Report from the Executive Committee

Andreas S. Kronfeld Fermilab

USQCD All Hands' Meeting Jefferson Lab I May 1–2, 2020





USQCD Executive Committee

- Richard Brower (until June 30) ۲
- Norman Christ
- Carleton DeTar
- Will Detmold
- Robert Edwards (Deputy)
- Anna Hasenfratz
- Andreas Kronfeld (Chair \Leftrightarrow Spokesperson) until September 30, 2021
- Christoph Lehner (elected junior member)
- Swagato Mukherjee
- Kostas Orginos ٠
- David Richards (ex officio, SPC Chair)

Tom Blum (starting July 1)

Chair October 1, 2021

2020 Election

USQCD Executive Committee

- Richard Brower (until June 30)
- Norman Christ
- Carleton DeTar
- Will Detmold
- Robert Edwards (Deputy)
- Anna Hasenfratz
- Andreas Kronfeld (Chair ⇔ Spokesperson) unt
- Christoph Lehner (elected junior member)
- Swagato Mukherjee
- Kostas Orginos
- David Richards (ex officio, SPC Chair)

Tom Blum (starting July 1)

Chair October 1, 2021

until September 30, 2021

2020 Election



Thanks, Rich!

Scientific Program Committee

- Alexei Bazavov
- Tanmoy Bhattacharya (Deputy)
- Jack Laiho
- Meifeng Lin
- Keh-Fei Liu
- Ethan Neil
- David Richards (Chair)
- Aida—thank you for your work on the SPC the past few cycles, particularly as Chair for two years.

- Type A proposals: this Call.
- Type B proposals: submit to David any time; response in ~1 week.
- Type C proposals: submit to site contacts; response asap:
 - BNL: Peter Boyle;



- Fermilab: Jim Simone;
- JLab: Robert Edwards.



• No response? Send follow-up.

Structure of USQCD

- Executive Committee started with SciDAC support to develop software, and soon became steward of a QCDOC and dedicated clusters.
- It now encompasses
 - LQCD ext. 3 research program;
 - NPPLC initiative;

Same SPC Overlapping hardware committees— (R. Edwards, R. Mawhinney, J. Osborn)

- INCITE allocations;
- SciDAC (NP+HEP for several cycles; now NP only);
- Exascale Computing Project (in practice, has subsumed Software Committee).

Nag, Nag, Nag

- When you (as PI) submit a proposal, you tacitly agree that, should you receive an allocation,
 - you and all active users^{*} on your project fill out the User Survey;
 - you will set up a web page describing the project's progress and publications;
 - you will acknowledge USQCD resources in publications.
- "Computations for this work were carried out with resources provided by the USQCD Collaboration, [other sources]. USQCD resources are acquired and operated thanks to funding from the Office of Science of the U.S. Department of Energy."

Confidentiality and Transparency

- The All Hands' Meeting is a collaboration meeting:
 - everything discussed here is collaboration confidential;
 - applies particularly and especially to scientific ideas and plans.
- From the CfP:

•

- "The investigators whose proposals have been selected by the Scientific Program Committee for a possible award of USQCD resources shall agree to have their proposals posted on a password protected website, available only to our Collaboration, for consideration during the All Hands' Meeting."
- Posting proposals and allocations necessary for transparency. Obviously must be treated as collaboration confidential.

Jargon

- LQCD refers to an infrastructure project; lattice QCD means the science.
- HEP refers to the Office of HEP; particle physics means the science.
- NP refers to the Office of NP; nuclear physics means the science.
- In lattice QCD, the distinction between particle physics and nuclear physics is blurry and can be both unhelpful and helpful.
- We are accustomed to periodic boundary conditions and have to cope with stovepipe boundary conditions.

Outline

- Not in this talk:
 - inventory of all USQCD computing resources (see David's talk, Bill's talk, Robert's talk, the Call for Proposals); ECP Software (see Carleton's talk and Saturday software sessions).
- In this talk:
 - HEP proposal & review for FY2020-2024 funding;
 - jeopardy policy;
 - APS Division of Particles & Fields (DPF) "Snowmass" planning;
 - diversity and inclusion;
 - INCITE.

