



Introduction to Python on ASU's HPC systems

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Core Research Facilities

Getting Started



- To use ASU's Agave system, create an account:
 - Go to <http://links.asu.edu/getHPC>
 - For "Affiliated Faculty":
 - If faculty, list yourself
 - If a student or student worker, list your professor or supervisor
 - If other, list the speaker of this presentation or ask rtshelp@asu.edu for help

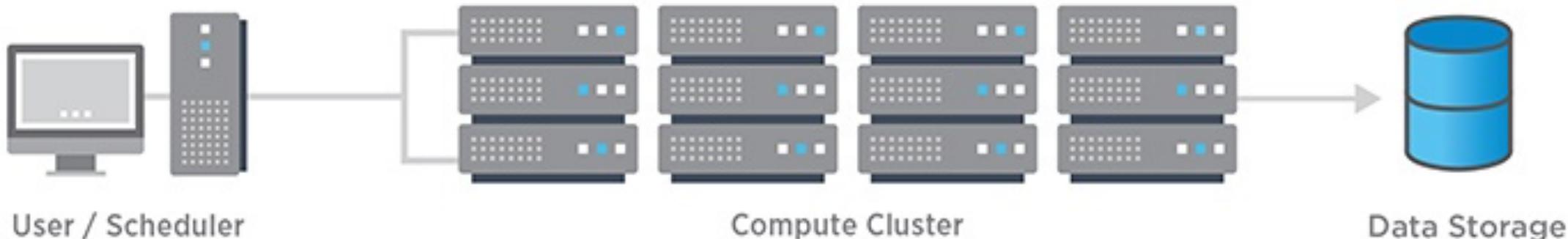


-
- For access outside ASU campuses, download the VPN:
 - Go to sslvpn.asu.edu and install the Cisco AnyConnect Client
 - In the connect window, enter "sslvpn.asu.edu"
 - Sign in with ASURITE and password
 - Faculty and staff may also need [Duo Two-Factor Authentication](#)

