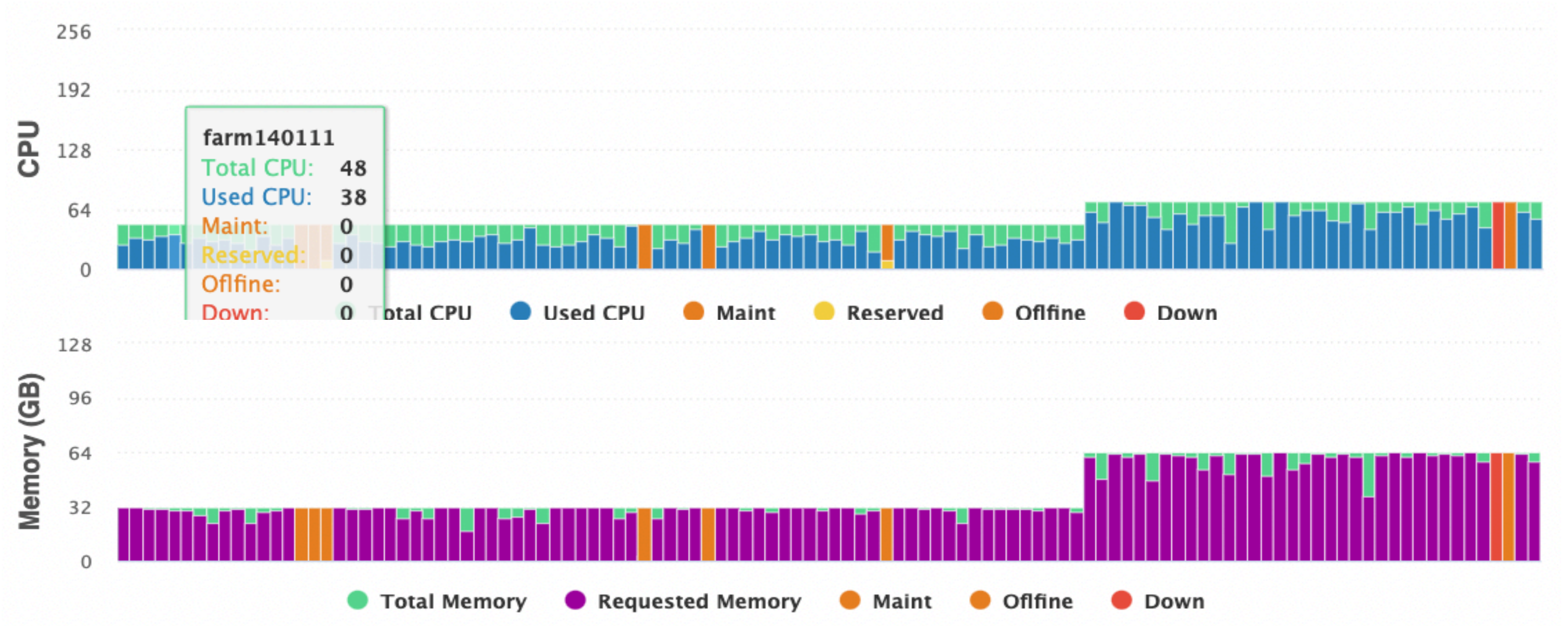
Computing and HPS

N. Baltzell - HPS Collaboration Meeting - June 2024

JLab Batch Jobs

FAQ/Reminders



- scicomp.jlab.org !!!
- SLURM
    - The base job scheduler at JLab and an industry standard
    - Requires you being added to the `hallb` SLURM account in order to submit jobs
        - Normally happens when you get added to the corresponding UNIX groups, but sometimes it gets overlooked ...
- SWIF
    - A JLab frontend to SLURM, currently also supporting a couple remote sites
    - Also knows about the JLab tape library and can stage data to disk and automatically submit to SLURM when ready
        - If you need to read data off tape at JLab, you probably should use SWIF, especially if that data is large, many TB
        - Although we can "pin" optimized skims for physics analysis on `/cache`, so you don't have to read from tape
    - Also supports workflows of jobs with complex inter-dependencies, which we leverage in the workflows CLAS12 chefs use
- The main source of underutilization of the farm is dry queues and still sometimes memory requests/requirements
    - Make sure your requests are appropriate for your jobs' requirements!
    - Can run a few test jobs and see how much memory they used, or run them interactively and check with `htop`.