HEP Funding for 2020–2024

Budget Outlook

- A year ago, we were encouraged to submit a Field Work Proposal from Fermilab to secure funding for institutional clusters at BNL & Fermilab:
 - budget guidance \$2.03M in FY2020, *= 1.03 escalation each year;
 - presentations to HEP July 9, 10, Cambria Hotel (Rockville, MD);
 - narrative to review panel 4–5 weeks beforehand:
 - based on the 2019 white papers;
 - available at https://www.usqcd.org/collaboration.html;
 - presentations by ASK (4), Robert Edwards, Ruth Van de Water, Zohreh Davoudi, Ethan Neil, Bill Boroski (2).

Charge

- The critical issues to be examined in the July 9-10 review include:
 - What is the scientific case for continuing simulations of [QCD] in high energy physics past 2019? Are the goals of the proposed research program aligned with the experimental and theoretical physics goals of HEP for the period 2020-2024?
 - What is the impact and interplay of lattice QCD simulations on the experimental and theoretical programs of HEP? Will the value of our experimental and theoretical programs be measurably enhanced by such simulations? Give specific examples where LQCD calculations impact the experimental program and add value to its experimental results.
 - Why is an extended project needed if the Office of Advanced Scientific Computing Research is providing the lattice community access to Leadership Class machines? In particular, is mid-scale hardware, such as CPU or GPU Institutional Clusters, essential and cost effective in such an environment? What is the optimal mix of machines, Leadership Class and mid-scale clusters, given realistic budget scenarios?
 - What are the plans at Fermilab and Brookhaven for LQCD Institutional Cluster computing? How are these plans incorporated into your proposal for the LQCD research program in 2020-2024?

Reviewers

- Maarten Golterman, San Francisco State (pheno and lattice QCD)
- Katrin Heitmann, ANL (computational cosmology)
- Patrick Huber, Virginia Tech (neutrino theory)
- Kevin McFarland, Rochester (neutrino experiment)
- Alexey Petrov, Wayne State (flavor physics theory)
- Laura Reina, Florida State (pQCD and collider pheno)
- Lee Roberts, Boston U. (Muon g-2 experimentalist)

Letters of Support

- Ed Blucher & Stefan Söldner-Rembold, Spokespersons of DUNE
- Joel Butler, Ex-spokesperson of CMS
- David Hertzog, Ex-spokesperson of Muon g 2
- Graham Kribs, Theory expert on physics beyond the Standard Model
- Fred Olness, Theory expert on parton distribution functions
- Alan Schwartz, Chair of Belle II Institutional Board
- Patricia Vahle & Peter Shanahan, Spokespersons of NOvA
- Mike Williams, Member of LHCb
- Kerstin Kleese van Dam, Director, Computational Science Initiative Brookhaven National Laboratory
- Elizabeth Sexton-Kennedy, Chief Information Office, Fermilab Directorate

Agenda

July 9					
08:30	Executive session (30 min)				
09:00	Logistics and Introductions (10 min) – John Kogut & Bill Boroski				
09:10	Overview of Scientific Program (15 min) – Andreas Kronfeld				
09:25	USQCD Governance and NP-HEP Cooperation (30 min)-Robert Edwards				
09:55	Science Talk 1: Quark and Lepton Flavor Physics (40 min) – Ruth Van de Water				
10:35	Break (20 min)				
10:55	Science Talk 2: Neutrino-Nucleus Scattering (40 min) – Andreas Kronfeld				
11:35	Science Talk 3: Fundamental Symmetries (40 min) – Zohreh Davoudi				
12:15	Working Lunch				
1:15	Science Talk 4: Beyond the Standard Model (40 min) - Ethan Neil				
1:55	LQCD-ext II: 2019 Accomplishments and Performance (40 min) - Bill Boroski				
2:35	LQCD-III: Computational Requirements and Milestones (40 min) - Andreas Kronfeld				
3:15	Break (20 min)				
3:35	LQCD-ext III: Institutional Cluster Computing & Operations Model (40 min) - Bill Boroski				
4:15	Summary (15 min) – Andreas Kronfeld				
4:30	Executive Session (60 min)				
5:30	Committee request for additional information – John Kogut / Proposal Leadership				
5:45	Adjourn				

How did it go?

