Advanced Cluster Usage

FAS Research Computing

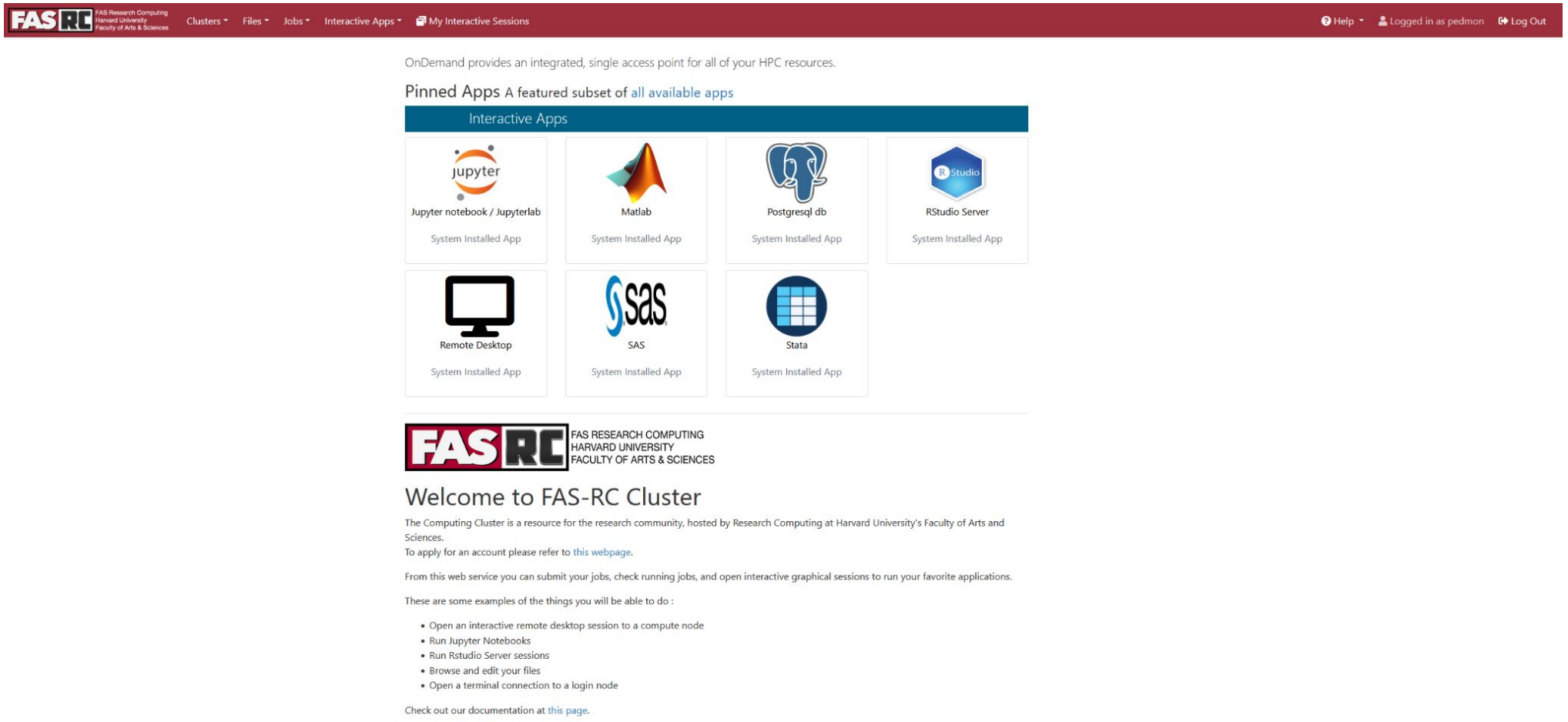
Outline

- Job Submission
- Job Resource Requirements
- Job/Partition/Queue Monitoring
- Job Checkpointing
- Fairshare
- Storage Workflow

