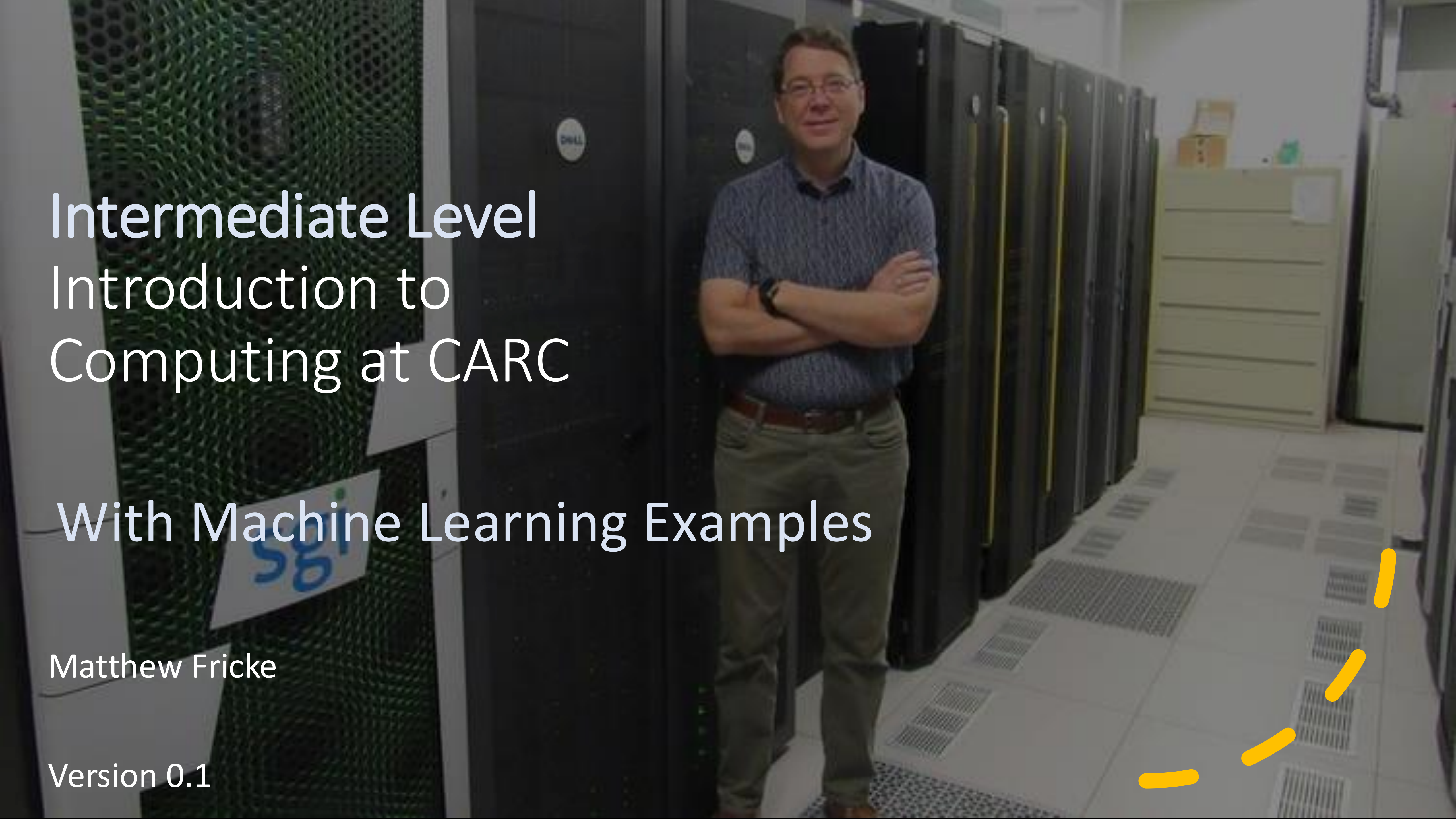


# Intermediate Level Introduction to Computing at CARC

## With Machine Learning Examples

Matthew Fricke

Version 0.1

## Goals

- 1) SLURM scheduler literacy
- 2) Run Machine Learning Tools on CARC Systems
  - Random Forests
  - Support Vector Machine
  - Multi-Layer Perceptron
  - Convolutional Neural Network
- We wont cover file transfer, storage systems, module system, conda, PBS. (These are all covered in depth in the video tutorials)

## Logging into Hopper

First login to the Linux **workstation** in front of you. Your CARC username is on the sign in sheet.

