Advanced Cluster Usage

FAS Research Computing
Outline

• Job Submission

• Job Resource Requirements

• Job/Partition/Queue Monitoring

• Job Checkpointing

• Fairshare

• Storage Workflow
Job Submission - Interactive

- `salloc -p test --mem=4G -t 0-01:00`
  - Gives back a shell prompt on a compute node
  - Uses
    - Testing code
    - Working interactively on the cluster without resource contention
- Limitations
  - Session stall
  - Ties up prompt
  - Not great for GUI applications
  - If submitting to a busy partition `salloc` may take a while to respond
Job Submission - Interactive

Job Submission - Interactive

On Demand provides an integrated, single access point for all of your HPC resources.

Pinned Apps: A featured subset of all available apps

Interactive Apps

- **Jupyter**: System Installed App
- **Matlab**: System Installed App
- **Postgres DB**: System Installed App
- **RStudio Server**: System Installed App
- **Remote Desktop**: System Installed App
- **SAS**: System Installed App
- **Shark**: System Installed App

Welcome to FAS-RC Cluster

The FAS Research Computing Cluster is a resource for the research community, hosted by Research Computing at Harvard University in the Faculty of Arts and Sciences.

To apply for an account please refer to this webpage.

From this web service you can submit your jobs, check running jobs, and open interactive graphical sessions to run your favorite applications.

Here are some examples of the things you will be able to do:
- Open an interactive remote desktop session to a compute node
- Run Jupyter Notebooks
- Run RStudio Server sessions
- Browse and edit your files
- Open a terminal connection to a login node

Check out our documentation at this page:

https://vdi.rc.fas.harvard.edu (VPN Required)
Job Submission - Interactive
#!/bin/bash
#SBATCH -J hybridtest
#SBATCH -n 32
#SBATCH -c 4
#SBATCH -p shared
#SBATCH -t 1-12:00:00
#SBATCH --mem-per-cpu=8G
#SBATCH -o hybrid_%A.out
#SBATCH -o hybrid_%A.err

module load intel/23.0.0-fasrc01 openmpi/4.1.4-fasrc01

srun -c $SLURM_CPUS_PER_TASK -n $SLURM_NTASKS --mpi=pmix ./wombat.x

sbatch runscript.slurm

Submits list of instructions and commands as a script to the scheduler
Does not require an open prompt

Types
Serial
Array (--array)
Thread
Rank
Hybrid

Useful Options (not exhaustive)
--contiguous
--constraint/--prefer
--dependency
--exclusive[={user|mcs}]
--gpu/--gres
Job Resource Requirements

[User@boslogin01 home]# seff 1234567
Job ID: 1234567
Cluster: odyssey
User/Group: user/user_lab
State: COMPLETED (exit code 0)
Nodes: 8
Cores per node: 64
CPU Utilized: 37-06:17:33
CPU Efficiency: 23.94% of 155-16:02:08 core-walltime
Job Wall-clock time: 07:17:49
Memory Utilized: 1.53 TB (estimated maximum)
Memory Efficiency: 100.03% of 1.53 TB (195.31 GB/node)

- Know your Code
  - Numerical Methods
  - Size of Data
  - Type of Parallelism

- Experimentation
  - Validate Memory Size Requirements
  - Scaling Tests
  - Profiling
  - sstat vs. sacct

- Select Appropriate Partition and Hardware
Job Resource Requirements - Scaling

Strong Scaling
Size of Computation Constant While Number of Cores Increases (log-log)