Job Submission - Interactive

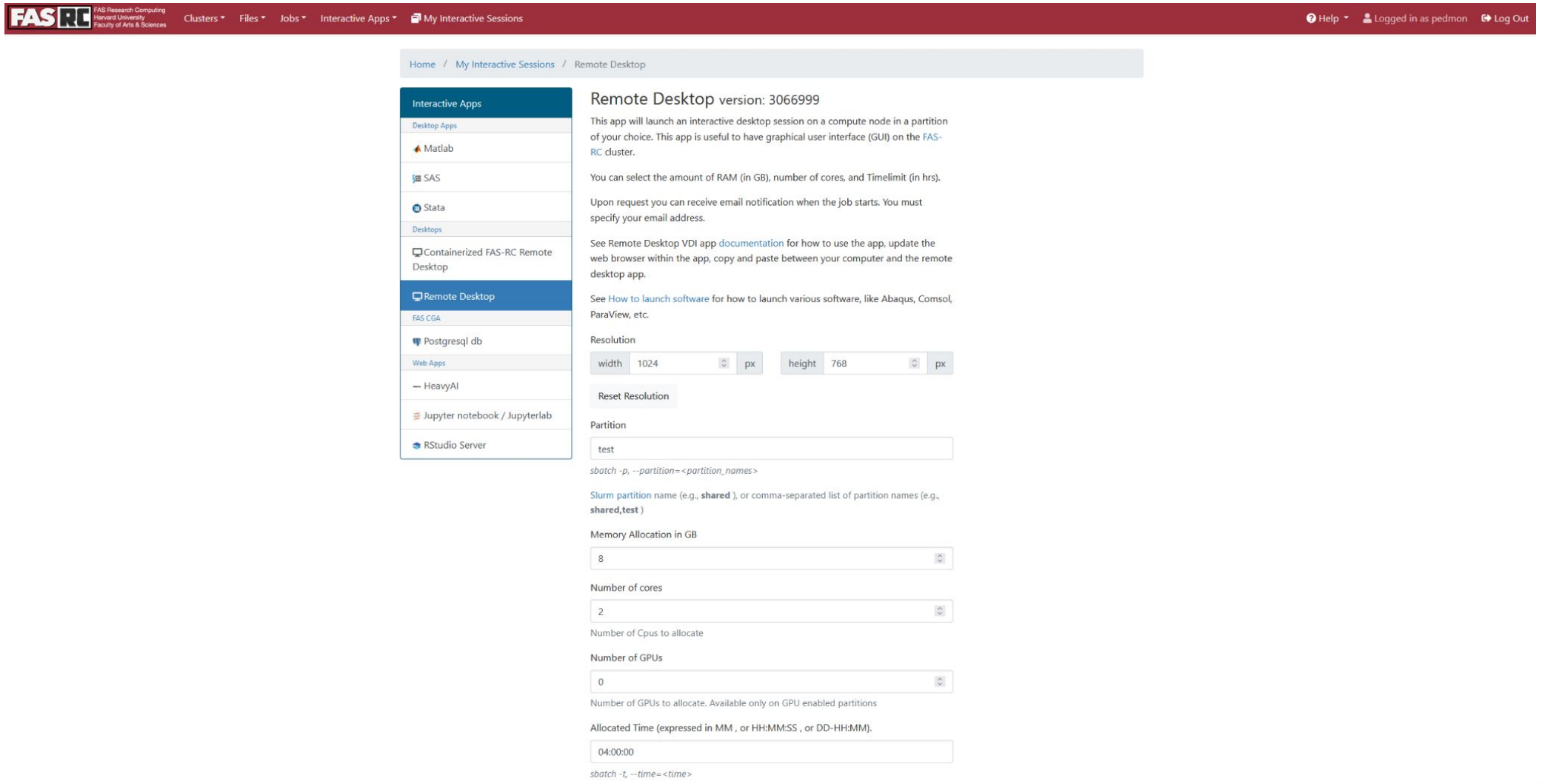
- salloc -p test --mem=4G -t 0-01:00
  - Gives back a shell prompt on a compute node
  - Uses
    - Testing code
    - Working interactively on the cluster without resource contention
  - Limitations
    - Session stall
    - Ties up prompt
    - Not great for GUI applications
    - If submitting to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

