Getting Started on DARWIN

IT-RCI

Fall 2024

University of Delaware

Getting Started on DARWIN

Required Prerequisites

- Introduction to Linux Workshop
- Active DARWIN Account
  - UD or ACCESS
- SSH Client installed on your system (and know how to use it)
  - i.e. PuTTY for Windows

Suggested Prerequisites

- Familiarity with Coding
  - python
  - C / C++
  - Fortran
- Introduction to HPC at UD

DARWIN Cluster

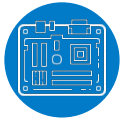
- ➔ Allocation Cluster
  - ◆ Research groups apply for allocations based on resources needed
    - Start up
    - Research
    - Education
  - ◆ PI of allocation requests accounts to be added
  - ◆ SU's are required to run jobs
  - ◆ CPU, GPU and Storage
  - ◆ Free to use

Workshop Overview

Connecting with SSH

Software and VALET

Joining Workgroups



Setting up Jobs

File Systems & Storage

SUs & Accounting

Collecting Data

Running and Monitoring Jobs with Slurm

Connecting with SSH

How to connect with SSH

- Windows
  - PuTTY
  - WSL
  - PowerShell
  - Terminal Emulator
- Linux/Mac OS
  - Terminal

```
mkyle@ITRC-G92D633:~$ ssh <user_name>@darwin.hpc.udel.edu
```

Connecting with SSH

How to connect with SSH

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  - PuTTY
  - WSL
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- Linux/Mac OS
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```
mkyle@ITRC-G92D633:~$ ssh mkyle@darwin.hpc.udel.edu
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Connecting with SSH

How to connect with SSH

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  - PuTTY
  - WSL
  - PowerShell
  - Terminal Emulator
- Linux/Mac OS
  - Terminal

```
mkyle@ITRC-G92D633:~$ ssh mkyle@darwin.hpc.udel.edu
Last login: Fri Sep 20 10:20:29 2024 from net10-7-191-11.host.udel.edu
[mkyle@login00.darwin ~]$
```

Joining Your Workgroup

How you join your workgroup?

- Finding workgroup(s)
  - **`workgroup --menu`**
  - `workgroup -q workgroups`
- Joining Workgroups
  - `workgroup -g [workgroup_name]`

```
[mkyle@login00.darwin ~]$ workgroup --menu
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Joining Your Workgroup

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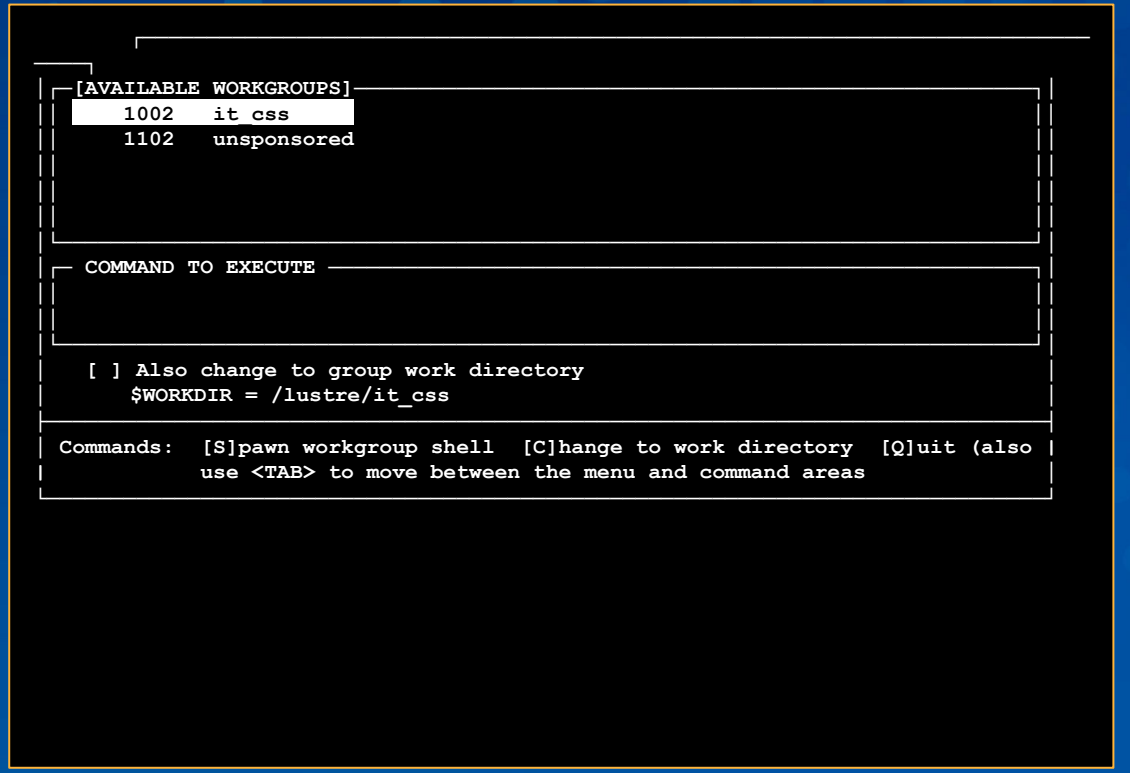

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[(it_css:mkyle)@login00.darwin ~]$ workgroup -q workgroups
```

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```
[mkyle@login00.darwin ~]$ workgroup --menu
[(it_css:mkyle)@login00.darwin ~]$ workgroup -q workgroups
 1002  it_css
 1102  unsponsored
[(it_css:mkyle)@login00.darwin ~]$
```

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[mkyle@login00.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login00.darwin ~]$
```

File Systems & Storage

Home Storage

- 20GB
- Personal use files
- `/home/<user_id>`
- `$HOME`

Lustre Storage

- 1.1PB
- Omni-path Infiniband

General Information

- > 13.5 TB Mem
- 100 GBit/s
- **No Back Ups!!**

Workgroup Storage

- >= 1TB
- Shared within workgroup
- `/lustre/<workgroup_name>/`
- `$WORKDIR`

Compute Node

- < 2TB
- Temporary job storage
- `$TMPDIR`

File Systems & Storage

- Workgroup
  - **$WORKDIR**
  - /lustre/<workgroup_name>
- Home
  - Login Landing path
  - $HOME
  - ~/
- Storage Usage Levels
  - df -h $HOME
  - my_quotas

```
[(it_css:mkyle)@login01.darwin ~]$ echo $WORKDIR
```

File Systems & Storage

- Workgroup
  - **$WORKDIR**
  - **/lustre/<workgroup_name>**
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```
[(it_css:mkyle)@login01.darwin ~]$ echo $WORKDIR
/lustre/it_css
[(it_css:mkyle)@login01.darwin ~]$
```

File Systems & Storage

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[(it_css:mkyle)@login01.darwin ~]$ echo $WORKDIR
/lustre/it_css
[(it_css:mkyle)@login01.darwin ~]$ cd $WORKDIR
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File Systems & Storage

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File Systems & Storage

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[(it_css:mkyle)@login01.darwin ~]$ echo $WORKDIR
/lustre/it_css
[(it_css:mkyle)@login01.darwin ~]$ cd $WORKDIR
[(it_css:mkyle)@login01.darwin it_css]$ echo $HOME
/home/2179
[(it_css:mkyle)@login01.darwin it_css]$
```

File Systems & Storage

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[(it_css:mkyle)@login01.darwin ~]$
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[(it_css:mkyle)@login01.darwin it_css]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ df -h $HOME
Filesystem                Size  Used Avail Use% Mounted on
nfs0-ib:/beagle/home/2179   20G  6.7G   14G  34% /home/2179
[(it_css:mkyle)@login01.darwin ~]$
```

File Systems & Storage

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[(it_css:mkyle)@login01.darwin ~]$ my_quotas
Type  Path                    In-use / kiB Available / kiB  Pct
----- --------------------- ------------- --------------- ----
user  /home/2179                  6953984        20971520  33%
group /lustre/it_css           1625031711      3026866824  53%
[(it_css:mkyle)@login01.darwin ~]$
```

File Systems & Storage

Exercise #1

- Home
  - path?
  - storage amount?
- Workgroup
  - path?
  - storage amount?

```
mkyle@ITRC-G92D633:~$
```

File Systems & Storage

Exercise #1

- Home
  - path?
  - storage amount?
- Workgroup
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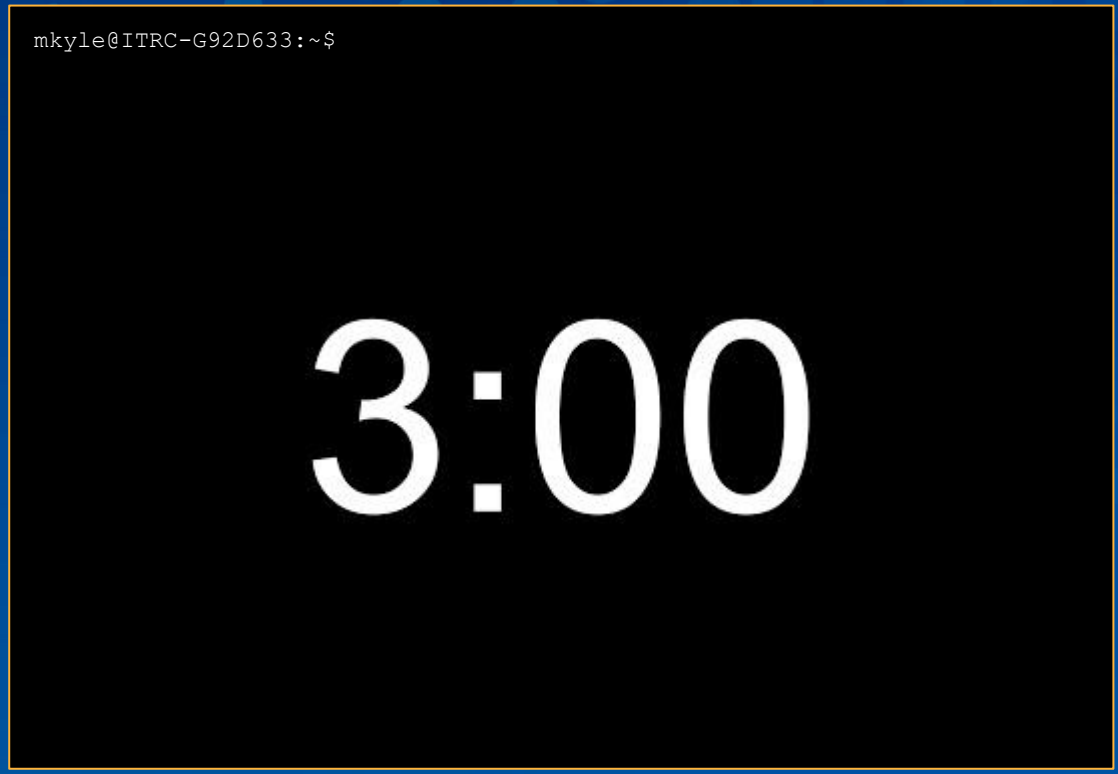

File Systems & Storage

Exercise #1

- **Home**
  - **path?**
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- Workgroup
  - path?
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[(it_css:mkyle)@login01.darwin ~]$ echo $HOME
/home/2179
[(it_css:mkyle)@login01.darwin ~]$
```

File Systems & Storage

Exercise #1

- **Home**
  - path?
  - **storage amount?**
- Workgroup
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[(it_css:mkyle)@login01.darwin ~]$ df -h $HOME
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File Systems & Storage

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  - storage amount?
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  - **path?**
  - storage amount

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[(it_css:mkyle)@login01.darwin ~]$ df -h $HOME
Filesystem                Size  Used Avail Use% Mounted on
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[(it_css:mkyle)@login01.darwin ~]$ echo $WORKDIR
/lustre/it_css
[(it_css:mkyle)@login01.darwin ~]$
```

File Systems & Storage

Exercise #1

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  - path?
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- **Workgroup**
  - path?
  - **storage amount?**

```
[(it_css:mkyle)@login01.darwin ~]$ echo $HOME
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[(it_css:mkyle)@login01.darwin ~]$ df -h $HOME
Filesystem                Size  Used Avail Use% Mounted on
nfs0-ib:/beagle/home/2179   20G  6.7G   14G  34% /home/2179
[(it_css:mkyle)@login01.darwin ~]$ echo $WORKDIR
/lustre/it_css
[(it_css:mkyle)@login01.darwin ~]$ my_quotas
Type  Path                In-use / kiB Available / kiB    Pct
----- -------------------- ------------ --------------- ----
user  /home/2179             6953984          20971520    33%
group /lustre/it_css         1625031711      3026866824    53%
[(it_css:mkyle)@login01.darwin ~]$
```

