Scientific Computing

Experimental Physics

Lattice QCD

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12GeV Software and Computing Review

Overview

- Scientific Computing at Jefferson Lab
- Software and Hardware Systems
  - Mass Storage
  - Clusters
  - Filesystems
  - Network
  - Infrastructure
- Management
- 12GeV Requirements
  - Cores
  - Disk
  - Tape
- Staffing
- Summary

Scientific Computing

Compute Clusters

- Experimental Physics: 2 racks
  - Data Analysis “Farm”: 1200 cores, adding 500 this month
- Theoretical Physics (outside the scope of this review; for context only)
  - Lattice Quantum Chromo Dynamics, part of the USQCD national collaboration
  - High Performance Computing: 37 racks
    - Infiniband: 10,000 cores, adding 1100 next month
    - GPUs – disruptive technology – 530 gpus, 200,000 cores
      - » Adding 6 racks this fall (GPU or MIC)

Mass Storage

- Tape Library
  - Raw experimental physics data, processed results
  - Other lab-supported efforts, mostly LQCD

Staffing

10 FTE: 1 Manager, 1 Physicist, 4 Development, 4 Operations

Mass Storage System

Tape Library- IBM TS3500, LTO5 tape drives, >1GB/s aggregate bandwidth

- 12 frames, 6800 slots; Capacity ~10PB
  - expandable to 16 frames, 1300 slots/frame, additional 7.8PB
- 8 LTO5 drives – all writes, copying LTO4s and duplicate raw data tapes
  - 1.5 TB/tape, 140MB/s
- 4 LTO4 drives – can be replaced
  - 1TB/tape, 120MB/s

JASMine software - JLab written; modular, distributed architecture; scalable

- manages data on tape plus 50TB disk cache

12GeV projections include 2nd tape library procurement in 2014

- expecting ~15PB yearly storage requirements in full 12GeV production
- LTO6 drives and media expected FY14, in advance of 12GeV turn-on
  - 3.2 TB /tape, 210MB/s
- 15-frame library with 1300 slots each = 19,500 slots x 3.2TB ea = ~60PB
- Upgrade to LTO7 expected in FY18
  - 6.4TB/tape, 300MB/s = ~120PB capacity

Scale-out solution – add more datamovers if more bandwidth needed

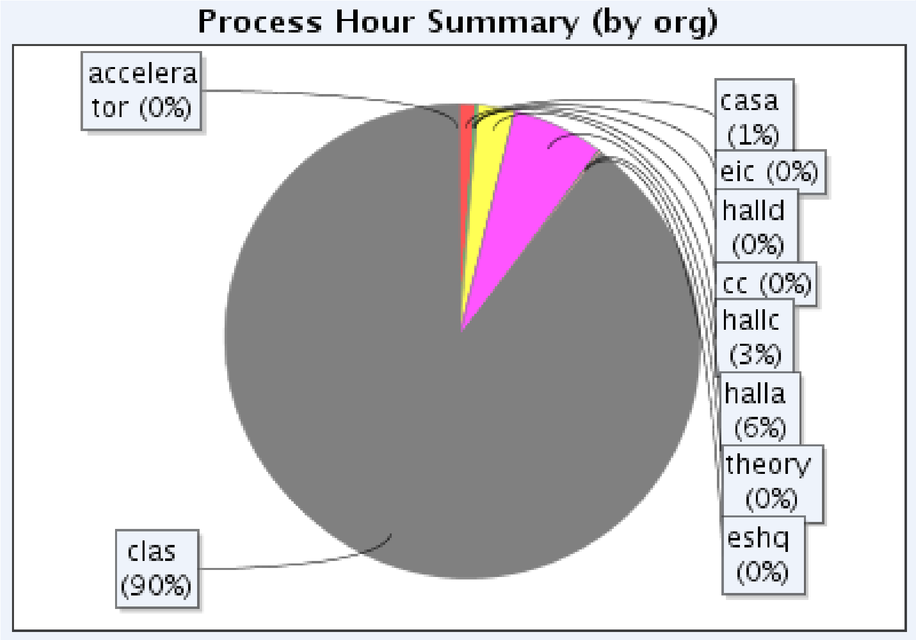
Data Analysis Cluster

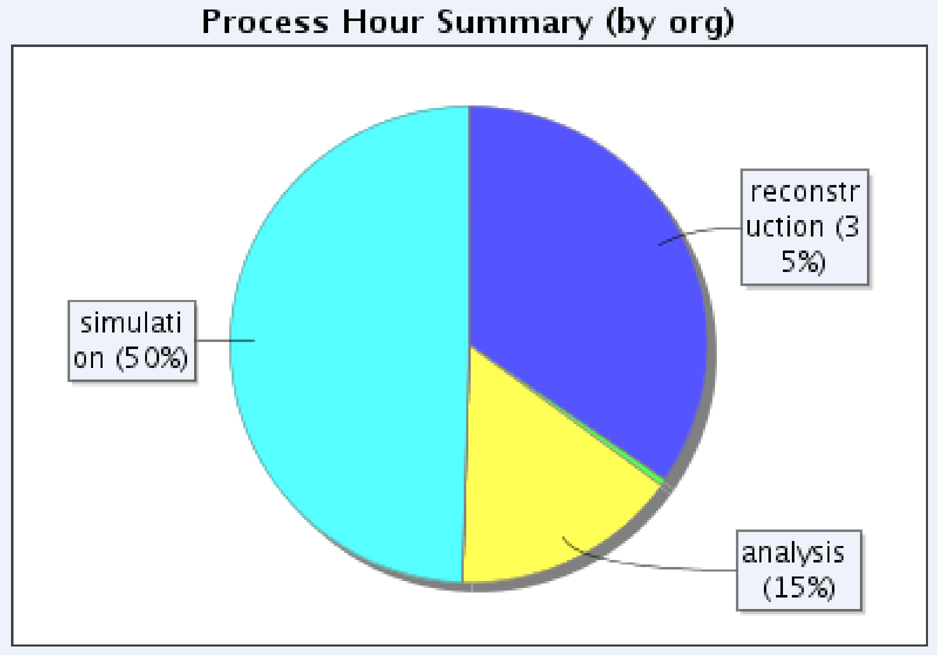
- **Auger** - Jlab written software for user interface, job management
- **Maui/PBS** open source resource manager/scheduler
- **Mysql** open source database
- 100 compute nodes, 1200 cores – CentOS 5.3 64-bit
  - mostly dual quad-core Nehalem, 24GB RAM
  - also 6 quad eight-core Opteron, 64GB RAM
    - support move to multithreaded codes
  - New this month: 32 16-core Sandy Bridge, 32GB RAM

