

USQCD All-Hands Meeting 2012

Report from the Scientific Program Committee

Robert Edwards

Outline

- Allocations 2011-2012
- Resources 2012-2013
- Requests 2012-2013
- New leadership facilities
- Projects emphasizing use of leadership resources

Scientific Program Committee

Simon Catterall

Robert Edwards (chair)

Taku Izubuchi

Peter Petreczky (replaced Frithjof Karsch)

Martin Savage

Doug Toussaint

Ruth Van de Water (replaced Junko Shigemitsu)

Allocation process

The Scientific Program Committee (SPC) advises the Executive Committee (EC)

- The SPC advises the EC on science priorities for USQCD
- The SPC recommends projects for leadership resources
- The SPC suggests to the EC allocations of computer time on the USQCD facilities (FNAL+JLab+BNL) as well as INCITE

INCITE Allocations 2011-2012

- INCITE:
 - 2nd half 1st year: July 1, 2011 – Dec. 31, 2011
 - 1st half 2nd year: Jan. 1, 2012 – Jun. 30, 2012
- [July 1, 2011 – June 30, 2012]
 - BG/P at Argonne ALCF:
 - 27M Jpsi (50M BG/P): regular
 - 45M Jpsi (83M BG/P): “zero-priority”
 - Cray X[EK]6 at Oak Ridge OLCF
 - 15M Jpsi (30M Cray): regular
 - Possible “over-burn” time

USQCD Allocations 2011-2012

- USQCD facilities:
 - Clusters: 262.3M Jpsi
 - 181.3M Jpsi: FNAL [Ds, Jpsi]
 - 81.0M Jpsi: JLab [10q, 9q, 7n]
 - GPUs: 4.2M
 - 0.78M Fermi/Tesla: FNAL
 - 3.46M GT285/480/580; C20Tesla: JLab

2012-2013 call for proposals

- INCITE:
 - 2nd half 2nd year: July 1, 2012 – Dec. 31, 2012
 - 1st half 3rd year: Jan. 1, 2013 – Jun. 30, 2013
- [July 1, 2012 – June 30, 2013]
 - BG/P at Argonne ALCF:
 - 27M Jpsi (50M BG/P): regular
 - 50M Jpsi (93M BG/P): “zero-priority”
 - Cray X[EK]6 at Oak Ridge OLCF
 - 22.5M Jpsi (45M Cray): regular
 - Possible “over-burn” time

2012-2013 call for proposals

- USQCD facilities:

- Clusters: 283.9M Jpsi

- 181.3M Jpsi: FNAL [Ds, Jpsi]
- 102.6M Jpsi: JLab [12s, 10q, 9q]

- GPUs: 4.7M [Fermi/Tesla]

- 1.09M Fermi/Tesla: FNAL
- 3.61M Fermi/Tesla [GT285/480/580; C20Tesla]: JLab
- <redefinition of a GPU-hour>

- BG/Q: 737K BG/Q node-hrs [~ 16M Jpsi]

- 10% of a BNL-owned (DDR2) rack

Proposal classifications

- Redefined Type A & B proposal classification
- Intent is to change (back) Type B to be for “development”
 - no “flying under the radar”
- Type A proposals
 - Address goals of USQCD collab.
 - Critical needs of USQCD – some described in SciDAC-3 proposals
 - No minimum time
 - Eligible for INCITE resources
- Type B
 - Address goals of USQCD collab.
 - Development of methodology for future (larger) proposals
 - No maximum time
 - Not eligible for INCITE resources

Proposals 2012-2013

- 24 type-A; 11 type-B proposals [22+15 last year]
- Type-A proposals:
 - 8 INCITE
 - 20 cluster
 - 7 GPU
 - 2 BNL/BG-Q
- Type-B proposals: [requested 6.5% of available time]
 - 8 cluster
 - 3 GPU
- Subscription
 - BNL BG/Q: small requests – will make resource freely available
 - Cluster: 1.7x over-subscribed
 - GPUs: 1.7x over-subscribed
 - INCITE (reg): 1.24x over-subscribed
 - INCITE (zero): 0.95x under-subscribed

Allocation requests

WME

INCITE: 34M
Cluster: 140M
GPU: 787K

Mackenzie
Mawhinney
Shigemitsu
Sugar
Witzel
Ishikawa
Sharpe

BSM

INCITE: 16M
Cluster: 60M
GPU: 775K

DeGrand
Fleming
Hasenfratz
Kuti
Neil
Catterall
Giedt

New Tests SM

INCITE: 0M
Cluster: 45M
GPU: 0K

Aubin
Izubuchi
Lin
Shintani

NP

INCITE: 42M
Cluster: 185M
GPU: 5300K

DeTar
Detmold
Edwards
Liu
Negele
Orginos
Richards
Alexandru
Engelhardt-1
Engelhardt-2
Osborn
Renner

