

Report from the Executive Committee

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USQCD All Hands' Meeting
Brookhaven
April 19-20, 2013

Happening this year

- LQCD-ext underway, LQCD-3 being considered by DoE.
- SciDAC-3 underway.
- New leadership class hardware.
 - Mira, Titan, Blue Waters
 - 10x more powerful
- New USQCD white papers; evolving experimental and experimental facilities landscape.
- Priorities and organization of USQCD



The LQCD Project

- LQCD-ext is well underway
 - \$18.5 M over five years.
 - 2010-2014
 - Sited at Fermilab, JLab, BNL
 - In 2013, installed 21.9 TF 1/2 rack BG/Q at BNL for mid-sized jobs; 12.6 TF node Infiniband cluster being purchased at Fermilab.
 - Brings total of LQCD-ext and LQCD-ARRA to 153.3 TF + GPUs.
- LQCD-ARRA at JLab is ended.
 - \$4.96 M.
 - Sited at JLab.
 - Hardware installation is completed, operations subsumed into LQCD-ext.



The LQCD Project

- Annual QCD-ext hardware review is at JLab in three weeks.
 - Need 2012 project web pages for all Class A projects. (See <http://www.usqcd.org/projects2012.html> to see if Alicia (alicia@fnal.gov) has a link to your project page.)
- LQCD-3, extension of the project in 2015-19 is beginning consideration by DoE.
 - Proposal just submitted.
- New white papers setting forth the scientific case for lattice calculations in the next five years. See <http://www.usqcd.org/collaboration.html> .
 - New look at scientific priorities. (More later.)



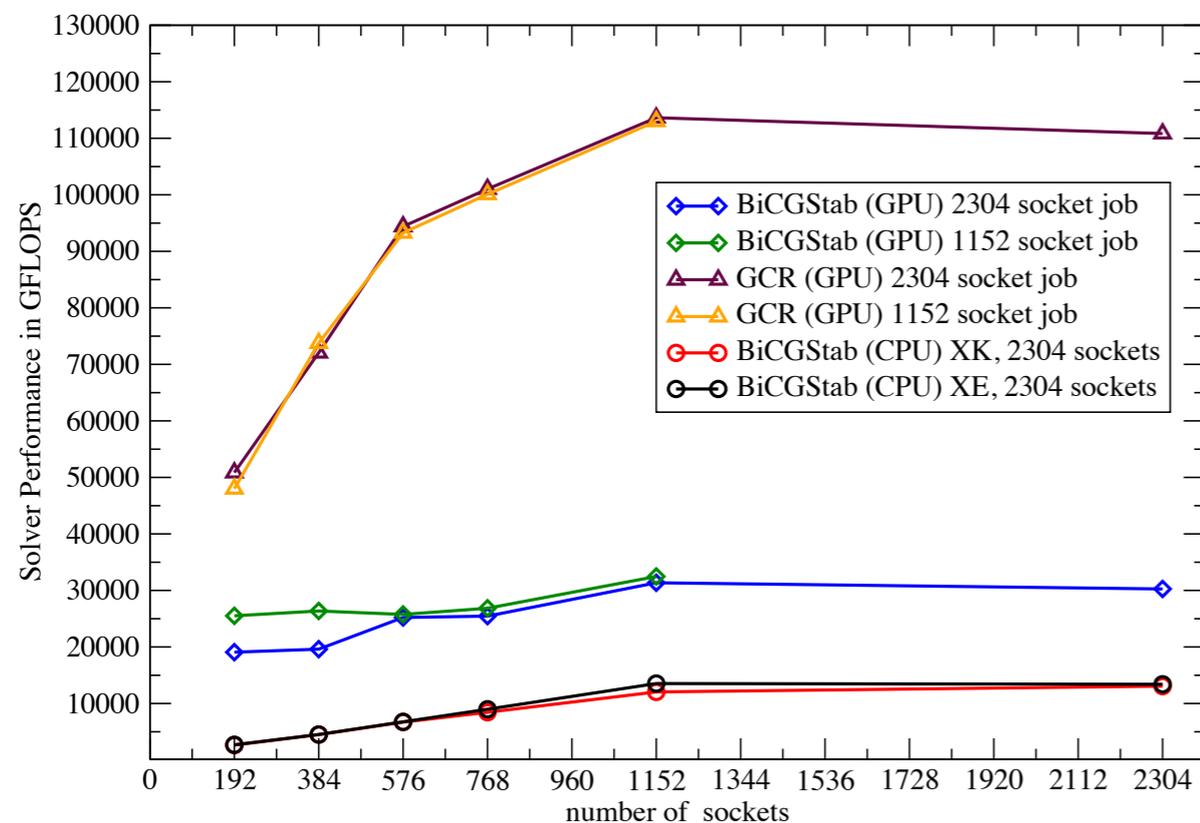
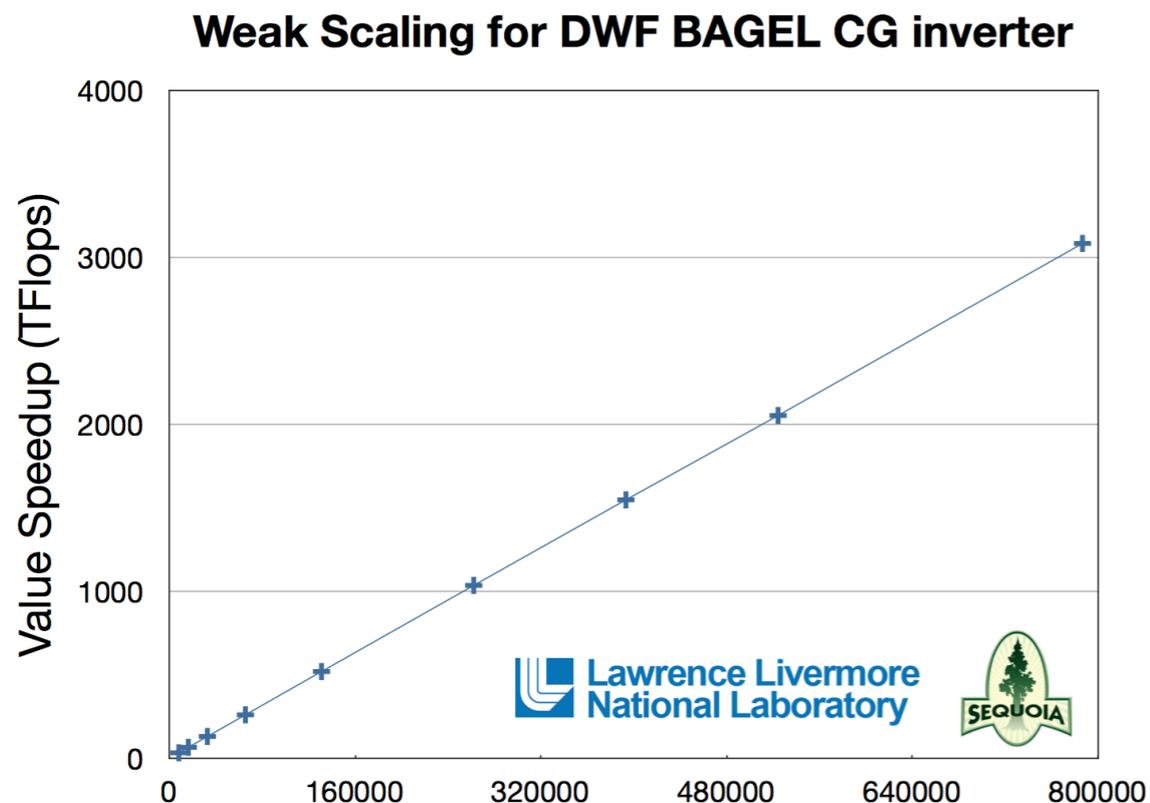
New leadership class hardware