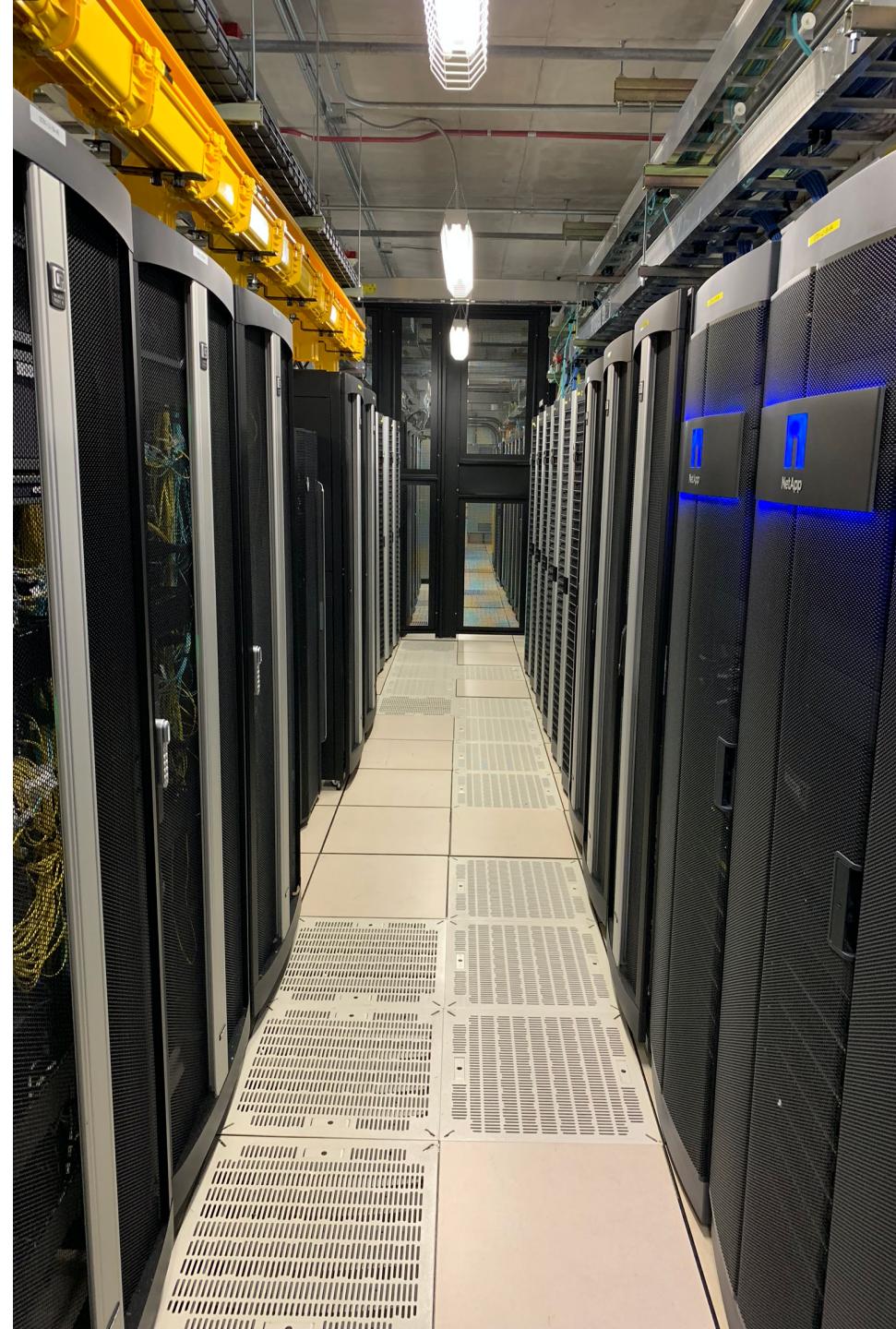
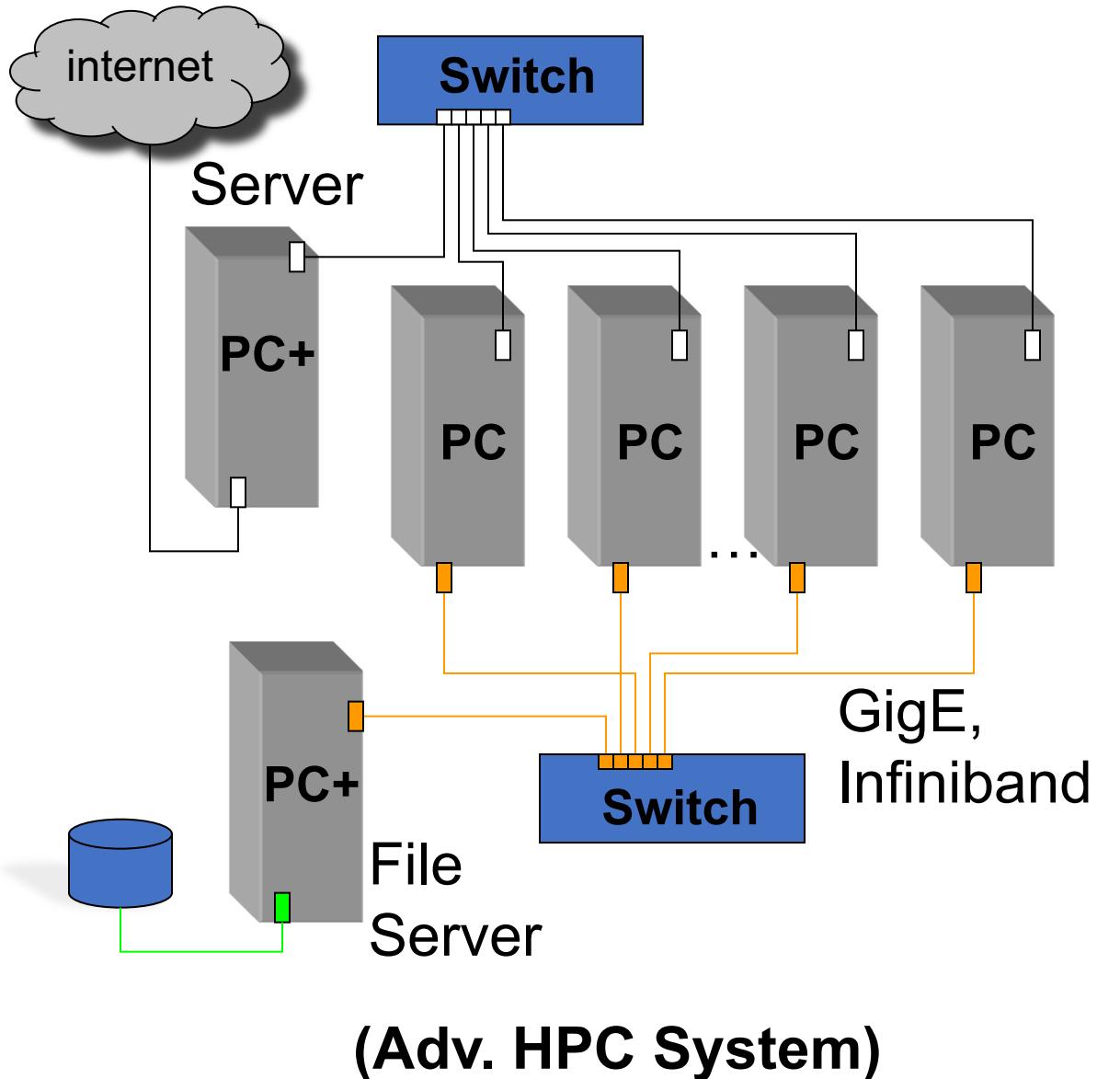
What is Agave?



- Agave is a High-Performance Computing (HPC) cluster
- This cluster architecture uses thousands of compute servers, also called nodes, to help users optimize their research
- This optimization can happen in several ways:
 - Free the researcher's local machine by running the program on a separate server
 - Allow for parallelization or for multiple operations, or "jobs", to run in parallel
 - Access to graphics processing units (GPUs)
 - Access to high memory computation and storage
 - Overall greater and more refined research through HPC



How Does a Cluster Work?