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - **scp**
  - wget
  - curl
  - rsync
- Advanced
  - rclone
  - Globus

```
[(it_css:mkyle)@login01.darwin ~]$ cd $HOME
```

HPC Wiki: Transferring files to/from DARWIN

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```
[(it_css:mkyle)@login01.darwin ~]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir workshop
```

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```
[(it_css:mkyle)@login01.darwin ~]$ mkdir workshop
[(it_css:mkyle)@login01.darwin ~]$ cd workshop
[(it_css:mkyle)@login01.darwin workshop]$  scp <file_to_copy> <destination>
```

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[(it_css:mkyle)@login01.darwin ~]$ cd workshop
[(it_css:mkyle)@login01.darwin workshop]$  scp <file_to_copy> <destination>
```

Note:
SCP can work between different systems, IE your laptop to a cluster, or to/from cluster to cluster

```
$ scp mkyle@caviness.hpc.udel.edu:~/file1.txt ~/
$ scp fileX.txt mkyle@darwin.hpc.udel.edu:~/workshop
```

Collecting Data On DARWIN

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```
[(it_css:mkyle)@login01.darwin ~]$ mkdir workshop
[(it_css:mkyle)@login01.darwin ~]$ cd workshop
[(it_css:mkyle)@login01.darwin workshop]$ scp
/opt/shared/help/DARWIN-Workshop/DARWIN_WrkShp.txt .
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

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  - **scp**
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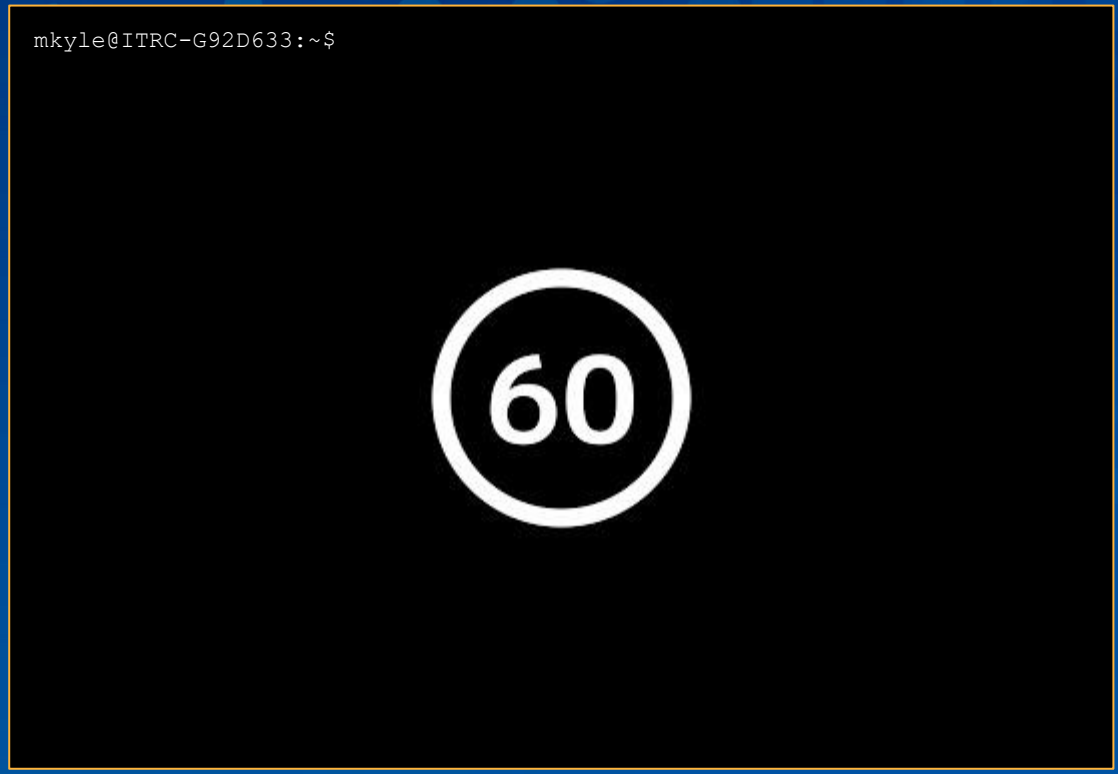
```
[(it_css:mkyle)@login01.darwin ~]$ mkdir workshop
[(it_css:mkyle)@login01.darwin ~]$ cd workshop
[(it_css:mkyle)@login01.darwin workshop]$ scp
/opt/shared/help/DARWIN-Workshop/DARWIN_WrkShp.txt .
[(it_css:mkyle)@login01.darwin workshop]$ ls
DARWIN_WrkShp.txt
[(it_css:mkyle)@login01.darwin workshop]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Exercise #1

- ➔ Open a second SSH session on DARWIN
- ➔ Use a text editor (nano, vim, etc) to open **`DARWIN_WrkShp.txt`**



Collecting Data On DARWIN

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[(it_css:mkyle)@login01.darwin ~]$ cd workshop
[(it_css:mkyle)@login01.darwin workshop]$ scp
/opt/shared/help/DARWIN-Workshop/DARWIN_WrkShp.txt .
[(it_css:mkyle)@login01.darwin workshop]$ ls
DARWIN_WrkShp.txt
[(it_css:mkyle)@login01.darwin workshop]$
[(it_css:mkyle)@login01.darwin workshop]$ wget <URL_TO_FILE>
```

Collecting Data On DARWIN

Data Transfer Methods

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DARWIN_WrkShp.txt
[(it_css:mkyle)@login01.darwin workshop]$
[(it_css:mkyle)@login01.darwin ~]$ wget
https://www.udel.edu/content/dam/udelImages/main/graphics/udelLogoImages/
logo-udel.png
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

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DARWIN_WrkShp.txt
[(it_css:mkyle)@login01.darwin workshop]$
[(it_css:mkyle)@login01.darwin ~]$ wget
https://www.udel.edu/content/dam/udelImages/main/graphics/udelLogoImages/
logo-udel.png
--2024-10-02 10:49:43--
https://www.udel.edu/content/dam/udelImages/main/graphics/udelLogoImages/
logo-udel.png
Resolving www.udel.edu (www.udel.edu)... 3.227.14.55, 34.207.18.216
Connecting to www.udel.edu (www.udel.edu)|3.227.14.55|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 31627 (31K) [image/png]
Saving to: 'logo-udel.png.1'

100%[=============================================================================
==============================>] 31,627        --.-K/s   in 0s

2024-10-02 10:49:43 (419 MB/s) - 'logo-udel.png' saved [31627/31627]
[(it_css:mkyle)@login01.darwin ~]$
```

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```
Resolving www.udel.edu (www.udel.edu)... 3.227.14.55, 34.207.18.216
Connecting to www.udel.edu (www.udel.edu)|3.227.14.55|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 31627 (31K) [image/png]
Saving to: 'logo-udel.png'

100%[=====================================================================
==============================>] 31,627        --.-K/s   in 0s

2024-10-02 10:49:43 (419 MB/s) - 'logo-udel.png' saved [31627/31627]
[(it_css:mkyle)@login01.darwin ~]$ ls
DARWIN_WrkShp.txt   logo-udel.png
[(it_css:mkyle)@login01.darwin workshop]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - `scp`
  - `wget`
  - **`curl`**
  - `rsync`
- Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin ~]$ ls
DARWIN_WrkShp.txt   logo-udel.png
[(it_css:mkyle)@login01.darwin workshop]$ mkdir sst_data
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - scp
  - wget
  - **curl**
  - rsync
- ➔ Advanced
  - rclone
  - Globus

```
[(it_css:mkyle)@login01.darwin ~]$ ls
DARWIN_WrkShp.txt   logo-udel.png
[(it_css:mkyle)@login01.darwin workshop]$ mkdir sst_data
[(it_css:mkyle)@login01.darwin workshop]$ cd sst_data
[(it_css:mkyle)@login01.darwin sst_data]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - `scp`
  - `wget`
  - **`curl`**
  - `rsync`
- Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin ~]$ ls
DARWIN_WrkShp.txt   logo-udel.png
[(it_css:mkyle)@login01.darwin workshop]$ mkdir sst_data
[(it_css:mkyle)@login01.darwin workshop]$ cd sst_data
[(it_css:mkyle)@login01.darwin sst_data]$ curl
https://downloads.psl.noaa.gov/Datasets/noaa.oisst.v2.highres/sst.day.anom.[1981-1982].nc -O
```

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - scp
  - wget
  - **curl**
  - rsync
- Advanced
  - rclone
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ curl
https://downloads.psl.noaa.gov/Datasets/noaa.oisst.v2.highres/sst.day.ano
m.[1981-1982].nc -O

[1/2]:
https://downloads.psl.noaa.gov/Datasets/noaa.oisst.v2.highres/sst.day.ano
m.1981.nc --> sst.day.anom.1981.nc
--_curl_--https://downloads.psl.noaa.gov/Datasets/noaa.oisst.v2.highres/s
st.day.anom.1981.nc
  % Total    % Received % Xferd  Average Speed   Time    Time     Time
Current
                                 Dload  Upload   Total   Spent    Left
Speed
100  182M  100  182M    0     0  3790k      0  0:00:49  0:00:49
--:--:-- 35.2M

[2/2]:
https://downloads.psl.noaa.gov/Datasets/noaa.oisst.v2.highres/sst.day.ano
m.1982.nc --> sst.day.anom.1982.nc
--_curl_--https://downloads.psl.noaa.gov/Datasets/noaa.oisst.v2.highres/s
st.day.anom.1982.nc
100  547M  100  547M    0     0  11.5M      0  0:00:47  0:00:47
--:--:-- 51.1M
[(it_css:mkyle)@login01.darwin sst_data]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- ➔ Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- ➔ Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$ cp
/opt/shared/help/DARWIN-Workshop/fileCreate.sh ./
[(it_css:mkyle)@login01.darwin sample]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$ cp
/opt/shared/help/DARWIN-Workshop/fileCreate.sh ./
[(it_css:mkyle)@login01.darwin sample]$ ls
fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$ cp
/opt/shared/help/DARWIN-Workshop/fileCreate.sh ./
[(it_css:mkyle)@login01.darwin sample]$ ls
fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ chmod 744 fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$ cp
/opt/shared/help/DARWIN-Workshop/fileCreate.sh ./
[(it_css:mkyle)@login01.darwin sample]$ ls
fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ chmod 744 fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ sh fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - scp
  - wget
  - curl
  - **rsync**
- Advanced
  - rclone
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$ cp
/opt/shared/help/DARWIN-Workshop/fileCreate.sh ./
[(it_css:mkyle)@login01.darwin sample]$ ls
fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ chmod 744 fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ sh fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ ls
file1.txt    file14.txt  file2.txt   file25.txt  file30.txt  file36.txt
file41.txt  file47.txt  file52.txt  file58.txt  file63.txt  file69.txt
file74.txt  ... MORE FILES REMOVED FOR SPACING ... fileCreate.sh
file13.txt   file19.txt  file24.txt  file3.txt   file35.txt  file40.txt
file46.txt  file51.txt  file57.txt  file62.txt  file68.txt  file73.txt
file79.txt  file84.txt  file9.txt   file95.txt
[(it_css:mkyle)@login01.darwin sample]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- ➔ Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$ cp
/opt/shared/help/DARWIN-Workshop/fileCreate.sh ./
[(it_css:mkyle)@login01.darwin sample]$ ls
fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ chmod 744 fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ sh fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ ls
file1.txt    file14.txt  file2.txt   file25.txt  file30.txt  file36.txt
file41.txt  file47.txt  file52.txt  file58.txt  file63.txt  file69.txt
file74.txt  ... MORE FILES REMOVED FOR SPACING ... fileCreate.sh
file13.txt   file19.txt  file24.txt  file3.txt   file35.txt  file40.txt
file46.txt  file51.txt  file57.txt  file62.txt  file68.txt  file73.txt
file79.txt  file84.txt  file9.txt   file95.txt
[(it_css:mkyle)@login01.darwin sample]$ cd ../workshop/
[(it_css:mkyle)@login01.darwin workshop]$
```

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - scp
  - wget
  - curl
  - **rsync**
- Advanced
  - rclone
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$ cp
/opt/shared/help/DARWIN-Workshop/fileCreate.sh ./
[(it_css:mkyle)@login01.darwin sample]$ ls
fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ chmod 744 fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ sh fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ ls
file1.txt    file14.txt  file2.txt   file25.txt  file30.txt  file36.txt
file41.txt  file47.txt  file52.txt  file58.txt  file63.txt  file69.txt
file74.txt  ... MORE FILES REMOVED FOR SPACING ... fileCreate.sh
file13.txt   file19.txt  file24.txt  file3.txt   file35.txt  file40.txt
file46.txt  file51.txt  file57.txt  file62.txt  file68.txt  file73.txt
file79.txt  file84.txt  file9.txt   file95.txt
[(it_css:mkyle)@login01.darwin sample]$ cd ../workshop/
[(it_css:mkyle)@login01.darwin workshop]$ mkdir dataFiles
[(it_css:mkyle)@login01.darwin workshop]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin sst_data]$ cd $HOME
[(it_css:mkyle)@login01.darwin ~]$ mkdir sample
[(it_css:mkyle)@login01.darwin ~]$ cd sample
[(it_css:mkyle)@login01.darwin sample]$ cp
/opt/shared/help/DARWIN-Workshop/fileCreate.sh ./
[(it_css:mkyle)@login01.darwin sample]$ ls
fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ chmod 744 fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ sh fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ ls
file1.txt    file14.txt  file2.txt   file25.txt  file30.txt  file36.txt
file41.txt  file47.txt  file52.txt  file58.txt  file63.txt  file69.txt
file74.txt  ... MORE FILES REMOVED FOR SPACING ... fileCreate.sh
file13.txt   file19.txt  file24.txt  file3.txt   file35.txt  file40.txt
file46.txt  file51.txt  file57.txt  file62.txt  file68.txt  file73.txt
file79.txt  file84.txt  file9.txt   file95.txt
[(it_css:mkyle)@login01.darwin sample]$ cd ../workshop/
[(it_css:mkyle)@login01.darwin workshop]$ mkdir dataFiles
[(it_css:mkyle)@login01.darwin workshop]$ cd dataFiles
[(it_css:mkyle)@login01.darwin dataFiles]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- Basic
  - scp
  - wget
  - curl
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- Advanced
  - rclone
  - Globus

