Advanced Cluster Usage

FAS Research Computing
FASRC User Survey 2024

Please fill it out! Your feedback is important.

https://harvard.az1.qualtrics.com/jfe/form/SV_e3AmuOrrmBOHTCu

Runs until April 12th
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
Welcome to FAS-RC Cluster

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

To apply for an account please refer to this webpage.

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

These 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:
Remote Desktop version: 3006999

This app will launch an interactive desktop session on a computer node in a partition of your choice. This app is useful to have a graphical user interface (GUI) on the FAS RC cluster.

You can select the amount of RAM (in GB), number of cores, and partition. Upon request, you will receive an email notification when the job starts. You must specify your email address.

See Remote Desktop VDI app documentation for how to use the app, update the web browser within the app, copy and paste between your computer and the remote desktop app.

See How to Launch software for how to launch various software, like Anaconda, Conda, Posix, etc.

Resolution

- width: 1024 px
- height: 768 px

Reset Resolution

Partition

- test
- [partition=partition name]

Run partition name (e.g., shared), or comma-separated list of partition names (e.g., shared, test).

Memory Allocation in GB

- 8

Number of cores

- 2

Number of CPUs to allocate

- 2

Number of GPUs to allocate

- 0

Number of GPUs to allocate. Available only on GPU-enabled partitions.

Allocated Time (expressed in Mins, or HH:MM:SS, or DD:HH:MM)

