## Jefferson Lab Scientific Computing Infrastructure Update

CLAS Collaboration Meeting November 2023

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#### Jefferson Lab's High Throughput Computing – The Farm

- In FY23 3072 EPYC 7763 AMD "Milan" cores added to the farm
- FY19 FY21 Were EPYC 7502 "Rome"
- 140 Million Core Hours (Using 7502 as normal)
- Farm14 nodes are being decommissioned now
  - Oldest HW, nodes reused for ad-hoc projects and/or excessed
- The farm is routinely busy, Utilization is almost always over 80%
- FairShare allocations are used to balance consumption between the halls
  - B&D ~40% each
  - A&C ~20% each
  - Bursts beyond share when cycles are free
  - CLAS routinely claims free cycles.
  - NB: Hall A data volumes and analysis requirements are rising to Hall B/D levels (SBS program, Moller)
    - Allocations will need rebalancing in 2024/5





#### **Off-Site Computing: Open Science Grid use by CLAS12**

- CLAS12 consumed an additional 37M Core Hours on the Open Science Grid in FY23
  - This is MC load that would not be achievable on the JLab farm without scheduling pressure
- We are moving to a model with the OSG where each Project (CLAS12, GlueX, ePIC, Moller) have their own OSG servers
  - Enables pilot job tuning and data storage strategies that match the collaboration's needs.
- NERSC has cycles available on Perlmutter at no cost (but must apply); Lawrencium not 'free' but arrangements can be made
  - -Code in SWIF already supports NERSC
  - -If interested, email brads@jlab.org





#### Farm Operating System Upgrade

- The Farm is presently running CentOS 7.9, which is approaching EOL.
- The next OS for the Farm will be AlmaLinux9
  - CentOS project was disbanded by RH; replacement distributions are similar, but not "bug for bug" identical to RHEL
  - Switch to Alma9 aligns with CERN, OSG, and other HEP/NP groups
- The Farm will be upgraded slowly, starting with early access to an Alma 9 partition
  - -Alma9 farm partition (and ifarm node) will be made available within weeks for testing
  - -The size of the Alma9 partition will grow over time
  - -As an incentive, the best CPUs (ie. farm23 nodes) will move first.
- Containerization as a strategy for legacy code using Apptainer (formerly Singularity)

-More on this later...

- We are gradually pruning legacy dependencies on CUE filesystems that have cybersecurity or operational gaps (e.g. /u/scratch)
  - -We will do this in small, announced steps
  - -Removing: /site, /u/scratch
  - -Deprecating (but still supporting): /apps



- There is strong demand for more disk. This is an explicit priority for for us.
  - High performance, reliable disk and associated infrastructure is still expensive and has been long lead...
  - -We are trying to get "ahead of the curve" on disk with FY23, and FY24 purchases
- Lustre Storage is good for large files, streaming, large block I/O, production farm runs.
- Lustre is not good for small files, high IOPS, and frequent metadata operations (worst case: open,write 1kB, close, loop)
- /work will not scale for large farm campaigns.
- Node-local /scratch is good for jobs with high IOPS to working files.
  - -MSS files are automatically copied to node-local working directory
- We are reevaluating the role of /work areas as legacy NFS spinning disk storage.

-More on this later...

Path	Best Use	FS Type	Deletion	backup
/cache	Bulk I/O, Migration to tape	Lustre	Once on tape	/mss
/volatile	Bulk I/O Temporary storage	Lustre	auto	NO
/work	User Managed	NFS+ ZFS	manual	NO
/home	Dot files, personal documents, etc	NFS ssd	manual	YES
/farm_out	Farm job stdout/stderr	NFS ssd	auto	NO
/group or /scigroup	Code	NFS ssd	Manual	YES
/scratch	Farm job I/O to node local disk	ssd	auto	NO
/u/scratch	CUE scratch. Deprecated.			
/cvmfs	Software stack. Configuration.			