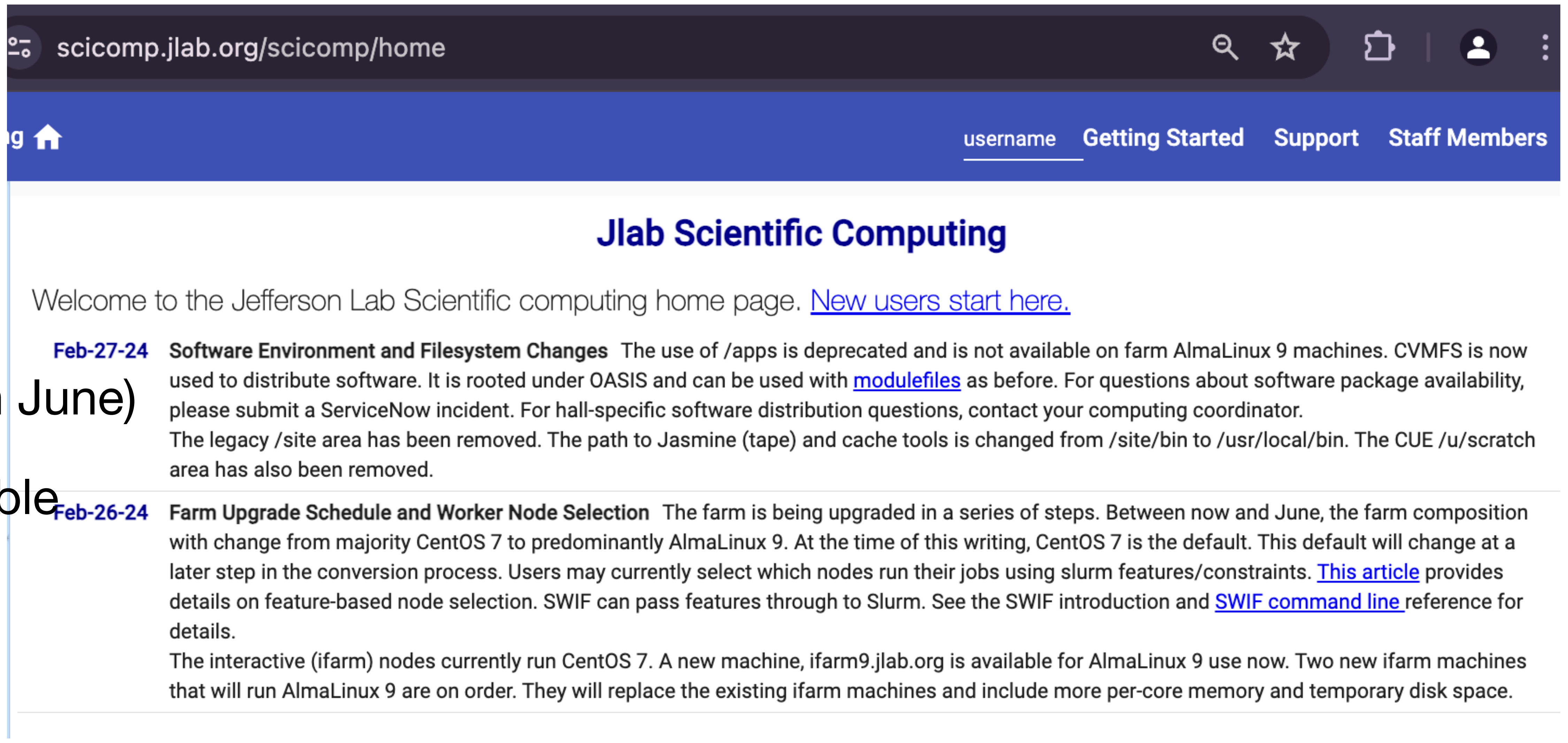
JLab Filesystems

FAQ/Reminders

- scicomp.jlab.org !!!!
- `/work/hallb/hps` - ZFS - **25 TB**
    - one single, hard quota, manually managed, no automatic deletion
    - live snapshots at `/work/hallb/hps.zfs`
    - not ideal for large I/O from many batch jobs simultaneously
        - clas12 chefs do not use it for any data
        - the conventional place for collaborators to store their more "personal", somewhat permanent, physics data and large software
- `/volatile/hallb/hps` - Lustre - **30-190 TB**
    - one single, "soft" quota. with auto-deletion queue based on file modification times FIFO
        - generally a 2-month lifetime for CLAS12
        - if you copy something there and it gets deleted prematurely, you might have copied it with old timestamps, e.g., `rsync -p`
    - no backups of any kind
    - ideal for large I/O from many batch jobs
    - bad for lots of small IOPS, e.g., streaming log files, and tons of small files' metadata
- `/cache/hallb/hps` - Lustre - **70-140 TB**
    - Very similar to /volatile, but serves as a disk mirror of tape, and generally has a lifetime of many months
        - e.g. `jcache get /mss/clas12/...` writes data from tape to disk
    - Files written there are also guaranteed to be copied to tape automatically before automatic deletion, except files smaller than 1 MB!
    - The main filesystem used during large-scale processing for HPS data that should be stored permanently and used for publications
    - Data on tape should be associated to an experiment, not individual users, so we coordinate with the run group's analysis coordinator when we want to write more "personal" data to tape for permanent storage
- `/mss/hallb/hps` - pseudo-filesystem
    - just the metadata of all files on tape, cannot write to it directly
- `/farm_out/$USER` - SSD
    - few-GB per-user, hard quotas (can cause jobs to crash!)
    - good for small IOPS and the ***only*** place for log files from batch jobs
- `/home/$USER` - SSD
    - few-GB per-user, hard quotas, see cc.jlab.org for values
    - live snapshots at `.snapshot` at every level in the directory tree, plus regularly backed up to tape
- `/group` - SSD
    - generally only written to by group coordinators, admins, for official software builds, databases, web interfaces, etc.
    - same snapshot/backup policy as /home

AlmaLinux 9

- JLab has replaced CENTOS with AlmaLinux (started early this year, finishing in June)
    - RHEL(9) remains for non-scientific computing at JLab, binary compatible
- Various changes, as centos7/RHEL7 was very old ....
    - gcc 11, ~~python2~~, system libraries like ssl
        - for us, this should really just be maintenance and removing kludges to support old stuff
    - `/tmp` is mounted noexec, which can break various software unless configured for an alternative /tmp, e.g. apptainer, Java sqlite, maven
        - here's an example workaround: https://github.com/JeffersonLab/clas12-env/blob/0229b9ef71af3398fc1e527c2aa19656fc5218c6/modulefiles/tmpfs#L11-L17
    - default umask is less permissive (user only, no group/world access), probably want to set it in your login setup with `umask 22`
- `/site` and `/apps` are gone on scicomp machines (separation from non-scicomp IT resources)
    - this breaks old environment setups unless testing for existence, e.g., `[-e /site] && source /site/...`
    - `/cvmfs/oasis.opensciencegrid.org/jlab/scicomp/sw` is the replacement for IT-provided physicsy software, e.g. cernlib/2023, ROOT
    - `/usr/local/bin` is now the location for in-house system utilities, e.g. swif2, jasmine, transparent to the user
- /group is still available for software builds, databases
    - although CLAS12 switched to `/cvmfs/oasis.opensciencegrid.org/jlab/hallb/clas12/sw`