Job Submission - Interactive

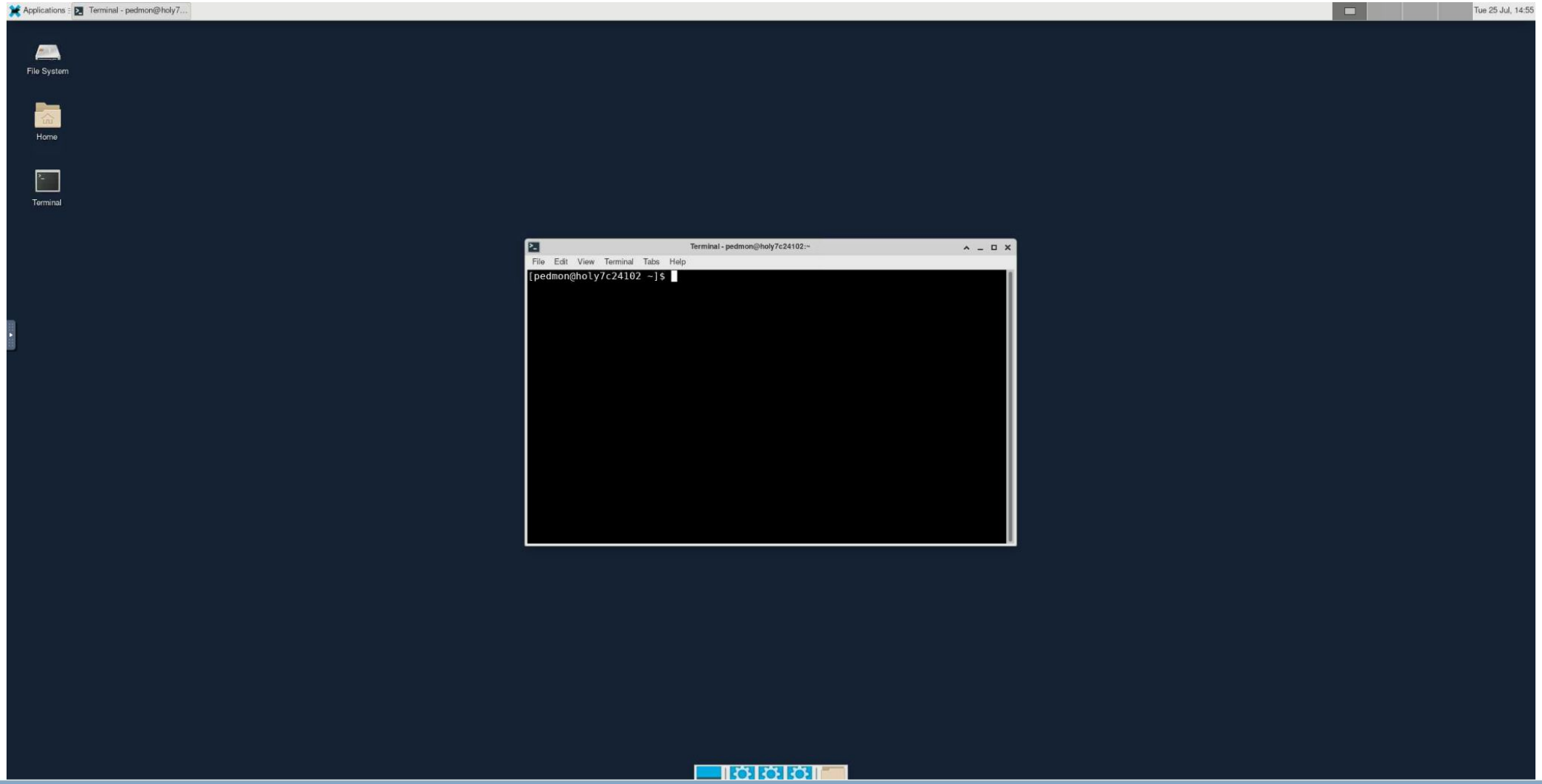


https://vdi.rc.fas.harvard.edu (VPN Required)