```
[(it_css:mkyle)@login01.darwin sample]$ ls
fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ chmod 744 fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ sh fileCreate.sh
[(it_css:mkyle)@login01.darwin sample]$ ls
file1.txt    file14.txt  file2.txt   file25.txt  file30.txt  file36.txt
file41.txt  file47.txt  file52.txt  file58.txt  file63.txt  file69.txt
file74.txt  ... MORE FILES REMOVED FOR SPACING ... fileCreate.sh
file13.txt   file19.txt  file24.txt  file3.txt   file35.txt  file40.txt
file46.txt  file51.txt  file57.txt  file62.txt  file68.txt  file73.txt
file79.txt  file84.txt  file9.txt   file95.txt
[(it_css:mkyle)@login01.darwin sample]$ cd ../workshop/
[(it_css:mkyle)@login01.darwin workshop]$ mkdir dataFiles
[(it_css:mkyle)@login01.darwin workshop]$ cd dataFiles
[(it_css:mkyle)@login01.darwin dataFiles]$ rsync -azP ~/sample/*.txt ./
file71.txt
              0 100% 0.00kB/s     0:00:00 (xfr#70, to-chk=30/100)
file72.txt
              0 100% 0.00kB/s     0:00:00 (xfr#71, to-chk=29/100)
file73.txt ... MORE FILES REMOVED FOR SPACING ...
              0 100% 0.00kB/s     0:00:00 (xfr#99, to-chk=1/100)
file99.txt
              0 100% 0.00kB/s     0:00:00 (xfr#100, to-chk=0/100)
[(it_css:mkyle)@login01.darwin dataFiles]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- ➔ Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin dataFiles]$ ls
file1.txt    file18.txt  file27.txt  file36.txt  file45.txt  file54.txt
file63.txt  file72.txt  file81.txt  file90.txt
file10.txt   file19.txt  file28.txt  file37.txt  file46.txt  file55.txt
file64.txt  file73.txt  file82.txt  file91.txt
file100.txt  file2.txt   file29.txt
... MORE FILES REMOVED FOR SPACING ...
[(it_css:mkyle)@login01.darwin dataFiles]$ cd ~/sample/
[(it_css:mkyle)@login01.darwin sample]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- ➔ Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin dataFiles]$ ls
file1.txt    file18.txt  file27.txt  file36.txt  file45.txt  file54.txt
file63.txt  file72.txt  file81.txt  file90.txt
file10.txt   file19.txt  file28.txt  file37.txt  file46.txt  file55.txt
file64.txt  file73.txt  file82.txt  file91.txt
file100.txt  file2.txt   file29.txt
... MORE FILES REMOVED FOR SPACING ...
[(it_css:mkyle)@login01.darwin dataFiles]$ cd ~/sample/
[(it_css:mkyle)@login01.darwin sample]$ nano file1.txt
[(it_css:mkyle)@login01.darwin sample]$ nano file2.txt
[(it_css:mkyle)@login01.darwin sample]$ nano file100.txt
[(it_css:mkyle)@login01.darwin sample]$
```

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- ➔ Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin dataFiles]$ ls
file1.txt    file18.txt  file27.txt  file36.txt  file45.txt  file54.txt
file63.txt  file72.txt  file81.txt  file90.txt
file10.txt   file19.txt  file28.txt  file37.txt  file46.txt  file55.txt
file64.txt  file73.txt  file82.txt  file91.txt
file100.txt  file2.txt   file29.txt
... MORE FILES REMOVED FOR SPACING ...
[(it_css:mkyle)@login01.darwin dataFiles]$ cd ~/sample/
[(it_css:mkyle)@login01.darwin sample]$ nano file1.txt
[(it_css:mkyle)@login01.darwin sample]$ nano file2.txt
[(it_css:mkyle)@login01.darwin sample]$ nano file100.txt
[(it_css:mkyle)@login01.darwin sample]$ cd ../workshop/dataFiles
[(it_css:mkyle)@login01.darwin dateFiles]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - `scp`
  - `wget`
  - `curl`
  - **`rsync`**
- ➔ Advanced
  - `rclone`
  - Globus

```
[(it_css:mkyle)@login01.darwin dataFiles]$ ls
file1.txt    file18.txt  file27.txt  file36.txt  file45.txt  file54.txt
file63.txt  file72.txt  file81.txt  file90.txt
file10.txt   file19.txt  file28.txt  file37.txt  file46.txt  file55.txt
file64.txt  file73.txt  file82.txt  file91.txt
file100.txt  file2.txt   file29.txt
... MORE FILES REMOVED FOR SPACING ...
[(it_css:mkyle)@login01.darwin dataFiles]$ cd ~/sample/
[(it_css:mkyle)@login01.darwin sample]$ nano file1.txt
[(it_css:mkyle)@login01.darwin sample]$ nano file2.txt
[(it_css:mkyle)@login01.darwin sample]$ nano file100.txt
[(it_css:mkyle)@login01.darwin sample]$ cd ../workshop/dataFiles
[(it_css:mkyle)@login01.darwin dateFiles]$ rsync -azP ~/sample/*.txt .
sending incremental file list
file1.txt
              7 100% 0.00kB/s     0:00:00 (xfr#1, to-chk=99/100)
file100.txt
             12 100%   11.72kB/s 0:00:00 (xfr#2, to-chk=97/100)
file2.txt
             10 100%       9.77kB/s      0:00:00 (xfr#3, to-chk=87/100)
[(it_css:mkyle)@login01.darwin dataFiles]$
```

HPC Wiki: Transferring files to/from DARWIN

Collecting Data On DARWIN

Data Transfer Methods

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  - `rsync`
- ➔ Advanced
  - **`rclone`**
  - Globus

Popular Rclone Storage Systems

- Amazon S3
- Box
- Dropbox
- FTP
- Google Cloud/Drive*
- Azure Blob/File Storage
- OneDrive
- SFTP

* Currently there is issue with Google Drive connections

Collecting Data On DARWIN

Data Transfer Methods

- ➔ Basic
  - `scp`
  - `wget`
  - `curl`
  - `rsync`
- ➔ Advanced
  - `rclone`
  - **Globus**

Globus

Globus is a web based file transfer application that allows resilient, unattended file transfers between two Globus endpoints.

- Good for small and large transfers
- Web browser and or CLI
- Parallel transfers
- Encryption
- Performance tuning automatically
- Failed transfers automatically restart
- UD IT covers the subscription
- Globus is on Caviness and DARWIN
  - https://docs.hpc.udel.edu/software/globus/globus

Software and VALET

VALET

UD-developed software to help configure your environment for all IT-installed software packages.

- Similar to Modules used on other clusters, however VALET offers other features such as preventing conflicts of software versions being loaded
- Changes environment variables such as PATH, LD_LIBRARY_PATH and MANPATH
- Changes software development environment variables such as LDFLAGS and CPPFLAGS

```
[(it_css:mkyle)@login01.darwin workshop]$ cd
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET

UD-developed software to help configure your environment for all IT-installed software packages.

- Similar to Modules used on other clusters, however VALET offers other features such as preventing conflicts of software versions being loaded
- Changes environment variables such as PATH, LD_LIBRARY_PATH and MANPATH
- Changes software development environment variables such as LDFLAGS and CPPFLAGS

```
[(it_css:mkyle)@login01.darwin workshop]$ cd
[(it_css:mkyle)@login01.darwin ~]$ man valet
VALET(7)
       VALET User Manual
       VALET(7)

NAME
       valet - VALET Automates Linux Environment Tasks

DESCRIPTION
       One  particularly annoying aspect of cluster computing for most
users is getting the environment setup properly given a set of requisite
libraries and applications. Quite often in a cluster environment there
are multiple versions of a library available at any one time, and knowing
which to use when running a  program  can  often  mean  the  difference
       between  predictable, correct results and a flawed or even failed
execution.  A piece of software called (quite simply) "modules" has been
around for quite some time to
Manual page valet(7) line 1 (press h for help or q to quit)
```

Software and VALET

VALET commands

- **vpkg_list**
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- vpkg_rollback [all/#]
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ vpkg_list
Available packages:
  in /opt/shared/valet/2.1/etc
       alphafold
       amd-rocm
       amd-uprof
       anaconda
       aocl
       arpack
       atlas
       autoconf
       binutils
       blacs
       blis
       boost
       charm
       cmake
       cryosparc
       cuda
       cudnn
       ... many more ...
```

Software and VALET

VALET commands

- vpkg_list
- **vpkg_versions <package_name>**
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- vpkg_rollback [all/#]
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ vpkg_versions intel-python
Available versions in package (* = default version):

[/opt/shared/valet/2.1/etc/intel-python.vpkg_yaml]
intel-python        Intel Distribution for Python
  2021              alias to intel-python/2021.4.0
  2021.1.1          2021 update 1 (Python 3.7)
  2021.1.1:unaltered  2021 update 1 (Python 3.7) ORIGINAL INSTALL
  2021.4.0          2021 update 4 (Python 3.7)
* 2022              alias to intel-python/2022.1.0
  2022.1.0          2022 update 1 (Python 3.9)
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- **vpkg_info <package_name>**
- vpkg_require <package_name>
- vpkg_history
- vpkg_rollback [all/#]
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ vpkg_info intel-python
[intel-python] {
  contexts: all
  flags: no-development-env,no-standard-paths
  actions: {
       executable(source, succeedThenFail, success=0) {
       sh : /opt/shared/valet/2.1/libexec/intel-python.sh
       } (contexts: all)
       SHADOW_PREFIX=${VALET_PATH_PREFIX} (contexts: all)
       INTEL_DASH_PYTHON_PREFIX=${VALET_PATH_PREFIX} (contexts:
development)
  }
  Intel Distribution for Python
  prefix: /opt/shared/intel-python
  source file: /opt/shared/valet/2.1/etc/intel-python.vpkg_yaml
  default version: intel-python/2022
  versions: {
         ...SKIPPING LINES..
       [intel-python/2022.1.0] {
       contexts: all
       2022 update 1 (Python 3.9)
       prefix: /opt/shared/intel-python/2022.1.0
       }
  }
}
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- **vpkg_require <package_name>**
- vpkg_history
- vpkg_rollback [all/#]
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- **vpkg_require <package_name>**
- vpkg_history
- vpkg_rollback [all/#]
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require intel-python/2022.1.0
Adding package `intel-python/2022.1.0` to your environment
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- **vpkg_history**
- vpkg_rollback [all/#]
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require intel-python/2022.1.0
Adding package `intel-python/2022.1.0` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- **vpkg_rollback [all/#]**
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require intel-python/2022.1.0
Adding package `intel-python/2022.1.0` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require gcc
Adding package `gcc/4.8.5` to your environment
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- **vpkg_rollback [all/#]**
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require intel-python/2022.1.0
Adding package `intel-python/2022.1.0` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require gcc
Adding package `gcc/4.8.5` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[standard]
  gcc/4.8.5
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- **vpkg_rollback [all/#]**
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require intel-python/2022.1.0
Adding package `intel-python/2022.1.0` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require gcc
Adding package `gcc/4.8.5` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[standard]
  gcc/4.8.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_rollback 1
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- **vpkg_rollback [all/#]**
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require intel-python/2022.1.0
Adding package `intel-python/2022.1.0` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require gcc
Adding package `gcc/4.8.5` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[standard]
  gcc/4.8.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_rollback 1
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- **vpkg_rollback [all/#]**
- vpkg_help

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require intel-python/2022.1.0
Adding package `intel-python/2022.1.0` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require gcc
Adding package `gcc/4.8.5` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[standard]
  gcc/4.8.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_rollback 1
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$ vpkg_rollback all
[(it_css:mkyle)@login01.darwin ~]$
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- vpkg_rollback [all/#]
- **vpkg_help**

