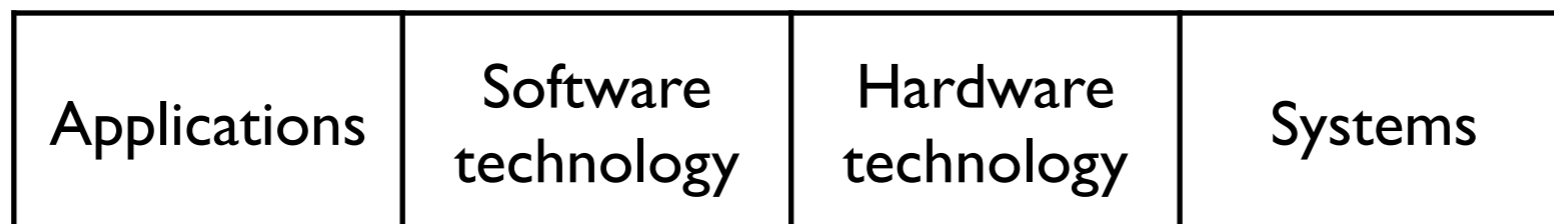
Lattice QCD
& couple dozen
other applications

- ASCR mandated a lab-based organizational structure.

- USQCD's Exascale effort is led by a steering committee which is in charge of several sub-groups:

  - Rich Brower - solvers.

  - Norman Christ - critical slowing down.

  - Carleton DeTar- software.

  - Robert Edwards - contractions

  - Paul Mackenzie (PI).

- Effort is aimed at producing application software and algorithms to run Exascale computers of ~2023 a factor of 50X faster than today's leadership-class computers Mira and Titan.

  - We're working on specific figures of merit to define this: how long does it take to create a decorrelated gauge configuration.

SciDAC

- Exascale is aimed at long-term code development, not at today's computers and calculations.

- For the immediate science program SciDAC continues to be very important.

- SciDAC 3 is ending this year.

  - We've had ~1.0 M/year from NP and 0.55 M/year from HEP.

  - We've submitted HEP and NP SciDAC 4 proposals.

Organization

Scientific Program Committee

- Current members

  - Anna Hasenfratz (chair)

  - Aida El-Khadra (chair, 2018)

  - Tom Blum

  - Steve Gottlieb

  - Swagato Mukherjee

  - David Richards (replacing Kostas)

  - Keh-Fei Liu (replacing Will)

- Rotates at a rate of about two/year.

- Class B and C proposals

  - A few got lost this year, per the user survey free form comments.

  - Class C proposals are approved by Mackenzie, Watson, or Mawhinney. Should take a few couple days to turn around.

  - Class B proposals can go to the SPC anytime. Should take a week or two to turn around.

  - If it takes longer, email to find out why.

Executive Committee

- Current members
    - Paul Mackenzie (chair),
    - Rich Brower,
    - Norman Christ,
    - Carleton DeTar (replacing Bob Sugar)
    - Will Detmold
    - Robert Edwards,
    - Anna Hasenfratz (replacing Julius Kuti)
    - Frithjof Karsch,
    - Kostas Orginos,
    - Martin Savage
- 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.

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.

- Last year we 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.

  - Will Detmold's election was announced at the last AHM. He will be replaced in another election next year.

- We are also asking the SPC chair to join the SPC while in office.

  - Goal is to improve communication between the EC and the SPC.

  - Starting in the fall, will be Aida El-Khadra.