

Central Computing at Jefferson Lab

Alexander Austregesilo

GlueX Software Tutorial
May 23, 2022



Outline

1 The Common User Environment (CUE)

- Interactive and batch nodes
- Recommendations for File Storage

2 The GlueX Software Stack

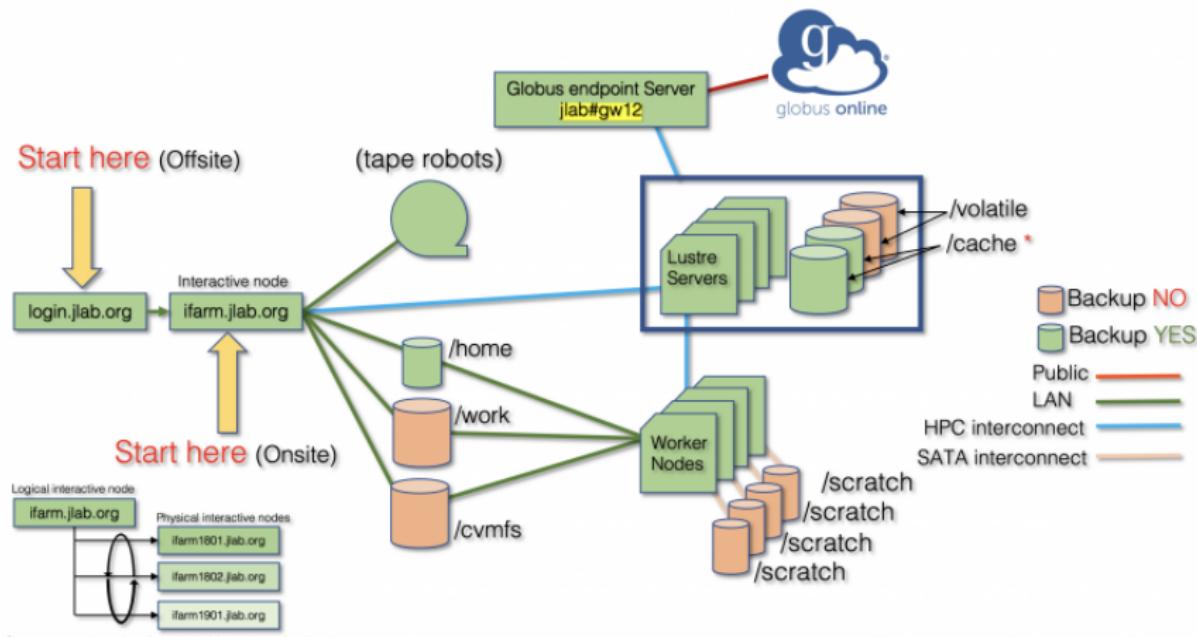
- Packages
- Default: Using the current release
- Developer mode

3 Batch Workflow Management

- SWIF2
- Batch Submission Scripts
- Example: How to run a plugin?
- Example: How to submit DSelector jobs?

4 How to Ask for Help

CUE Overview



* Backed to tape. Excludes small files.

https://scicomp.jlab.org/docs/getting_started

Computing Resources



Interactive nodes

- Login to ifarm1801, ifarm1802 or ifarm1901
- For software development and testing
- From offsite, only reachable through login.jlab.org

Batch farm

- Different nodes with 32-128 cores, 32-256BG RAM

Nodes with GPUs

- 4 NVidia TitanRTX and 40 T4 cards
- Accessible thorough slurm

https://halldweb.jlab.org/wiki/index.php/HOWTO_use_AmpTools_on_the_JLab_farm_GPUs

File Storage

/home/USER

- Very small
- Use for scripts (environment, batch, ...)

/work/halld/home/USER

- Shared workspace, 400TB total
- Use for software builds
- **Do not use for analysis output**

/volatile/halld/home/USER

- Shared temporary storage, 250TB total
- Files are deleted after 6 months, possibly earlier if above quota

/cache/halld/home/USER

- "Write-through" cache, 1.5PB
- Files > 1MB migrated to tape
- Backed-up files deleted when full
- **Overwrite produces conflicts**

/mss/halld/home/USER

- Representation of tape library
- Use jcache command (next slide)

/farm_out/USER

- Optimized for batch log files

More info: <https://scicomp.jlab.org/docs/node/632>

Cache and Tape

Useful Commands



/cache/halld/home/USER

- jcache pin (-D X): keep on disk (for X days, default 7, max 60)
- jcache put: force to tape