```
[(it_css:mkyle)@login01.darwin ~]$ python --version
Python 2.7.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require intel-python/2022.1.0
Adding package `intel-python/2022.1.0` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$ vpkg_require gcc
Adding package `gcc/4.8.5` to your environment
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[standard]
  gcc/4.8.5
[(it_css:mkyle)@login01.darwin ~]$ vpkg_rollback 1
[(it_css:mkyle)@login01.darwin ~]$ vpkg_history
[standard]
  intel-python/2022.1.0
[(it_css:mkyle)@login01.darwin ~]$ vpkg_rollback all
[(it_css:mkyle)@login01.darwin ~]$ vpkg_help
```

Software and VALET

VALET commands

- vpkg_list
- vpkg_versions <package_name>
- vpkg_info <package_name>
- vpkg_require <package_name>
- vpkg_history
- vpkg_rollback [all/#]
- **vpkg_help**

```
VALET(7)                                                    VALET User Manual                                                    VALET(7)

NAME
       valet - VALET Automates Linux Environment Tasks

DESCRIPTION
       One  particularly annoying aspect of cluster computing for most users is getting the environment setup properly given a set of
       requisite libraries and applications. Quite often in a cluster environment there are multiple versions of a library  available
       at  any  one  time, and knowing which to use when running a program can often mean the difference between predictable, correct
       results and a flawed or even failed execution.  A piece of software called (quite simply) "modules" has been around for  quite
       some  time  to address the complexities of environment configuration for users. The tool itself is fairly complex, both in the
       commands it offers the user and the manner by which environment modifications  are  specified  (a  modulefile).   valet  --  a
       recursive acronym for VALET Automates Linux Environment Tasks -- is an alternative that strives to be as simple as possible to


Manual page valet(7) line 1 (press h for help or q to quit)
```

Setting Up Jobs

Job Templates

- ➔ **/opt/shared/templates/slurm/**
  - ◆ applications/
    - R
    - comsol
    - abaqus
    - gaussian
    - lammps
    - matlab
    - tensorflow
  - ◆ generic/
    - serial.qs
    - thread.qs
    - mpi/

```
[(it_css:mkyle)@login01.darwin ~]$ cd /opt/shared/templates/slurm/
[(it_css:mkyle)@login01.darwin slurm]$
```

Setting Up Jobs

Job Templates

- ➔ **/opt/shared/templates/slurm/**
  - ◆ applications/
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    - abaqus
    - gaussian
    - lammps
    - matlab
    - tensorflow
  - ◆ generic/
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```
[(it_css:mkyle)@login01.darwin ~]$ cd /opt/shared/templates/slurm/
[(it_css:mkyle)@login01.darwin slurm]$ ls
README.md  applications  generic
[(it_css:mkyle)@login01.darwin slurm]$
```

Setting Up Jobs

Job Templates

- ➔ **/opt/shared/templates/slurm/**
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[(it_css:mkyle)@login01.darwin ~]$ cd /opt/shared/templates/slurm/
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README.md  applications  generic
[(it_css:mkyle)@login01.darwin slurm]$  cd applications
[(it_css:mkyle)@login01.darwin applications]$
```

Setting Up Jobs

Job Templates

- ➔ /opt/shared/templates/slurm/
  - ◆ **applications/**
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```
[(it_css:mkyle)@login01.darwin ~]$ cd /opt/shared/templates/slurm/
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README.md  applications  generic
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RStudio-Server.qs  abaqus.qs  comsol.qs  gaussian.qs  gromacs.qs
lammps.qs  matlab-mcr.qs  matlab.qs  nwchem.qs  tensorflow.qs
[(it_css:mkyle)@login01.darwin applications]$
```

Setting Up Jobs

Job Templates

- ➔ /opt/shared/templates/slurm/
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[(it_css:mkyle)@login01.darwin ~]$ cd /opt/shared/templates/slurm/
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lammps.qs  matlab-mcr.qs  matlab.qs  nwchem.qs  tensorflow.qs
[(it_css:mkyle)@login01.darwin applications]$ cd ../generic/
[(it_css:mkyle)@login01.darwin generic]$
```

Setting Up Jobs

Job Templates

- ➔ /opt/shared/templates/slurm/
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    - **thread.qs**
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```
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RStudio-Server.qs  abaqus.qs  comsol.qs  gaussian.qs  gromacs.qs
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[(it_css:mkyle)@login01.darwin generic]$ ls
mpi  serial.qs  threads.qs
[(it_css:mkyle)@login01.darwin generic]$
```

Setting Up Jobs

Job Templates

- ➔ /opt/shared/templates/slurm/
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```
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RStudio-Server.qs  abaqus.qs  comsol.qs  gaussian.qs  gromacs.qs
lammps.qs  matlab-mcr.qs  matlab.qs  nwchem.qs  tensorflow.qs
[(it_css:mkyle)@login01.darwin applications]$ cd ../generic/
[(it_css:mkyle)@login01.darwin generic]$ ls
mpi  serial.qs  threads.qs
[(it_css:mkyle)@login01.darwin generic]$ mkdir ~/workshop/job && cp
serial.qs ~/workshop/job/
[(it_css:mkyle)@login01.darwin generic]$
```

Setting Up Jobs

Job Templates

- ➔ /opt/shared/templates/slurm/
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```
[(it_css:mkyle)@login01.darwin ~]$ cd /opt/shared/templates/slurm/
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mpi  serial.qs  threads.qs
[(it_css:mkyle)@login01.darwin generic]$ mkdir ~/workshop/job && cp
serial.qs ~/workshop/job/
[(it_css:mkyle)@login01.darwin generic]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$
```

Setting Up Jobs

Job Templates

- ➔ /opt/shared/templates/slurm/
  - ◆ applications/
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[(it_css:mkyle)@login01.darwin ~]$ cd /opt/shared/templates/slurm/
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mpi  serial.qs  threads.qs
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serial.qs ~/workshop/job/
[(it_css:mkyle)@login01.darwin generic]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$ ls
serial.qs
[(it_css:mkyle)@login01.darwin job]$
```

Setting Up Jobs

Job Templates

- ➔ /opt/shared/templates/slurm/
  - ◆ applications/
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    - tensorflow
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    - **serial.qs**
    - thread.qs
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```
[(it_css:mkyle)@login01.darwin ~]$ cd /opt/shared/templates/slurm/
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README.md  applications  generic
[(it_css:mkyle)@login01.darwin slurm]$  cd applications
[(it_css:mkyle)@login01.darwin applications]$ ls
RStudio-Server.qs  abaqus.qs  comsol.qs  gaussian.qs  gromacs.qs
lammps.qs  matlab-mcr.qs  matlab.qs  nwchem.qs  tensorflow.qs
[(it_css:mkyle)@login01.darwin applications]$ cd ../generic/
[(it_css:mkyle)@login01.darwin generic]$ ls
mpi  serial.qs  threads.qs
[(it_css:mkyle)@login01.darwin generic]$ mkdir ~/workshop/job && cp
serial.qs ~/workshop/job/
[(it_css:mkyle)@login01.darwin generic]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$ ls
serial.qs
[(it_css:mkyle)@login01.darwin job]$ less serial.qs
```

Setting Up Jobs

Job Templates

- ➔ /opt/shared/templates/slurm/
  - ◆ applications/
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    - matlab
    - tensorflow
  - ◆ generic/
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    - thread.qs
    - mpi/

```
#!/bin/bash -l
#
# DARWIN job script template, generated 2022-05-05T10:14:37-0400
#
# Sections of this script that can/should be edited are delimited by a
# [EDIT] tag.  All Slurm job options are denoted by a line that starts
# with "#SBATCH " followed by flags that would otherwise be passed on
# the command line.  Slurm job options can easily be disabled in a
# script by inserting a space in the prefix, e.g. "# SLURM " and
# reenabled by deleting that space.
#
# This is a batch job template for a program using a single processor
# core/thread (a serial job).
#
#SBATCH --nodes=1 --ntasks=1 --cpus-per-task=1
#
# [EDIT] All jobs have memory limits imposed.  The default is 1 GB per
#      CPU allocated to the job.  The default can be overridden either
#      with a per-node value (--mem) or a per-CPU value (--mem-per-cpu)
#      with unitless values in MB and the suffixes K|M|G|T denoting
#      kibi, mebi, gibi, and tebibyte units.  Delete the space between
#      the "#" and the word SBATCH to enable one of them:
#
# SBATCH --mem=8G
# SBATCH --mem-per-cpu=1024M
```

Setting Up Jobs

- **Getting Jobs Files & Data**
- Creating a Copy
- Customizing Job Script

```
[(it_css:mkyle)@login01.darwin job]$ cp
/opt/shared/help/DARWIN-Workshop/stockLRM.py .
[(it_css:mkyle)@login01.darwin job]$
```

HPC Wiki: DARWIN Slurm Job Script Templates

Setting Up Jobs

- **Getting Jobs Files & Data**
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- Customizing Job Script

```
[(it_css:mkyle)@login01.darwin job]$ cp
/opt/shared/help/DARWIN-Workshop/stockLRM.py .
[(it_css:mkyle)@login01.darwin job]$ tail -n1 ../DARWIN_WrkShp.txt
curl
'https://docs.google.com/spreadsheets/d/1upReABmkz8I-7X1RbqWzE6IlCiUUbbqs
L9LiQ6F8lQ8/gviz/tq?tqx=out:csv' -o sp500.csv
[(it_css:mkyle)@login01.darwin job]$
```

Setting Up Jobs

- **Getting Jobs Files & Data**
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- Customizing Job Script

```
[(it_css:mkyle)@login01.darwin job]$ cp
/opt/shared/help/DARWIN-Workshop/stockLRM.py .
[(it_css:mkyle)@login01.darwin job]$ tail -n1 ../DARWIN_WrkShp.txt
curl
'https://docs.google.com/spreadsheets/d/1upReABmkz8I-7X1RbqWzE6IlCiUUbbqs
L9LiQ6F8lQ8/gviz/tq?tqx=out:csv' -o sp500.csv
[(it_css:mkyle)@login01.darwin job]$ curl
'https://docs.google.com/spreadsheets/d/1upReABmkz8I-7X1RbqWzE6IlCiUUbbqs
L9LiQ6F8lQ8/gviz/tq?tqx=out:csv' -o sp500.csv
% Total      % Received % Xferd  Average Speed   Time       Time   Time
Current
                                 Dload  Upload   Total   Spent    Left
Speed
100  152k     0  152k       0      0  48948      0 --:--:--  0:00:03
--:--:-- 48953
[(it_css:mkyle)@login01.darwin job]$
```