- Hard questions about management:
 - If it is not a "project", why do you need Bill and Jo?
 - Theorists unsuited for negotiating Memoranda of Understanding.
 - What do you do if a lab loses interest?
 - Vigorous, heartfelt support from BNL (Eric Lançon, on behalf of Kerstin Kleese van Dam) and Fermilab (Liz Sexton-Kennedy).
- Hard questions about science during talks, but none for homework.
- Alternative budget scenarios: if +10% or so, it would be worthwhile to procure large archival storage (10s of PBytes).

Outcome (quoting Executive Summary)

"..., the review team was asked to either endorse the present funding scenario of \$2M/year (with annual escalations tied to inflation) or modify this level based on additional needs or deficiencies of the LQCD effort. The review team was very favorably impressed by the LQCD-ext III proposal and the presentations at the July 9-10 review. The review team unanimously endorsed the proposed \$2M/year plan but directed HEP to consider additional funds for storage needs at an approximate level of \$200,000/year. This recommendation was based on information provided by USQCD at the review which demonstrated the value to the world wide lattice gauge theory community of sharing lattice configurations in an open fashion. Although the physics goals of the next five years will be considerably different from those of the past five years, the LQCD-ext III team convinced the reviewers that their plans presented in their proposal were well aligned with the HEP experimental program and would, in fact, be unique and vital to those interests. The computational strategy of the team was strongly endorsed by the reviewers and the essential need of mid-scale computing resources to analyze the gauge configurations produced by simulations on Leadership Class machines was validated."

Recommendations & Reactions

- "For Fermilab/BNL: We urge both laboratories to keep ensuring that USQCD has sufficient input into the design decisions for the [institutional clusters] so that they will continue to provide the best possible computing environment for their projects."
- "For DOE: We recommend funding at the requested level for the proposed duration of the project."
- "..., the DOE should consider the possibility of increasing the USQCD budget for specific new research efforts during this grant period."
- John Kogut immediately directed us to modify the FWP to \$2.2M/year to include the proposed storage facility.
- In September 2019, DOE-HEP provided \$2.5M/year for FY2020–2024.

Jeopardy Policy

Problem & Solution

- The Allocation Year (AY) starts July 1 difficult to change.
- July and August almost always suffer from under-usage:
 - new users (at a given site) need time to ramp up;
 - Independence Day holiday (?) and summer travel.
- Fixes:
 - rolling start in June—as soon as SPC announces allocations each site gives its new users a Type C project;
 - fewer nodes contracted in July & August w/ BNL & Fermilab;
 - jeopardy policy: run at pace or you will lose allocation;
 - start AY July 15 (useful?).

Remarks

- A cycle lost is a cycle lost:
 - It is inefficient to stop running to look for ~20% better performance.
 - It is the site managers' job to enforce fairness in the queue.
 - If run problems arise, notify the helpline!
 - Take your run plan (the one in your proposal) seriously—it tells you what to do until exceptional circumstances arise:
 - revise it when you learn your allocation (as requested by SPC);
 - "We will use 25% of our allocation each quarter" \neq run plan.
 - Especially in the "institutional cluster" model, lost cycles review poorly.

DPF Planning aka "Snowmass"

DPF "Snowmass" Study

- The APS is embarking on a ~year-long long-range planning exercise.*
 - Will be followed by a DOE-NSF Particle Physics Project Prioritization Panel.
- Kick-off meeting at Fermilab November 4–6, 2020.
- Website with lots of information: Snowmass2021.
- Ten frontiers:
 - Energy Frontier
 - Rare and Precision Frontier
 - Theory Frontier
 - Instrumentation Frontier
 - Underground Facilities

- Neutrino Physics Frontier
- Cosmic Frontier
- Accelerator Frontier
- Computational Frontier
- Community Involvement

*Until early 2000s, such Studies often centered on a three-week workshop in Snowmass, CO.