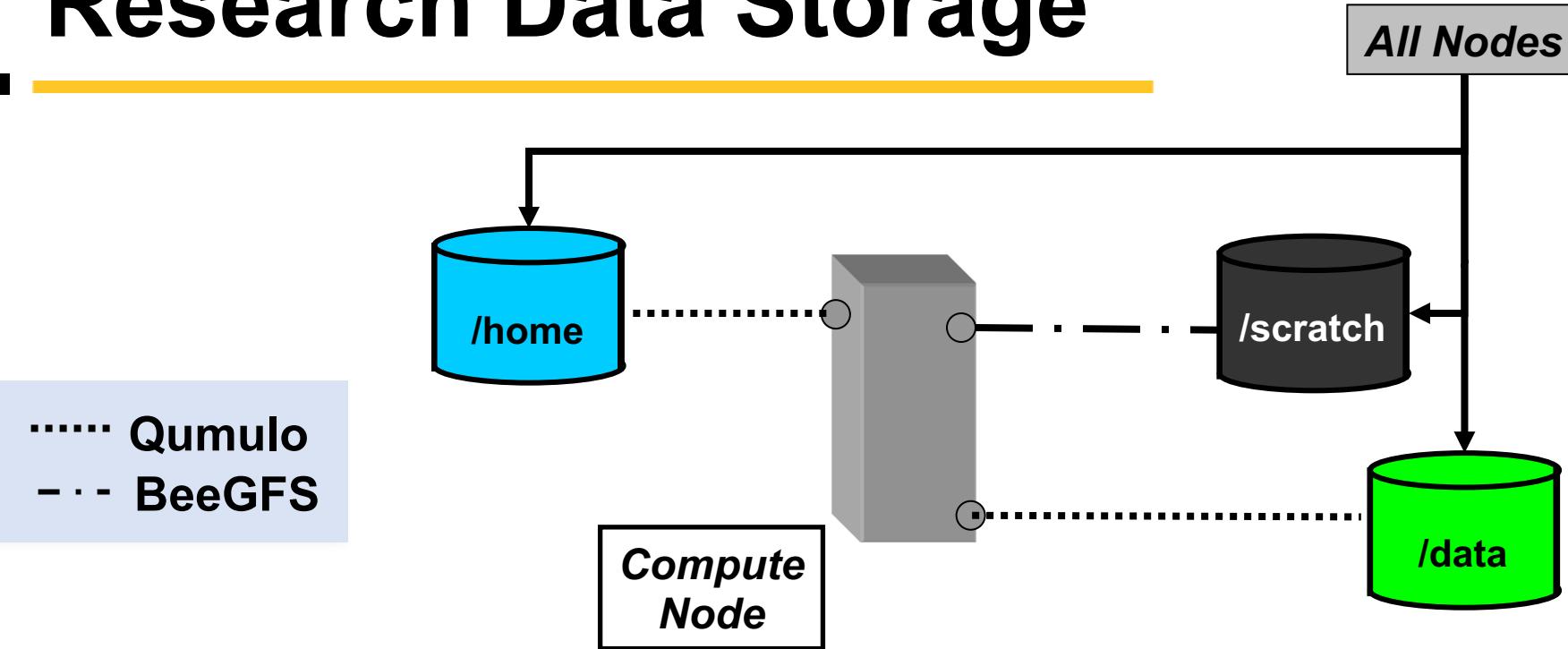


Agave System Information

- Agave ~7.5K networked Broadwell cores (Intel CPU)
 - >300 trillion (theoretical) floating point operations/s (TFLOPs)
 - >34TB aggregate RAM
 - >6PB aggregate disk
 - Omnipath Interconnect – 100Gb/s
 - Located in ISTB1
- Additional ~3K cores in various partitions
- ~5K Xeon Phi cores
- GPU partitions (~300 GPUs)
- High memory nodes (1TB, 1.5TB, 2TB)
- Remember, Agave is a true **cluster** architecture
 - Each Broadwell node has 28 processors and 128GB of RAM (~4.5GB/CPU).
 - Programs needing more resources **must** use parallel programming
 - Normal, single processor applications **do not go faster** on Agave