- 00:00:00

[Submit]
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 -e 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
--tmp
Job Resource Requirements - `seff`

```
[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
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 - seff-account

[root@holy7c22501 ~]# seff-account -u user

Job Information
Names: interactive, column_integration, stilt
Cluster: odyssey
Users: user
Account: user_lab
Start Time: now-1days
End Time: now
Average Requested CPUs: 7.89 cores on 1.00 node(s)
Average Requested Memory: 123.52G
Average Requested Time: 86248.08s

Job Status
CANCELLED by 0: 3004
COMPLETED: 59
FAILED: 2237
PREEMPTED: 8

Finished Job Statistics
(excludes pending, running, and cancelled jobs)
Average CPU Efficiency 15.74%
Average Memory Usage 3.43G
Average Run-time 2386.95s

CPU Efficiency (%)
--------------------------------------
+0.00e+00 - +1.00e+01  [2619]  █████████████▌
+1.00e+01 - +2.00e+01  [ 75]  ▏
+2.00e+01 - +3.00e+01  [  0]
+3.00e+01 - +4.00e+01  [882]  ▏
+4.00e+01 - +5.00e+01  [131]  ▏
+5.00e+01 - +6.00e+01  [ 10]
+6.00e+01 - +7.00e+01  [ 3]  ▏
+7.00e+01 - +8.00e+01  [10]  ▏
+8.00e+01 - +9.00e+01  [10]  ▏
+9.00e+01 - +1.00e+02  [ 3]  ▏

Memory Efficiency (%)
--------------------------------------
+0.00e+00 - +1.00e+01  [3448]  ████████████████████████████████████████
+1.00e+01 - +2.00e+01  [265]  ▏
+2.00e+01 - +3.00e+01  [ 3]  ▏
+3.00e+01 - +4.00e+01  [ 1]
+4.00e+01 - +5.00e+01  [ 2]
+5.00e+01 - +6.00e+01  [ 6]
+6.00e+01 - +7.00e+01  [10]
+7.00e+01 - +8.00e+01  [ 5]
+8.00e+01 - +9.00e+01  [ 1]
+9.00e+01 - +1.00e+02  [42]

Time Efficiency (%)
--------------------------------------
+0.00e+00 - +1.00e+01  [3769]  ████████████████████████████████████████
+1.00e+01 - +2.00e+01  [ 4]
+2.00e+01 - +3.00e+01  [ 5]
+3.00e+01 - +4.00e+01  [ 0]
+4.00e+01 - +5.00e+01  [ 0]
+5.00e+01 - +6.00e+01  [ 0]
+6.00e+01 - +7.00e+01  [ 4]
+7.00e+01 - +8.00e+01  [ 1]
+8.00e+01 - +9.00e+01  [ 0]
+9.00e+01 - +1.00e+02  [ 0]

Options
- -u user
- -a account (will not show data for jobs outside your user)
- -S start time
- -E end time
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

<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>6391161</td>
<td>train_liif</td>
<td>gpu</td>
<td>pfister_l+</td>
<td>14</td>
<td>TIMEOUT</td>
<td>0:0</td>
</tr>
<tr>
<td>6391161.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>pfister_l+</td>
<td>14</td>
<td>CANCELLED</td>
<td>0:15</td>
</tr>
<tr>
<td>6391161.ex+</td>
<td>extern</td>
<td>pfister_l+</td>
<td>pfister_l+</td>
<td>14</td>
<td>COMPLETE</td>
<td>0:0</td>
</tr>
<tr>
<td>63911755</td>
<td>train_liif</td>
<td>gpu</td>
<td>pfister_l+</td>
<td>14</td>
<td>TIMEOUT</td>
<td>0:0</td>
</tr>
<tr>
<td>63911755.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>pfister_l+</td>
<td>14</td>
<td>CANCELLED</td>
<td>0:15</td>
</tr>
<tr>
<td>63911755.ex+</td>
<td>extern</td>
<td>pfister_l+</td>
<td>pfister_l+</td>
<td>14</td>
<td>COMPLETE</td>
<td>0:0</td>
</tr>
<tr>
<td>63971094</td>
<td>train_liif</td>
<td>gpu</td>
<td>pfister_l+</td>
<td>14</td>
<td>COMPLETE</td>
<td>0:0</td>
</tr>
<tr>
<td>63971094.ba+</td>
<td>batch</td>
<td>pfister_l+</td>
<td>pfister_l+</td>
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<td>63971094.ex+</td>
<td>extern</td>
<td>pfister_l+</td>
<td>pfister_l+</td>
<td>14</td>
<td>COMPLETE</td>
<td>0:0</td>
</tr>
</tbody>
</table>

- Default shows data from last day
- Options
  - --starttime/--endtime
  - --format
  - --parsable2
  - --partition
  - --state
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=0:0
RunTime=1-21:52:05 TimeLimit=3-00:00:00 TimeMin=N/A
AccrueTime=2023-07-25T13:45:18
StartTime=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:Sid=0.0.0.0:2677159
ReqNodeList=(null) ExcNodeList=(null)
NodeList=holygpu7c26101 BatchHost=holygpu7c26101
NumNodes=1 NumCPUs=14 NumTasks=1 CPUs/Task=14 RegB:S:C:T=0:0:::*
TRES=cpu=14,mem=490G,node=1,billing=926,gpus/cpu=4,gpus/gpu:nvidia_a100-sxm4-40gb=4
Socks/Node=* NtasksPerNode:S:C=0:0:::* 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/Lab/coxfs01/pfister_lab2/Lab/mngo/vu-master-thesis/liif/slurm/job_train_iter.sh
WorkDir=/n/holylfs05/LABS/pfister_lab/Lab/coxfs01/pfister_lab2/Lab/mngo/vu-master-thesis/liif
StdErr=/n/holylfs05/LABS/pfister_lab/Lab/coxfs01/pfister_lab2/Lab/mngo/vu-master-thesis/liif/slurm/outputs/myerrors_64063319.err
StdOut=/n/holylfs05/LABS/pfister_lab/Lab/coxfs01/pfister_lab2/Lab/mngo/vu-master-thesis/liif/slurm/outputs/myoutput_64063319.out
Power=MemPerTres=gpu:100 TresPerNode=gpus:gpus:4
```
**Partition Monitoring - showq**