If you have logged in before use your existing password

Otherwise, your initial password is Welcome2CARC

This is an “important step” so don’t let me move on until you have logged in

## Logging into Hopper

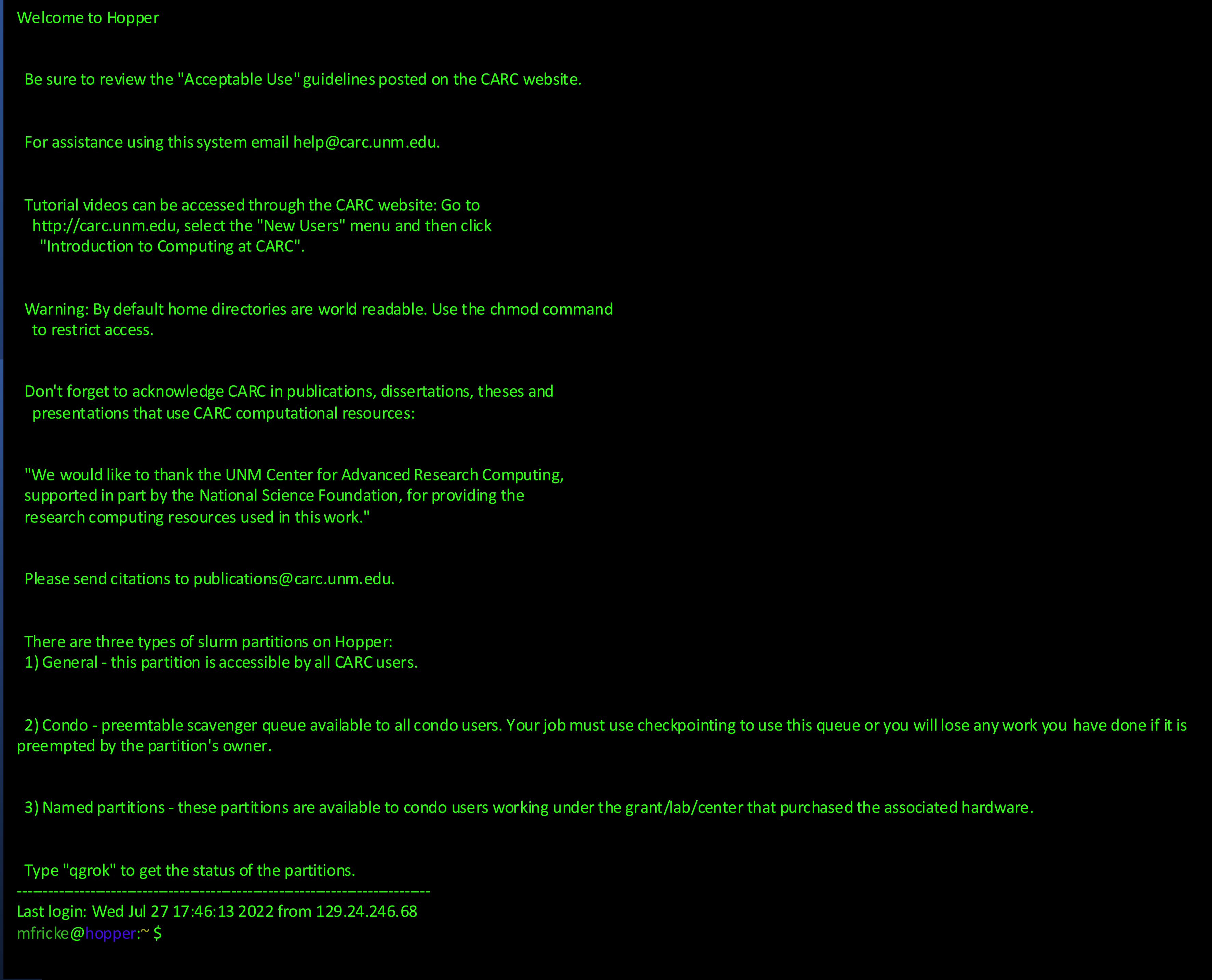
```
ssh vanilla@hopper.alliance.unm.edu
```

Should prompt you for a password…

Don’t let me move on until you are able to login.