Jlab Scientific Computing

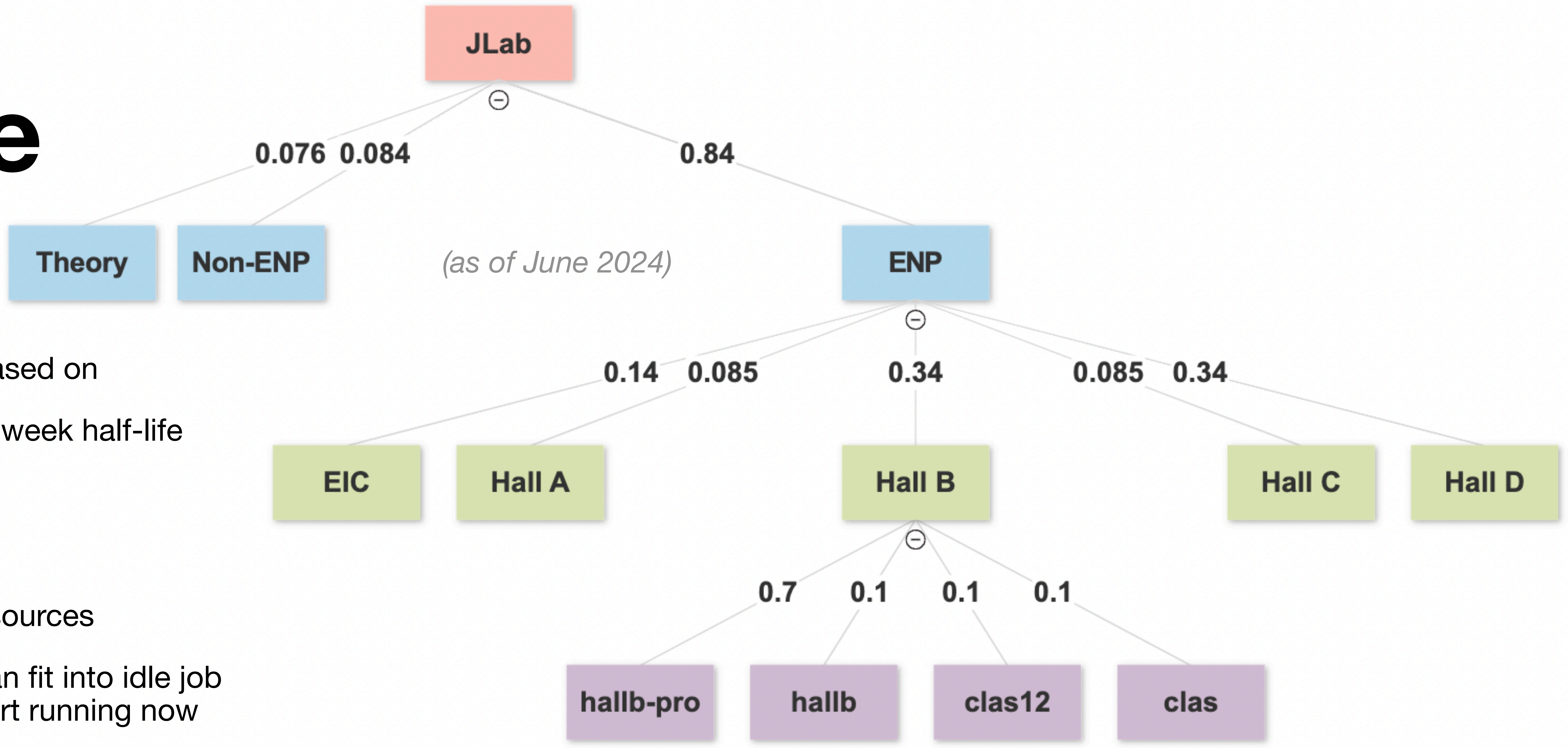
Welcome to the Jefferson Lab Scientific computing home page. New users start here.

Feb-27-24 **Software Environment and Filesystem Changes** The use of /apps is deprecated and is not available on farm AlmaLinux 9 machines. CVMFS is now used to distribute software. It is rooted under OASIS and can be used with modulefiles as before. For questions about software package availability, please submit a ServiceNow incident. For hall-specific software distribution questions, contact your computing coordinator.
The legacy /site area has been removed. The path to Jasmine (tape) and cache tools is changed from /site/bin to /usr/local/bin. The CUE /u/scratch area has also been removed.

Feb-26-24 **Farm Upgrade Schedule and Worker Node Selection** The farm is being upgraded in a series of steps. Between now and June, the farm composition with change from majority CentOS 7 to predominantly AlmaLinux 9. At the time of this writing, CentOS 7 is the default. This default will change at a later step in the conversion process. Users may currently select which nodes run their jobs using slurm features/constraints. This article provides details on feature-based node selection. SWIF can pass features through to Slurm. See the SWIF introduction and SWIF command line reference for details.
The interactive (ifarm) nodes currently run CentOS 7. A new machine, ifarm9.jlab.org is available for AlmaLinux 9 use now. Two new ifarm machines that will run AlmaLinux 9 are on order. They will replace the existing ifarm machines and include more per-core memory and temporary disk space.