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

```bash
[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 48</td>
<td>0</td>
<td></td>
<td></td>
<td>167:46:27 Thu Jul 20 11:29:20</td>
</tr>
<tr>
<td>60897570</td>
<td>cm_afm.sh</td>
<td>joonholee</td>
<td>Running 48</td>
<td>0</td>
<td></td>
<td></td>
<td>196:29:26 Fri Jul 21 16:12:19</td>
</tr>
<tr>
<td>60897572</td>
<td>cm_afm.sh</td>
<td>joonholee</td>
<td>Running 48</td>
<td>0</td>
<td></td>
<td></td>
<td>247:54:04 Sun Jul 23 19:36:17</td>
</tr>
<tr>
<td>61589362</td>
<td>skin-W5_sy</td>
<td>csxue</td>
<td>Running 1</td>
<td>0</td>
<td></td>
<td></td>
<td>215:50:42 Fri Jul 21 09:33:35</td>
</tr>
<tr>
<td>62421778</td>
<td>.fasrcood/</td>
<td>verstyuk</td>
<td>Running 1</td>
<td>0</td>
<td></td>
<td></td>
<td>244:49:17 Fri Jul 14 17:32:10</td>
</tr>
<tr>
<td>63128424</td>
<td>sbatch</td>
<td>dverbart</td>
<td>Running 64</td>
<td>0</td>
<td></td>
<td></td>
<td>63:18:07 Sat Jul 22 03:10:00</td>
</tr>
<tr>
<td>63268630</td>
<td>sbatch</td>
<td>dverbart</td>
<td>Running 64</td>
<td>0</td>
<td></td>
<td></td>
<td>123:59:12 Mon Jul 24 15:42:05</td>
</tr>
<tr>
<td>63884205</td>
<td>S110-6K</td>
<td>yrupan</td>
<td>Waiting 40</td>
<td>0</td>
<td></td>
<td></td>
<td>27:44:14 Thu Jul 13 03:43:17</td>
</tr>
<tr>
<td>63885231</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting 10</td>
<td>0</td>
<td></td>
<td></td>
<td>336:00:00 Sun Jul 23 11:23:48</td>
</tr>
<tr>
<td>63885232</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting 10</td>
<td>0</td>
<td></td>
<td></td>
<td>336:00:00 Sun Jul 23 11:23:48</td>
</tr>
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<td></td>
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<td>Waiting 10</td>
<td>0</td>
<td></td>
<td></td>
<td>336:00:00 Sun Jul 23 11:23:48</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>SI10-6K</td>
<td>yrupan</td>
<td>Waiting 40</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>63885231</td>
<td>BAYES2_N30</td>
<td>agarciasoto</td>
<td>Waiting 10</td>
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<td>agarciasoto</td>
<td>Waiting 10</td>
<td>0</td>
<td></td>
<td></td>
<td></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
```bash
[user1@holyitc01 ~]$ sshare --account=test_lab -a
```

<table>
<thead>
<tr>
<th>Account</th>
<th>User</th>
<th>RawShares</th>
<th>NormShares</th>
<th>RawUsage</th>
<th>EffectvUsage</th>
<th>FairShare</th>
</tr>
</thead>
<tbody>
<tr>
<td>test_lab</td>
<td></td>
<td>244</td>
<td>0.001363</td>
<td>4556082</td>
<td>0.000572</td>
<td>0.747627</td>
</tr>
<tr>
<td>test_lab</td>
<td>user1</td>
<td></td>
<td>0.001363</td>
<td>82028750</td>
<td>0.000572</td>
<td>0.747627</td>
</tr>
<tr>
<td>test_lab</td>
<td>user2</td>
<td></td>
<td>0.001363</td>
<td>248820</td>
<td>0.000572</td>
<td>0.747627</td>
</tr>
<tr>
<td>test_lab</td>
<td>user3</td>
<td></td>
<td>0.001363</td>
<td>163318</td>
<td>0.000572</td>
<td>0.747627</td>
</tr>
<tr>
<td>test_lab</td>
<td>user4</td>
<td></td>
<td>0.001363</td>
<td>18901027</td>
<td>0.000572</td>
<td>0.747627</td>
</tr>
<tr>
<td>test_lab</td>
<td>user5</td>
<td></td>
<td>0.001363</td>
<td>18050039</td>
<td>0.000572</td>
<td>0.747627</td>
</tr>
</tbody>
</table>

- **Default Raw Shares**
  - Cannon: 200
  - 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
```
[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

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 use 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?