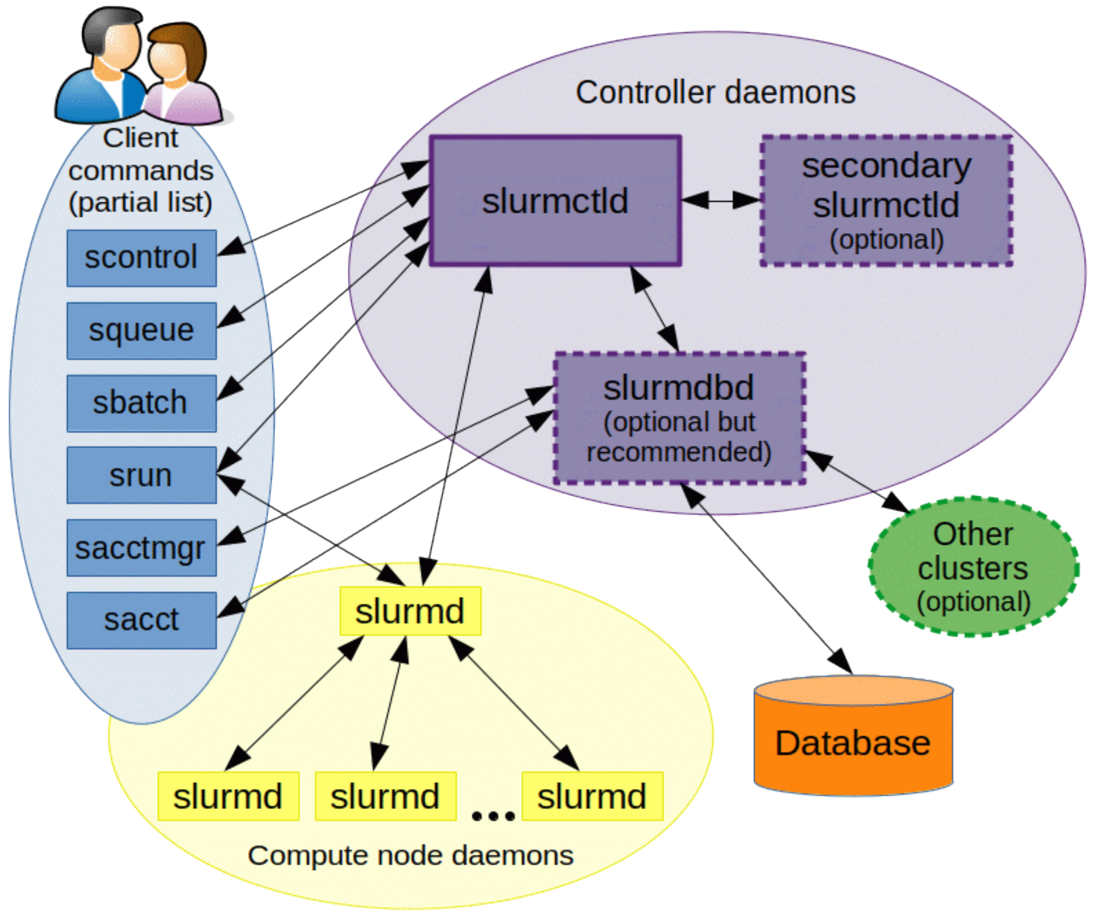
Replace vanilla with your name (unless your last name is Ice)

# Logging into Hopper



```
Welcome to Hopper


 Be sure to review the "Acceptable Use" guidelines posted on the CARC website.


 For assistance using this system email help@carc.unm.edu.


 Tutorial videos can be accessed through the CARC website: Go to
   http://carc.unm.edu, select the "New Users" menu and then click
     "Introduction to Computing at CARC".


 Warning: By default home directories are world readable. Use the chmod command
   to restrict access.


 Don't forget to acknowledge CARC in publications, dissertations, theses and
   presentations that use CARC computational resources:


 "We would like to thank the UNM Center for Advanced Research Computing,
 supported in part by the National Science Foundation, for providing the
 research computing resources used in this work."


 Please send citations to publications@carc.unm.edu.


 There are three types of slurm partitions on Hopper:
 1) General - this partition is accessible by all CARC users.


 2) Condo - preemtable scavenger queue available to all condo users. Your job must use checkpointing to use this queue or you will lose any work you have done if it is
preempted by the partition's owner.


 3) Named partitions - these partitions are available to condo users working under the grant/lab/center that purchased the associated hardware.


 Type "qgrok" to get the status of the partitions.
-------------------------------------------------------------------------------
Last login: Wed Jul 27 17:46:13 2022 from 129.24.246.68
mfricke@hopper:~ $
```

