Drexel UNIVERSITY

Intro. to Picotte

FITSUM ALEBACHEW

Overview

- What is Picotte?
- Using Picotte:
  - Logging into Picotte
  - Transferring files to/from Picotte
  - Creating/submitting job scripts
  - Viewing your results

What is Picotte?

Picotte is a high-performance computing cluster

- Operating System: Red-Hat Enterprise Linux 8 64-bit
- Default shell: Bash (Bourne Again Shell)
- Job scheduler: SLURM Workload Manager

Specifications: https://drexel.edu/core-facilities/facilities/research-computing/service/picotte/

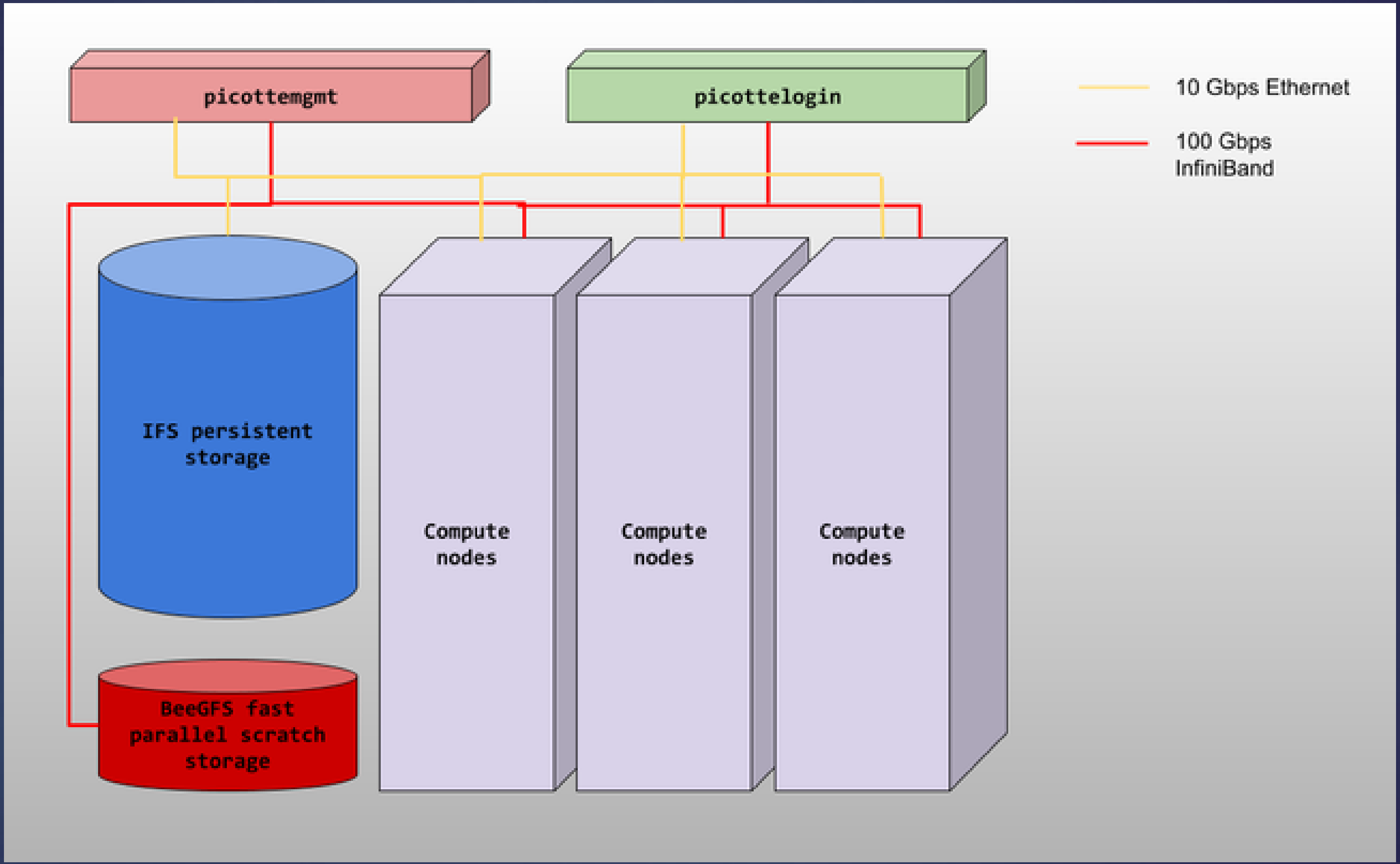
Picotte (Nodes)