USQCD Involvement

- Aida El-Khadra = Theory Frontier Convener
- Steve Gottlieb = Computing Frontier Convener
- Several topical group leaders:
 - Huey-Wen Lin (EF.PDFs), Swagato Mukherjee (EF.heavy-ions);
 - Stefan Meinel (RPF.HQ), Tom Blum (RPF.fun);
 - Zohreh Davoudi, Taku Izubuchi, Ethan Neil (TF.LGT), Simon Catterall (TF.QIS);
 - Peter Boyle (CF.theory), Phiala Shanahan (CF.ML), Martin Savage (CF.QC).
- Representative to "Snowmass Young" nominated.
- USQCD EC will submit "Letter of Interest" and a report based on WPs.

Diversity and Conclusion

Inclusion and Diversity

- We want every member of USQCD to feel welcome in every activity of the collaboration:
 - AHM (including the CfP) is the highest profile, but also, for example, we openly solicited participation in the white papers.
- Starting now, we are adopting a code of conduct based on the one adopted for Lattice 2019^{*}. *We apologize for not making it explicit during registration; please abide even so.
- We all work in collaborations that are diverse (often because of international connections)—
 - even so, many segments of US society are clearly underrepresented in the upper echelons of US academia.
 - Can USQCD attract US undergraduates to computational science as a springboard to careers in academia and industry?

Committee on Diversity and Inclusion

- Will Detmold (chair), Joel Giedt, Huey-Wen Lin, ASK (ex officio) plus:
 - some of you!
 - Will also chairs the Lattice^{*} Diversity and Inclusion Committee.
 - Joel secured an NSF grant to organize summer schools to attract undergrads to computational science, with explicit outreach to underrepresented communities.
 - Huey-Wen is the initiator of the "Women in Lattice QCD" luncheon.
- The committee does not yet have a charge—we want to hear from you before writing it: the committee (by definition) must be inclusive and seek a diversity of opinion!

i.e., the annual Symposium on Lattice Field Theory

Committee on Diversity and Inclusion

- Will Detmold (chair), Joel Giedt, Huey-Wen Lin, ASK (ex officio) plus:
 - some of you!
 - Will also chairs the Lattice* Diversity and Inclusion Committee.
 - Joel secured an NSF grant to organize summer schools to attract

Topic for following discussion

- Huey-Wen is the initiator of the "Women in Lattice QCD" luncheon.
- The committee does not yet have a charge—we want to hear from you before writing it: the committee (by definition) must be inclusive and seek a diversity of opinion!

i.e., the annual Symposium on Lattice Field Theory

INCITE

INCITE

- Innovative and Novel Computational Impact on Theory and Experiment
 - Allocates ~60% of computers at the DOE-ASCR Leadership Class Facilities, Argonne LCF and Oak Ridge LCF. (Rest via ALCC and ECP.)
 - ALCF: Theta, 4,392 64-core KNL nodes w/ Cray interconnect.
 - OLCF: Summit, the most powerful open computer in the U.S.:
 - 4,608 nodes;
 - each with 2 IBM Power9 CPUs and 6 NVIDIA Volta V100 GPUs;
 - Mellanox EDR 100G InfiniBand communications network.
- Open to researchers worldwide—focus on high-quality science (*cf.* ALCC, where high-quality science must also be DOE-mission oriented.

INCITE

- Innovative and Novel Computational Impact on Theory and Experiment
 - Allocates ~60% of computers at the DOE-ASCR Leadership Class Facilities, Argonne LCF and Oak Ridge LCF. (Rest via ALCC and ECP.)
 - ALCF: Theta, 4,392 64-core KNL nodes Aurora coming in 2021!
 - OLCF: Summit, the most powerful open

Frontier coming in 2021!

- 4,608 nodes;
- each with 2 IBM Power9 CPUs and 6 NVIDIA Volta V100 GPUs;
- Mellanox EDR 100G InfiniBand communications network.
- Open to researchers worldwide—focus on high-quality science (*cf.* ALCC, where high-quality science must also be DOE-mission oriented.

USQCD and INCITE

- USQCD Charter: "USQCD members should not appear as PIs or Co- PIs on competing proposals. These USQCD proposals can be found on the collaboration web site: http://www.usqcd.org/."
- In addition to the proposals for dedicated (or institutional) clusters, USQCD proposals have included proposals to INCITE, but not ALCC or NSF machines (except, for a while, Blue Waters at NCSA).
- For a long time, 3-year "omnibus" proposals covering flavor, BSM, hot, cold.
- 2018: additional proposal (Orginos, PI) on hadron structure.
- 2019: 5+1 proposals for Summit & Mira (ALCF BG/Q; third year of an omnibus proposal w/ Mackenzie, PI). PIs = Christ, Brower, Mukherjee, Edwards, Orginos.
- 2020: one omnibus again.