JLab Fairshare

Algorithm

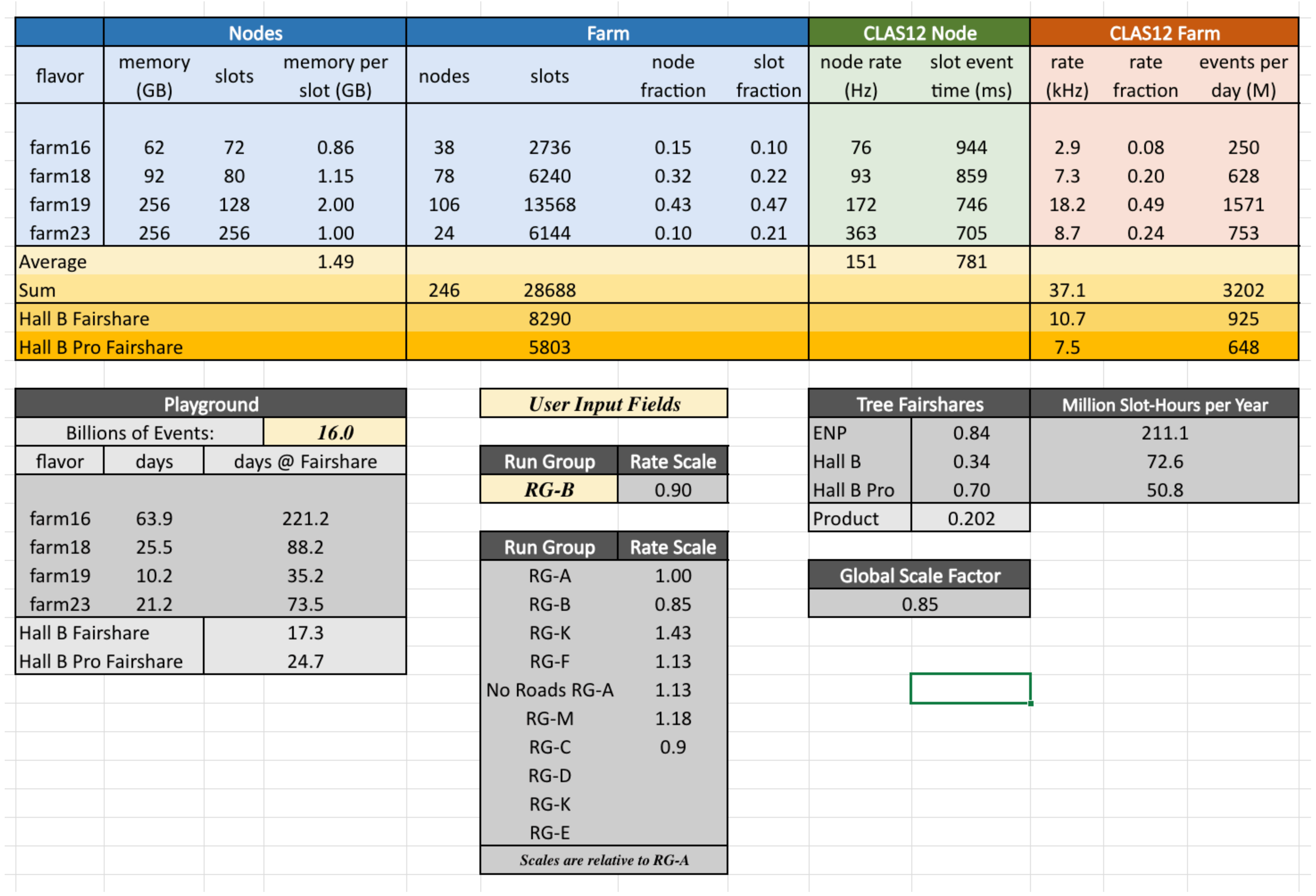


- JLab uses SLURM's *Fair Tree Fairshare* algorithm
  - Decides whose jobs to run first, priority, based on
    - wall hours used in the past, with a ~1-week half-life
    - the fairshare targets in the tree
    - queued jobs' wall time requests
  - Aims for 100% utilization of computing resources
    - If there's any jobs in the queue that can fit into idle job slots, someone's jobs are going to start running now
    - If a group doesn't submit enough jobs to utilize their fairshare, it can get absorbed by the other groups at the same level in the tree.
  - No preemption, i.e., no jobs ever get killed due to priority, only due to misuse of resources (over memory, disk, time limit).
- Entire tree not shown above, e.g., at the bottom of each branch are all individual users/accounts, all with equal fairshare
  - Current fairshares and priorities are available to all via the `sshare` command (used to be in graphical form at scicomp.jlab.org, presumably will return)
- hallb-pro is used for large-scale processing of real data, by special accounts for all Hall B experiments
  - It has a net fairshare of 0.84*0.34*0.7 → 20% of the entire farm (currently!)

CLAS12@JLab Fairshare

Calculations

- For a few years we've maintained calculations of the farm hardware distribution and benchmarks of CLAS12 software on each, stored on JLab's O365 and publicly accessible:
    - CLAS12 @ JLab Batch.xlsx
- Used to project how long it'll take to process each large data set on Jlab's farm
    - This works for steady-state running, when our queues are kept primed for days.
    - Sometimes you might hear other, much slower numbers, but those are probably for things like time for a few runs submitted for calibration, which includes large startup overhead if the farm is occupied (no preemption, waiting for other's jobs to finish).
- Also used for HPS by scaling, ~10 Hz (?)
- The "priority" portion of Hall B fairshare is currently ~50 million CPU hours per year, shared by all Hall B run groups.
- HPS is still small CPU compared to CLAS12



	Nodes			Farm				CLAS12 Node		CLAS12 Farm		
flavor	memory (GB)	slots	memory per slot (GB)	nodes	slots	node fraction	slot fraction	node rate (Hz)	slot event time (ms)	rate (kHz)	rate fraction	events per day (M)
farm16	62	72	0.86	38	2736	0.15	0.10	76	944	2.9	0.08	250
farm18	92	80	1.15	78	6240	0.32	0.22	93	859	7.3	0.20	628
farm19	256	128	2.00	106	13568	0.43	0.47	172	746	18.2	0.49	1571
farm23	256	256	1.00	24	6144	0.10	0.21	363	705	8.7	0.24	753
Average			1.49					151	781			
Sum				246	28688					37.1		3202
Hall B Fairshare					8290					10.7		925
Hall B Pro Fairshare					5803					7.5		648