Weak Scaling
Size of Computation Grows as Number of Cores Increases (log-linear)
### Job Monitoring - sacct

```bash
[root@holy7c22501 general]# sacct -u mngo

<table>
<thead>
<tr>
<th>JobID</th>
<th>JobName</th>
<th>Partition</th>
<th>Account</th>
<th>AllocCPUS</th>
<th>State</th>
<th>ExitCode</th>
</tr>
</thead>
<tbody>
<tr>
<td>63911611</td>
<td>train_liif</td>
<td>gpu pfister_l+</td>
<td>14</td>
<td>TIMEOUT</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>63911611.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>14</td>
<td>CANCELLED 0:15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>63911611.ex+</td>
<td>extern</td>
<td>pfister_l+</td>
<td>14</td>
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<td>0:0</td>
<td></td>
</tr>
<tr>
<td>63911755</td>
<td>train_liif</td>
<td>gpu pfister_l+</td>
<td>14</td>
<td>TIMEOUT</td>
<td>0:0</td>
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</tr>
<tr>
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<td>batch</td>
<td>pfister_l+</td>
<td>14</td>
<td>CANCELLED 0:15</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>extern</td>
<td>pfister_l+</td>
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<tr>
<td>63971094</td>
<td>train_liif</td>
<td>gpu pfister_l+</td>
<td>14</td>
<td>COMPLETED</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>63971094.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>14</td>
<td>COMPLETED</td>
<td>0:0</td>
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</tr>
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<td>extern</td>
<td>pfister_l+</td>
<td>14</td>
<td>COMPLETED</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
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<td>train_liif</td>
<td>gpu pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>64063319.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>64063319.ex+</td>
<td>extern</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
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<td>gpu pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
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<td>batch</td>
<td>pfister_l+</td>
<td>14</td>
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<td>extern</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
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<td>train_liif</td>
<td>gpu pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
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<td>64063331.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
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<td>extern</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>64078487</td>
<td>train_liif</td>
<td>gpu pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>64078487.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>64078487.ex+</td>
<td>extern</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>64078502</td>
<td>train_liif</td>
<td>gpu pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>64078502.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
<tr>
<td>64078502.ex+</td>
<td>extern</td>
<td>pfister_l+</td>
<td>14</td>
<td>RUNNING</td>
<td>0:0</td>
<td></td>
</tr>
</tbody>
</table>
```

- **Default shows data from last day**
- **Options**
  - `--starttime/--endtime`
  - `--format`
  - `--parsable2`
  - `--partition`
  - `--state`

---

**FAS Research Computing**

Division of Science

https://rc.fas.harvard.edu
Job Monitoring - scontrol

```
[root@holy7c22501 general]# scontrol show job 64063319
JobId=64063319 JobName=train_liif
UserId=mngo(63096) GroupId=pfister_lab(40134) MCS_label=N/A
Priority=17583 Nice=0 Account=pfister_lab QOS=normal
JobState=RUNNING Reason=None Dependency=(null)
Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0
RunTime=1:21:52.05 TimeLimit=3:00:00 TimeMin=N/A
AccrueTime=2023-07-25T13:45:18
Startime=2023-07-25T13:45:21 Endtime=2023-07-28T13:45:21 Deadline=N/A
SuspendTime=None SecsPreSuspend=0 LastSchedEval=2023-07-25T13:45:21 Scheduler=Main
Partition=gpu AllocNode:Std=0.0.0.0:267715
ReqNodeList=(null) ExcNodeList=(null)
NodeList=holygpu7c26101
BatchHost=holygpu7c26101
NumNodes=1 NumCPUs=14 NumTasks=1 CPUs/Task=14 ReqB:S:C:T=0:*:*:*
TRES=cpu=14,mem=490G,node=1,billing=926,gres/gpu=4,gres/gpu:nvidia_a100-sxm4-40gb=4
Socks/Node=* TaksPerN:B:S:C=0:*:*:* CoreSpec=* 
MinCPUsNode=14 MinMemoryCPU=35G MinTmpDiskNode=0
Features=(null) DelayBoot=00:00:00
OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
Command=/n/holylfs05/LABS/pfister_lab/Job/coxfs01/pfister_lab2/Lab/mngo/vu-master-thesis/liif/slurm/job_train_iter.sh
WorkDir=/n/holylfs05/LABS/lfisher_lab/Job/coxfs01/pfister_lab2/Lab/mngo/vu-master-thesis/liif
StdErr=/n/holylfs05/LABS/lfisher_lab/Job/coxfs01/pfister_lab2/Lab/mngo/vu-master-thesis/liif
StdOut=/n/holylfs05/LABS/lfisher_lab/Job/coxfs01/pfister_lab2/Lab/mngo/vu-master-thesis/liif
Power=
MemPerTres=gpu:100
TresPerNode=gres/gpu:4
```
### Partition Monitoring - showq