Thermo

INCITE: 17M
Cluster: 59M
GPU: 491K

Bazavov
Ding
Mukherjee
Maezawa
Mehta

Classification according to SciDAC3 proposals

Requested media storage

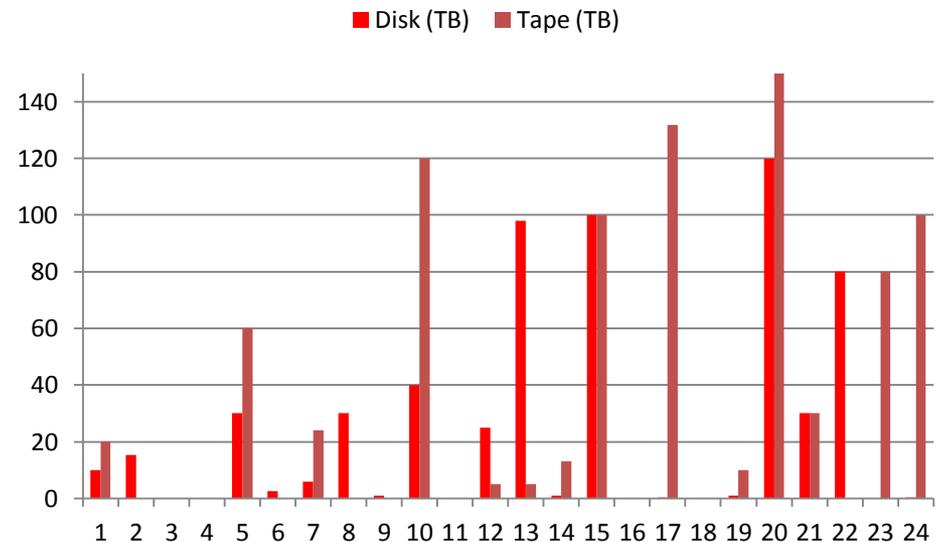
- Total request is significantly larger than year, which was significantly larger than the previous year
- Central values are increasing

- 2012-2013

- 625 TB disk
- 1448 TB tape

- 2011-2012

- 330 TB disk
- 915 TB tape



- In Jpsi units, request is < 10% of available cluster time
- Facilities project allocates ~6% of acquisitions for disk & tape
- Increasing media requirements have impact on facilities

Major upgrades in 2012-2013

- FY2012 - JLab
 - Cluster: expanded version of 12s [early fall 2012]
 - Accelerators: fall of 2012
- FY2013 - ???
 - Decision late summer
- Depending on outcomes (USQCD & national resources), SPC may issue a mid-year Call-for-proposals

Leadership facilities 2012-2013

- NSF BlueWaters:
 - USQCD has a “Petascale Resource Allocation” (PRAC) project started ~4 years ago for development on original IBM machine
 - Proposal designed an initial research direction centered on gauge generation at $T=0$ for projects in WME’s and hadronic physics (HISQ,DWF,Clover)
 - Both MILC and Chroma/QUDA used for acceptance tests of new Cray XE6 and XK6
- System installation proceeding in phases
 - Early Science periods – large scale resource but for very short time periods
 - Phase 1: charmonium spectroscopy on HISQ lattices
 - Phase 3: call sometime in summer

Leadership facilities 2012-2013

- INCITE:
 - CY2013 is 3rd (& last) year of INCITE allocation
 - Available number of hours has increased
 - ORNL:
 - 78% racks adding Kepler GPUs ~ 14k GPUs + 19k CPUs
 - Call suggests ~ 2x to 3x increase in allocation / project
 - Charge unit is XK6 node: 30 total cores = 16cpu+14gpu
 - ANL:
 - BG/P – available all of CY2013
 - BG/Q – avg. allocation: ~4x increase (?) in allocation / project
 - Request to Class A PI's for project suggestions
- ANL BG/Q Early-Science-Period time
 - USQCD has an allocation - not clear when it starts or how long.

Leadership facilities 2012-2013

- USQCD has several critical scientific goals as listed in SciDAC-3 proposals
 - HEP (WME's, BSM), NP(thermo, hadronic physics, nuclear structure)
 - Total project costs: gauge generation and valence analysis
 - Gauge generation becoming proportionally smaller in project cost (1X – 10X)
- Available resources and constraints
 - ~300M Jpsi in clusters and ~4.7M GPU in USQCD
 - ~50M Jpsi in leadership + 50M Jpsi zero-priority
 - Some gauge gen. on clusters & some analysis in zero-priority
 - Roughly 50M out of 400M available [not including GPUs] for gauge gen. -> only 1/6 to 1/4
 - Large scale gauge generation highly constrained both by available time and type of resources
- To achieve science goals: rough split
 - Gauge generation on leadership resources
 - USQCD facilities for analysis (many small-ish jobs, accelerators, etc.)

Projects on leadership facilities

- These projects are representative of broader programs which have requested leadership resources
 - Mawhinney(Christ) – [DWF and WME's]
 - Sugar(Toussaint) – [HISQ]
 - Mackenzie – [WME's]
 - Fleming – [BSM]
 - Bazavov – [HotQCD]
 - Richards – [aniso. clover for excited spectroscopy and structure]
 - Orginos – [isotropic clover for hadron and nuclear structure]