- **INCITE: Argonne Leadership Computing Facility (Mira)**
 - 40 rack BG/Q, ~ 10 PF Peak.
 - ALCF is looking for ~ 30 projects that can use ~20% of machine at a time; average allocation 100 M hours (ours is 250 M hours on BG/Q, 40 M on BG/P). Early Science has finished and allocated running is underway.
- **INCITE: Oak Ridge LCF (Titan)**
 - Cray, 18,688 GPUs, 300K cores. ~ 10 PF peak?
 - Similar allocation policies to ALCF. (Our allocation, 140 M hours. Allocated running is underway.)
- **NSF: NCSA (Blue Waters)**
 - Cray, 3072 GPUs, 380 K cores. ~ 10 PF peak?
 - Allocations policies opaque. Currently they are having us run on a proposal written in 2008, generating gauge configurations (HISQ and anisotropic clover. (We don't know long term proposal and allocation procedure.)



New leadership class hardware

Total performance on BG/Q



Performance/GPU on Titan



SciDAC-3

- SciDAC-3 began in 2013
 - NP, 2013-2017. \$1.00 M/yr.
 - HEP, 2013-2015. \$1.075 M/yr.
 - Goals and progress are coordinated to maximize the usefulness of both projects for both communities.
- Most pressing priorities this year are preparing codes for the new machines: BQ/Q, Titan...
- Other new priorities in SciDAC-3: software for BSM calculations, measurements.
- Discussion this afternoon: coherence of the software and hardware program with the physics program.
 - How do we optimized them? How are the results?