/mss/halld/home/USER

- jcache get: cache file

jcache -h: display all options

More info: <https://scicomp.jlab.org/docs/write-through-cache>

Software Stack

Active Development

- hdds: Hall D detector specifications
- halld_recon: reconstruction, monitoring, analysis
- halld_sim: generators, detector simulation, amplitudes
- hdgeant4: MC simulation
- AmpTools: amplitude analysis
- gluex_root_analysis: DSelector analysis
- gluex_MCWrapper: scripts to run all simulation
- hd_utilities: many useful scripts

All packages have repositories on github: Guide to Using Git Wiki

Dependencies

- ccdb, cernlib, diracxx, evio, evtgen, geant4, hepmc, jana, lapack, photon, rcdb, root, sqlite, sqlitecpp, xerces-c

All versions specified in xml file: `version.xml`

Default Scenario

bash and tcsh supported, this talk uses bash for all examples (.sh instead of .csh)

```
source /group/halld/Software/build_scripts/glueX_env_boot_jlab.sh
```

- Provides gxenv command and defines some directories
- Does not yet set up environment
- Add this to your .bashrc or .profile

gxenv

- Without argument: set up current default environment
Warning: default versions change over time
- Set up fixed version with xml file as argument, e.g.:
gxenv \$HALLD VERSIONS/version_5.7.1.xml
- gxclean: cleans environment

Developer Mode

\$BUILD_SCRIPTS/my_halld_build_jlab

- Use case: develop new features or debug existing software
- Starts with default version set
- Checks out local versions of (a subset of):
hdds, halld_recon, halld_sim, hdgeant4, gluex_root_analysis, amptools

\$BUILD_SCRIPTS/my_halld_update.py

- Update all private packages as identified in the xml file and build them

https://halldweb.jlab.org/docs/build_scripts_web/

Workflow Management

SWIF: Jefferson Lab's Scientific Workflow Indefatigable Factotem

- *it will work tirelessly on your behalf so that you need not expend unnecessary effort to make good use of the compute farm*
 - <https://scicomp.jlab.org/docs/swif2>

- Efficiently handles I/O with tape library
- Book-keeping, classification of errors, resubmission
- Possibility to handle job dependencies
- Submission to computing resources off-site, e.g. NERSC, PSC

Useful Commands

- `swif2 help` and `swif2 <command> help`
prints usage instructions
- `swif2 list (-archived)`
displays all your workflows (archived after 2 weeks)
- `swif2 status -workflow [WORKFLOW]`
shows more info about workflow, problem jobs
- `swif2 create -workflow [WORKFLOW]`
creates new workflow
- `swif2 add-job`
adds jobs to workflow, should be done with script
- `swif2 run -workflow [WORKFLOW]`
runs workflow
- `swif2 retry-jobs -workflow [WORKFLOW] -problems [PROBLEM]`
retries problems jobs

Possible problems

- SLURM_FAILED : your program crashed
- SLURM_TIMEOUT, SLURM_OUT_OF_MEMORY : check resources
- SITE_LAUNCH_FAIL, SWIF_INPUT_FAIL, SWIF_SYSTEM_ERROR : just retry
- `swif2 cancel -delete -workflow [WORKFLOW]`
deletes workflow

Scientific Computing

<https://scicomp.jlab.org/>

Scientific Computing 

username: aaustreg Getting Started Support Staff Members

Cluster Info

- Farm Nodes
- Slurm Jobs
- SWIF2 Jobs
- Usages

Jlab Scientific Computing

Welcome to the Jefferson Lab Scientific computing home page. [New users start here.](#)

Mar-04-22 **New auger-like slurm clients** After Auger retired, the auger clients, jsub, jkill and jobstat are disabled. But these auger-like slurm commands, `slurmHosts`, `slurmJobs` and `slurmQueues` are still available.

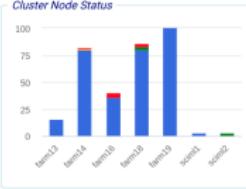
Feb-06-22 **Lustre usage tips for /cache and /volatile** 1) Avoid small or unbuffered writes to Lustre when possible. 2) Write log files to `/farm_out` when possible, which is tuned for high IOPS/small files. 3) Avoid file metadata operations in tight loops, such as hundreds of `open()` and `close()` operations per second. 4) Lustre perform best when reading or writing files using large buffers.