[root@holy7c22501 general]# showq -p intermediate -o

**SUMMARY OF JOBS FOR QUEUE: intermediate**

**ACTIVE JOBS**

<table>
<thead>
<tr>
<th>JOBID</th>
<th>JOBNAME</th>
<th>USERNAME</th>
<th>STATE</th>
<th>CORE</th>
<th>GPU</th>
<th>REMAINING</th>
<th>STARTTIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>60897569</td>
<td>cm_afm.sh</td>
<td>joonholee</td>
<td>Running</td>
<td>48</td>
<td>0</td>
<td>167:46:27</td>
<td>Thu Jul 20 11:29:20</td>
</tr>
<tr>
<td>60897570</td>
<td>cm_afm.sh</td>
<td>joonholee</td>
<td>Running</td>
<td>48</td>
<td>0</td>
<td>196:29:26</td>
<td>Fri Jul 21 00:12:19</td>
</tr>
<tr>
<td>60897572</td>
<td>cm_afm.sh</td>
<td>joonholee</td>
<td>Running</td>
<td>48</td>
<td>0</td>
<td>24:54:04</td>
<td>Sun Jul 23 19:36:57</td>
</tr>
<tr>
<td>61583962</td>
<td>skin_WS_syts</td>
<td>csxue</td>
<td>Running</td>
<td>1</td>
<td>0</td>
<td>21:50:42</td>
<td>Fri Jul 21 09:33:35</td>
</tr>
<tr>
<td>62497782</td>
<td>.fasrcood/verstyuk</td>
<td>dverbart</td>
<td>Running</td>
<td>1</td>
<td>0</td>
<td>24:49:17</td>
<td>Fri Jul 14 17:32:10</td>
</tr>
<tr>
<td>62497784</td>
<td>.fasrcood/verstyuk</td>
<td>dverbart</td>
<td>Running</td>
<td>1</td>
<td>0</td>
<td>24:49:59</td>
<td>Fri Jul 14 17:32:52</td>
</tr>
<tr>
<td>63128424</td>
<td>sbatch</td>
<td>dverbart</td>
<td>Running</td>
<td>64</td>
<td>0</td>
<td>63:18:07</td>
<td>Sat Jul 22 03:01:00</td>
</tr>
<tr>
<td>63128430</td>
<td>sbatch</td>
<td>dverbart</td>
<td>Running</td>
<td>64</td>
<td>0</td>
<td>123:59:12</td>
<td>Mon Jul 24 15:42:05</td>
</tr>
<tr>
<td>63268520</td>
<td>sbatch</td>
<td>dverbart</td>
<td>Running</td>
<td>64</td>
<td>0</td>
<td>144:02:24</td>
<td>Tue Jul 25 11:45:17</td>
</tr>
<tr>
<td>63884205</td>
<td>doParallelcdadams</td>
<td>dverbart</td>
<td>Running</td>
<td>64</td>
<td>0</td>
<td>27:44:41</td>
<td>Tue Jul 25 07:27:34</td>
</tr>
<tr>
<td>63885162</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>336:00:00</td>
<td>Sun Jul 23 11:23:49</td>
</tr>
<tr>
<td>63885172</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>302:55:15</td>
<td>Wed Jul 26 02:38:08</td>
</tr>
<tr>
<td>63885194</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>313:14:06</td>
<td>Wed Jul 26 12:56:59</td>
</tr>
<tr>
<td>63885224</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>323:24:06</td>
<td>Wed Jul 26 23:06:59</td>
</tr>
<tr>
<td>63885226</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>323:25:14</td>
<td>Wed Jul 26 23:08:07</td>
</tr>
</tbody>
</table>

28 active jobs: 539 of 576 cores (93.58%); 0 of 0 gpus (0.00%); 12 of 12 nodes (100.00%)