Picotte has a total of 90 nodes:

- 1 management node
- 1 login node
- 88 compute nodes:
  - 74 def nodes - 48 cores/node, 192 GB RAM/node
  - 12 gpu nodes - 48 cores/node, 192 GB RAM/node, 4 Nvidia Tesla V100-SXM2 32GB GPU devices/node
  - 2 bm nodes - 48 cores/node, 1.5 TB RAM/node

Total of 4224 compute cores, 19.1 TiB RAM

Picotte


picottemgmt
picottelogin
10 Gbps Ethernet
100 Gbps InfiniBand
IFS persistent storage
BeeGFS fast parallel scratch storage
Compute nodes
Compute nodes
Compute nodes

Logging In

- To get access to Picotte, you MUST initially be logged into Drexel's VPN or using the Drexel on-campus Wi-Fi.
- Logging into Drexel's VPN:
    - Download and install Cisco AnyConnect Secure Mobility Client
        - https://vpn.drexel.edu/
    - Launch Cisco AnyConnect Secure Mobility Client
    - Sign in with Drexel credentials

Detailed instructions: https://drexel.edu/it/help/a-z/VPN/

Logging In (cont.)

There are several ways to log into Picotte:

- OpenSSH (Windows) or Terminal (Mac)
  - ssh username@picottelogin@urcf.drexel.edu
- MobaXterm for GUI display
- SSH through Visual Studio Code
- Other SSH clients like PUTTY

More info:

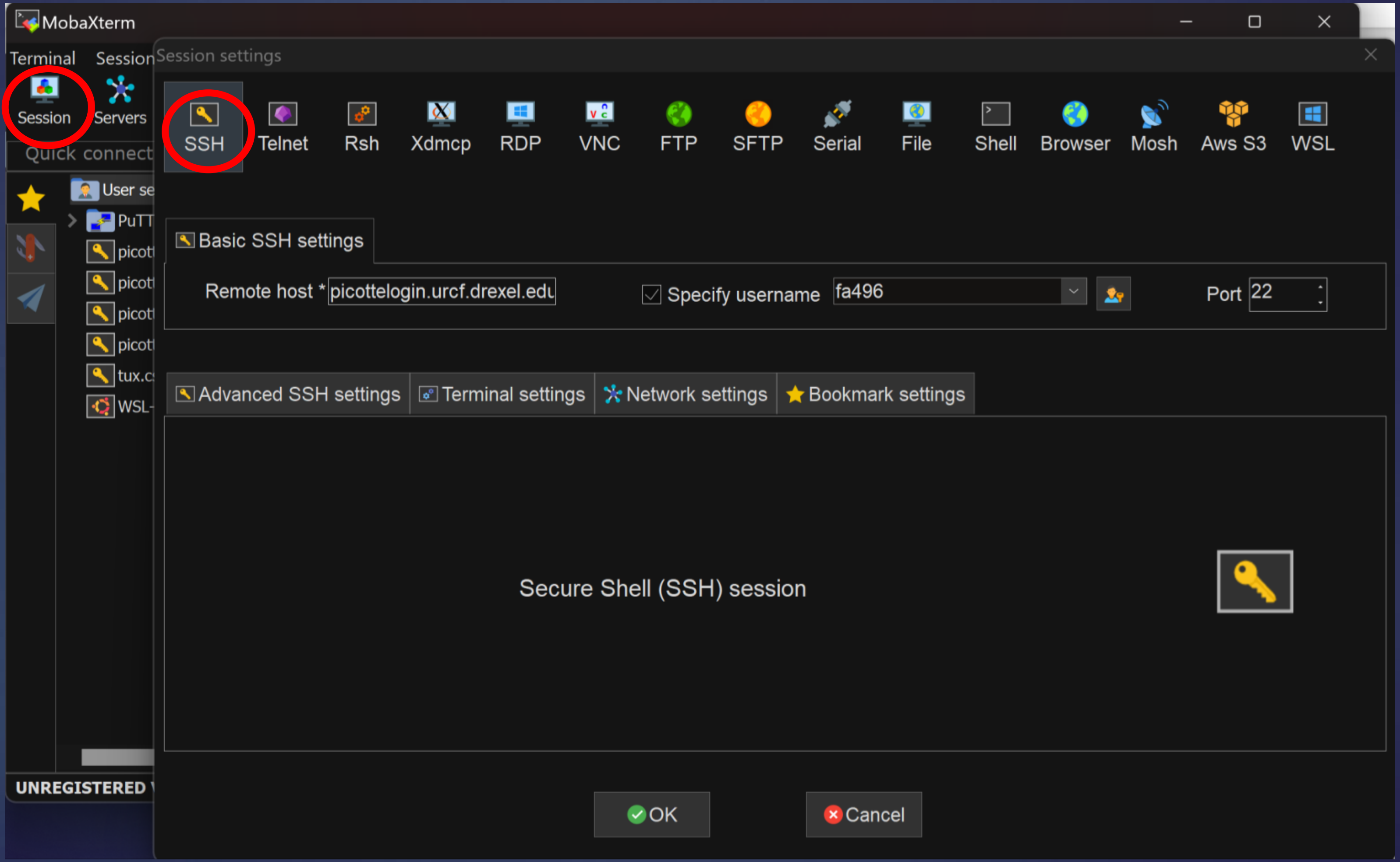
- Windows: https://proteusmaster.urcf.drexel.edu/urcfwiki/index.php/Tips_for_Windows_Users
- Mac: https://proteusmaster.urcf.drexel.edu/urcfwiki/index.php/Tips_for_macOS_Users

Logging in with MobaXterm

- Open MobaXterm application
- Click on ‘Session’ in the menu tab
- Choose SSH option
- Enter hostname and username
- Enter password

More info: https://mobaxterm.mobatek.net/

Logging in with MobaXterm



Remote host * picottelogin.urcf.drexel.edu

☑ Specify username fa496

Port 22

GUI Display on MobaXterm

You can use MobaXterm to display app GUIs like MATLAB, Jupyter Notebook, etc. on your local machine from Picotte:

- Log into Picotte using MobaXterm
- Load the modules for the applications you want to run
- Run the applications from the command line to open a new window containing the GUI.

Logging in with Visual Studio Code

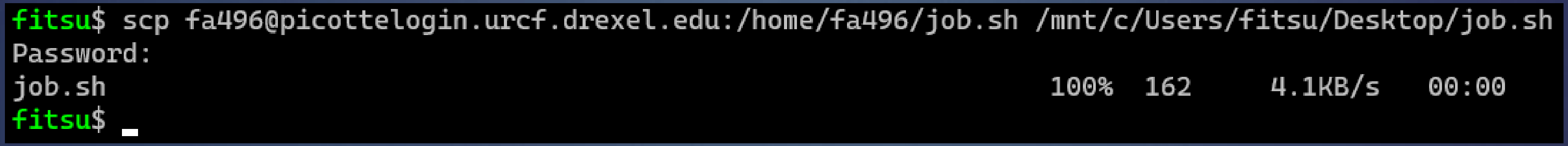
- Install an OpenSSH compatible SSH client on device
- Install ‘Remote Development’ extension pack on VS Code
- Go to the ‘Remote Explorer’ tab on VS Code and click on ‘Add new’
- Enter your username and hostname as ‘ssh username@hostname’
- Enter your password when prompted