Science goals

- The official science goals of USQCD are given in its white papers and proposals, organized by the Executive Committee, with inputs from the Scientific Program Committee and the broader lattice, particle physics, and nuclear physics communities.
- For the 2013 white papers, we solicited input on our proposed program from a kitchen cabinet of experimenters, phenomenologists, and theorists.
 - Going forward from 2013, we plan to formalize this process.
- At this meeting, we plan to discuss the methods and outcomes of the current process.



The EC and SPC members

- Current EC members are Paul Mackenzie (chair), Rich Brower, Norman Christ, Frithjof Karsch, Julius Kuti, John Negele, David Richards, Martin Savage, and Bob Sugar.
 - Steve Sharpe -> Martin Savage in 2013.
- Current SPC members are Robert Edwards (chair), Simon Catterall, Will Detmold, Taku Izubuchi, Doug Toussaint, Peter Petreczky, Ruth Van de Water.
 - Martin Savage -> Will Detmold in 2013.



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.



Scientific Priorities and Allocations: Current procedures

- The Scientific Program Committee (SPC) allocates all USQCD computing resources.
- It is the responsibility of the Executive Committee, in consultation with the SPC and the community, to put forward compelling physics programs in proposals.
- It is the responsibility of the SPC to accomplish the goals of a given proposal, bearing in mind the goals of the funders.
- E.g., [charge number 1](#) to the May 9-10, 2013, [LQCD annual review](#) panel is as usual to [evaluate](#):
“The continued significance and relevance of the LQCD-ext project, with an emphasis on its impact on the experimental programs’ support by the DOE Offices of High Energy Physics and Nuclear Physics;



Scientific Priorities and Allocations: Current procedures

- The Executive Committee consults with the SPC and the community to create a compelling program of physics for the proposal.
- USQCD does not apply as a collaboration for resources at NERSC or on NSF supercomputers less powerful than Blue Waters. Of course, sub-groups within USQCD can and do apply for these resources.



Evolving experimental landscape

- New five-year LQCD Project proposed
- Evolving experimental situation
 - LHC find no BSM, but a Higgs consistent with the SM
- Evolving experimental facilities situation
 - FRIB becoming closer
 - Flavor factories close
 - New search for BSM in muon $g-2$ getting closer
- How should USQCD program and organization react?



Evolution of USQCD organization

We have always informally sought experimental input in formulating our programs. We are now formalizing that.

- Planned Science Advisory Board
 - Roughly even mix of experimenters, phenomenologists, and representatives of the SPC. It will 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.
 - 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.
 - An experiment.



Discussion of scientific goals

- Current goals
 - At this year's All Hands Meeting, this SPC has asked members of the white paper committees to describe the goals in each area and the process by which they were set
 - These will be followed by reports from projects in each area.
 - A member of the SPC will then discuss how the current goals are reflected in this year's allocated program.
- Questions for discussion
 - Are the current stated goals in the white papers near optimal?
 - Are the goals optimally embodied in this year's scientific program?
 - If not, in either case, how could the process be improved.
 - Should the year's science program be more centrally mandated or more proposal driven?
 - Should the program of ensemble generation be more centralized?

Discussion tomorrow afternoon, Saturday.



Role of hardware and software programs

- How do the hardware and software programs function to advance the goals of the collaboration?
 - How is the current system working?
 - How could it be done better?

Discussion at 5:00 today, Friday.