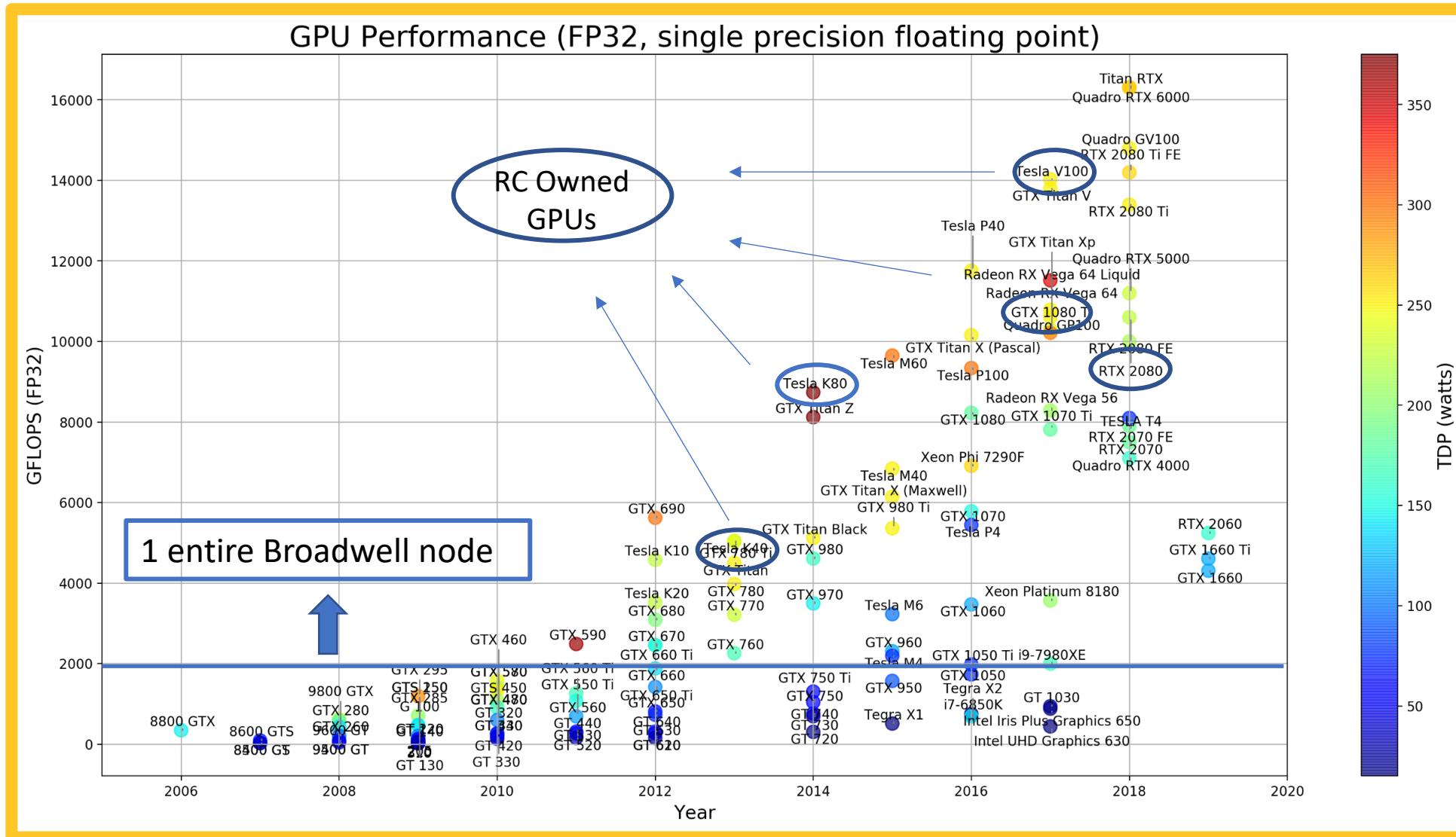


Research Data Storage



| Mount point | User Quota | Lifetime |
|-------------|------------|--------------|
| /home | 100 GB | Project |
| /scratch | None | 30 days |
| /data | Purchased | \$50/TB/year |

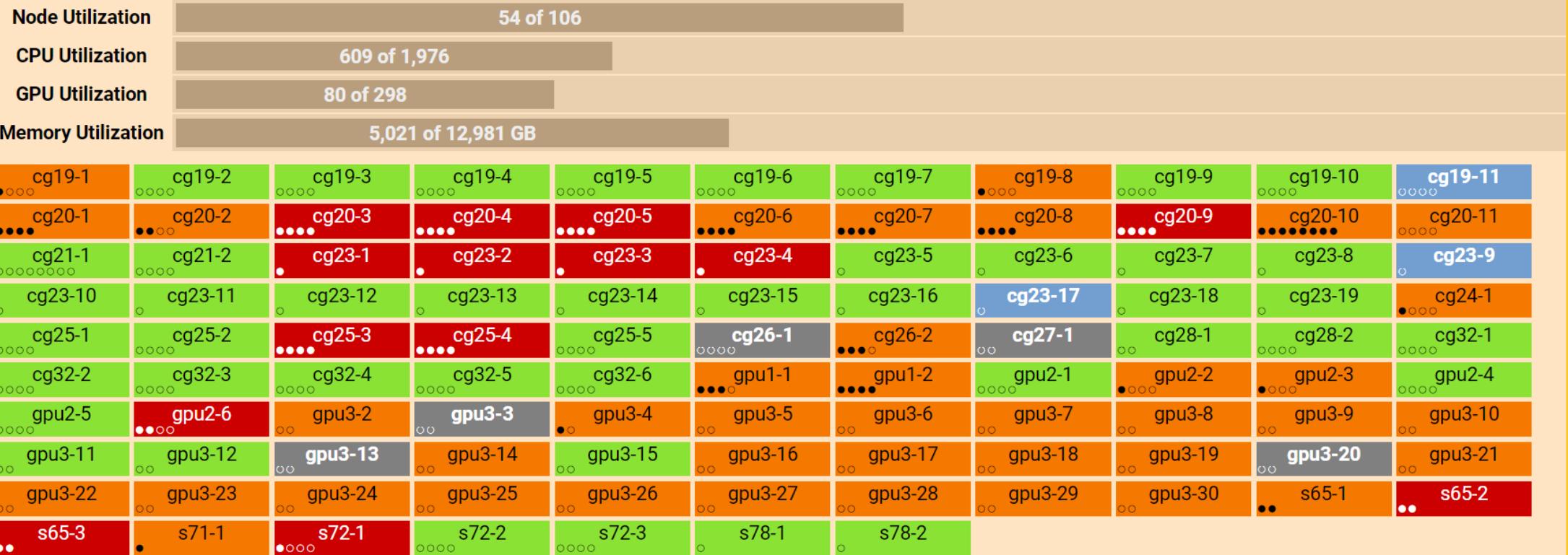
Graphical Processing Units (GPU) on Agave and Performance



Agave's GPU Nodes

GPU Nodes: [Click here for info on how to use these nodes](#)

| | | | | | | | | | |
|----------------------------------|----|----------------------------------|---|----------------------------------------|---|----------------------------------------|---|----------------------------------------------------|--|
| GPU Running Jobs | 25 | GPU Pending Jobs | 0 | Users Running GPU Jobs | 3 | Users Pending GPU Jobs | 0 | Users Pending not Running GPU Jobs | |
|----------------------------------|----|----------------------------------|---|----------------------------------------|---|----------------------------------------|---|----------------------------------------------------|--|



Legend:

● – node is free

○ – node is mixed between taken and free

● – node is taken

● – node is being drained

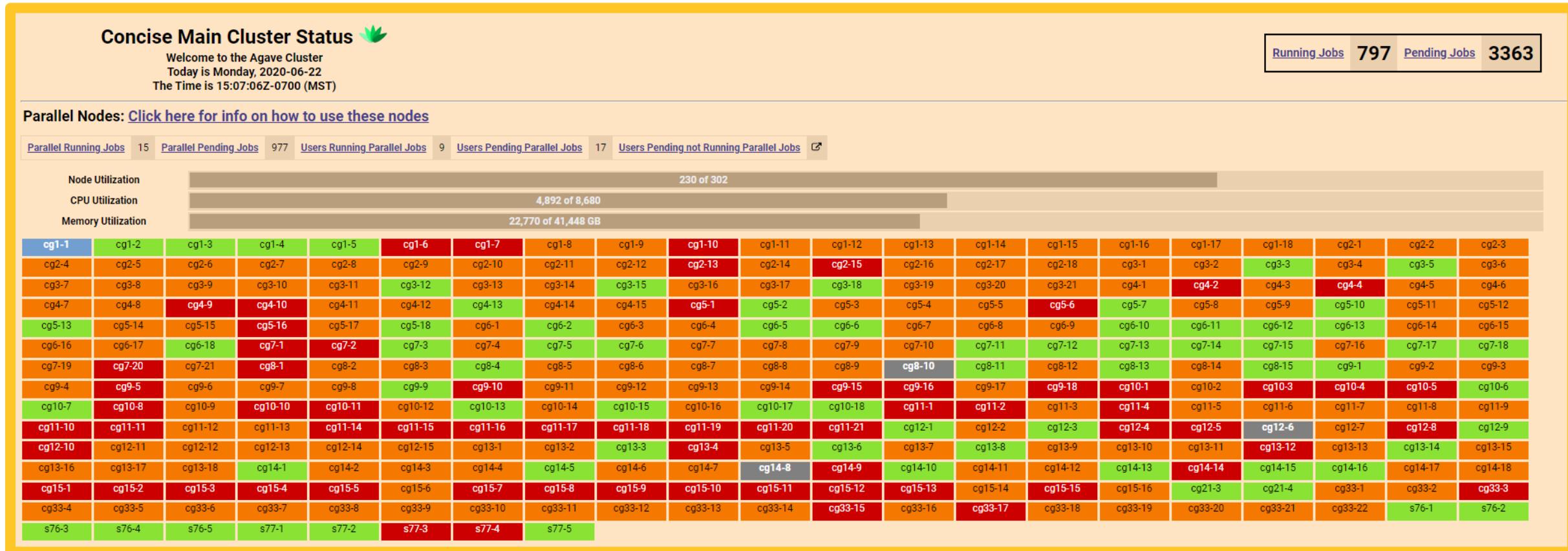
● – node is offline

● – GPU is taken

○ – GPU is free

Agave Status Page

- To see the status of Agave and to check which nodes are free, check out <http://links.asu.edu/status>



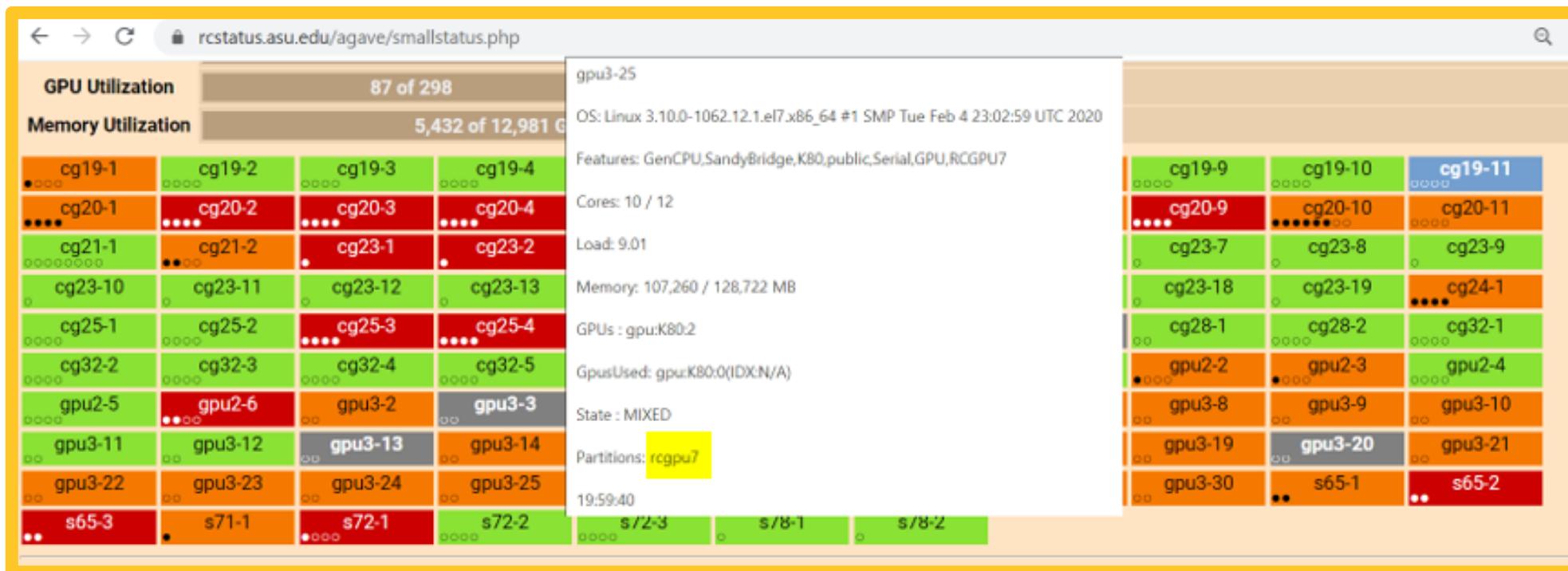
Legend:

Green – node is free **Orange** – node is mixed between taken and free **Red** – node is taken

Blue – node is being drained **Grey** – node is offline

More on Agave's GPU Nodes

- Currently, Research Computing's GPU partition contains over 100 GPU nodes with nearly 300 GPUs collectively
- This GPU partition is broken into two subpartitions:
 - 1) private GPUs
 - 2) public GPUs



Popular Python Software



Notebook



Py3-basic



atomate



DeepNeuro



keras



keras-gpu



keras-rmcnn



liligelab



Neuron



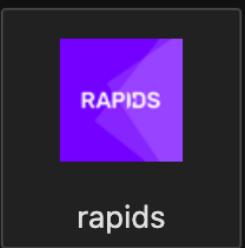
pyintel



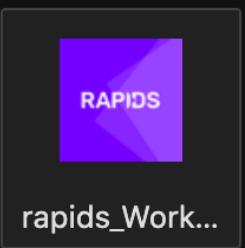
pytorch



pytorch-gpu



rapids



rapids_Work...