Moore’s Law holds true; replacing oldest ¼ compute nodes every 4 years keeps pace with increasing computing requirements.

Also, reallocate 4-year-old HPC compute nodes to the farm, after nodes don’t function well in large parallel system but are fine individually.

Data Analysis 2011





7,094,223 process hours delivered in FY11.

5,053,580 process hours delivered so far in FY12.

For comparison, LQCD has delivered 72M process hours in FY12.

Filesystems

- Traditionally, **zfs** filesystems exported via **NFS** (Network File System) over trunked gigabit Ethernet
  - Continue to use for work data; migrating to Infiniband
  - 110TB production total
    - 70TB for Experimental Physics

- Most recently added **Lustre** filesystem over Infiniband
  - Volatile scratch space, automanaged
  - 22 servers, scale-out solution
  - 500TB production total
    - 85TB for Experimental Physics
  - Improves scalability and I/O performance.
  - Require a specific kernel and Lustre client; no NFS.

Network

- Compute nodes
  - Oldest are gigabit Ethernet
  - Latest are 10gigabit Infiniband
- Fileservers
  - Trunked gigabit Ethernet fileservers, 4gb
  - Move almost complete to Infiniband, 10 - 40gb interfaces
- Data acquisition systems to Computing Center
  - 10 gigabit Ethernet
    - Plan to test 40gb Infiniband next year
      - 4x bandwidth, lower CPU load
- Wide area network
  - ESNet: DoE's Energy Sciences Network
  - 10 gigabit shared
    - can be assigned our own lambda when needed
  - Used for remote logins, offsite data transfers

Infrastructure

- Space
  - 7400 square feet today; 50% used
  - 2000 square foot conference room carved out; could be reclaimed if necessary
- Power
  - ~650KW, including PDU loss
  - can add another large UPS
  - Expect to increase power density 1.5x
- Cooling
  - Today: ~470KW; Fall: ~550KW with a new air handler
    - limited by 8” pipe
  - Fall 2014: >650KW with upgraded 12” pipe

Management

Information Technology

- The Scientific Computing Group is in JLab's Information Technology Division.
- IT/SciComp manages computing, disk and tape storage systems for Experimental Physics as a **Service Provider** (SP).
- **Funding** for staffing, hardware, and storage media are in the **Physics budget**.
- JLab's annual work plans (**AWP**) define labor, funding, and requirements.

Physics

- Physics computing requirements are gathered and conveyed by the **Physics Computing Coordinator,** Graham Heyes**,** to the **Head of Scientific Computing**.
- **Offline Computing Coordinators** for each hall manage their requirements.
  - Physics experiments/run groups communicates with their hall offline computing coordinator for resource allocation.
- **Regular meetings** occur with Physics and IT -- SciComp & CNI -- to ensure requirements are met and issues are addressed.

JLab

- **Users Group Board of Directors** includes a Computing coordinator, now Mark Ito.
- **JLab IT Steering Committee** includes Physics Computing Coordinator, the UGBoD Computing contact, and several physicists.

12GeV Requirements

Cores

- Based on 2011 Intel Westmere 2.533 core, $200

Hall\Year	2014	2015	2016
A	20	40	100
B	550	4400	11,000
C	20	40	100
D	500	5000	10,000
Total	1090	9480	21,200
Cost/core	$80	$50	$35

#cores/node	32	32	64
#nodes/rack	64	64	64

Base spending plan includes $50K/yr on computing.

At 12GeV operations in 2016, 7 racks.

12GeV Requirements

Storage – Tape (TB)/year

	2014	2015	2016
A	170	410	660
B	150	5200	9500
C	600	250	1750
D	200	1800	3600
Total	1120	7660	15510
Cost/tape	$ 40+30 (LTO5)	$60+30 (LTO6)	$45+30 (LTO6)

12GeV Requirements

Storage – Disk (TB)/year

$300/TB in 2012

	2014	2015	2016
A	20	50	110
B	90	1300	2700
C	60	125	175
D	50	750	2000
Total	220	2225	4985
Cost/TB	$160	$120	$90

Staffing

Staffing (FTEs)

- Today:

CPU servers:	1.5
Disk servers:	0.5
Robots:	0.5
Services:	0.5
User Support:	0.5

- 12 GeV:
  - + 0.5 computing
  - < 0.5 all else

No new staff; absorb LQCD as their footprint shrinks (constant dollars)

Summary

Experimental Physics' data analysis computing cluster and mass data storage system are sized appropriately for current needs.

Funding and staffing resources are appropriate at present.

The future growth of both systems is requirements driven, and is based on information provided by the Halls and funded by Physics.

Ample space, cooling, and power are available for 12GeV era computing and storage needs in CEBAF Center F112, the IT Data Center.

12GeV IT requirements for scientific computing need to be revisited and updated by Physics on a regular basis as 12GeV approaches.