Detailed instructions: https://code.visualstudio.com/docs/remote/ssh

Transferring Files

There are also several ways to transfer files to and from Picotte:

- Shell commands like scp, sftp, pscp
  - scp <source address> <destination address>
  - address format (remote): username@hostname:<working directory>



```
fitsu$ scp fa496@picottelogin.urcf.drexel.edu:/home/fa496/job.sh /mnt/c/Users/fitsu/Desktop/job.sh
Password:
job.sh                                                            100%  162     4.1KB/s   00:00
fitsu$ _
```

- MobaXterm/VS Code
  - To copy from Picotte to local machine:
    - Right click on file in explorer and click on download
  - To copy from local machine to Picotte:
    - Open directory in file explorer and drag file from local machine to file explorer

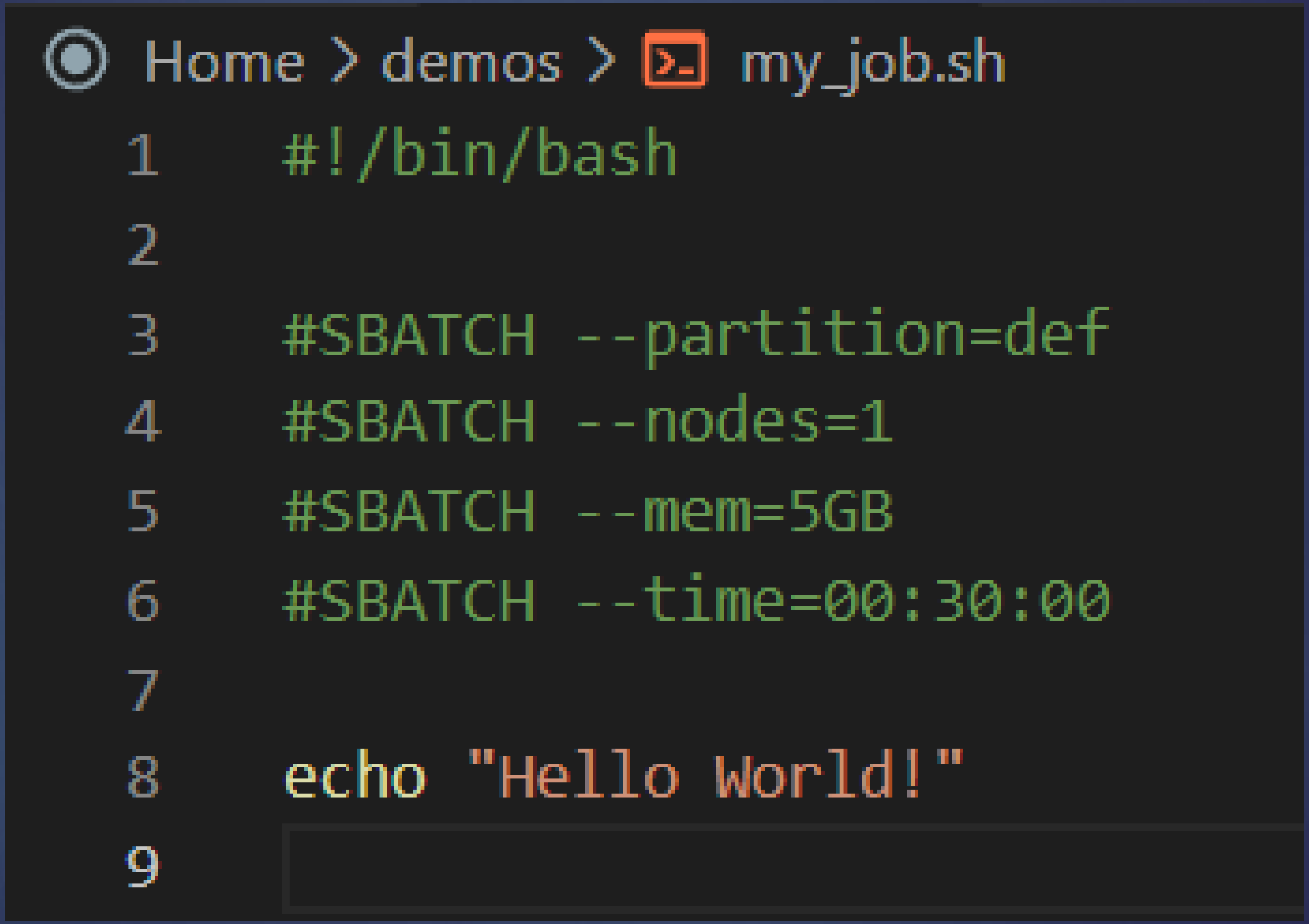
Creating/Submitting Job Scripts

Job scripts are shell scripts that specify the details/options to the job:

- Always start with shebang - #!/bin/bash
- Use ‘#SBATCH’ to set options