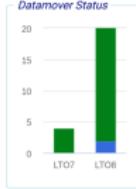
Slurm Job (Outstanding jobs)

Running	Pending	Held	Other
4,406	33,348	8	13

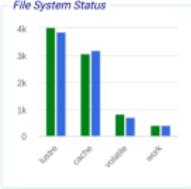
Slurm Job (past 24 Hrs finished jobs)

Success	Failed	Cancelled	Timedout	OverMemory	NodeFail
61,344	10,371	159	1,754	233	40

Cluster Node Status


Datamover Status


LTO7	LTO8
~2	~18

File System Status


File System	Value
File System 1	~4k
File System 2	~18k
File System 3	~15k
File System 4	~10k
File System 5	~5k

Job Info Last 24 Hrs


Date Time	Value
00:00	~50K
01:00	~45K
02:00	~48K
03:00	~40K
04:00	~42K
05:00	~44K
06:00	~46K
07:00	~48K
08:00	~45K
09:00	~47K
10:00	~49K
11:00	~46K
12:00	~48K
13:00	~45K
14:00	~47K
15:00	~44K
16:00	~46K
17:00	~43K
18:00	~45K
19:00	~47K
20:00	~44K
21:00	~46K
22:00	~43K
23:00	~45K
24:00	~42K

- Useful information about
 - Batch jobs and SWIF2 (more details coming soon)
 - File system and tape library
 - Usage statistics




A. Austregesilo (aaustreg@jlab.org) — Central Computing

12/18

Scientific Computing

<https://scicomp.jlab.org/>



- Overview of current farm usage
- Click on node to see individual jobs

Scientific Computing

<https://scicomp.jlab.org/>



Scientific Computing

username: aaustreg

Getting Started Support Staff Members

Outstanding (Pending/Active) Batch Farm Jobs

	Outstanding Jobs	Recent Jobs	Jobs query	Slurm Info	Slurm Account	Job Limit
Filter						
	User Name	Account	Pending	Running	Holding	Other
	acschick	halld	0	1	2,457	13
	almaeen	f4thy	0	1	0	0
File System	barryp	jam	0	769	0	0
	bparris	enp	0	1	0	0
Lustre	bruker	casa	0	1	0	0
Cache	ccocuzzza	jam	0	243	0	0
Volatile	churaman	halld	315	194	0	0
Work	clas12	halib-pro	0	80	10	0
	clas12-3	halib-pro	611	85	0	0
Tape Library	devita	clas12	0	100	0	0
	efuchey	hallia	0	404	0	0
Jobs	gluex	halld	0	80	10	0

- User specific information by “log-in” in the box on the top right
- Click on lines to see individual jobs

GlueX Scripts



https://github.com/JeffersonLab/hd_utilities/tree/master/launch_scripts/launch

https://github.com/JeffersonLab/hd_utilities/tree/master/launch_scripts/root_analysis

- Easy-to-use framework
- In use for official production and analysis launches
- Can also be used for DSelector analysis
- Actively supported

- `launch.py` : generic python program to submit jobs to workflow
- `script.sh` : bash scripts handles I/O and running on farm node
- `jobs.config` : steered with simple config file, **only user modification here!**

Usage: `launch.py <job.config> <minrun> <maxrun>`

halld_recon on the farm

jobs_analysis_bggen.config file



/group/halld/Software/gluex_workshops/tutorial_2022/session2a/launch/jobs_analysis.config

```

# SCICOMP JOB ACCOUNTING
PROJECT          halld
TRACK           production
IOS              general
USER             # PUT YOUR USER NAME HERE !!!
# JOB RESOURCES
NCORES           6      # This has to match the NTHREADS in jana_analysis.config
DISK             50GB
RAM              6GB
TIMELIMIT        6hrs
# WORKFLOW DEFINITION
# RUNPERIOD, VERSION, & BATCH: Not needed by launch.py: Only used to replace variables in this config
RUNPERIOD        2017-01
VERSION          03
BATCH            01
WORKFLOW         bggen_[RUNPERIOD]_ver[VERSION]_batch[BATCH]
# JOB, SCRIPT CONTROL
ENVFILE          analysis-2017_01-ver52.xml      # on the group disk
SCRIPTFILE        /group/halld/Software/workshops/tutorial_2022/session2a/launch/script.sh
RCDB_QUERY        "#is_production and @status_approved" # comment-out for all runs
JANA_CONFIG       /group/halld/Software/workshops/tutorial_2022/session2a/launch/jana_analysis.config
CACHE_PIN_DAYS    8      # max is 60, 0 or comment-out for none
# FILE INPUT, OUTPUT BASE DIRECTORIES
INDATA_TOPDIR    /cache/halld/gluex_simulations/REQUESTED_MC/2017_bggen_batch01_ver03_31_20220210010210pm/hddm/
# FOR FULL RECON LAUNCHES
OUTDIR_LARGE     /volatile/halld/home/[USER]/bggen/RunPeriod-[RUNPERIOD]/ver[VERSION]
OUTDIR_SMALL      /farm_out/[USER]/bggen/RunPeriod-[RUNPERIOD]/ver[VERSION]/batch[BATCH]/          # REST, skims, hists, trees
                                                # log files