Playground		
Billions of Events:		*16.0*
flavor	days	days @ Fairshare
farm16	63.9	221.2
farm18	25.5	88.2
farm19	10.2	35.2
farm23	21.2	73.5
Hall B Fairshare		17.3
Hall B Pro Fairshare		24.7

User Input Fields

Run Group	Rate Scale
RG-B	0.90

Run Group	Rate Scale
RG-A	1.00
RG-B	0.85
RG-K	1.43
RG-F	1.13
No Roads RG-A	1.13
RG-M	1.18
RG-C	0.9
RG-D	
RG-K	
RG-E	

Scales are relative to RG-A

Tree Fairshares		Million Slot-Hours per Year
ENP	0.84	211.1
Hall B	0.34	72.6
Hall B Pro	0.70	50.8
Product	0.202	

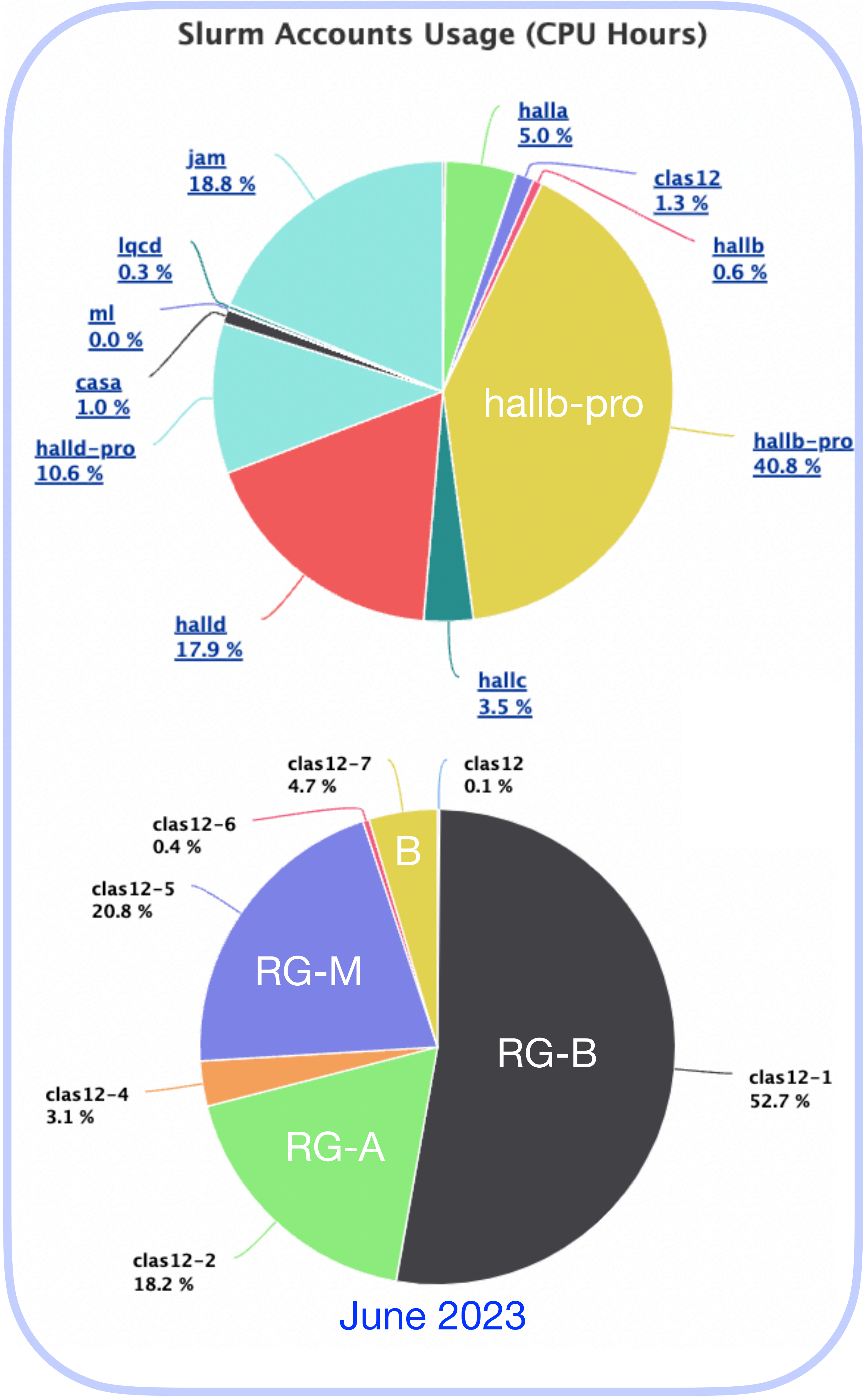
Global Scale Factor
0.85

CLAS12@JLab

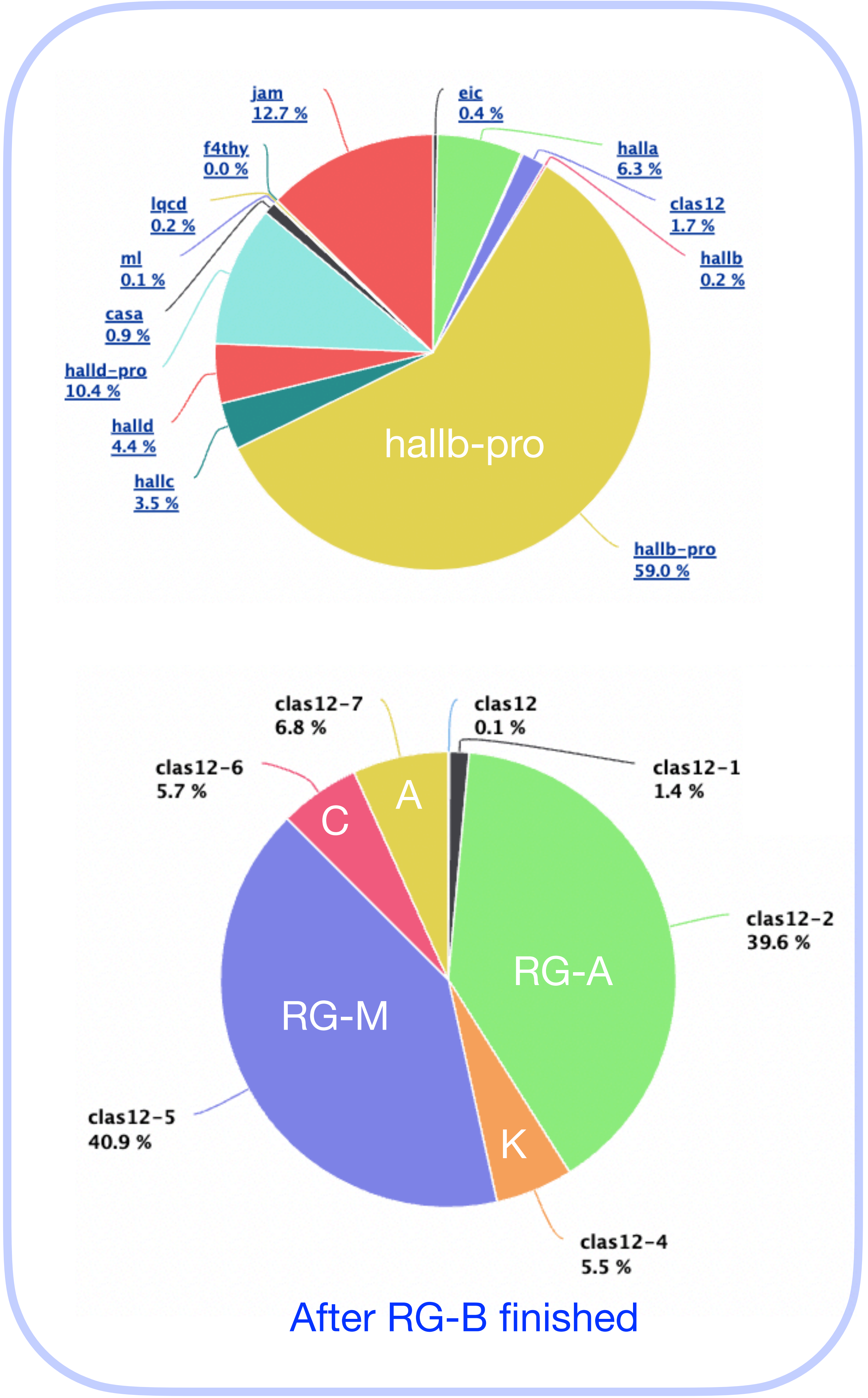
Reality

- RG-B's pass-2 ran for 30 days, start to finish
  - If we take the fraction of the farm clas12-1 really used during that time, and scale by the ratio of the expected hallb-pro fairshare of 20%, the 37-day projection from the previous slide turns into 30 days. 👍
  - The same assessment was done for RG-A/B's pass-1s, with similar agreement.
- You can also see RG-A/M's full passes coming online later in June, otherwise clas12-1's 53% would have been a much higher fraction of Hall-B's June usage, and then RG-A/M getting equal shares after RG-B finished.
- Meanwhile, calibration jobs are coming in from other run groups, and due to their much lower recent usage, immediately take priority over the full passes.
- So far, we have not (and do not want to!) manually managed any fairshares or job submissions to prioritize run groups or calibrations. All have equal fairshare.

Account Name	Current Purpose
clas12	admin
clas12-1	RG-B
clas12-2	RG-A
clas12-3	RG-F
clas12-4	RG-K
clas12-5	RG-M
clas12-6	RG-C
clas12-7	parallel calibrations
clas12-8	RG-D
clas12-9	RG-E
hps	HPS