Job Submission - Interactive



Job Submission - Interactive



Job Submission - Batch

```
#!/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)

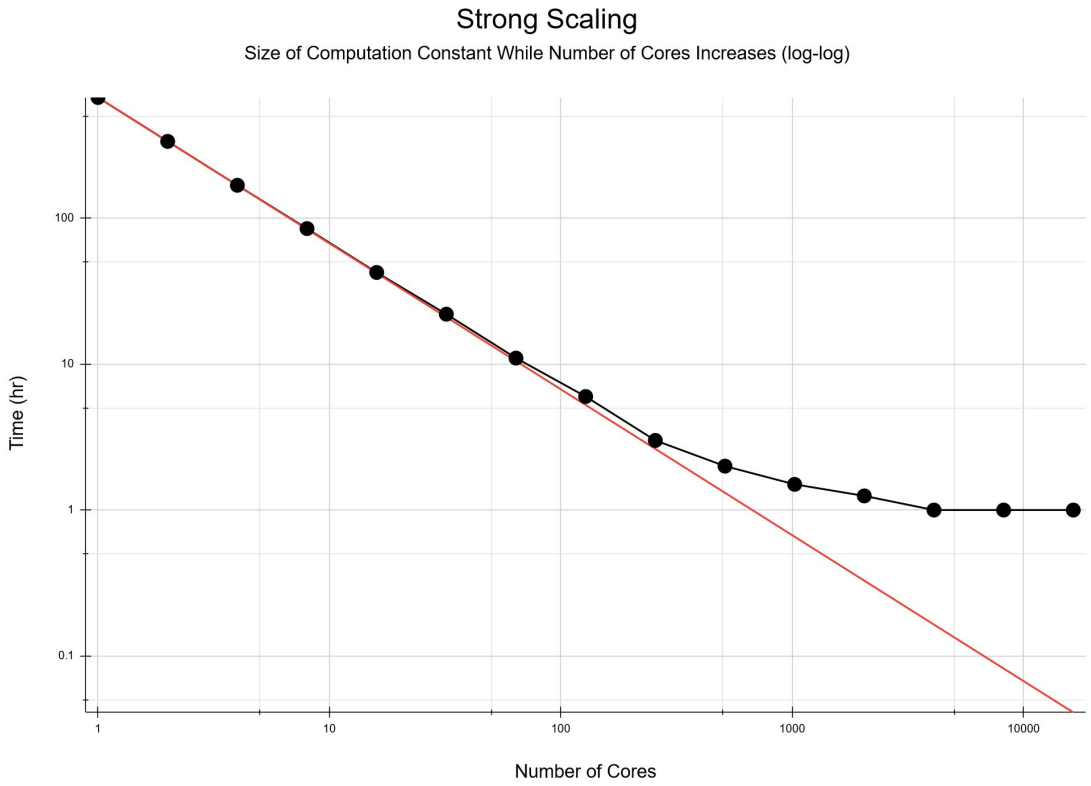
- --contiguous
- --constraint/--prefer
- --dependency
- --exclusive[={user|mcs}]
- --gpu/--gres

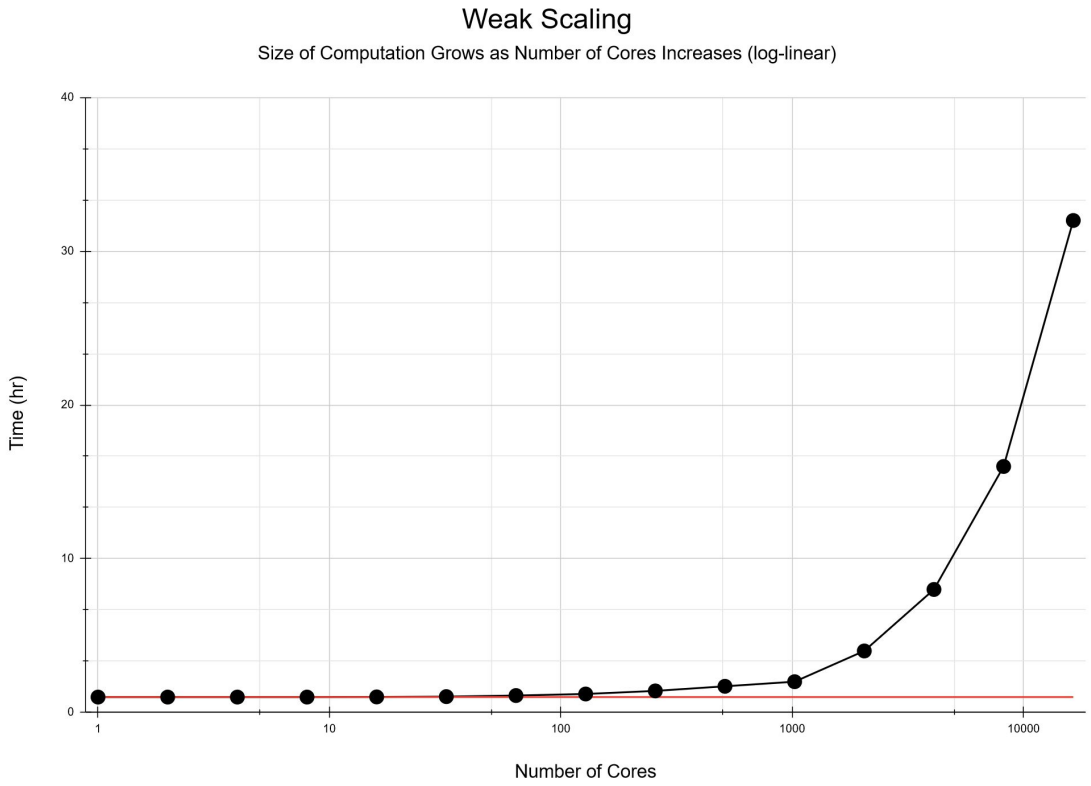
Job Resource Requirements