# Simple Linux Utility for Resource Management


Client commands (partial list)
scontrol
squeue
sbatch
srun
sacctmgr
sacct
Controller daemons
slurmctld
secondary slurmctld (optional)
slurmdbd (optional but recommended)
Other clusters (optional)
Database
slurmd
slurmd
slurmd
...
slurmd
Compute node daemons

ENJOY
Slurm
SODA
IT'S HIGHLY ADDICTIVE!
VOTED #1 SOFT DRINK OF THE 31st CENTURY!
SLURMS MCKENZIE

```
[vanilla@hopper ~]$ qgrok
queues    free  busy  offline  jobs  nodes  CPUs  GPUs  CPUs/node  GPUs/node  Memory/node  time_limit  CPU_limit
-----     -----  -----  -----   -----  -----  -----  -----  -----     -----      -----       -----       -----
general   4     6     0       4     10    320   0     32        0         93G        2-00:00:00   64
debug     2     0     0       0     2     64    0     32        0         93G        4:00:00      8
condo     22    25    4       7     51    1632  28    32        2         93G-1.5T   2-00:00:00   192
bugs      2     0     0       0     2     64    0     32        0         93G        7-00:00:00
```

```
vanilla@hopper:~ $ qgrok
queues     free  busy  offline  jobs  nodes  CPUs  GPUs
-----      ----- ----- -----    ----- -----  ----- -----
general    1     9     0        7     10     320   0
debug      2     0     0        0     2      64    0
condo      18    19    1        7     38     1216  8
bugs       0     2     0        0     2      64    0
pcnc       1     1     0        0     2      64
pathogen   1     0     0        0     1
tc         5     5     0        3     10     32
gold       2     0     0        0     2      6
fishgen    0     1     0        0     1
neuro-hsc  8     6     0        0     14
cup-ecs    0     2     0        2     2
tid        0     1     0        0     1      32
biocomp    0     1     0        0     1
chakra     1     0     0        0     1
pna        0     0     1        0     1      3
totals:    19    28    1        14    48     1
```

**Open partitions for use by everyone with a CARC account.**

**Purchased by the Office for the Vice President for Research.**

```
vanilla@hopper:~ $ qgrok
queues     free  busy  offline  jobs  nodes  CPUs  GPUs
-----      ----- ----- -----    ----- ----- ----- -----
general    1     9     0        7     10     320   0
debug      2     0     0        0     2      64    0
condo      18    19    1        7     38     1216  8
bugs       0     2     0        0     2      64    0
pcnc       1     1     0        0     2      64    0
pathogen   1     0     0        0     1      32    0
tc         5     5     0        3     10     320   0
gold       2     0     0        0     2      64    0
fishgen    0     1     0        0     1      32    0
neuro-hsc  8     6     0        0     14     448   0
cup-ecs    0     2     0        2     2      64    4
tid        0     1     0        0     1      32    2
biocomp    0     1     0        0     1      32    1
chakra     1     0     0        0     1      32    1
pna        0     0     1        0     1      32    0
totals:    19    28    1        14    48     1536  8
```

```
vanilla@hopper:~ $ qgrok
queues     free  busy  offline  jobs  nodes  CPUs  GPUs
-----      ----- ----- -----    ----- ----- ----- -----
general    1     9     0        7     10    320   0
debug      2     0     0        0     2     64    0
condo      18    19    1        7     38    1216  8
bugs       0     2     0        0     2     64    0
pcnc       1     1     0        0     2     6
pathogen   1     0     0        0     1
tc         5     5     0        3     10    3
gold       2     0     0        0     2     6
fishgen    0     1     0        0     1
neuro-hsc  8     6     0        0     14
cup-ecs    0     2     0        2     2
tid        0     1     0        0     1     32
biocomp    0     1     0        0     1
chakra     1     0     0        0     1
pna        0     0     1        0     1     3
totals:    19    28    1        14    48    1
```