```

- RESOURCES : modify for efficient use of farm
- CACHE_PIN_DAYS : only effective if OUTDIR_LARGE on cache disk

halld_recon on the farm

Example

/group/halld/Software/gluex_workshops/tutorial_2022/session2a/launch/

1 Set up workflow:

```
swif create bggen_2017-01_ver03_batch01
```

Name has to match entry in jobs.config exactly

2 Register jobs:

```
./launch.py jobs_analysis_bggen.config 30274 31057 -f '00[0-4]',
```

with runs in range 30274 - 31057 that fulfil RCDB query

-f : optional, only first five files in this example

3 Run workflow:

```
swif run -workflow bggen_2017-01_ver03_batch01
```

4 Periodically check workflow:

- swif2 list and swif2 status bggen_2017-01_ver03_batch01
- <https://scicomp.jlab.org/>
- output folder

To avoid interference, copy config file and edit USER

DSelector on the farm

jobs_root_analysis.config file

```
/group/halld/Software/workshops/tutorial_2022/session2a/root_analysis/jobs_root_analysis.config
```

```
# SCICOMP JOB ACCOUNTING
PROJECT          halld
TRACK           production
OS               general
USER             # PUT YOUR USER NAME HERE !!!
# JOB RESOURCES
NCORES           4
DISK             50GB
RAM              8GB
TIMELIMIT        1hrs
# WORKFLOW DEFINITION
# RUNPERIOD, VERSION, & BATCH: Not needed by launch.py: Only used to replace variables in this config
RUNPERIOD        2017-01
VERSION          53
BATCH            01
WORKFLOW         dselector_[RUNPERIOD]_ver[VERSION]_batch[BATCH]
# JOB_SCRIPT CONTROL
ENVFILE          version.xml # latest release
SCRIPTFILE        /group/halld/Software/gluex_workshops/tutorial_2022/session2a/root_analysis/script.sh
# ROOT CONFIG
ROOT_SCRIPT      /group/halld/Software/gluex_workshops/tutorial_2022/session2a/root_analysis/Run_Selector.C
TREE_NAME         pi0eta_B4_M17_M7_Tree
SELECTOR_NAME    /group/halld/Software/gluex_workshops/tutorial_2022/session2c/DSelector_etapi      # Leave .C off of the end!
# FILE INPUT, OUTPUT BASE DIRECTORIES
INDATA_TOPDIR   /cache/halld/RunPeriod-2017-01/analysis/ver52/tree_pi0eta_B4_M17_M7/merged/
# FILE OUTPUT
OUTDIR_LARGE    /volatile/halld/home/[USER]/root_analysis/RunPeriod-[RUNPERIOD]/ver[VERSION]          # tree, hist
OUTDIR_SMALL     /farm_out/[USER]/root_analysis/RunPeriod-[RUNPERIOD]/ver[VERSION]/batch[BATCH]/          # log files
```

- TREE_NAME : name of tree in input file
- SELECTOR_NAME : your DSelector (without .C)

DSelector on the farm

Example

/group/halld/Software/workshops/tutorial_2022/session2a/root_analysis/

- ➊ Set up workflow:

```
swif2 create dselector_2017-01_ver52_batch01
```

Name has to match entry in jobs.config exactly

- ➋ Register jobs (same executable as before):

```
.. /launch/launch.py jobs.root_analysis.config 30274 31057
```

with runs in range 30274 - 31057 that fulfil RCDB query

- ➌ Run workflow:

```
swif2 run -workflow dselector_2017-01_ver52_batch01
```

- ➍ Periodically check workflow:

- swif2 list and swif2 status dselector_2017-01_ver52_batch01
- <https://scicomp.jlab.org/>
- output folder

To avoid interference, copy config file and edit USER

How to Ask for Help

- Useful wiki pages:
 - Getting Started at GlueX : lots of useful info for starters
 - Software Overview : description of all analysis steps
 - Offline Software : detailed info about software
 - Offline HOWTO : guides to various specific tasks
 - Analysis HOWTO : guides to common analysis tasks
- Computer Center, SciComp websites and Service Now ticket system
- halld-offline email list and glueX software google group
- Slack for quick feedback, Open Analysis discussion meetings every Tuesday
- Github issues for problem with specific package



Report inconsistencies, fix bugs, contribute to the documentation efforts!

Best Practise for Bug Report

- As much information as possible: environment, software versions, recent changes
- Accessible location of program, script, input files, ...
- Ideal: minimal example with all necessary parts to reproduce problem