- Load modules being used
- Run program executable/command
- Submit your script with the command ‘sbatch myjob.sh’

More info: https://proteusmaster.urcf.drexel.edu/urcfwiki/index.php/Writing_Slurm_Job_Scripts

Creating/Submitting Job Scripts

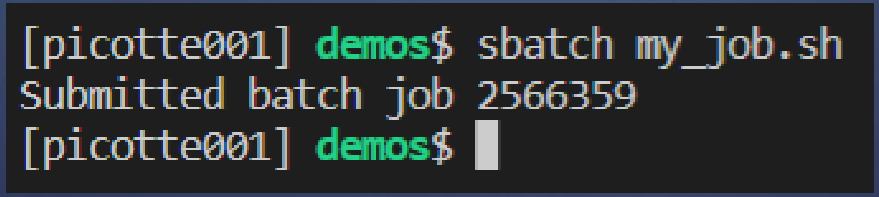


```
#!/bin/bash

#SBATCH --partition=def
#SBATCH --nodes=1
#SBATCH --mem=5GB
#SBATCH --time=00:30:00

echo "Hello World!"

```

SLURM commands

Some important SLURM commands:

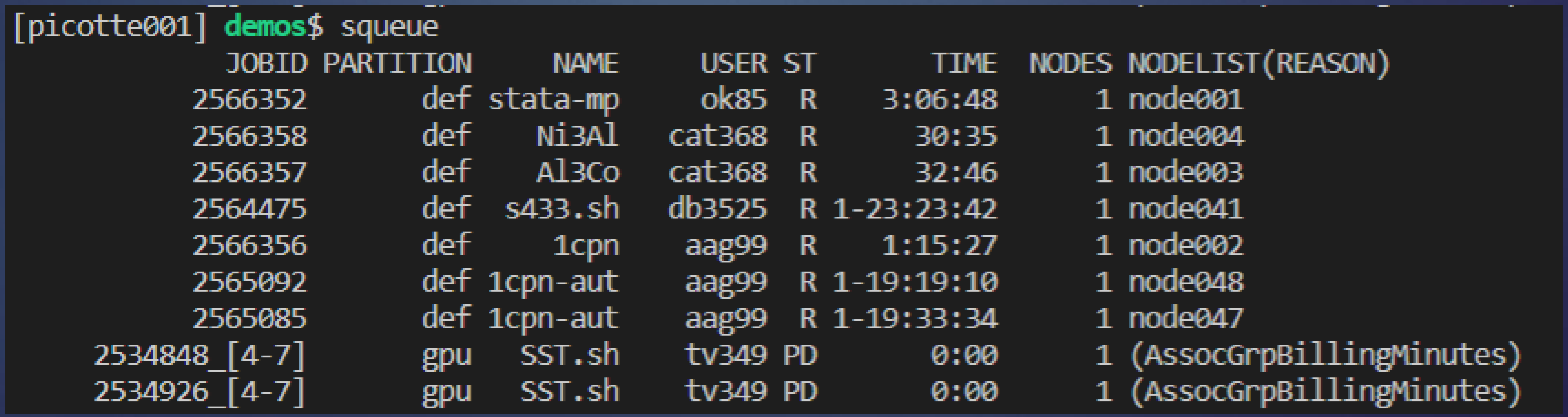
- sbatch: submit a job script to Slurm
  - -p, --partition=par – specify partition to run job (def by default)
  - -N, --nodes=numOfNodes – specify how many nodes to allocate (1 by default)
  - -t, --time=hh:mm:ss – specify a time limit for the job (30min by default)
  - --mem=size – specify required memory per node (4GB by default)
  - --mail-user=user@host – send job status to email (none by default)



```
[picotte001] demos$ sbatch my_job.sh
Submitted batch job 2566359
[picotte001] demos$
```