## Private partitions

- Reserved for use by the purchaser.
- Request access by emailing support@carc.unm.edu and CC the partition owner.

```
mfricke@hopper:~ $ qgrok
queues     free  busy  offline  jobs  nodes  CPUs  GPUs
-----      ----- ----- -----    ----- ----- ----- -----
general    1     9     0        7     10    320   0
debug      2     0     0        0     2     64    0
condo      18    19    1        7     38    1216  8
bugs       0     2     0        0     2     64    0
pcnc       1     1     0        0     2     64
pathogen   1     0     0        0     1
tc         5     5     0        3     10    32
gold       2     0     0        0     2     6
fishgen    0     1     0        0     1
neuro-hsc  8     6     0        0     14
cup-ecs    0     2     0        2     2
tid        0     1     0        0     1     32
biocomp    0     1     0        0     1
chakra     1     0     0        0     1
pna        0     0     1        0     1     3
totals:    19    28    1        14    48    1
```

**Condo "scavenger" partition**

- Allows you to use compute nodes purchased by another group that are currently idle.
- May be interrupted at any time if the owners start to use it.

```
[vanilla@hopper ~]$ quotas
Home Directory (/users/vanilla):
quota: Cannot resolve mountpoint path /root/.spack: Permission denied
Disk quotas for user vanilla (uid 659):
    Filesystem  space  quota  limit  grace  files  quota  limit  grace
chama:/home/homes
              1527M   100G   200G         14913  4295m  4295m
---------------------------
Centerwide user scratch (/carc/scratch/users/mfricke)

Quota information for storage pool Default (ID: 1):

     user/group     ||          size          ||    chunk files
    name      |  id  ||    used     |    hard    ||  used    |  hard
--------------|------||------------|------------||---------|---------
      mfricke|  1512||  592.71 GiB | 1024.00 GiB ||    32784|unlimited

Centerwide scratch quota for project mfricke2016174 (/carc/scratch/projects/mfricke2016174)

Quota information for storage pool Default (ID: 1):
     user/group     ||          size          ||    chunk files
    name      |  id  ||    used     |    hard    ||  used    |  hard
--------------|------||------------|------------||---------|---------
mfricke2016174|2016142||  190.97 GiB| 1024.00 GiB||    23704|unlimited
```

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

sinfo reports information about partitions

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

The debug queues are intended for testing your programs.

And for interactive jobs.

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

Name

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

You can run a “job” for up to 4 hrs.

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

There are two nodes in this partition.

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

The names of the nodes in the partition

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

The names of the nodes in the partition

```
[vanilla@hopper ~]$ sinfo --partition general
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
general*     up 2-00:00:00      9  alloc hopper[001-009]
general*     up 2-00:00:00      1   idle hopper010
```

Hopper001 through 009 are running jobs.

Hopper010 is waiting to be used.

```
[vanilla@hopper ~]$ hostname
hopper
[vanilla@hopper ~]$
```

Running on the Head Node.

The head node’s name is “hopper”.

```
[vanilla@hopper ~]$ hostname
hopper
[vanilla@hopper ~]$ man hostname
```

```
[vanilla@hopper ~]$ hostname
hopper
[vanilla@hopper ~]$ man hostname
(‘q’ to quit)

[vanilla@hopper ~]$ man man
(‘q’ to quit)
```

## [vanilla@hopper ~]$ man sinfo

```
sinfo(1)                    Slurm Commands                    sinfo(1)

NAME
     sinfo - View information about Slurm nodes and partitions.

SYNOPSIS
     sinfo [OPTIONS...]

DESCRIPTION
     sinfo is used to view partition and node information for a system running Slurm

OPTIONS
     -a, --all
          Display  information  about  all partitions. This causes information to be displayed about partitions that are
configured as hidden and partitions that are unavailable to the user's group.
```

```
[vanilla@hopper ~]$ sinfo --all
```

```
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
general*     up 2-00:00:00      9  alloc hopper[001-009]
general*     up 2-00:00:00      1   idle hopper010
debug        up    4:00:00      2   idle hopper[011-012]
condo        up 2-00:00:00      1  down* hopper045
condo        up 2-00:00:00      3    mix hopper[018-020]
condo        up 2-00:00:00     16  alloc hopper[013-015,028-036,049-052]
condo        up 2-00:00:00     18   idle hopper[016-017,021-027,037-044,053]
bugs         up 7-00:00:00      2  alloc hopper[013-014]
pcnc         up 7-00:00:00      1  alloc hopper015
pcnc         up 7-00:00:00      1   idle hopper016
pathogen     up 7-00:00:00      1   idle hopper017
tc           up 7-00:00:00      3    mix hopper[018-020]
tc           up 7-00:00:00      2  alloc hopper[029-030]
tc           up 7-00:00:00      5   idle hopper[021-025]
gold         up 7-00:00:00      2   idle hopper[026-027]
fishgen      up 7-00:00:00      1  alloc hopper028
neuro-hsc    up 7-00:00:00      6  alloc hopper[031-036]
neuro-hsc    up 7-00:00:00      8   idle hopper[037-044]
cup-ecs      up 7-00:00:00      2  alloc hopper[049-050]
tid          up 7-00:00:00      1  alloc hopper051
biocomp      up 7-00:00:00      1  alloc hopper052
chakra       up 7-00:00:00      1   idle hopper053
pna          up 7-00:00:00      1  down* hopper045
```

```
[vanilla@hopper ~]$ srun --partition debug hostname
```