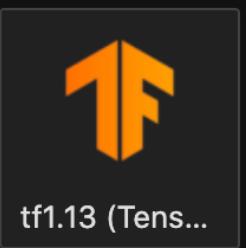
smcpp



tf1.12 (Tens...



tf1.12-gpu (...



tf1.13 (Tens...

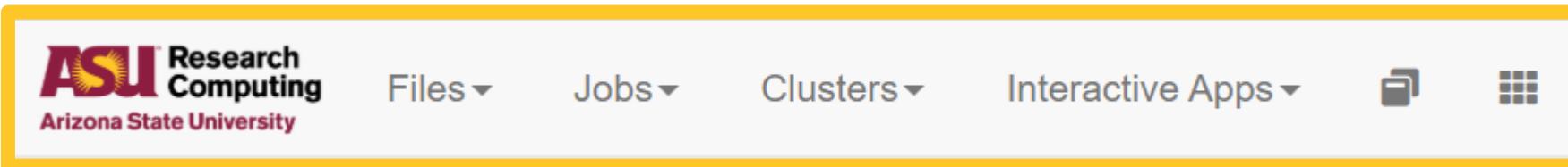


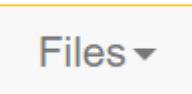
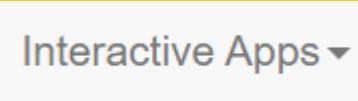
tf1.13-gpu (...



tf2.0-gpu (T...

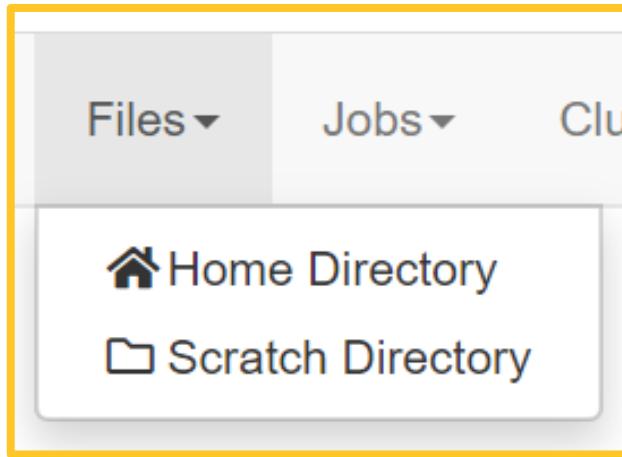
Using Agave through OnDemand



- Supercomputing through the web
- Once connected to VPN: go to <https://login.rc.asu.edu>
- Single sign on with ASURITE and password
- From here users can:
 - Manage file systems 
 - Create and monitor jobs 
 - Access the shell 
 - Access interactive apps 
 - View and manage interactive sessions 
 - View all apps 
 - Request help 

Browser-Based File Management

- Manage files between local machine, home, and scratch with click and drop interface
- See more under [Available File Systems](#)



A screenshot of the main file management interface. It features a toolbar at the top with buttons for 'Go To...', 'Open in Terminal', 'New File', 'New Dir', 'Upload', 'Show Dotfiles', and 'Show Owner/Mode'. Below this is a breadcrumb path showing the current directory as '/home/ASURITE/'. At the bottom is another toolbar with buttons for 'View', 'Edit', 'Rename/Move', 'Download' (which is highlighted in blue), 'Copy', 'Paste', '(Un)Select All', and 'Delete'. The entire interface is highlighted with a yellow box.