SLURM commands (cont.)

- scancel <jobId>: cancel a job that is pending/running
- squeue: display a list of running jobs
  - --me option to show only your jobs
  - -j <jobId> for a specific job



```
[picotte001] demos$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           2566352       def stata-mp     ok85  R    3:06:48      1 node001
           2566358       def    Ni3Al   cat368  R      30:35      1 node004
           2566357       def    Al3Co   cat368  R      32:46      1 node003
           2564475       def  s433.sh   db3525  R 1-23:23:42      1 node041
           2566356       def     1cpn    aag99  R    1:15:27      1 node002
           2565092       def 1cpn-aut    aag99  R 1-19:19:10      1 node048
           2565085       def 1cpn-aut    aag99  R 1-19:33:34      1 node047
     2534848_[4-7]       gpu   SST.sh    tv349 PD       0:00      1 (AssocGrpBillingMinutes)
     2534926_[4-7]       gpu   SST.sh    tv349 PD       0:00      1 (AssocGrpBillingMinutes)
```

SLURM commands (cont.)

- sacct: show account information on active/completed jobs
- sinfo: display status of nodes in Picotte
- seff <jobId>: report efficiency statistics on a job

More info: https://proteusmaster.urcf.drexel.edu/urcfwiki/index.php/Slurm_Quick_Start_Guide#Commands

SLURM commands (slurm_util)

These commands have the same behavior and options as their base commands but display output with some added detail.

Run the command “module load slurm_util” to use (consider adding the line to ~/.bashrc file to do it automatically on log-in:

- squeue_detail (squeue_long)
- sinfo_detail
- sacct_detail
- seff_array

Picotte (Storage)

Picotte has 3 levels of storage, each better suited for different uses:

- Persistent (NFS): for long-lived data (includes /home and /ifs)
    - 649 TB, 10 Gbps Ethernet (big and slow)
    - Main storage for most data, avoid using if you have lots of I/O
- Local Scratch (TMP) : internal drives in nodes (/tmp)
    - 854 GB, 12 Gbps SAS SSD (per node)
    - Fast, but not shared, ideal for single node jobs
    - $TMP variable to access from within a job
- Fast Parallel Shared Scratch (BeeGFS): shared memory b/n nodes (/beegfs)
    - 175 TB, 100 Gbps Infiniband Network
    - Fast and shared, ideal for intensive I/O operations across multiple nodes
    - $BEEGFS_TMPDIR variable to access from within a job

Viewing your Results

- The standard output of the program will be redirected to a new file named ‘slurm-jobId.out’ in the same directory as job script.
- Any file outputs will be saved in the same directory as job script with same name.

Questions?

- Feel free to attend my office hours every weekday 2 - 3 pm (any changes will be reflected on the URCF wiki main page): https://proteusmaster.urcf.drexel.edu/urcfwiki/index.php/Main_Page#Talks_and_Workshops