OLD

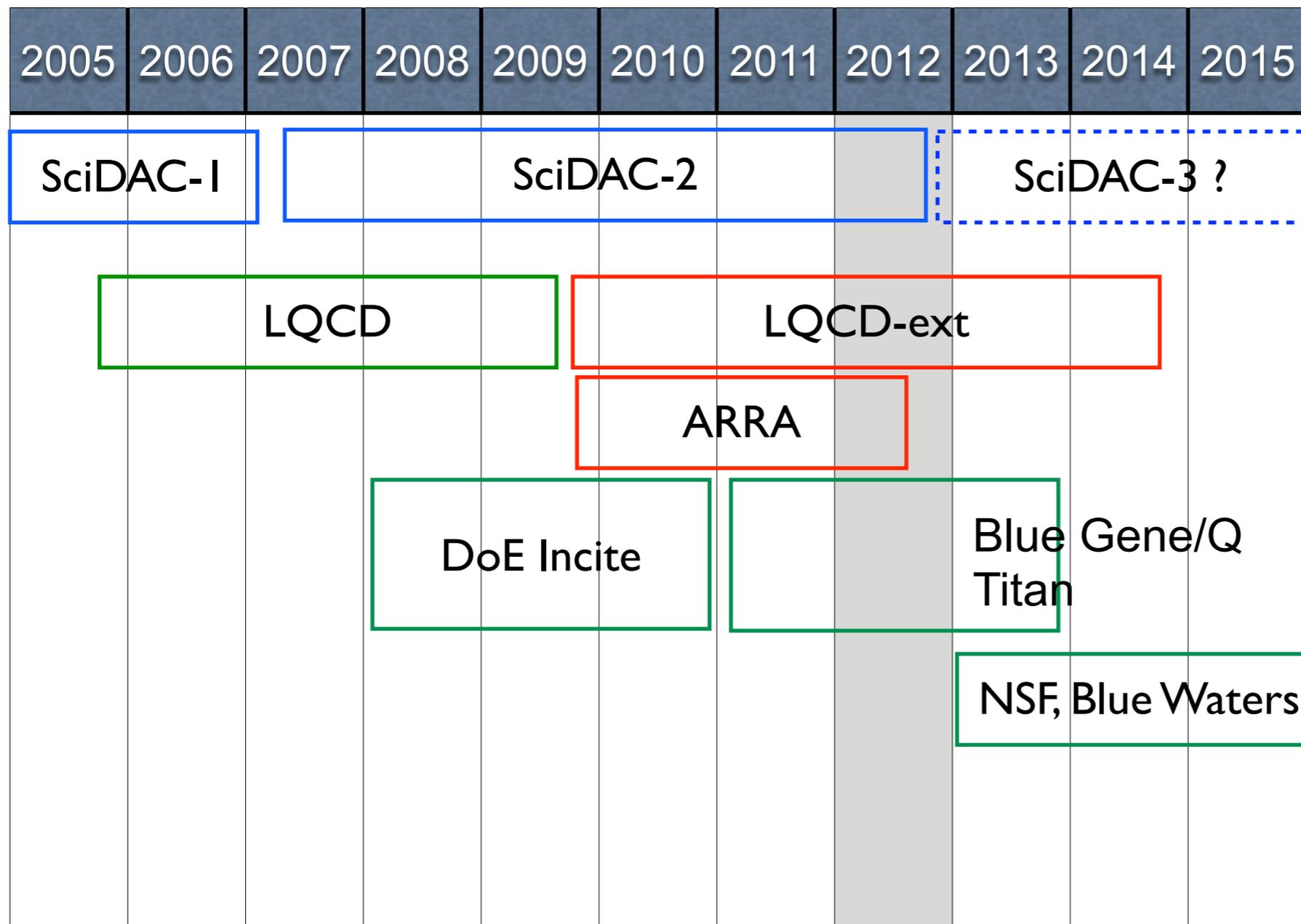


Outline

- LQCD-ext Project, 2010-2014
- LQCD-ARRA Project, 2009-2012
- Current INCITE Grant
- SciDAC-2 Grant, 2006-2011
- Surveys
- Travel Funds
- Coming INCITE and NSF resources



USQCD projects



Software

Capacity hardware

Capability hardware



The LQCD-ext Project, 2010-2014

- Project budget of \$18.15 M over five years.
- Areas of scientific emphasis
 - Fundamental parameters of the Standard Model, and precision tests of it.
 - The spectrum, internal structure and interactions of hadrons.
 - Strongly interacting matter under extreme conditions of temperature and density.
 - Theories for physics beyond the Standard Model.
- The proposal envisioned access to the DOE's leadership class computers as an essential component of the full program.



The LQCD-ext Project, 2010-2014

- 2010/11 hardware at Fermilab.
 - Ds: 421-node, 13,440-core, quad-socket, 8-core Infiniband cluster.
 - Dsg: 76 nodes, 152 Fermi GPUs. (Don's talk.)
- 2012 hardware at JLab.
 - 12s: 212 nodes, each dual-socket eight-core 2.0 GHz Intel,
 - additional mixture of nodes and Kepler (we hope) GPUs. (Chip's talk.)
- 2012 hardware at BNL
 - Use of 10% of a Blue Gene/Q rack at BNL. (Bob M.'s talk.)
- 2012 Project annual review in two weeks at BNL.
 - We need from each physics project PI
 - updated publication lists,
 - updated project web pages.