```
[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





Job Monitoring - sacct

```
[root@holy7c22501 general]# sacct -u mngo
JobID           JobName  Partition       Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
63911611        train_liif        gpu pfister_l+         14    TIMEOUT      0:0
63911611.ba+    batch             pfister_l+         14  CANCELLED 0:15
63911611.ex+    extern            pfister_l+         14  COMPLETED      0:0
63911755        train_liif        gpu pfister_l+         14    TIMEOUT      0:0
63911755.ba+    batch             pfister_l+         14  CANCELLED 0:15
63911755.ex+    extern            pfister_l+         14  COMPLETED      0:0
63971094        train_liif        gpu pfister_l+         14  COMPLETED      0:0
63971094.ba+    batch             pfister_l+         14  COMPLETED      0:0
63971094.ex+    extern            pfister_l+         14  COMPLETED      0:0
64063319        train_liif        gpu pfister_l+         14    RUNNING      0:0
64063319.ba+    batch             pfister_l+         14    RUNNING      0:0
64063319.ex+    extern            pfister_l+         14    RUNNING      0:0
64063323        train_liif        gpu pfister_l+         14    RUNNING      0:0
64063323.ba+    batch             pfister_l+         14    RUNNING      0:0
64063323.ex+    extern            pfister_l+         14    RUNNING      0:0
64063331        train_liif        gpu pfister_l+         14    RUNNING      0:0
64063331.ba+    batch             pfister_l+         14    RUNNING      0:0
64063331.ex+    extern            pfister_l+         14    RUNNING      0:0
64078487        train_liif        gpu pfister_l+         14    RUNNING      0:0
64078487.ba+    batch             pfister_l+         14    RUNNING      0:0
64078487.ex+    extern            pfister_l+         14    RUNNING      0:0
64078502        train_liif        gpu pfister_l+         14    RUNNING      0:0
64078502.ba+    batch             pfister_l+         14    RUNNING      0:0
64078502.ex+    extern            pfister_l+         14    RUNNING      0:0
```