Tell slurm to run a program on a compute node…

```
[vanilla@hopper ~]$ srun --partition debug hostname
```

Run the program on a compute node in the debug partition.

```
[vanilla@hopper ~]$ srun --partition debug hostname
```

The program to run.

```
[vanilla@hopper ~]$ srun --partition debug hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest
project
You have not been allocated GPUs. To request GPUs, use the -G option in your
submission script.
hopper011
```

```
[vanilla@hopper ~]$ squeue
```

```
[vanilla@hopper ~]$ squeue
  JOBID PARTITION     NAME     USER ST       TIM
  4314    general      PRE erowland PD      0:00
  4315    general      PRE erowland PD      0:00
  4317    general      PRE erowland PD      0:00
  4318    general      PRE erowland PD      0:00          2 (QOSMaxCpuPerUserLimit)
               4319    general      PRE erowland PD      0:00       2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
                                                                    2 (QOSMaxCpuPerUserLimit)
               4337    general      PRE erowland PD      0:00       2 (QOSMaxCpuPerUserLimit)
```

**PD means programs that are waiting their turn.**

**Shows you what the slurm scheduler is doing right now.**

**Here we can see that user ’erowland’ has a lot of programs waiting to run.**

```
[vanilla@hopper ~]$ squeue
  JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             4314   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
             4315   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
             4317   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
             4318   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
                                                                 2 (QOSMaxCpuPerUserLimit)
```

**The reason these jobs are not running is that ‘erowland’ is already using the maximum number of CPUs they are allowed.**

```
[vanilla@hopper ~]$ squeue -t R --all
         JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          4405     condo    2ndMA  mfricke  R 1-07:48:30      6 hopper[031-036]
          5208     condo       NN      kgu  R    5:48:49      1 hopper015
          5210     condo       NN      kgu  R    6:30:13      1 hopper014
          5209     condo       NN      kgu  R    6:31:13      1 hopper013
          5206     condo       NN      kgu  R    6:32:13      1 hopper051
          5207     condo       NN      kgu  R    6:32:13      1 hopper052
          5205     condo       NN      kgu  R    6:32:43      1 hopper028
          4595   cup-ecs golConfi aalasand  R 2-06:51:59      1 hopper050
          4594   cup-ecs golConfi aalasand  R 2-06:52:03      1 hopper049
          5120   general jupyterh   jacobm  R   11:45:47      1 hopper007
          4313   general      PRE erowland  R    1:17:29      2 hopper[003-004]
          5111   general    1stMA  mfricke  R   11:15:28      2 hopper[005-006]
          5025   general      c2n    jxzuo  R       1:50      1 hopper001
          5024   general      c2n    jxzuo  R      31:28      1 hopper002
          5203   general       NN      kgu  R    6:37:50      1 hopper009
          5201   general       NN      kgu  R    6:38:14      1 hopper008
          4390        tc UCsTpCyd lepluart  R 2-15:18:18      3 hopper[018-020]
          5198        tc       NN      kgu  R    6:40:19      1 hopper030
          5196        tc       NN      kgu  R    6:40:31      1 hopper029
```

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest project
You have not been allocated GPUs. To request GPUs, use the -G option in your submission
script.
hopper011
hopper011
```

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest project
You have not been allocated GPUs. To request GPUs, use the -G option in your submission
script.
hopper011
hopper011
```

**You ran two copies of your program.**

**ntasks is the number of copies to run.**

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 8 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest project
hopper011
hopper011
hopper011
You have not been allocated GPUs. To request GPUs, use the -G option in your submission
script.
hopper011
hopper011
hopper011
hopper011
hopper011
```

**You ran eight copies of your program.**

**ntasks is the number of copies to run.**

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 8 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest project
hopper011
hopper011
hopper011
You have not been allocated GPUs. To request GPUs, use the -G option in your submission
script.
hopper011
hopper011
hopper011
hopper011
hopper011
```