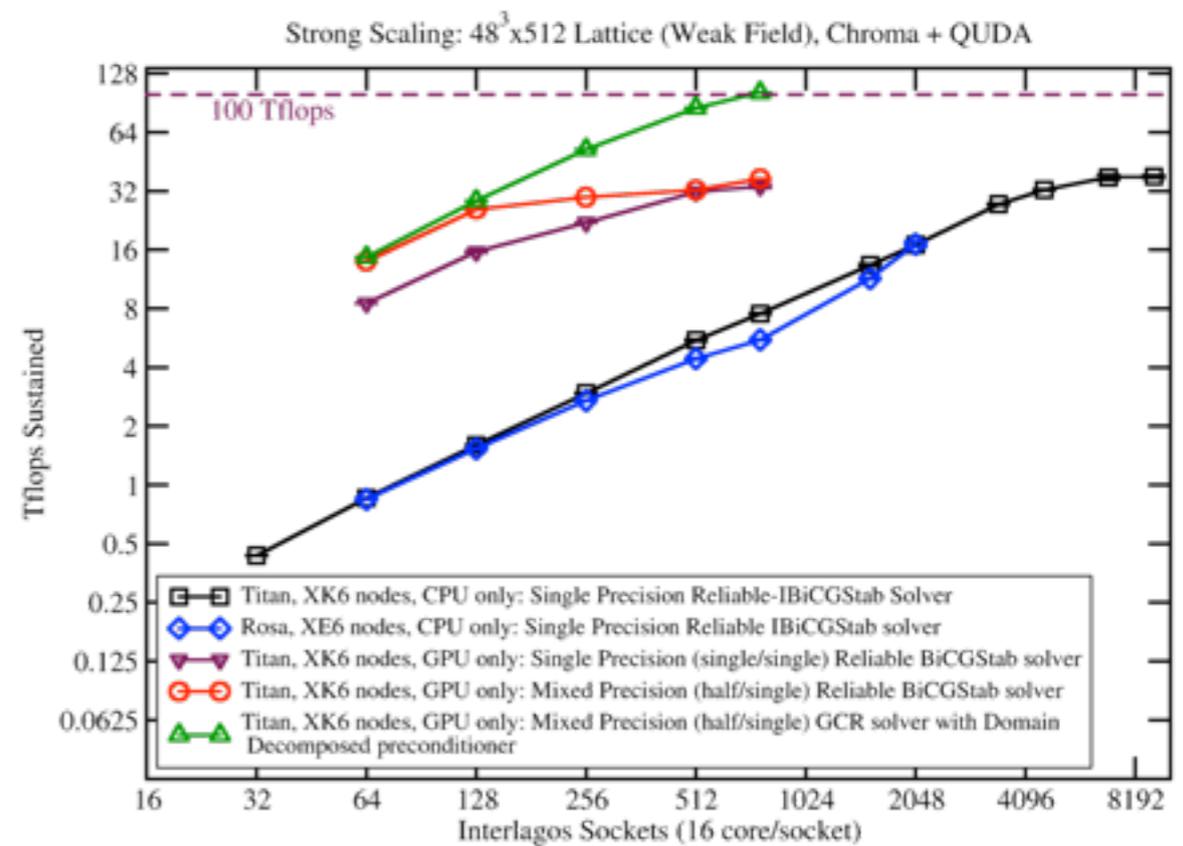


The LQCD-ARRA Project

- Separate project from LQCD-ext;
 - project management have been separate and parallel to LQCD-ext.
 - Resources have been managed for science as a coherent whole.
 - Project will be brought to close in 2012, operations folded into LQCD-ext.
- Sited at JLab, budget of \$4.96 M.
 - Combined budgets for the LQCD-ext and LQCD-ARRA projects around \$23 M, as we originally proposed. (Compared with ~\$9.2 M for LQCD Project.)
- Infiniband clusters 9q and 10q.
 - ~500 nodes, dual quad core Infiniband cluster.
- GPUs
 - 480 GPUs of several types.
 - Both Tesla (scientific) and gaming cards