Setting Up Jobs

- **Getting Jobs Files & Data**
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```
[(it_css:mkyle)@login01.darwin job]$ cp
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[(it_css:mkyle)@login01.darwin job]$ tail -n1 ../DARWIN_WrkShp.txt
curl
'https://docs.google.com/spreadsheets/d/1upReABmkz8I-7X1RbqWzE6IlCiUUbbqs
L9LiQ6F8lQ8/gviz/tq?tqx=out:csv' -o sp500.csv
[(it_css:mkyle)@login01.darwin job]$ curl
'https://docs.google.com/spreadsheets/d/1upReABmkz8I-7X1RbqWzE6IlCiUUbbqs
L9LiQ6F8lQ8/gviz/tq?tqx=out:csv' -o sp500.csv
% Total      % Received % Xferd  Average Speed   Time       Time   Time
Current
                                 Dload  Upload   Total   Spent    Left
Speed
100  152k    0  152k      0      0  48948      0 --:--:--  0:00:03
--:--:-- 48953
[(it_css:mkyle)@login01.darwin job]$ ls
serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$
```

Setting Up Jobs

- Getting Jobs Files & Data
- **Creating a Copy**
- Customizing Job Script

```
[(it_css:mkyle)@login01.darwin job]$ ls
serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ cp serial.qs ${USER}_Stock.qs
[(it_css:mkyle)@login01.darwin job]$
```

Setting Up Jobs

- ➔ Getting Jobs Files & Data
- ➔ Creating a Copy
- ➔ **Customizing Job Script**

```
[(it_css:mkyle)@login01.darwin job]$ ls
serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ cp serial.qs ${USER}_Stock.qs
[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ nano mkyle_Stock.qs
```

Setting Up Jobs

- Getting Jobs Files & Data
- Creating a Copy
- **Customizing Job Script**

```
#!/bin/bash -l
#
# DARWIN job script template, generated 2022-05-05T10:14:37-0400
#
# Sections of this script that can/should be edited are delimited by a
# [EDIT] tag.  All Slurm job options are denoted by a line that starts
# with "#SBATCH " followed by flags that would otherwise be passed on
# the command line.  Slurm job options can easily be disabled in a
# script by inserting a space in the prefix, e.g. "# SLURM " and
# reenabled by deleting that space.
#
# This is a batch job template for a program using a single processor
# core/thread (a serial job).
#
#SBATCH --nodes=1 --ntasks=1 --cpus-per-task=1
#
# [EDIT] All jobs have memory limits imposed.  The default is 1 GB per
#      CPU allocated to the job.  The default can be overridden either
#      with a per-node value (--mem) or a per-CPU value (--mem-per-cpu)
#      with unitless values in MB and the suffixes K|M|G|T denoting
#      kibi, mebi, gibi, and tebibyte units.  Delete the space between
#      the "#" and the word SBATCH to enable one of them:
#
# SBATCH --mem=8G
# SBATCH --mem-per-cpu=1024M
```

Setting Up Jobs

- Getting Jobs Files & Data
- Creating a Copy
- **Customizing Job Script**

```
#!/bin/bash -l
#
# DARWIN job script template, generated 2022-05-05T10:14:37-0400
#
# Sections of this script that can/should be edited are delimited by a
# [EDIT] tag.  All Slurm job options are denoted by a line that starts
# with "#SBATCH " followed by flags that would otherwise be passed on
# the command line.  Slurm job options can easily be disabled in a
# script by inserting a space in the prefix, e.g. "# SLURM " and
# reenabled by deleting that space.
#
# This is a batch job template for a program using a single processor
# core/thread (a serial job).
#
#SBATCH --nodes=1 --ntasks=1 --cpus-per-task=1
#
# [EDIT] All jobs have memory limits imposed.  The default is 1 GB per
#      CPU allocated to the job.  The default can be overridden either
#      with a per-node value (--mem) or a per-CPU value (--mem-per-cpu)
#      with unitless values in MB and the suffixes K|M|G|T denoting
#      kibi, mebi, gibi, and tebibyte units.  Delete the space between
#      the "#" and the word SBATCH to enable one of them:
#
#SBATCH --mem=1G # template default 8G
# SBATCH --mem-per-cpu=1024M
```

Setting Up Jobs

- ➔ Getting Jobs Files & Data
- ➔ Creating a Copy
- ➔ **Customizing Job Script**

```
# [EDIT] Each node in the cluster has local scratch disk of some sort
#      that is always mounted as /tmp.  Per-job temporary directories
#      are automatically created and destroyed by Slurm and can be
#      referenced via the $TMPDIR environment variable.  To ensure a
#      minimum amount of free space when your job is scheduled, the
#      --tmp option can be used; it has the same behavior unit-wise as
#      --mem and --mem-per-cpu.  Delete the space between the "#" and the
#      word SBATCH to enable:
#
# SBATCH --tmp=24G
#
# [EDIT] It can be helpful to provide a descriptive (terse) name for
#      the job (be sure to use quotes if there's whitespace in the
#      name):
#
#SBATCH --job-name=stockLRM # Changed from serial_job
#
#
# [EDIT] The partition determines which nodes can be used and with what
#      maximum runtime limits, etc.  Partition limits can be displayed
#      with the "sinfo --summarize" command.
#
#
#      PLEASE NOTE:  On DARWIN every job is **required** to include the
#                   --partition flag in its submission!
#
```

Setting Up Jobs

- ➔ Getting Jobs Files & Data
- ➔ Creating a Copy
- ➔ **Customizing Job Script**

```
#SBATCH --partition=idle #standard
# [EDIT] Jobs that will run in one of the GPU partitions can request GPU
#      resources using ONE of the following flags:
#
#             --gpus=<count>
#             <count> GPUs total for the job, regardless of node count
#             --gpus-per-node=<count>
#             <count> GPUs are required on each node allocated to the job
#             --gpus-per-socket=<count>
#             <count> GPUs are required on each socket allocated to the
#             job
#             --gpus-per-task=<count>
#             <count> GPUs are required for each task in the job
#
#      PLEASE NOTE:  On DARWIN the --gres flag should NOT be used to
#                    request GPU resources.  The GPU type will be
#                    inferred from the partition to which the job is
#                    submitted if not specified.
#
# SBATCH --gpus=1
# SBATCH --gpus-per-task=1
# SBATCH --gpus=1
# SBATCH --gpus-per-task=1
# SBATCH --gpus-per-node=1
# SBATCH --gpus-per-socket=2
```

Setting Up Jobs

- Getting Jobs Files & Data
- Creating a Copy
- **Customizing Job Script**

```
# [EDIT] The maximum runtime for the job; a single integer is interpreted
#      as a number of minutes, otherwise use the format
#            d-hh:mm:ss
#      Jobs default to the default runtime limit of the chosen partition
#      if this option is omitted.
#SBATCH --time=0-00:05:00
#
#      You can also provide a minimum acceptable runtime so the scheduler
#      may be able to run your job sooner.  If you do not provide a
#      value, it will be set to match the maximum runtime limit (discussed
#      above).
#
#SBATCH --time-min=0-00:02:00
#
# [EDIT] By default SLURM sends the job's stdout to the file
"slurm-<jobid>.out"
#      and the job's stderr to the file "slurm-<jobid>.err" in the working
#      directory.  Override by deleting the space between the "#" and the
#      word SBATCH on the following lines; see the man page for sbatch
#      for special tokens that can be used in the filenames:
#
#SBATCH --output=%x-%j.out
#SBATCH --error=%x-%j.out
```

Setting Up Jobs

- Getting Jobs Files & Data
- Creating a Copy
- **Customizing Job Script**

```
# [EDIT] Slurm can send emails to you when a job transitions through
various
#      states: NONE, BEGIN, END, FAIL, REQUEUE, ALL, TIME_LIMIT,
#      TIME_LIMIT_50, TIME_LIMIT_80, TIME_LIMIT_90, ARRAY_TASKS.  One or
more
#      of these flags (separated by commas) are permissible for the
#      --mail-type flag.  You MUST set your mail address using
#      --mail-user
#      for messages to get off the cluster.
#
# SBATCH --mail-user='my_address@udel.edu'
# SBATCH --mail-type=END,FAIL,TIME_LIMIT_90
#
# [EDIT] By default we DO NOT want to send the job submission environment
#      to the compute node when the job runs.
#
#SBATCH --export=NONE
#
#
# [EDIT] If you're not interested in how the job environment gets setup,
#      uncomment the following.
#
#UD_QUIET_JOB_SETUP=YES
```

Setting Up Jobs

- ➔ Getting Jobs Files & Data
- ➔ Creating a Copy
- ➔ **Customizing Job Script**

```
# [EDIT] Define a Bash function and set this variable to its
#      name if you want to have the function called when the
#      job terminates (time limit reached or job preempted).
#
#      PLEASE NOTE:  when using a signal-handling Bash
#      function, any long-running commands should be prefixed
#      with UD_EXEC, e.g.
#
#                    UD_EXEC mpirun vasp
#
#      If you do not use UD_EXEC, then the signals will not
#      get handled by the job shell!
#
#job_exit_handler() {
#  # Copy all our output files back to the original job directory:
#  cp * "$SLURM_SUBMIT_DIR"
#
#  # Don't call again on EXIT signal, please:
#  trap - EXIT
#  exit 0
#}
#export UD_JOB_EXIT_FN=job_exit_handler
```

Setting Up Jobs

- ➔ Getting Jobs Files & Data
- ➔ Creating a Copy
- ➔ **Customizing Job Script**

```
#
# [EDIT] By default, the function defined above is registered
#      to respond to the SIGTERM signal that Slurm sends
#      when jobs reach their runtime limit or are
#      preempted.  You can override with your own list of
#      signals using this variable -- as in this example,
#      which registers for both SIGTERM and the EXIT
#      pseudo-signal that Bash sends when the script ends.
#      In effect, no matter whether the job is terminated
#      or completes, the UD_JOB_EXIT_FN will be called.
#
#export UD_JOB_EXIT_FN_SIGNALS="SIGTERM EXIT"

#
# [EDIT] Slurm only sets SLURM_MEM_PER_CPU when the --mem-per-cpu option
is
#      used.  The job template system will attempt to set the missing
#      SLURM_MEM_PER_CPU when --mem was used and the job has a uniform
number
#      of tasks per node (the only case when per-node memory yields a
#      uniform memory per task/cpu) if this variable is set:
#UD_PREFER_MEM_PER_CPU=YES
```

Setting Up Jobs

- Getting Jobs Files & Data
- Creating a Copy
- **Customizing Job Script**

```
#      Uncomment the following variable if the job mandates a per-CPU
memory
#      limit to be present or calculable when UD_PREFER_MEM_PER_CPU is
set:
#UD_REQUIRE_MEM_PER_CPU=YES

#
# If you have VALET packages to load into the job environment,
# uncomment and edit the following line:
#
#vpkg_require intel/2019
vpkg_require intel-python/2022.1.0
#
# Do general job environment setup:
#
. /opt/shared/slurm/templates/libexec/common.sh

#
# [EDIT] Add your script statements hereafter, or execute a script or
program
#      using the srun command.
#
#srun date
python --version
python stockLRM.py
```

Setting Up Jobs

- Getting Jobs Files & Data
- Creating a Copy
- **Customizing Job Script**

```
[(it_css:mkyle)@login01.darwin job]$ ls
serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ cp serial.qs ${USER}_Stock.qs
[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ nano mkyle_Stock.qs
[(it_css:mkyle)@login01.darwin job]$
```

Before we run the job…

Let's check our allocations SU's

SUs and Accounting

sproject

- **allocations**
  - --detail
- projects
- jobs
- failures

```
[(it_css:mkyle)@login00.darwin job]$ sproject allocations -w <workgroup>
```

SUs and Accounting

sproject

- **allocations**
  - --detail
- projects
- jobs
- failures

```
[(it_css:mkyle)@login00.darwin job]$  sproject allocations -w it_css
Project id Alloc id Alloc descr Category RDR Start date            End date
---------- -------- ---------- -------- --- -------------------------
-------------------------
       2       3 it_css::cpu startup  cpu 2021-07-12 00:00:00-04:00 2021-07-25
23:59:59-04:00
       2       4 it_css::gpu startup  gpu 2021-07-12 00:00:00-04:00 2021-07-25
23:59:59-04:00
       2      43 it_css::cpu startup  cpu 2021-07-26 00:00:00-04:00 2023-07-31
00:00:00-04:00
       2      44 it_css::gpu startup  gpu 2021-07-26 00:00:00-04:00 2023-07-31
00:00:00-04:00
       2     512 it_css::cpu startup  cpu 2023-08-01 00:00:00-04:00 2024-08-31
00:00:00-04:00
       2     514 it_css::gpu startup  gpu 2023-08-01 00:00:00-04:00 2025-08-31
00:00:00-04:00
[(it_css:mkyle)@login00.darwin job]$
```

SUs and Accounting

sproject

- **allocations**
  - **--current-only**
  - --detail
- projects
- jobs
- failures