#### Disk Update Coming for Lustre (/cache, /volatile)

- The Current Lustre System ("Lustre19") for /cache and /volatile is End of Life; Replacement on order
- The new Lustre23 system
  - Target: Double sustained I/O to >40GB/sec.
  - -HDR InfiniBand (200Gbit/sec)
  - -Build out in two steps
    - 4PB in FY23 (HW finally arriving!)
    - +5PB in FY24
    - Aim to double current capacity
- Down-cycle old HW to support *non* user-visible 'read-cache' and backing-store applications
- At right: example full load performance
  - -20GB/sec reads
  - -Now stable server uptime
  - -IOPS monitoring

lustre19 server uptime ~						
scmds1901:9100						
scmds1902:9100						
scoss1901:9100						
scoss1902:9100						
scoss1903;9100						
scoss1904:9100		10.967 week				
scoss1905:9100						
scoss1906/9100						
scoss1907:9100						
scoss1908:9100						
scoss1909:9100						
scoss1910:9100						
scoss1911:9100		10.983 week				
scoss1912:9100		0.974 week				
✓ Objects lustre19 bandwidth: smoothed, divided, and #field	Top IO Operations/sec users - Lur	stre19				
5 GBs	20.0 K		max+ current			
		gxproj4	16.81 K 25			
	1754	jboyd	766 635			
08		- clas12-1	487 98			
		clas12-6	140 0			
	15.0 K	- alobus20	125 0			
		clar_12.5	90 0			
-5 GBs		50 6				
	125K		35 40			
		stayto	30 0			
2 - 10 GBs	10.0 K	gmat	2/ 0			
		— dilks	13 0			
		— jrsteven	3 1			
8 15 GBs	7.5 K	— — richcap	1 0			
	— manavb	0 0				
	tianye	0 0				
		— rahmans	0 0			
20 68s 25 68s 11:35 11:40 11:45 11:50 11:55 12:00 12:05 12:10 12:15 12:20 12:25 12:30	25K 0 11.40 11.50 12.00 12.10 12.20 12.30					



#### **/volatile User Experience Issues**

- Working on improving user experience for /volatile
  - People get surprised when files in /volatile disappear on them
  - Option: Remove/discourage the 'over-subscription' ("High Quota") feature.
    - Can lead to rapid 'purges' when other groups fill their 'unused space' and trigger an unexpected purge
  - Option: need HW, under investigation
    - Provide a modest 'Recovery Pool' area where purged files go for a week before they are really gone.
      - 200TB would seem to provide a ~7 day buffer at current volumes
    - "Best effort" fall-back, not guaranteed

Project Name	High Quota (GB)	Guarantee (GB)	Used (GB)	Used/Quota	Small File(MB)	SmallFileCount
▶ halla	162,350	120,750	106,573	65.64%	78,922	921,93
▼ hallb	465,400	187,050	479,168	<b>102.96</b> %	423,024	3,713,57
clas12	361,000	150,500	377,393	104.54%	388,283	3,499,49
clase1-6	500	250	0	0%	0	
clase2	100	50	3	3.00%	1	
claseg2	1,000	500	0	0%	29	8,01
claseg3	500	200	0	0%	39	63
claseg4	100	50	0	0%	0	
claseg6	500	200	120	24.00%	21,337	116,29
clasg10	2,000	1,000	714	35.70%	5	e
clasg11	1,000	500	0	0%	0	
clasg12	2,000	1,000	0	0%	0	
clasg13	500	250	0	0%	0	
clasg14	2,000	1,000	2,235	111.75%	0	
hps	94,000	31,500	98,498	104.79%	9,745	51,03
prad	200	50	205	102.50%	3,585	38,04
	465,400	187,050	479,168	0%	423,024	3,713,57
▶ hallc	60,500	27,500	28,695	47.43%	9,494	113,90
cebaf24gev	10,000	5,000	83	0.83%	0	
CIS	1,000	500	0	0%	0	
cteqX	500	200	0	0%	0	
eic	20,000	10,000	5,304	26.52%	9,590	196,87
halld	230,000	100,000	100,010	43.48%	249,268	1,822,88
JAM	10,000	2,000	223	2.23%	105,348	1,070,29
	959.750	453.000	720.056		875.646	7,839.4