- 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
   SubmitTime=2023-07-25T13:45:18 EligibleTime=2023-07-25T13:45:18
   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 ReqB:S:C:T=0:0:*:*
   TRES=cpu=14,mem=490G,node=1,billing=926,gres/gpu=4,gres/gpu:nvidia_a100-sxm4-40gb=4
   Socks/Node=* NtasksPerN:B: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
   StdIn=/dev/null
   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=gres:gpu:4
```

Partition Monitoring - showq

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

SUMMARY OF JOBS FOR QUEUE: <intermediate>

ACTIVE JOBS--------------------
JOBID     JOBNAME  USERNAME      STATE  CORE  GPU   REMAINING  STARTTIME
================================================================================
60897569  cm_afm.sh  joonholee   Running 48           0          167:46:27  Thu Jul 20 11:29:20
60897570  cm_afm.sh  joonholee   Running 48           0          196:29:26  Fri Jul 21 16:12:19
60897572  cm_afm.sh  joonholee   Running 48           0          247:54:04  Sun Jul 23 19:36:57
61583962  skin-WS_sy csxue       Running 1            0          21:50:42  Fri Jul 21 09:33:35
62497782  .fasrcood/ verstyuk    Running 1            0          24:49:17  Fri Jul 14 17:32:10
62497784  .fasrcood/ verstyuk    Running 1            0          24:49:59  Fri Jul 14 17:32:52
63128424  sbatch     dverbart    Running 64           0          63:18:07  Sat Jul 22 03:01:00
63128430  sbatch     dverbart    Running 64           0          123:59:12  Mon Jul 24 15:42:05
63268520  sbatch     dverbart    Running 64           0          144:02:24  Tue Jul 25 11:45:17
63884205  doParallel cdadams     Running 1            0          27:44:41  Tue Jul 25 07:27:34
63885162  BAYES2_N30 agarciasoto  Running 10          0          288:14:43  Tue Jul 25 11:57:36
63885172  BAYES2_N30 agarciasoto  Running 10          0          302:55:15  Wed Jul 26 02:38:08
63885194  BAYES2_N30 agarciasoto  Running 10          0          313:14:06  Wed Jul 26 12:56:59
63885224  BAYES2_N30 agarciasoto  Running 10          0          323:24:06  Wed Jul 26 23:06:59
63885226  BAYES2_N30 agarciasoto  Running 10          0          323:25:14  Wed Jul 26 23:08:07

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

WAITING JOBS------------------------
JOBID     JOBNAME  USERNAME      STATE  CORE  GPU   WCLIMIT  QUEUETIME
================================================================================
62277463  S110-6K    yrupan      Waiting 40           0          336:00:00  Thu Jul 13 03:45:48
63885231  BAYES2_N30 agarciasoto  Waiting 10          0          336:00:00  Sun Jul 23 11:23:48
63885232  BAYES2_N30 agarciasoto  Waiting 10          0          336:00:00  Sun Jul 23 11:23:48
63885233  BAYES2_N30 agarciasoto  Waiting 10          0          336:00:00  Sun Jul 23 11:23:48
63885234  BAYES2_N30 agarciasoto  Waiting 10          0          336:00:00  Sun Jul 23 11:23:48
63885235  BAYES2_N30 agarciasoto  Waiting 10          0          336:00:00  Sun Jul 23 11:23:48
63885236  BAYES2_N30 agarciasoto  Waiting 10          0          336:00:00  Sun Jul 23 11:23:49
63885237  BAYES2_N30 agarciasoto  Waiting 10          0          336:00:00  Sun Jul 23 11:23:49
63885238  BAYES2_N30 agarciasoto  Waiting 10          0          336:00:00  Sun Jul 23 11:23:49
```