```
[(it_css:mkyle)@login00.darwin job]$ sproject allocations -w it_css
Project id Alloc id Alloc descr Category RDR Start date                    End
date
---------- -------- ---------- -------- --- -------------------------
-------------------------
       2       3 it_css::cpu startup  cpu 2021-07-12 00:00:00-04:00 2021-07-25
23:59:59-04:00
       2       4 it_css::gpu startup  gpu 2021-07-12 00:00:00-04:00 2021-07-25
23:59:59-04:00
       2       43 it_css::cpu startup  cpu 2021-07-26 00:00:00-04:00 2023-07-31
00:00:00-04:00
       2       44 it_css::gpu startup  gpu 2021-07-26 00:00:00-04:00 2023-07-31
00:00:00-04:00
       2       512 it_css::cpu startup  cpu 2023-08-01 00:00:00-04:00 2024-08-31
00:00:00-04:00
       2       514 it_css::gpu startup  gpu 2023-08-01 00:00:00-04:00 2025-08-31
00:00:00-04:00
[(it_css:mkyle)@login00.darwin job]$  sproject allocations -w it_css
--current-only
Project id Alloc id Alloc descr Category RDR Start date             End date
---------- -------- ---------- -------- --- -------------------------
-------------------------
       2       680 it_css::cpu startup  cpu 2024-10-04 00:00:00-04:00 2025-09-30
00:00:00-04:00
       2       681 it_css::gpu startup  gpu 2024-10-04 00:00:00-04:00 2025-09-30
00:00:00-04:00
```

SUs and Accounting

sproject

- **allocations**
  - --current-only
  - **--detail**
- projects
- jobs
- failures

```
[(it_css:mkyle)@login00.darwin job]$  sproject allocations -w it_css --detail
Project id Alloc id Alloc descr Category RDR Credit Run+Cmplt Debit Balance
---------- -------- ----------- -------- --- ------ --------- ----- -------
         2        3 it_css::cpu startup  cpu 108500           0 -1678  106822
         2        4 it_css::gpu startup  gpu    417           0   -16     401
         2       43 it_css::cpu startup  cpu  33333           0  -433   32900
         2       44 it_css::gpu startup  gpu  33333           0   -22   33311
         2      512 it_css::cpu startup  cpu  33333         -72 -6467   26794
         2      514 it_css::gpu startup  gpu  33333          -3    -8   33322
         2      680 it_css::cpu startup  cpu  33333           0     0   33333
         2      681 it_css::gpu startup  gpu  33333           0     0   33333
[(it_css:mkyle)@login00.darwin job]$
```

HPC Wiki: Job Accounting on DARWIN

SUs and Accounting

sproject

- **allocations**
  - **--current-only**
  - **--details**
- projects
- jobs
- failures

```
[(it_css:mkyle)@login00.darwin job]$ sproject allocations -w it_css --detail
Project id Alloc id Alloc descr Category RDR Credit Run+Cmplt Debit Balance
---------- -------- ----------- -------- --- ------ --------- ----- -------
         2        3 it_css::cpu startup  cpu 108500           0 -1678  106822
         2        4 it_css::gpu startup  gpu    417           0   -16     401
         2       43 it_css::cpu startup  cpu  33333           0  -433   32900
         2       44 it_css::gpu startup  gpu  33333           0   -22   33311
         2      512 it_css::cpu startup  cpu  33333         -72 -6467   26794
         2      514 it_css::gpu startup  gpu  33333          -3    -8   33322
         2      680 it_css::cpu startup  cpu  33333           0     0   33333
         2      681 it_css::gpu startup  gpu  33333           0     0   33333
[(it_css:mkyle)@login00.darwin job]$  sproject allocations -w it_css --detail
--current-only
Project id Alloc id Alloc descr Category RDR Credit Run+Cmplt Debit Balance
---------- -------- ----------- -------- --- ------ --------- ----- -------
         2      680 it_css::cpu startup  cpu  33333           0     0   33333
         2      681 it_css::gpu startup  gpu  33333           0     0   33333
[(it_css:mkyle)@login00.darwin job]$
```

SUs and Accounting

sproject

- allocations
- **projects**
  - --current-only
  - --detail
- jobs
- failures

```
[(it_css:mkyle)@login00.darwin job]$  sproject projects -w it_css
Project id Account Group id Group name  Creation date
---------- ------- -------- ----------  -------------------------
         2 it_css       1002 it_css     2021-07-12 14:51:57-04:00
[(it_css:mkyle)@login00.darwin job]$
```

SUs and Accounting

sproject

- allocations
- **projects**
  - **--detail**
- jobs
- failures

```
[(it_css:mkyle)@login00.darwin job]$ sproject projects -w it_css
Project id Account Group id Group name  Creation date
---------- ------- -------- ----------  ------------------------
       2 it_css       1002 it_css    2021-07-12 14:51:57-04:00
[(it_css:mkyle)@login00.darwin job]$  sproject projects -w it_css --detail
Project id Account Group id Group name Allocation id Category RDR Start date
       End date                          Creation date
---------- ------- -------- ---------- ------------ -------- ---
------------------------- -------------------------  -------------------------
       2 it_css       1002 it_css                    3 startup  cpu 2021-07-12
00:00:00-04:00 2021-07-25 23:59:59-04:00  2021-07-12 15:00:46-04:00
                                                     4 startup  gpu 2021-07-12
00:00:00-04:00 2021-07-25 23:59:59-04:00  2021-07-12 15:00:54-04:00
                                                    43 startup  cpu 2021-07-26
00:00:00-04:00 2023-07-31 00:00:00-04:00  2021-07-26 14:47:56-04:00
                                                    44 startup  gpu 2021-07-26
00:00:00-04:00 2023-07-31 00:00:00-04:00  2021-07-26 14:47:56-04:00
                                                   512 startup  cpu 2023-08-01
00:00:00-04:00 2024-08-31 00:00:00-04:00  2023-08-04 10:03:08-04:00
                                                   514 startup  gpu 2023-08-01
00:00:00-04:00 2024-08-31 00:00:00-04:00  2023-08-04 10:03:08-04:00
                                                   680 startup  cpu 2024-10-04
00:00:00-04:00 2025-09-30 00:00:00-04:00  2024-10-04 15:26:13-04:00
                                                   681 startup  gpu 2024-10-04
00:00:00-04:00 2025-09-30 00:00:00-04:00  2024-10-04 15:26:13-04:00
[(it_css:mkyle)@login00.darwin job]$
```

SUs and Accounting

sproject

- allocations
- projects
- **jobs**
- failures

```
[(it_css:mkyle)@login00.darwin job]$  sproject jobs -w it_css
sproject jobs -w it_css
Activity id Alloc id Alloc descr  Job id Owner       Status  Amount Modification
date           Creation date
----------- -------- ----------- ------- -------- --------- ------
------------------------- -------------------------
       13:06:30-04:00 2024-06-25 12:31:28-04:00
       4647038        514 it_css::gpu 5212043 thuachen completed   -1 2024-06-25
13:34:30-04:00 2024-06-25 12:59:09-04:00
       4647047        514 it_css::gpu 5212053 thuachen completed   -1 2024-06-25
14:13:30-04:00 2024-06-25 13:38:30-04:00
       4648461        514 it_css::gpu 5213473 thuachen completed   0 2024-06-25
15:28:44-04:00 2024-06-25 15:27:58-04:00
       4648462        514 it_css::gpu 5213474 thuachen completed   0 2024-06-25
15:30:37-04:00 2024-06-25 15:30:06-04:00
       4648464        514 it_css::gpu 5213476 thuachen completed   0 2024-06-25
15:53:32-04:00 2024-06-25 15:31:10-04:00
       4697342        512 it_css::cpu 5264839 bkang completed      -24 2024-07-23
10:43:14-04:00 2024-07-23 10:17:58-04:00
       4697340        512 it_css::cpu 5264836 bkang completed      0 2024-07-23
10:16:50-04:00 2024-07-23 10:16:44-04:00
       4697368        512 it_css::cpu 5264893 bkang completed      -24 2024-07-23
13:11:17-04:00 2024-07-23 12:46:19-04:00
       4697390        512 it_css::cpu 5264953 bkang completed      -23 2024-07-23
14:19:05-04:00 2024-07-23 13:55:17-04:00
```

SUs and Accounting

sproject

- ➔ allocations
- ➔ projects
- ➔ jobs
- ➔ **failures**

`--help` Can be used with all the above

```
[(it_css:mkyle)@login00.darwin job] $ sproject failures -w it_css
 Job id Error message
------- ------------------------------------------------------------
5063695 Requested allocation has insufficient balance: 1612159 < 6451200
5063937 Requested allocation has insufficient balance: 1612159 < 6451200
[(it_css:mkyle)@login00.darwin job] $
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ **`workgroup -g <workgroup_name>`**

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g <workgroup>
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ **`workgroup -g <workgroup_name>`**

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login01.darwin ~]$
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ **`workgroup -g <workgroup_name>`**

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login01.darwin ~]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin ~]
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ **`workgroup -g <workgroup_name>`**

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login01.darwin ~]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job] $
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - **`sbatch <job_script>`**
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login01.darwin ~]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ sbatch ${USER}_Stock.qs
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - **`sbatch <job_script>`**
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login01.darwin ~]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ sbatch ${USER}_Stock.qs
Submitted batch job 5321840
[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - **`sbatch <job_script>`**
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login01.darwin ~]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ sbatch ${USER}_Stock.qs
Submitted batch job 5321840
[(it_css:mkyle)@login01.darwin job]$ ls
meanSquareError.png  mkyle_Stock.qs  serial.qs  sp500.csv
stockLRM-5321840.out  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

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  - **`sbatch <job_script>`**
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```
[mkyle@login01.darwin ~]$ workgroup -g it_css
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[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ sbatch ${USER}_Stock.qs
Submitted batch job 5321840
[(it_css:mkyle)@login01.darwin job]$ ls
meanSquareError.png  mkyle_Stock.qs  serial.qs  sp500.csv
stockLRM-5321840.out  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ display meanSquareError.png
```

Running & Monitoring Jobs

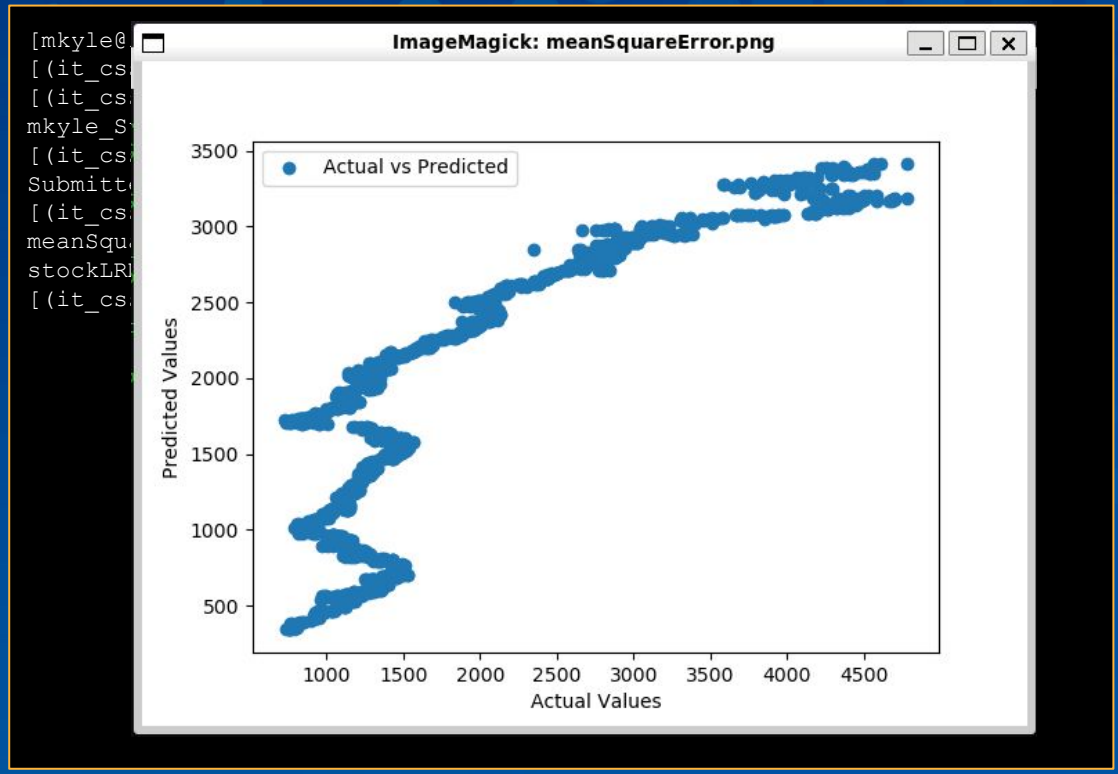
Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - **`sbatch <job_script>`**
- Interactive Jobs
  - `salloc`
  - `slurm options`



Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - **`sbatch <job_script>`**
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login01.darwin ~]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ sbatch ${USER}_Stock.qs
Submitted batch job 5321840
[(it_css:mkyle)@login01.darwin job]$ ls
meanSquareError.png  mkyle_Stock.qs  serial.qs  sp500.csv
stockLRM-5321840.out  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ display meanSquareError.png
[(it_css:mkyle)@login01.darwin job]$ nano stockLRM-5321840.out
```