Browser-Based Job Submission

Submit Script

main_job.sh

Script contents:

```
#!/bin/bash
#SBATCH -p parallel ## Parallel Partition
#SBATCH -N 1 ## 1 Node
#SBATCH -n 1 ## 1 core
#SBATCH --time=0-1:00 ## 0 days, 1 hour, and 0 minutes
#SBATCH --job-name=batchtools_test
#SBATCH --error=slurm.%j.err
#SBATCH --output=slurm.%j.out

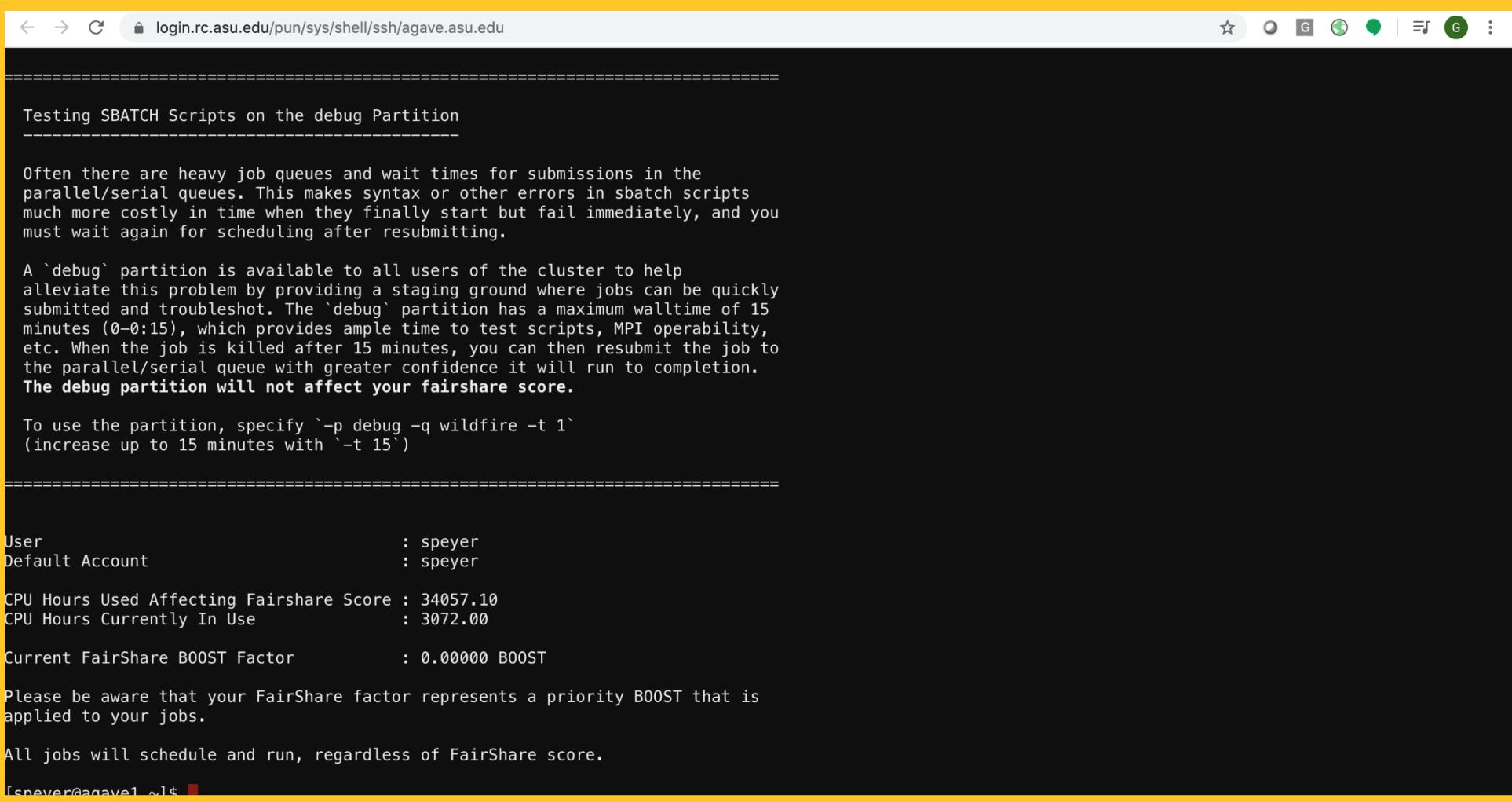
cd $HOME/agave_R_test ## Specifying directory

module purge ## Purging any previous modules
module load r/latest ## Loading latest version of R

R --no-save --quiet --slave < batchtools_test.R ## Running R
```

[Open Editor](#) [Open Terminal](#) [Open Dir](#)

Browser-Based Shell



The screenshot shows a browser window with a terminal-like interface. The URL in the address bar is `login.rc.asu.edu/pun/sys/shell/ssh/agave.asu.edu`. The terminal content is as follows:

```
=====
Testing SBATCH Scripts on the debug Partition
-----
Often there are heavy job queues and wait times for submissions in the
parallel/serial queues. This makes syntax or other errors in sbatch scripts
much more costly in time when they finally start but fail immediately, and you
must wait again for scheduling after resubmitting.

A `debug` partition is available to all users of the cluster to help
alleviate this problem by providing a staging ground where jobs can be quickly
submitted and troubleshooted. The `debug` partition has a maximum walltime of 15
minutes (0-0:15), which provides ample time to test scripts, MPI operability,
etc. When the job is killed after 15 minutes, you can then resubmit the job to
the parallel/serial queue with greater confidence it will run to completion.
The debug partition will not affect your fairshare score.

To use the partition, specify `-p debug -q wildfire -t 1`
(increase up to 15 minutes with `-t 15`)

=====
User : speyer
Default Account : speyer

CPU Hours Used Affecting Fairshare Score : 34057.10
CPU Hours Currently In Use : 3072.00

Current FairShare BOOST Factor : 0.00000 BOOST

Please be aware that your FairShare factor represents a priority BOOST that is
applied to your jobs.

All jobs will schedule and run, regardless of FairShare score.

[never@agave1 ~]$
```