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

Job Checkpointing

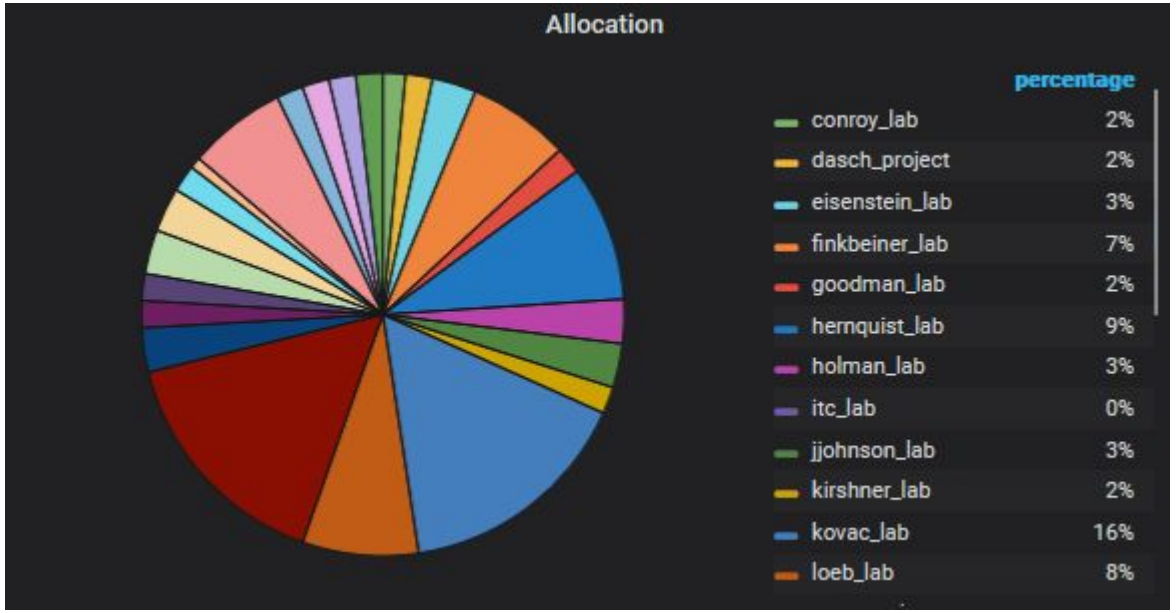
- Creates a save point for your job to pick up from where it left off
  - Also Known As: Checkpointing, Save File, Restart File

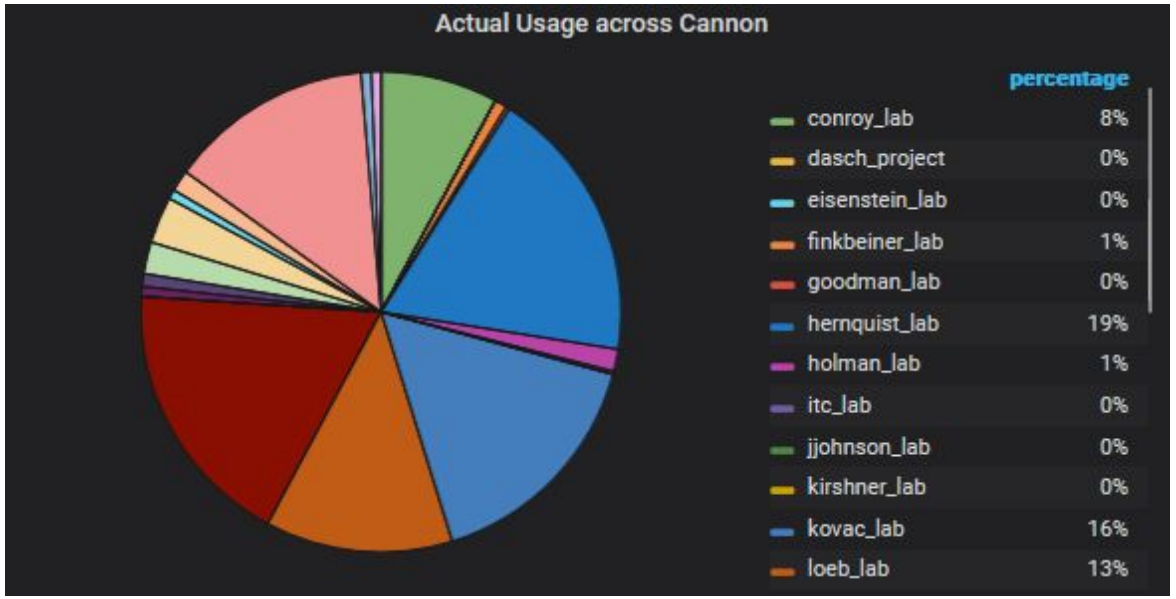
- Useful for:
  - Long running jobs
  - Jobs that error out
  - Jobs that need midstream tweaking
  - Leveraging requeue partitions