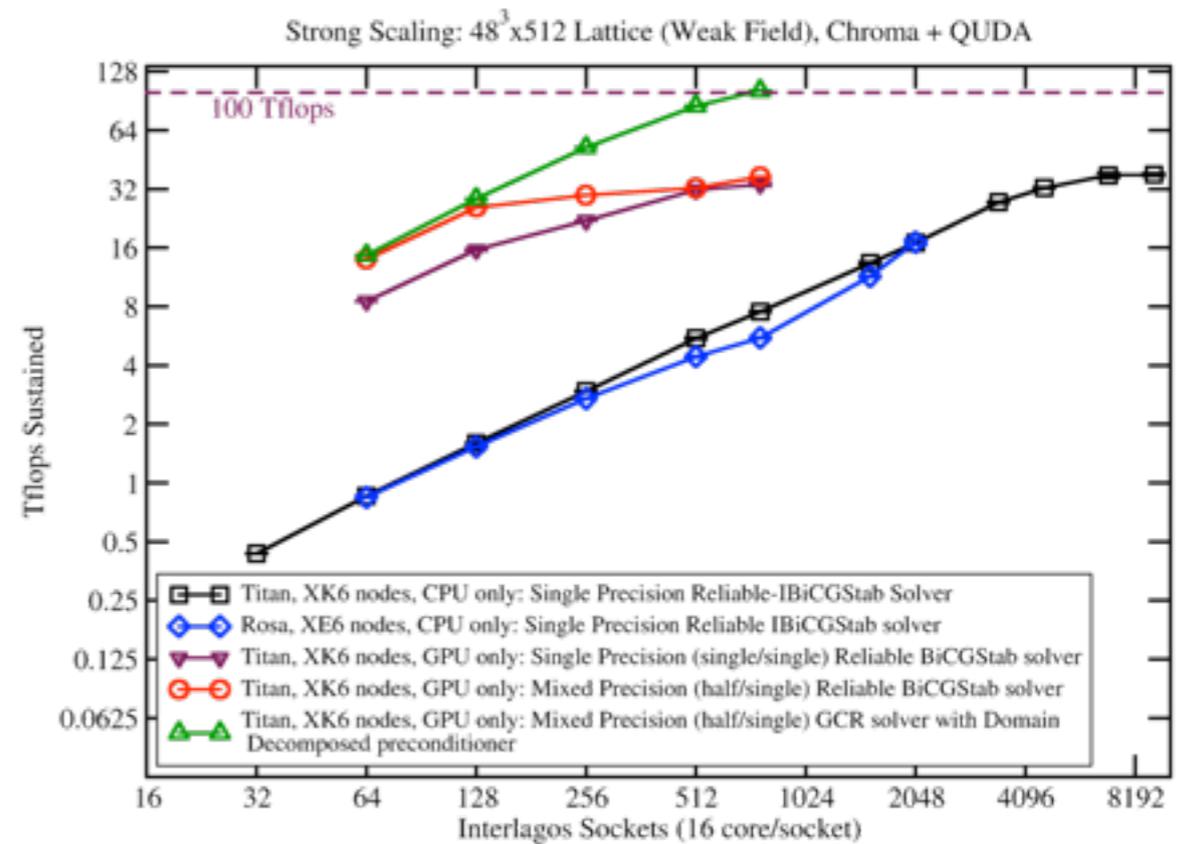
GPU progress



Clark and Joo, ACS Symposium, 2012

- Much progress with GPU codes this year.
 - Decent strong scaling on $48^3 \times 512$ run with 4-D decomposition.
- It's clear that GPUs can handle part of our capacity needs very well. How big is that part?
 - Current plan is for the FY12 12s to be supplemented with additional GPUs.
 - FY13 purchase could include clusters, accelerated clusters, or BG/Q. Benchmarking information by June would have maximum usefulness.

GPU progress



Clark and Joo, ACS Symposium, 2012

- The Project needs community input on metrics for several GPU-related quantities:
 - What fraction of GPU-enabled hardware should be contained in new purchases?
 - Moving target now as GPU use is just ramping up.
 - How should GPUs be related to CPUs in allocations?
 - Charge units could be based on current price of hardware.
 - How should we report the CPU power of a system including GPUs to the DoE?
 - Effective core-hours delivered by GPUs could be based on core-hours that would have been required to do the same calculation on CPUs.

USQCD INCITE Award

- Time on the DOE's leadership class computers, the Cray XT5 at ORNL and the BlueGene/P at ANL, is allocated through the INCITE Program.
- USQCD has a three-year grant from Jan. 1, 2011 to Dec. 31, 2013.
- Ours is one of the three largest allocations for 2012. It consists of:
 - 50 M core-hours on the ANL BlueGene/P, plus zero-priority time (130 M ch in 2012),
 - 46 M core-hours on the ORNL Cray XT5.
- In 2011 the Cray is being used to generate anisotropic–Clover gauge configurations. The BG/P has been used to generate Asqtad and DWF gauge configurations and to do analysis on those configurations.
- New INCITE-managed resources coming in 2013 (later).



USQCD INCITE Award

- At ALCF in 2008, USQCD was one of first projects ready to go, only one with three-year program mapped out.
- In one year we accomplished a three-year program of asqtad ensemble generation and the creation of DWF ensembles with a second, fine lattice spacing. We used 359 M core-hours in '08 (~1/3 of BG/P cycles), 279 M in '09, 187 M in '10, 180 M in '11.
- Thanks Software Committee: James Osborn, Chulwoo Jung, Balint Joo ...