Running & Monitoring Jobs

Running Jo

Required to

➔ workgr

<workq

Job types

- Batch J
  - s
  - <
- Interac
  - s
  - s

```
  GNU nano 2.3.1                                File: stockLRM-5321840.out

Adding package `intel-python/2022.1.0` to your environment
Python 3.9.10 :: Intel Corporation
 Intel(R) Extension for Scikit-learn* enabled (https://github.com/intel/scikit-learn-intelex)
Mean Squared Error: 310439.05366691446
Predicted closing price for 2023-02-15: 3289.6151191285753

                                [ Read 5 lines ]
^G Get Help  ^O WriteOut  ^R Read File  ^Y Prev Page  ^K Cut Text  ^C Cur
Pos |  ^X Exit  ^J Justify  ^W Where Is  ^V Next Page  ^U UnCut Text
^T To Spell
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - **`sbatch <job_script>`**
- Interactive Jobs
  - `salloc`
  - `slurm options`

```
[mkyle@login01.darwin ~]$ workgroup -g it_css
[(it_css:mkyle)@login01.darwin ~]$ cd ~/workshop/job
[(it_css:mkyle)@login01.darwin job]$ ls
mkyle_Stock.qs  serial.qs  sp500.csv  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ sbatch ${USER}_Stock.qs
Submitted batch job 5321840
[(it_css:mkyle)@login01.darwin job]$ ls
meanSquareError.png  mkyle_Stock.qs  serial.qs  sp500.csv
stockLRM-5321840.out  stockLRM.py
[(it_css:mkyle)@login01.darwin job]$ display meanSquareError.png
[(it_css:mkyle)@login01.darwin job]$ nano stockLRM-5321840.out
[(it_css:mkyle)@login01.darwin job]$ clear
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - **`salloc`**
  - `slurm options`

```
[(it_css:mkyle)@login01.darwin ~]$ salloc --partition=<partition>
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - **`salloc`**
  - `slurm options`

```
[(it_css:mkyle)@login01.darwin ~]$ salloc --partition=standard
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - **`salloc`**
  - `slurm options`

```
[(it_css:mkyle)@login01.darwin ~]$ salloc --partition=standard
salloc: Granted job allocation 5322677
salloc: Waiting for resource configuration
salloc: Nodes r1n02 are ready for job
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - **`salloc`**
  - `slurm options`

```
[(it_css:mkyle)@login01.darwin ~]$ salloc --partition=standard
salloc: Granted job allocation 5322677
salloc: Waiting for resource configuration
salloc: Nodes r1n02 are ready for job
[(it_css:mkyle)@r1n02 job]$
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - **`salloc`**
  - `slurm options`

```
[(it_css:mkyle)@login01.darwin job]$ salloc --partition=standard
salloc: Granted job allocation 5322677
salloc: Waiting for resource configuration
salloc: Nodes r1n02 are ready for job
[(it_css:mkyle)@r1n02 job]$ exit
logout
salloc: Relinquishing job allocation 5322677
salloc: Job allocation 5322677 has been revoked.
[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Running Jobs

Required to join workgroup

➔ `workgroup -g <workgroup_name>`

Job types

- Batch Jobs
  - `sbatch <job_script>`
- Interactive Jobs
  - `salloc`
  - **`slurm options`**

```
# [EDIT] The maximum runtime for the job; a single integer is interpreted
#      as a number of minutes, otherwise use the format
#            d-hh:mm:ss
#      Jobs default to the default runtime limit of the chosen partition
#      if this option is omitted.
#SBATCH --time=0-00:05:00
#
#      You can also provide a minimum acceptable runtime so the scheduler
#      may be able to run your job sooner.  If you do not provide a
#      value, it will be set to match the maximum runtime limit (discussed
#      above).
#
#SBATCH --time-min=0-00:02:00
#
# [EDIT] By default SLURM sends the job's stdout to the file
"slurm-<jobid>.out"
#      and the job's stderr to the file "slurm-<jobid>.err" in the working
#      directory.  Override by deleting the space between the "#" and the
#      word SBATCH on the following lines; see the man page for sbatch
#      for special tokens that can be used in the filenames:
#
#SBATCH --output=%x-%j.out
#SBATCH --error=%x-%j.out
```

Running & Monitoring Jobs

Running Jobs

Exercise #3:

Change the stockLRM.py file's Random Seed value and rerun the program using slurm's sbatch or salloc method to run the job.

The goal is to get a lower Mean Squared Error: 310439.053

```
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error
import matplotlib.pyplot as plt

# Read the CSV file into a DataFrame
df = pd.read_csv('sp500.csv')

# Convert the 'Date' column to datetime and extract the year and month
df['Date'] = pd.to_datetime(df['Date'])
df['Year'] = df['Date'].dt.year
df['Month'] = df['Date'].dt.month

# Create a linear regression model
X = df[['Year', 'Month']]  # Features
y = df['Close']  # Target variable

# Split the data into training and testing sets
#X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
random_state=42)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
random_state=3338)
```

Running & Monitoring Jobs

Running Jobs

Exercise:

Change the stockLRM.py file's Random Seed value and rerun the program using slurm's sbatch or salloc method to run the job.

The goal is to get a lower Mean Squared Error: 310439.053

```
[(it_css:mkyle)@login01.darwin job]$ salloc --partition=standard
salloc: Granted job allocation 5322677
salloc: Waiting for resource configuration
salloc: Nodes r1n02 are ready for job
[(it_css:mkyle)@r1n02 job]$ exit
logout
salloc: Relinquishing job allocation 5322677
salloc: Job all
[(it_css:mkyle)
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ **squeue**
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ `sacct`
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ squeue
 JOBID   PARTITION     NAME USER     ST    TIME    NODES NODELIST(REASON)
 5322549 gpu-v100 MetSRGAN xsedeu35  R   22:37:54          1   r2v01
 5322589 gpu-v100 NNtrainL xsedeu31  R   15:01:46          1   r2v00
 5322606 idle     openmpi_  ruiqihu  PD  0:00        1   (QOSMaxCpuPerUserLimit)
 5322641 idle     openmpi_  ruiqihu  PD  0:00        1   (QOSMaxCpuPerUserLimit)
 5322686 idle     interact    mkyle  R   11:32       1   r2112
 5322055 idle          mv  msnouri   R   2-03:38:57        1   r2x00
 5322645 idle     interact    shard  R   3:58:01     1   r2112
 5322665 idle         df      shard  R   2:37:09     1   r2121
 5322626 idle     gromacs_  tianren  R   5:33:29     1   r2126
[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ **squeue**
- ➔ ssqueue (Pretty)

Ended Jobs

- ➔ sacct
- ➔ ssacct (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ squeue
 JOBID  PARTITION     NAME USER     ST    TIME    NODES NODELIST(REASON)
 5322549 gpu-v100 MetSRGAN xsedeu35  R   22:37:54          1   r2v01
 5322589 gpu-v100 NNtrainL xsedeu31  R   15:01:46          1   r2v00
 5322606 idle     openmpi_  ruiqihu  PD  0:00        1   (QOSMaxCpuPerUserLimit)
 5322641 idle     openmpi_  ruiqihu  PD  0:00        1   (QOSMaxCpuPerUserLimit)
 5322686 idle     interact    mkyle  R   11:32       1   r2112
 5322055 idle          mv  msnouri   R   2-03:38:57        1   r2x00
 5322645 idle     interact    shard  R   3:58:01     1   r2112
 5322665 idle         df      shard  R   2:37:09     1   r2121
 5322626 idle     gromacs_  tianren  R   5:33:29     1   r2126
[(it_css:mkyle)@login01.darwin job]$
[(it_css:mkyle)@login01.darwin job]$ squeue -j 5322686
 JOBID PARTITION NAME         USER    ST      TIME  NODES NODELIST(REASON)
 5322686  idle   interact     mkyle   R      20:13  1      r2112
[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ **squeue**
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ `sacct`
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ squeue
 JOBID  PARTITION     NAME USER     ST    TIME    NODES NODELIST(REASON)
 5322549 gpu-v100 MetSRGAN xsedeu35  R   22:37:54          1   r2v01
 5322589 gpu-v100 NNtrainL xsedeu31  R   15:01:46          1   r2v00
 5322606 idle     openmpi_  ruiqihu  PD  0:00        1   (QOSMaxCpuPerUserLimit)
 5322641 idle     openmpi_  ruiqihu  PD  0:00        1   (QOSMaxCpuPerUserLimit)
 5322686 idle     interact    mkyle  R   11:32       1   r2112
 5322055 idle          mv  msnouri   R   2-03:38:57        1   r2x00
 5322645 idle     interact    shard  R   3:58:01     1   r2112
 5322665 idle         df      shard  R   2:37:09     1   r2121
 5322626 idle     gromacs_  tianren  R   5:33:29     1   r2126
[(it_css:mkyle)@login01.darwin job]$
[(it_css:mkyle)@login01.darwin job]$ squeue -j 5322686
 JOBID PARTITION NAME                USER    ST      TIME  NODES NODELIST(REASON)
 5322686  idle   interact     mkyle   R      20:13  1       r2112
[(it_css:mkyle)@login01.darwin job]$
[(it_css:mkyle)@login01.darwin job]$ squeue -u mkyle
 JOBID   PARTITION    NAME       USER  ST    TIME  NODES NODELIST(REASON)
 5322686 idle         interact   mkyle R     22:34   1    r2112
[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ **squeue**
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ `sacct`
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ squeue --help
Usage: squeue [OPTIONS]
  -A, --account=account(s)     comma separated list of accounts
                               to view, default is all accounts
  -a, --all                    display jobs in hidden partitions
      --array-unique                  display one unique pending job array
                               element per line
  -D, --delimiter=DELIM        print DELIM between each output field
      --federation                    Report federated information if a member
                               of one
  -h, --noheader               no headers on output
      --hide                          do not display jobs in hidden partitions
  -i, --iterate=seconds        specify an interation period
  -j, --job=job(s)             comma separated list of jobs IDs
                               to view, default is all
      --local                         Report information only about jobs on the
                               local cluster. Overrides --federation.
  -l, --long                   long report
...More Information was skipped...
Help options:
  --help                       show this help message
  --usage                      display a brief summary of squeue options
[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ **`ssqueue`** (Pretty)

Ended Jobs

- ➔ `sacct`
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ ssqueue
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ **`ssqueue`** (Pre

Ended Jobs

- ➔ `sacct`
- ➔ `ssacct` (Prett

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST
5322756	gpu-v100	NNtrainLSTM01	xsedeu3108	R	9:29:32	1	r2v00
5322774	idle	bulk	ruiqihu	PD	0:00	2	(QOSMaxCpuPerUserLimit)
5322055	idle	mv	msnouri	R	21:44:01	1	r2x00
5322744	idle	df_reduce	shard	R	12:06:30	1	r2l00
5322645	idle	jupyter	shared	R	22:03:05	1	r2l12
5322768	idle	gromacs_elp	tianren	R	2:02:15	1	r2l04
5322769	idle	gromacs_elp	tianren	R	2:02:15	1	r2l09
5322760	idle	gromacs_elp	tianren	R	2:02:16	1	r2l00
5322761	idle	gromacs_elp	tianren	R	2:02:16	1	r2l01
5322773	idle	openmpi_job	ruiqihu	R	51:27	1	r2l20