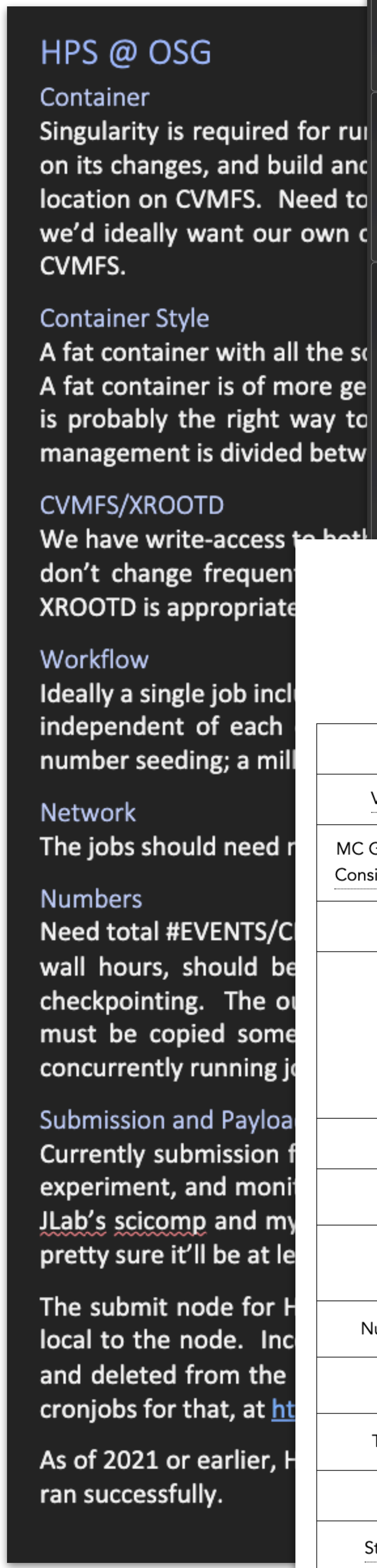
June 2023



After RG-B finished

Open Science Grid

- CLAS12 runs 99% of simulations on OSG, ~doubling available CPU resources relative to JLab's farm
    - Various machinery in place to automate for the collaboration's independent users, but HPS doesn't need all that
    - Timelines: https://clasweb.jlab.org/clas12offline/osg/
    - Submission portal: https://gemc.jlab.org/web_interface/index.php
- JLab has one submit node per ~hall, and submissions must go through HTCondor (not SWIF/SLURM) locally on that particular node
- Currently no mechanism other than HTCondor's built-in to get output data back from the job, and the submit nodes are DMZ'd, so it's staged locally on the submit node, and transferred manually to networked filesystems at JLab before manual deletion to ensure the local staging filesystem doesn't fill up.
- Large-scale stuff should be centrally managed by HPS, i.e., only one person submitting/managing jobs at a time.
- This writeup was distributed a couple years ago with some preparatory information and questions (data volume, job independence/atomicity, CPU hours) for HPS simulations on OSG
    - [HPS @ OSG.docx]()



HPS @ OSG

Container

Singularity is required for ru
on its changes, and build and
location on CVMFS. Need to
we'd ideally want our own c
CVMFS.

Container Style

A fat container with all the s
A fat container is of more ge
is probably the right way to
management is divided betw

CVMFS/XROOTD

We have write-access to both
don't change frequen
XROOTD is appropriate

Workflow

Ideally a single job incl
independent of each
number seeding; a mil

Network

The jobs should need r

Numbers

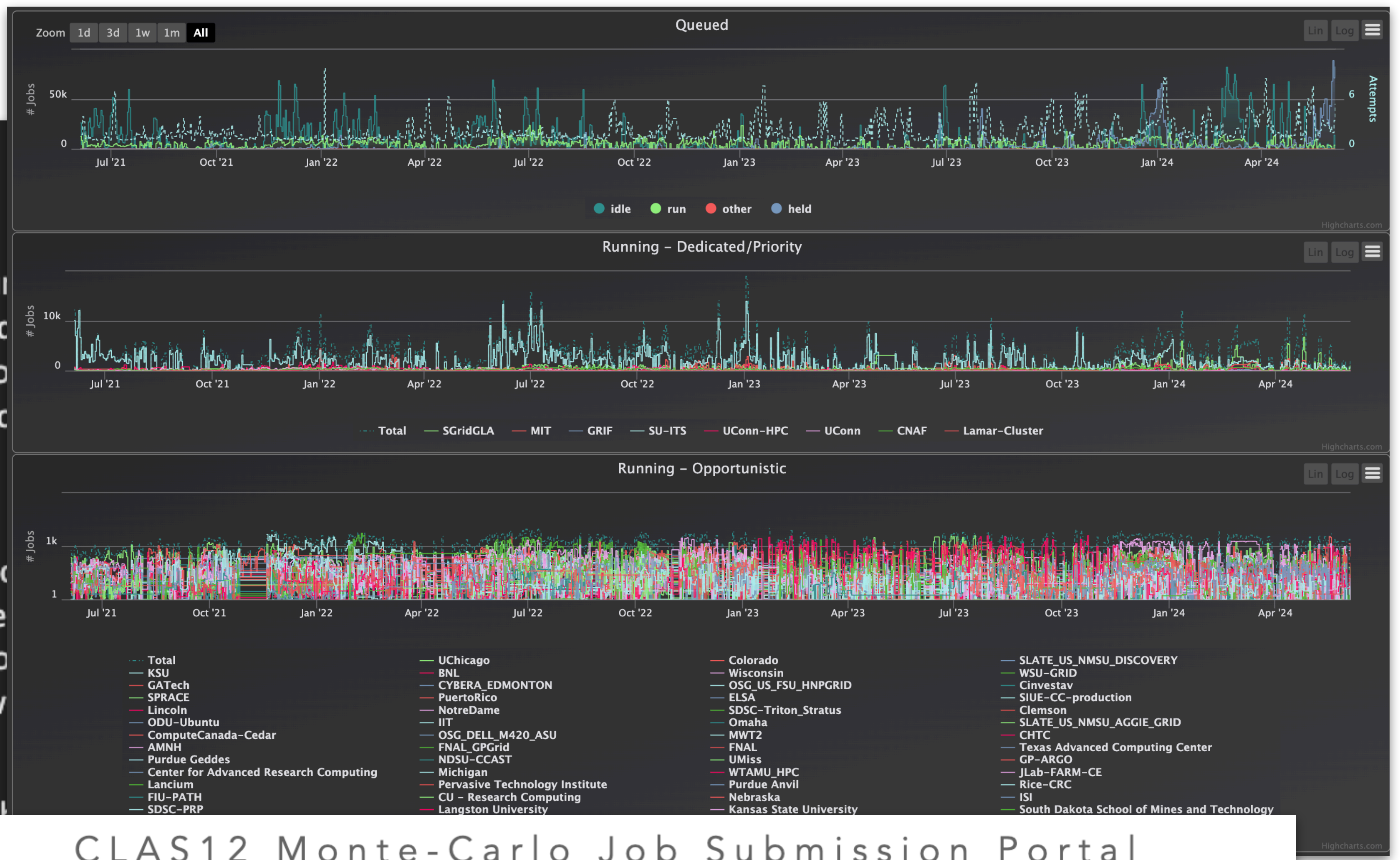
Need total #EVENTS/C
wall hours, should be
checkpointing. The o
must be copied some
concurrently running j