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Committee Members

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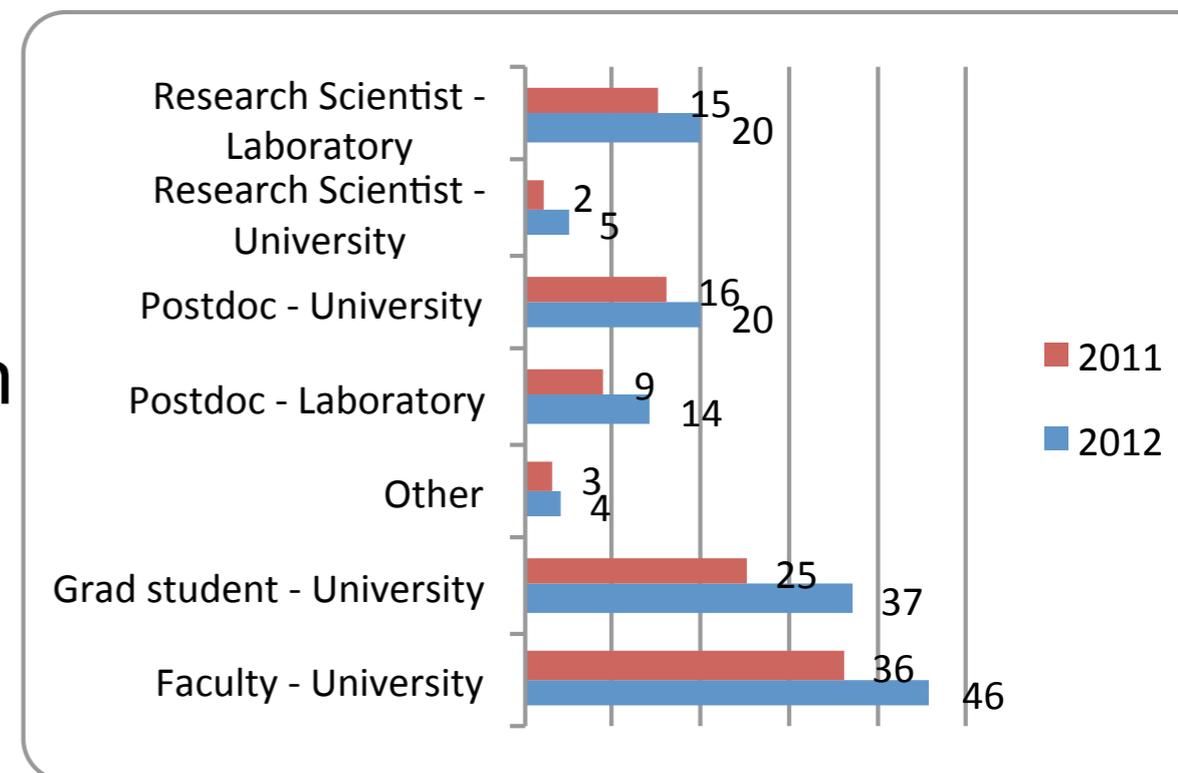
SciDAC-2 Grant

- Grant runs from 2006-2012.
- We received \$1,817,000 this year.
- Recent efforts have focused on USQCD codes for the BlueGene/P and Cray XTs as well as methods to meet the challenges of GPU and many-core hardware and multi-level algorithms. Rich Brower will give an overview of these activities for the Software Committee.
- SciDAC-3 beginning in late 2012 is under review. Project was split into an HEP project and an NP project. News is expected soon.



Membership, demographic, and user surveys

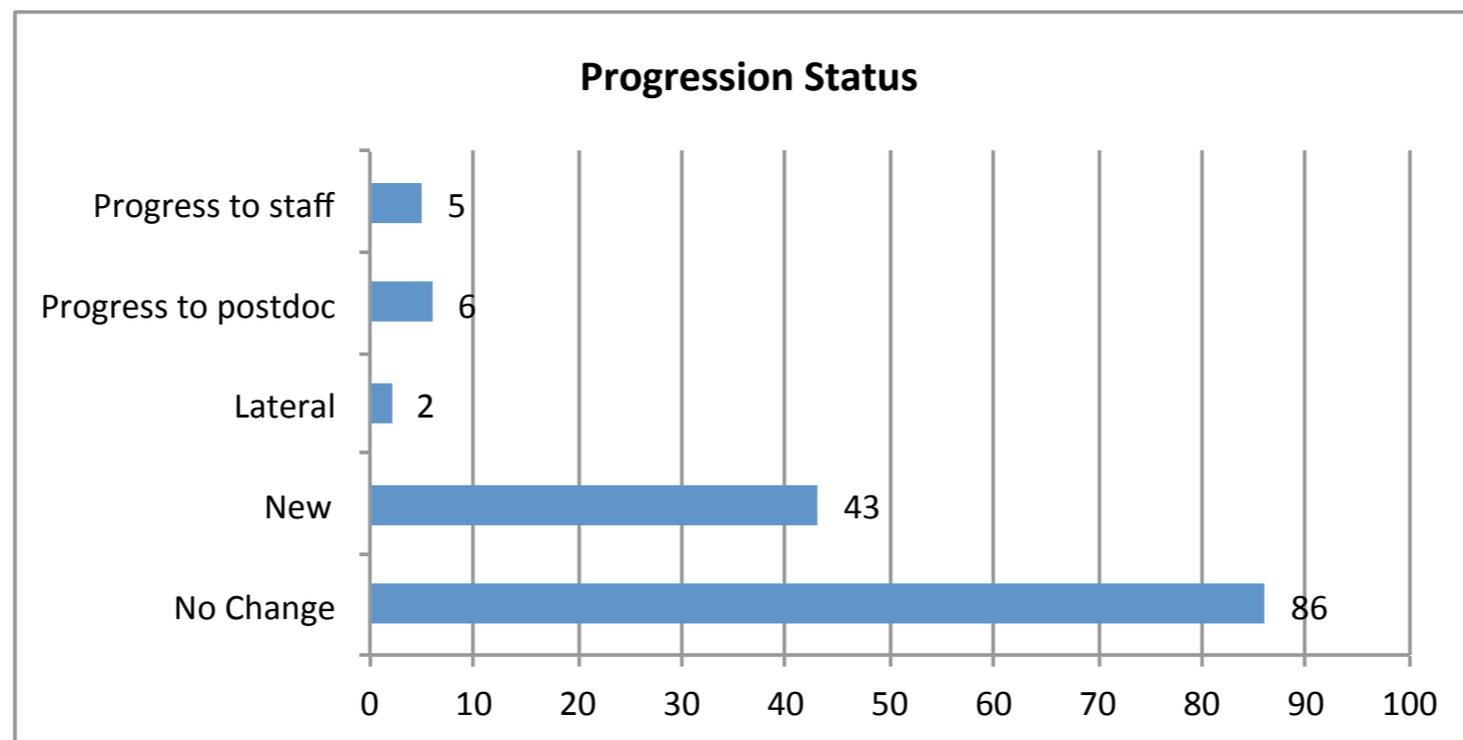
- DoE asks the collaboration to take regular surveys on various topics.
 - We understand that this is a pain in the neck, but the information is important to the DoE.
- DoE has asked the project to keep regularly updated **demographic information** on our field. New postdocs and students, new faculty members is a measure of the health of a field.