Scicomp Volatile Disk 820 (TB)

/volatile disk pool policy

\* Small file counts all files less than 1ME



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### **Disk Update Coming for /work**

- Working on a plan to augment /work filesystem
  - Perhaps new "/project" space?
    - Deprecate "/work" name in favor of SciComp manged "/project" space that merges in the Exp Phys "/group" space
  - Upgraded hardware and increase storage
    - +1 PB with modern SSD-backed storage
      - Purchased in FY23; awaiting delivery
  - Tuned for fast, random I/O
  - Consistent backup policy
    - snapshots and nightly backups
  - Roll out in 2024
    - Details to be worked out with Hall Compute Coordinators
    - DO express concerns, wishlists to them and/or me!



#### Scicomp /work Disk Pool Usage History

Date

) halla 🔵 hallb 🔵 hallc 🔵 halld 💛 eic 🔵 general

Project Name	Quota (GB)	Used (GB)	Used/Quota
▶ eic	523,629	377,068	72.01%
▶ general	102,509	53,226	51.92%
▶ halla	69,272	49,753	71.82%
▼ hallb	262,118	178,404	68.06%
clas	46,077	40,206	87.26%
clas12	169,963	104,203	61.31%
hps	25,598	19,787	77.30%
prad	16,384	12,225	74.61%
primex	4,096	1,983	48.42%
	262,118	178,404	
▶ hallc	25,224	19,960	79.13%
▶ halld	409,600	340,222	83.06%
	1,392,352	1,018,633	



#### Tape Library Strategy: Write Once, Read Rarely.

- Historically, access to Tape has been a bottleneck; This is no longer true
  - -Consolidation of data to LTO8
  - -Use of SWIF for data+cpu co-scheduling
  - -Expansion of disk storage
- We are at an articulation point where it is becoming possible to cache "hot" data and avoid repeated round-trip churn to tape
- Implementation of a system Read Only Cache (distinct from user-visible cache)
  - -Keep all small files disk resident
  - -Aggressively cache hot files
  - -Use XRootD storage
  - -Repurpose EOL storage for RO Cache
  - RO cache failures well-tolerated since storage is not POSIX or user-facing. Worst case, go to tape for the file again.





## Networking

- The Lab's Internet is being upgraded from 2x10Gbit/sec to 2x100Gbit/sec by ESNet
- Installation delays due to external work and long lead on 100Gig optical switch gear.
  - Hardware finally arrived and being installed in November
- Current forecast is for 100Gbit operations before the end of 2023
- Once connected, we will have 100Gbit connectivity directly to the scientific computing resources, including data transfer nodes for Globus, XRootD, and OSG.





## Rucio

- Distributed data management system
  - Initially developed for ATLAS
  - Highly scalable & modular
- Features
  - Basic data operations
    - Storage, transfer, deletion
  - Policy based replication (automatic)
  - Designed with distributed storage and 'protocol agnostic' data transfer methods in mind
- Can serve as a Replica/File catalog and metadata service
  - Can search its DB and present files matching names, metadata, etc

- "Beta" JLab Rucio Instance under development
  - Initial customers will be EIC group
    - JLab ↔ BNL automated file registration and transport
  - GlueX (modest sub-project)
  - Load testing, solve authentication challenges, develop policy and namespace conventions
  - Integrate relevant metadata from RunDB and other sources
- Goal is progressive, but full fledged roll-out in 2024
  - Transparent Jasmine/tape integration
  - Full offsite DB query and data transport functionality
  - Backfill from existing tape library as needed