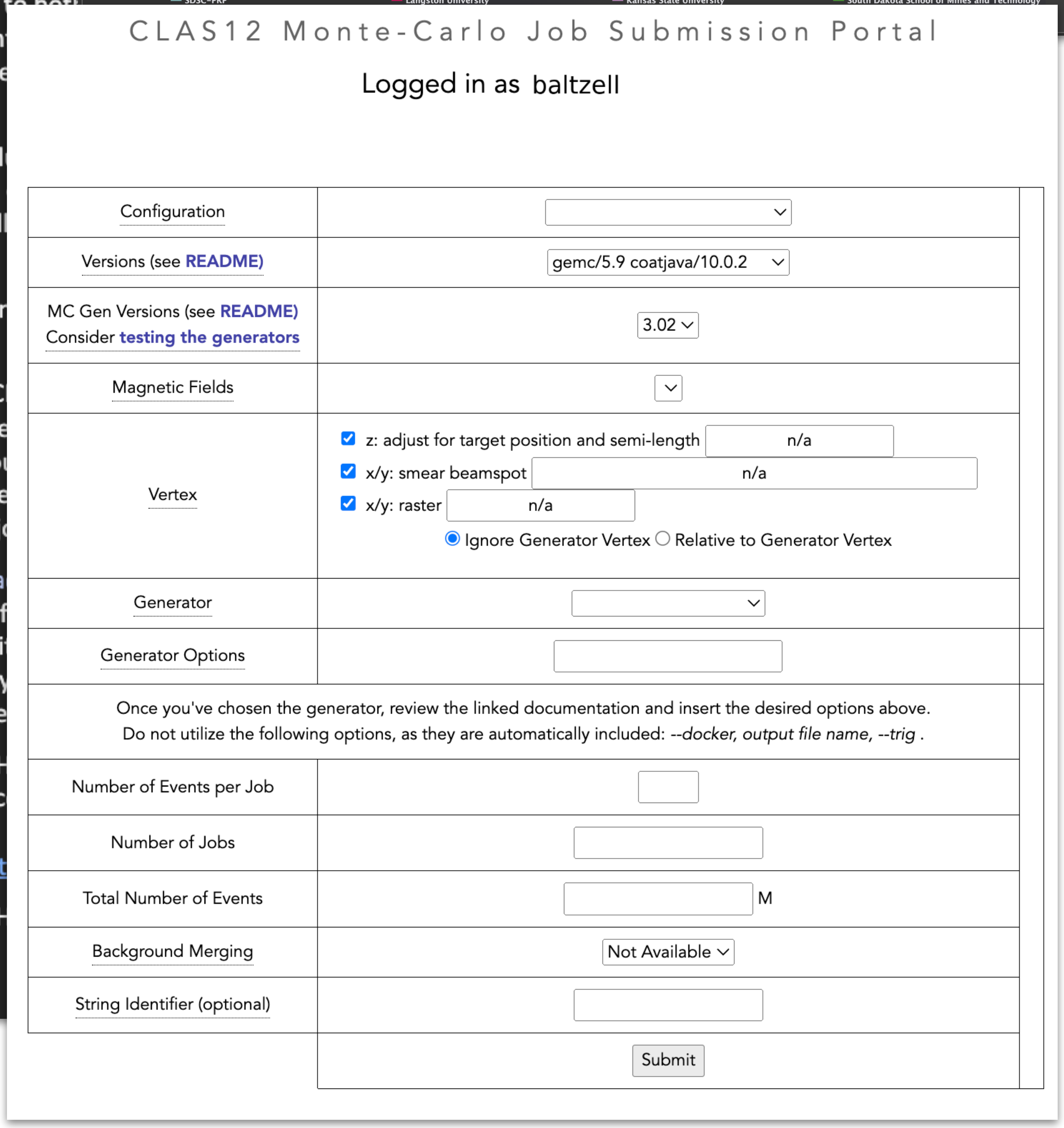
Submission and Payloa

Currently submission f
experiment, and moni
JLab's scicomp and my
pretty sure it'll be at le

The submit node for H
local to the node. Inc
and deleted from the
cronjobs for that, at ht

As of 2021 or earlier, H
ran successfully.





CLAS12 Monte-Carlo Job Submission Portal

Logged in as baltzell

Configuration	
Versions (see README)	gemc/5.9 coatjava/10.0.2
MC Gen Versions (see README) Consider testing the generators	3.02
Magnetic Fields	
Vertex	☑ z: adjust for target position and semi-length n/a ☑ x/y: smear beamspot n/a ☑ x/y: raster n/a ◉ Ignore Generator Vertex ○ Relative to Generator Vertex
Generator	
Generator Options	
Once you've chosen the generator, review the linked documentation and insert the desired options above. Do not utilize the following options, as they are automatically included: *--docker, output file name, --trig* .	
Number of Events per Job	
Number of Jobs	
Total Number of Events	M
Background Merging	Not Available
String Identifier (optional)	
	Submit

HPS Computing

- One critical thing for the larger 2019/2021 HPS runs is data volume.
    - With O(PB) raw data we cannot afford anywhere close to the output volume used for the 2015/2016 data sets (5x larger than the input EVIO!)

Coming Soon @ JLab

- RUCIO: https://rucio.cern.ch/
    - data catalog, searching, transferring
    - EIC pushed for it, GlueX is the next customer, then maybe CLAS12
- gitlab: https://code.jlab.org
    - in-house gitlab deployment, CI/CD imminent, infinite private repos
    - no sign JLab's github is going away, but we're grandfathered into our current plan and upgrading is expensive
- And much more ...