**WAITING JOBS**

<table>
<thead>
<tr>
<th>JOBID</th>
<th>JOBNAME</th>
<th>USERNAME</th>
<th>STATE</th>
<th>CORE</th>
<th>GPU</th>
<th>WCLIMIT</th>
<th>QUEUETIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>62277463</td>
<td>S110-6K</td>
<td>yrupan</td>
<td>Waiting</td>
<td>40</td>
<td>0</td>
<td>336:00:00</td>
<td>Thu Jul 13 03:45:48</td>
</tr>
<tr>
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<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>336:00:00</td>
<td>Sun Jul 25 11:23:48</td>
</tr>
<tr>
<td>63885223</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>336:00:00</td>
<td>Sun Jul 23 11:23:48</td>
</tr>
<tr>
<td>63885233</td>
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<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>336:00:00</td>
<td>Sun Jul 23 11:23:48</td>
</tr>
<tr>
<td>63885234</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>336:00:00</td>
<td>Sun Jul 23 11:23:48</td>
</tr>
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<td>10</td>
<td>0</td>
<td>336:00:00</td>
<td>Sun Jul 23 11:23:48</td>
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<td>agarciasoto</td>
<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>336:00:00</td>
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<tr>
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<td>336:00:00</td>
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<td>Waiting</td>
<td>10</td>
<td>0</td>
<td>336:00:00</td>
<td>Sun Jul 23 11:23:49</td>
</tr>
</tbody>
</table>

---

- **Shows queue state**
- **Options**
  - `-p`: partition
  - `-o`: order by priority
  - `-U`: username
  - `-s`: only summary information
Job Checkpointing

- Creates a save point for your job to pick up from where it left off
  - Also Known As: Checkpointing, Save File, Restart File

- Useful for:
  - Long running jobs
  - Jobs that error out
  - Jobs that need midstream tweaking
  - Leveraging requeue partitions

- How?
  - Build it into your code
  - DMTCP: Distributed MultiThreaded Checkpointing
  - Leverage --dependency
  - Make code aware to check for checkpoint when requeued
Fairshare

1. A method for ensuring the equitable use of a cluster
2. The fraction of the cluster a user/group gets
3. The score assigned by Slurm to a user/group based on usage
4. Priority that users/groups get based on usage
Fairshare - sshare

```
[user1@holyitc01 ~]$ sshare --account=test_lab -a

Account User RawShares NormShares RawUsage EffectvUsage FairShare
--------------------------------------------------------------------
test_lab 244 0.001363 45566082 0.000572 0.747627
test_lab user1 parent 0.001363 82028750.000572 0.747627
test_lab user2 parent 0.001363 248820 0.000572 0.747627
test_lab user3 parent 0.001363 163318 0.000572 0.747627
test_lab user4 parent 0.001363 18901027 0.000572 0.747627
test_lab user5 parent 0.001363 18050039 0.000572 0.747627
```

- **Default Raw Shares**
  - Cannon: 120
  - FASSE: 100

- **Fairshare Regimes:**
  - \( f = 1 \): Unused
  - \( 1.0 > f > 0.5 \): Underutilized
  - \( 0.5 \): Average utilization
  - \( 0.5 > f > 0 \): Over-utilized
  - \( f = 0 \): No share left
Fairshare - scalc

[root@holy7c22501 ~]# scalc
What do you want to calculate?
1) Projected FairShare Based on New RawShare
2) Additional RawShare Need for FairShare Score
3) Projected Time to Reach FairShare Score Assuming No New Jobs
4) Projected Usage and Fairshare Based on Job
5) Calculate New RawShare Based on Additional Hardware
Option: 4

4

We will now calculate how much TRES your jobs will cost as well as how it will impact the specified account's usage and fairshare.
First we need to know what account you want to calculate for: rc_admin
Next we need the partition you want to submit to: shared
How many cores will you use per job: 1024
How much memory in GB will you use per job: 4000
How many total GPUs will you user per job: 0
How long will the job run for (DD-HH:MM:SS): 1-00:00:00
How many jobs (or array elements) will you run of this type: 1
rc_admin has a current Raw Usage of 9725230 a Normalized Usage of 0.000026 a Normalized Allocation of 0.000759 and Fairshare of 0.976085
This partition has a TRES charge per second of CPU: 1.0 | Mem (per GB): 0.25 | GPU (per GPU): 0
This set of jobs has a total TRES usage of: 174873600.0
For rc_admin this will give a new Normalized Usage of 0.0004935173337802807 and a Fairshare of 0.6371829348127839
Storage Workflow
Questions, Comments, Concerns?