#### **Containerization Support**

- CST is developing formal containerization support for Users
  - Documentation
    - ie. Easy 'on-ramp' / how-to for common use cases
  - "Official" Infrastructure support
    - Apptainer / Singularity
    - Docker, Podman support for image building and deployment
    - JLab GitLab Container Registry
- Among other benefits, Containers can provide
  - 'Plug and play' software configurations
  - SW version / configuration snapshots
  - Ability to run 'custom' software frameworks on other datacenters, computers, laptops
- Will also support/streamline upcoming Farm transition from RHELX  $\rightarrow$  Alma9

- New JLab GitLab instance
  - Public facing; support internal and remote users
  - Direct support for GitLab Container Registry
    - Image deployment
    - Automated container builds
  - Full CI/CD support
  - Federated authentication
- Note: Existing GitHub subscription will not vanish
  - Current Github 'seat-based' subscription model gets very expensive for our
    - Our current 'legacy' plan is based on private repo count, not #users
      - "cheap", but not upgradable and we are bouncing off its limits...
  - Folks will be encouraged to use the GitLab instance
    - Using carrot not a stick! Goal is to make GitLab a win for the Users
  - Automated GitHub  $\rightarrow$  GitLab repo migration tools exist



#### Hall ESX Virtual Machine Cluster

- VMs within the Hall experimental enclave are available now
  - High-uptime infrastructure explicitly targeted to support Hall operations, etc.
  - Update policy, downtime scheduling for VMs defined by Hall Compute Coords as usual.
  - Ex: Slow control systems
    - EPICS softIOCs
    - Windows/Rockwell control systems
      - ie. Hall C: cmagnets, skylla10
    - PXE boot hosts/services
  - Ex: Data-base hosts
    - RCDB, CCDB hosts
  - Ex: "Remote CH" support hosts

- VM hosts functionally operate within the Hall subnets (no firewall issues)
  - Direct access within respective subnets
  - 2-factor hop (via. hallgw) as with any existing Hall hosts
- Take advantage of VM flexibility
  - snapshotting / backups
  - auto-failover on HW issues
  - advantages wrt "cloning", load balancing, etc
- Keep this in mind for future deployments, HW upgrades, etc
  - Cheaper / better than HW for many applications



#### JLab (internal) SciComp Director's Review 2024

- Tentative dates:
  - First week of Feb, 2024
  - Formal Charge and dates distributed soon (have draft charge in hand!)
- Nominal 2-day review following historical pattern
  - Dec 2021 Review Indico

[Access Key: "JLAB2021"]

• See <u>Review Report</u> and <u>Responses</u> documents on that page

- Will require updates on
  - Scientific Computing Systems
    - incl. OSG / NERSC usage/plans
  - EPSCI Report
  - Hall Reports/Projections
  - Data Science Report
  - EIC, Theory Reports/Projections
- Possible special topics
  - SRO status and plans
  - AI/ML progress
  - HPDF status and pre-planning(?)



- What are the problems / pain-points in your workflows?
- Other question / comments?



# Thank you!



- Slurm is the standard for batch processing, both HTC and HPC.
- SWIF is the Jlab workflow tool that coschedules data and orchestrates workflows
- SWIF guarantees that data and jobs are scheduled together to increase farm utilization and throughput.
- SWIF pre-stages data for users and SLURM FairShare scheduling matches the jobs to resources
- Reference Guide
  <u>https://scicomp.jlab.org/docs/swif2</u>



#### **Documentation and Services**

- Online Documentation
  - Experimental Physics Users Guide: <u>https://scicomp.jlab.org/docs/FarmUsersGuide</u>
  - -Linked from the portal at <a href="https://scicomp.jlab.org/scicomp/home">https://scicomp.jlab.org/scicomp/home</a>
- ServiceNow Expansion: Service Portal
  - -<u>https://jlab.servicenowservices.com/scicomp</u>
  - -Moving documentation to Knowledge Base Articles
  - Working to make articles more discoverable, both from on-site search and from search engines.