- 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

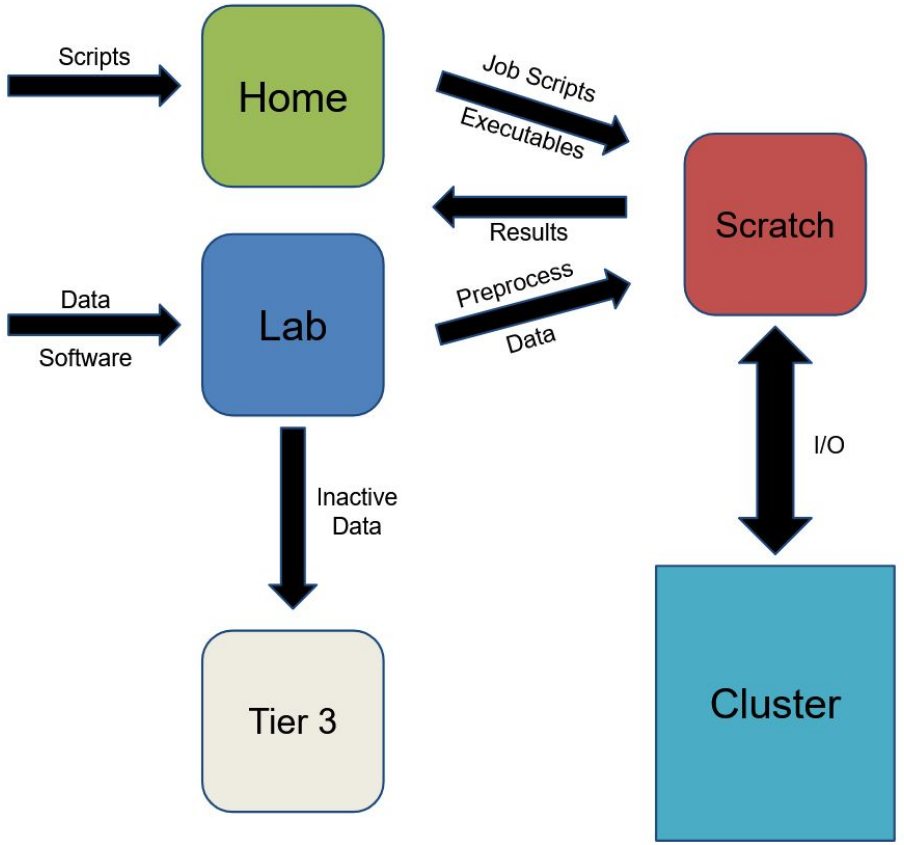
```
[user1@holyitc01 ~]$ sshare --account=test_lab -a
Account  User  RawShares NormShares RawUsage  EffectvUsage FairShare
----------------------------------------------------------------------
test_lab       244      0.001363   45566082     0.000572    0.747627
test_lab user1 parent   0.001363   82028750.000572    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?