[Q]uit [P]rev/[N]ext page Page [L]eft/[R]ight [E]nd/[B]eginning of list

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ **`sacct`**
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ sacct -j <job_id>
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ **`sacct`**
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ sacct -j 5322667
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ **`sacct`**
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ sacct -j 5322667
       JobID   JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
5322667        stockLRM       idle    it_css          1  COMPLETED    0:0
5322667.bat+   batch                  it_css          1  COMPLETED    0:0
5322667.ext+   extern                 it_css          1  COMPLETED    0:0
[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ **`sacct`**
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ sacct --helpformat
Account              AdminComment         AllocCPUS            AllocNodes
AllocTRES            AssocID              AveCPU               AveCPUFreq
AveDiskRead          AveDiskWrite         AvePages             AveRSS
AveVMSize            BlockID              Cluster              Comment
Constraints          ConsumedEnergy       ConsumedEnergyRaw    CPUTime
CPUTimeRAW           DBIndex              DerivedExitCode      Elapsed
ElapsedRaw           Eligible             End                  ExitCode
Flags                GID                  Group                JobID
JobIDRaw             JobName              Layout               MaxDiskRead
MaxDiskReadNode      MaxDiskReadTask      MaxDiskWrite         MaxDiskWriteNode
MaxDiskWriteTask     MaxPages             MaxPagesNode         MaxPagesTask
MaxRSS               MaxRSSNode           MaxRSSTask           MaxVMSize
MaxVMSizeNode        MaxVMSizeTask        McsLabel             MinCPU
MinCPUNode           MinCPUTask           NCPUS                NNodes
NodeList             NTasks               Priority             Partition
QOS                  QOSRAW               Reason               ReqCPUFreq
ReqCPUFreqMin        ReqCPUFreqMax        ReqCPUFreqGov        ReqCPUS
ReqMem               ReqNodes             ReqTRES              Reservation
ReservationId        Reserved             ResvCPU              ResvCPURAW
Start                State                Submit               Suspended
SystemCPU            SystemComment        Timelimit            TimelimitRaw
TotalCPU             TRESUsageInAve       TRESUsageInMax       TRESUsageInMaxNode
TRESUsageInMaxTask   TRESUsageInMin       TRESUsageInMinNode   TRESUsageInMinTask
TRESUsageInTot       TRESUsageOutAve      TRESUsageOutMax      TRESUsageOutMaxNode
TRESUsageOutMaxTask  TRESUsageOutMin      TRESUsageOutMinNode  TRESUsageOutMinTask
TRESUsageOutTot      UID                  User                 UserCPU
WCKey                WCKeyID              WorkDir
```

HPC Wiki: Managing Jobs on DARWIN

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ **`sacct`**
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$  sacct --format="jobid, jobname,
partition, account, user, state, alloccpus, totalcpu, elapsed" -j 5321840
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ **`sacct`**
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$  sacct --format="jobid, jobname, partition, account,
user, state, alloccpus, totalcpu, elapsed" -j 5321840
       JobID  JobName  Partition  Account  User  State      AllocCPUS   TotalCPU Elapsed
------------ -------- ---------- -------- ----- ---------- ---------- --------- ----------
5321840       stockLRM      idle   it_css   mkyle COMPLETED        1     00:02.195  00:00:04
5321840.bat+    batch             it_css         COMPLETED        1     00:02.194  00:00:04
5321840.ext+ extern               it_css         COMPLETED        1     00:00.001  00:00:04
[(it_css:mkyle)@login01.darwin ~]$
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ **`sacct`**
- ➔ `ssacct` (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$  sacct --format="jobid, jobname,
partition, account, user, state, alloccpus, totalcpu, elapsed" -j 5321840
       JobID   JobName  Partition    Account  User  State      AllocCPUS
TotalCPU Elapsed
------------ -------- ---------- -------- ----- ---------- ---------- ---------
----------
5321840        stockLRM       idle    it_css   mkyle COMPLETED       1
00:02.195  00:00:04
5321840.bat+    batch               it_css         COMPLETED       1
00:02.194  00:00:04
5321840.ext+   extern               it_css         COMPLETED       1
00:00.001  00:00:04
[(it_css:mkyle)@login01.darwin ~]$ sacct --help
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ `sacct`
- ➔ **`ssacct`** (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ sacct --help
sacct [<OPTION>]
       Valid <OPTION> values are:
       -a, --allusers:
              Display jobs for all users. By default, only the
              current user's jobs are displayed.  If ran by user root
              this is the default.
       -A, --accounts:
              Use this comma separated list of accounts to select jobs
              to display.  By default, all accounts are selected.
       -b, --brief:
              Equivalent to '--format=jobstep,state,error'.
       -c, --completion: Use job completion instead of accounting data.

       -X, --allocations:
              Only show statistics relevant to the job allocation
              itself, not taking steps into consideration.
       ...More Lines that are Skipped...

       Note, valid start/end time formats are...
              HH:MM[:SS] [AM|PM]
              MMDD[YY] or MM/DD[/YY] or MM.DD[.YY]
              MM/DD[/YY]-HH:MM[:SS]
              YYYY-MM-DD[THH:MM[:SS]]
              now[{+|-}count[seconds(default)|minutes|hours|days|weeks]]

[(it_css:mkyle)@login01.darwin job]$
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs
- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs
- ➔ `sacct`
- ➔ **`ssacct`** (Pretty)

```
[(it_css:mkyle)@login01.darwin job]$ ssacct -j 5321840
```

Running & Monitoring Jobs

Monitoring Jobs

Active Jobs

- ➔ `squeue`
- ➔ `ssqueue` (Pretty)

Ended Jobs

- ➔ `sacct`
- ➔ **`ssacct`** (Pretty)

```
JobID    | JobName  | Partition | Account | AllocCPUS | State    | ExitCode
---------|----------|-----------|---------|-----------|----------|---------
5321840  | stockLRM | idle      | it_css  |         1 | COMPLETE | 0:0
5321840  | batch    |           | it_css  |         1 | COMPLETE | 0:0
5321840n | extern   |           | it_css  |         1 | COMPLETE | 0:0

 [Q]uit   [P]rev/[N]ext page   Page [L]eft/[R]ight   [E]nd/[B]eginning of list
```

Monitoring Jobs

DARWIN Partitions

standard	Contains all 48 standard memory nodes (64 cores, 512 GiB memory per node)	• Maximum run time of 7 days • Maximum of 400 jobs per user per partition • Default no preemption
large-mem	Contains all 32 large memory nodes (64 cores, 1024 GiB memory per node)	• Maximum run time of 7 days • Maximum of 400 jobs per user per partition • Default no preemption
xlarge-mem	Contains all 11 extra-large memory nodes (64 cores, 2048 GiB memory per node)	• Maximum run time of 7 days • Maximum of 400 jobs per user per partition • Default no preemption
extended-mem	Contains the single extended memory node (64 cores, 1024 GiB memory + 2.73 TiB NVMe swap)	• Maximum run time of 7 days • Maximum of 400 jobs per user per partition • Default no preemption

Monitoring Partitions

DARWIN Partitions Part II

gpu-t4	Contains all 9 NVIDIA Tesla T4 GPU nodes (64 cores, 512 GiB memory, 1 T4 GPU per node)	• Maximum run time of 7 days • Maximum of 400 jobs per user per partition • Default no preemption
gpu-v100	Contains all 3 NVIDIA Tesla V100 GPU nodes (48 cores, 768 GiB memory, 4 V100 GPUs per node)	• Maximum run time of 7 days • Maximum of 400 jobs per user per partition • Default no preemption
gpu-mi50	Contains the single AMD Radeon Instinct MI50 GPU node (64 cores, 512 GiB memory, 1 MI50 GPU)	• Maximum run time of 7 days • Maximum of 400 jobs per user per partition • Default no preemption
gpu-mi100	Contains the single AMD Radeon Instinct MI100 GPU node (64 cores, 512 GiB memory, 1 MI100 GPU)	• Maximum run time of 7 days • Maximum of 400 jobs per user per partition • Default no preemption
idle	**Contains all nodes in the cluster, jobs on this partition can be preempted but are not charged against your allocation**	• **Preemption is enabled for all jobs** • **Maximum of 320 jobs per user** • **Maximum of 640 CPUs per user (across all jobs in the partition)**

Monitoring Jobs

Monitoring Jobs

- **sinfo**
  - Used to report status of all the nodes of cluster.
- scontrol

```
[(it_css:mkyle)@login01.darwin job]$ sinfo

PARTITION     AVAIL  TIMELIMIT  NODES  STATE NODELIST
standard*     up 7-00:00:00      1 drain* r1n10
standard*     up 7-00:00:00      1  down* r1n19
standard*     up 7-00:00:00      9      mix
r1n[00,02,04-05,24,37-38,42,45]
standard*     up 7-00:00:00     36  alloc
r1n[01,03,06-09,11-16,18,20-23,25-36,39-41,43-44,46-47]
large-mem     up 7-00:00:00      1  down* r2l31
large-mem     up 7-00:00:00      3      mix r2l[00,09,12]
large-mem     up 7-00:00:00     24  alloc
r2l[01-08,10-11,13-18,20,22-25,27-29]
large-mem     up 7-00:00:00      4   idle r2l[19,21,26,30]
xlarge-mem    up 7-00:00:00      1      mix r2x00
xlarge-mem    up 7-00:00:00      3  alloc r2x[04,06-07]
xlarge-mem    up 7-00:00:00      7   idle r2x[01-03,05,08-10]
extended-mem  up 7-00:00:00      1   idle r2e00
gpu-t4        up 7-00:00:00      2  alloc r1t[00,05]
gpu-t4        up 7-00:00:00      7   idle r1t[01-04,06-07],r2t08
gpu-v100      up 7-00:00:00      1      mix r2v00
gpu-v100      up 7-00:00:00      2   idle r2v[01-02]
gpu-mi50      up 7-00:00:00      1   idle r2m00
gpu-mi100     up 7-00:00:00      1   idle r0m01
```

Monitoring Jobs

Monitoring Jobs

- ➔ sinfo
- ➔ **scontrol**
  - ◆ Used for monitoring and modifying queued jobs, as well as holding and releasing jobs.

```
[(it_css:mkyle)@login01.darwin job]$ scontrol show job 5322641
   JobId=5322606 JobName=openmpi_job
   UserId=ruiqihu(2262) GroupId=mtg(1074) MCS_label=N/A
   Priority=90755271 Nice=0 Account=mtg QOS=normal
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=0 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   RunTime=12:28:21 TimeLimit=3-00:00:00 TimeMin=3-00:00:00
   SubmitTime=2024-10-07T07:34:43 EligibleTime=2024-10-07T07:34:43
   AccrueTime=2024-10-07T07:34:43
   StartTime=2024-10-08T01:29:08 EndTime=2024-10-11T01:29:08
Deadline=N/A
   PreemptEligibleTime=2024-10-08T01:39:08 PreemptTime=None
   SuspendTime=None SecsPreSuspend=0 LastSchedEval=2024-10-08T01:29:08
   Partition=idle AllocNode:Sid=r0login1:113063
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=r2127
   BatchHost=r2127
   NumNodes=1 NumCPUs=64 NumTasks=64 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   TRES=cpu=64,mem=448G,node=1,billing=1
   Socks/Node=* NtasksPerN:B:S:C=64:0:*:* CoreSpec=*
   MinCPUsNode=64 MinMemoryCPU=7G MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
```

Office Hours

- Research Computing Office Hours
  - Time: Tuesdays and Wednesdays @ 11am – noon
  - Location: 002C Smith Hall, Conference Room or via Zoom
- Research Software Engineering (RSE) Support For The College Of Arts And Science (CAS)
  - Time: Tuesdays and Wednesdays @ 1pm – 2pm
  - Location: Room 110 Sharp Lab or via Zoom

Upcoming Workshops

- IT-RCI Workshop Series October 17-31
  - Getting Started with DARWIN: 10/17 @ 2-3 pm, 10/18 @ 10-11:30 am
  - Introduction to Slurm: 10/21 @ 1:30-3:30 pm
  - Shell Scripting: 10/23 @ 1:30-3:30 pm
  - HPC Software Development and Installation: 10/31 @ 10 am-noon

Helpful HPC Resources

Scan 4 url's

hpc-ask

caviness-users

darwin-users

hpc-wiki

Help Desk
askit@udel.edu

Thank you!

For more information, contact:

askit@udel.edu