Browser-Based Virtual Desktops



Select Jupyter tricks

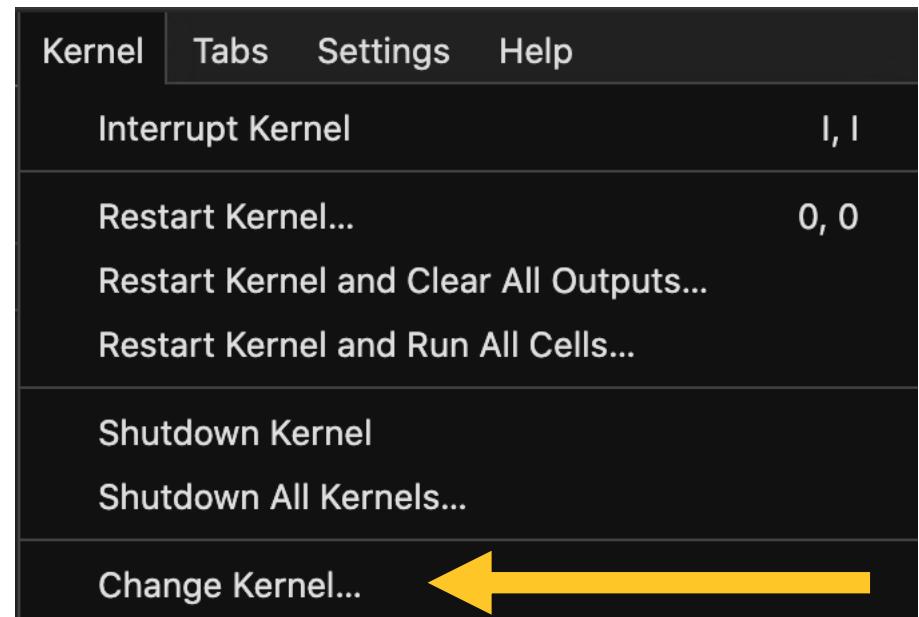
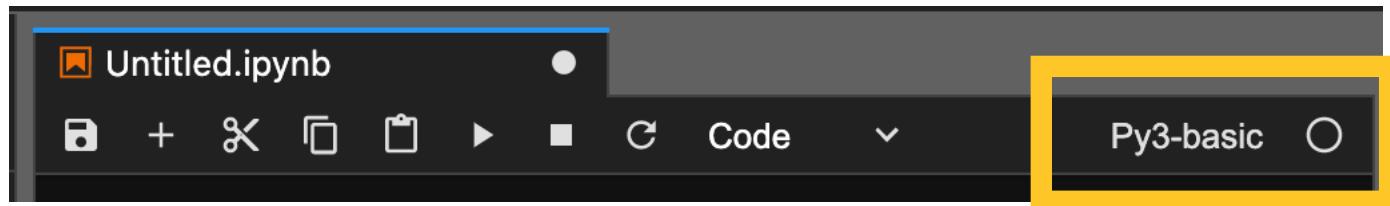
Change from Jupyter lab to notebook midsession:

<https://login.rc.asu.edu/node/cg1-2.agave.rc.asu.edu/38457/lab?>

->

<https://login.rc.asu.edu/node/cg1-2.agave.rc.asu.edu/38457/tree>

Change the kernel of a notebook:



Scheduling, Priority, and Fairshare

- Jobs in the queue are scheduled based on priority through the SLURM scheduler
- Priority is computed from a linear combination of factors: job age, job size, job quality of service, and FairShare with admin defined weights
- FairShare ranges from 0 (lowest priority) to 1 (highest priority)
- Calculated from usage

$$\text{FairShare} = 2^{-\text{usage}/(10,000 \text{ core hours})}$$

- *usage* decays exponentially, half-life of 1 week



Other Resources and Services



Additional advantages of Research Computing:

- Consultation in optimizing research
- Consultation and opportunities to purchase hardware through Research Computing--
 - Research Computing maintains the hardware, handles OS, and provides software installations for researchers
- Offers XSEDE Campus Champions allocations
- Offers in-depth workshops for HPC applications, XSEDE, and Carpentries

Contribute! (<http://links.asu.edu/services>)

Dell Pre-Approved Compute Nodes

| Compute Node Types | Processor | Core Count | RAM | GPU | Price |
|--------------------|--------------------|------------|---------|---------------|-------------|
| Standard Intel | Intel Cascade Lake | 52 cores | 192GB | N/A | \$9,555.87 |
| High Memory | Intel Cascade Lake | 52 cores | 1,536GB | N/A | \$20,801.46 |
| GPU Option 1 | Intel Cascade Lake | 52 cores | 192GB | (4) 16GB V100 | \$37,242.80 |
| GPU Option 2 | Intel Cascade Lake | 52 cores | 192GB | (4) 32GB V100 | \$43,331.73 |
| Standard AMD | AMD EPYC | 64 cores | 256GB | N/A | \$11,450.04 |

Fall Workshops (links.asu.edu/learn)

Introduction to Linux Command Line Interface:

- Aug 17, 3-4 PM, Zoom.
- October 19, 3-4 PM, Zoom.

Matlab for HPC and on GPU:

- Aug 24, 2-3 PM, Zoom.

Python HPC Applications Series:

- Aug 31, 2-3 PM, *Python Intro for HPC (Python 1)*, Zoom.
- Sep 8, 2-3 PM, *Python Data Handling for HPC (Python 2)*, Zoom.
- Oct 5, 3-4 PM, *Python Machine Learning for HPC (Python 3)*, Zoom.
- Nov 11, 2-3 PM, *Python Deep Learning for HPC (Python 4)*, Zoom.

Google Drive, Globus, and HPC:

- Aug 31, 3-4 PM, Zoom.

R for HPC and GPU Applications:

- Sep 14, 2-3 PM, Zoom.

General GPU Applications:

- Oct 5, 2-3 PM, Zoom.

Introduction to HPC and the Research Computing Cluster:

- Aug 17, 2-3 PM, Zoom.
- Sep 21, 2-3 PM, Zoom.
- Nov 30, 2-3 PM, Zoom.
- Dec 14, 2-3 PM, Zoom.

Quick Links

For assistance: rtshelp@asu.edu

Office Hours: 1-3:30 Tu (and W during Academic semesters)

Zoom: <https://asu.zoom.us/j/9598636843> Password: 456456

Slack Channel: #rc-support

Documentation Page: <http://links.asu.edu/docs>

Discourse Site (for common errors and fixes):

<http://links.asu.edu/discourse>

Agave Status Page:

<http://links.asu.edu/status>

Mailing List:

<http://links.asu.edu/MailingList>



Thank you

Please visit
researchcomputing.asu.edu
for more information



Arizona State University

August 31st 2020



Arizona State University

Core Research Facilities