Demographic progression

Our project managers at DoE have expressed particular interest in the progress and promotions of young people.

Our information collected so far is clearly incomplete; we will be interacting with you in the next week to try to get more complete information before the hardware review.



Membership, demographic, and user surveys

- Membership list and member email list.
- 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

- As was indicated at last year's All-hands Meeting, limited travel funds are available for use by USQCD members.
 - Main priorities are USQCD Collaboration business, such as traveling to another USQCD institution to work on SciDAC software or USQCD hardware, or representing USQCD at an ILDG meeting.
- Those wishing to make use of these funds should send email to mackenzie@fnal.gov.
- Highest priority will be given to junior members of USQCD.



Coming peta-scale hardware

We expect to have access to several very large resources in the next year.

- INCITE:
 - “Mira”, IBM BG/Q at Argonne
 - “Titan”, Cray with GPU accelerators at Oak Ridge
- The new INCITE Resources
 - are for projects that can run on 20% of the machine (a partition > full BG/P),
 - projects that can't be done on any smaller machine (like BG/P or Jaguar).
- NSF:
 - IBM Cray Blue Waters at NCSA



BG/Q at Argonne

- 48 racks, 48 K 16-core nodes.
- INCITE will allocate 0.768 B - 3 B ch in 2013, starting perhaps spring-summer 2013.
 - USQCD through Columbia involved in design. (Peter Boyle dslash was the first realistic code running on simulator. Chulwoo, James Osborn, ... working on higher level codes, QLA, QDP, ... on the BG/Q.)
- Early science proposal.
 - Awarded 150 M core-hours, beginning late 12.
- Prototype BG/Q hardware at BNL and Argonne now.



Oak Ridge 2012 machine, Titan

- Upgraded Jaguar, + Fermi (→Tesla) GPUs.
 - 299,088 AMD Interlagos cores + 14,592 GPUs.
 - Currently, TitanDEV has 960 nodes with Fermi GPUs.
- INCITE will allocate 2 B ch for 2013.
- Formal collaboration with NVIDIA to prepare for it.
 - Mike Clark, Ron Babich→NVIDIA.
 - NVIDIA has decided that lattice QCD is an application they should support.



NSF: Blue Waters at NCSA

- AMD “Interlagos” nodes, >380,000, >3,000 GPUs.
- Chroma and MILC have been run.
- Trial projects going on a small amount of early science time.
- Not much known as of now about how the NSF intends to allocate Blue Waters.
 - As we learn more, we’ll have to figure out how to apply in a way that maximizes our physics goals.



NSF PRAC Proposal for Blue Waters

- USQCD has submitted a proposal to Petascale Computing Resource Allocations (PRAC). We requested:
 - Travel funds to be used in the development and optimization of software for Blue Waters.
 - Early access to information regarding Blue Waters' architecture.
 - An early allocation of time on Blue Waters.
- The USQCD proposal has received a grant of \$40,000 for travel associated with code development.