INCITE and USQCD, Lattice QCD

Year	Approved	Summit node-hours	%-age	USQCD %-age	Lat QCD %-age
<u>2019</u> 30 awards,	USQCD Hot, dense	900,000 4th (tie)	6.4	12.4	17.4
totalling 14,064,000	USQCD Flavor	850,000 6th (tie)	6.0		
Summit node-hours	CalLat	700,000 9th (tie)	5.0	0	
<u>2020</u> 39 awards,	USQCD Omnibus	750,000 5th	3.9	3.9	
totalling 19,000,000	Ratti/Fodor Thermo	510,000 13th	2.7	0	9.3
Summit node-hours	CalLat	500,000 14th (tie)	2.6	0	

Remarks

- If the 2019 outcome was disappointing (no cold nuclear physics or BSM), 2020 was worse.
- We learned that the review panel learned to love reading several complete proposals rather than one super-terse one—
 - impossible to explain the USQCD program in 15 pages;
 - 2020 panelists unhappy: the plans weren't complete, but USQCD must receive an allocation;
 - unhappiness can be measured in the size of the allocation.
- The EC thus favors submitting $N_P \ge 4$ proposals this year:
 - N_P to be decided after consulting you at this AHM.

2021 Framework

- Quark & lepton flavor physics: Fermilab/MILC and RBC/UKQCD submitted joint ALCC proposal; one INCITE proposal (for this topic) also seems to optimize size and distribution of computing resources.
- BSM: reviews well but viewed as exploratory, which suggests aiming for Theta and, perhaps, a modest Summit allocation.
- Hot, dense QCD: INCITE always has a project in QCD thermodynamics; may as well be USQCD.
- Cold nuclear physics: best strategy not at all clear.

2021 Framework—Cold Nuclear Physics

- One proposal runs risk of being viewed as insufficiently specific, like the omnibus proposals.
- Several proposals will compete with each other (and CalLat), and leave most proposals unsuccessful.
- Clover ensemble generation serves most (all?) cold NP researchers in USQCD.
- CalLat's proposals focus on physics (using ensembles from MILC, Sierra, or Europe).
- Collaboration responsibilities (all and EC):
 - cold NP researchers have most at stake, hence most say;
 - others provide advice and support.

2021 Framework—Cold Nuclear Physics

- One proposal runs risk of being viewed as insufficiently specific, like the omnibus proposals.
- Several proposals will compete with each other (and CalLat), and leave most proposals unsuccessful.
- Clover ensemble generation serves most (all?) cold NP researchers in

Big topic for following discussion

Europe).

- Collaboration responsibilities (all and EC):
 - cold NP researchers have most at stake, hence most say;
 - others provide advice and support.

Thank you

Thank you



← Bob Mawhinney Dean of Science, Columbia U.

> Chip Watson → happily retired



Backup

Whitepaper Coordinators

- Hot-dense Lattice QCD
- Hadrons and Nuclei
- Fundamental Symmetries
- Neutrino-Nucleus Scattering
- Quark and Lepton Flavor Physics
- LGT for Physics BSM
- LGT Calculations: Exasale and Beyond

Frithjof Karsch & Swagato Mukherjee

Will Detmold & Robert Edwards

Zohreh Davoudi & Vincenzo Cirigliano

ASK & David Richards

Christoph Lehner & Stefan Meinel

Rich Brower, Anna Hasenfratz, Ethan Neil

Balínt Joó & Chulwoo Jung

USQCD Scientific Advisory Board

- Current members:
 - Ayana Arce (Duke, ATLAS)
 - Daniel Cebra (UC Davis, STAR)
 - Lawrence Gibbons (Cornell, mu2e)
 - Krishna Rajagopal (MIT, theory)
 - Alan Schwartz (Cincinnati, Belle 2)
 - Matthew Shepherd (Indiana, GlueX, BES III)
 - Jure Zupan (Cincinnati, theory)