**By default, each task (copy of your program) is allowed to use one CPU.**

**Many programs are able to use more than one CPU at a time.**

```
[vanilla@hopper ~]$ srun --partition debug --ntasks 2 --cpus-per-task 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest project
You have not been allocated GPUs. To request GPUs, use the -G option in your submission script.
hopper011
hopper011
```

**Here we are telling SLURM to run 2 copies of our program and let each copy of our program use 2 CPUs.**

```
[vanilla@hopper ~]$ srun --partition debug --nodes 2 --ntasks-per-node 4 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest project
hopper012
You have not been allocated GPUs. To request GPUs, use the -G option in your submission script.
hopper012
hopper011
hopper011
hopper012
hopper012
hopper011
hopper011
```

**Here we are telling SLURM to run 4 copies of our program on 2 different compute nodes.**

**This is useful when our programs need a bigger share of the compute node.**

```
[vanilla@hopper ~]$ srun --partition debug --nodes 2
--ntasks-per-node 2 --cpus-per-task 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest
project
hopper011
You have not been allocated GPUs. To request GPUs, use the -G option in your
submission script.
hopper011
hopper012
hopper012
```

**And we can combine all three.**

```
[vanilla@hopper ~]$ srun --partition debug --mem 4G
--nodes 2 --ntasks-per-node 2 --cpus-per-task 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest
project
hopper012
hopper012
You have not been all                                                          r
submission script.
hopper011
Hopper011
```

**And we can specify how much memory we want.**

**--mem 4G means give me 4 gigabytes of memory per node.**

```
[vanilla@hopper ~]$ srun --partition debug --mem 4G
--nodes 2 --ntasks-per-node 2 --cpus-per-task 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest
project
hopper012
hopper012
You have not been allo                                                          r
submission script.
hopper011
Hopper011
```

**Why does all this matter?**

**The purpose of SLURM is to provide you the hardware your programs need.**

**So you have to understand what those requirements are really well.**

```
[vanilla@hopper ~]$ srun --partition debug --mem 4G
--nodes 2 --ntasks-per-node 2 --cpus-per-task 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest
project
hopper012
hopper012
You have not been all                                                    r
submission script.
hopper011
Hopper011
```

1) **Can my program use multiple CPUs?**
2) **How much memory does my program need?**
3) **Can my program use multiple compute nodes (MPI*, GNU Parallel*)?**
4) **Can my program use GPUs?**

```
[vanilla@hopper ~]$ srun --partition debug --mem 4G
--nodes 2 --ntasks-per-node 2 --cpus-per-task 2 hostname
srun: Account not specified in script or ~/.default_slurm_account, using latest
project
hopper012
hopper012
You have not been alloca                                                        r
submission script.
hopper011
Hopper011
```

**This command is getting pretty long.**

**We can use shell scripts to automate all this in batch mode.**

## Interactive vs Batch Mode

### Interactive Mode

- Everything so far has been interactive. You request hardware, run your program, and get the output on your screen right away.

### Batch Mode

- Most programs at an HPC center are run in “batch” mode.
- Batch mode means we write a shell script that the SLURM scheduler runs for us. The script requests hardware just like we did with salloc and then runs the commands in the script.
- Whatever would have been written to the screen is saved to a file instead.

```
[vanilla@hopper ~]$ git clone https://lobogit.unm.edu/CARC/workshops.git
Cloning into 'workshops'...
remote: Enumerating objects: 132, done.
remote: Counting objects: 100% (75/75), done.
remote: Compressing objects: 100% (43/43), done.
remote: Total 132 (delta 33), reused 74 (delta 32), pack-reused 57
Receiving objects: 100% (132/132), 57.58 KiB | 3.60 MiB/s, done.
Resolving deltas: 100% (51/51), done.
```

**Rather than make you write shell scripts lets just download some we wrote for this workshop…**

```
[vanilla@hopper ~]$ tree workshops
workshops/
├── intro_workshop
│   ├── code
│   │   ├── calcPiMPI.py
│   │   ├── calcPiSerial.py
│   │   └── vecadd
│   │       ├── Makefile
│   │       ├── vecadd_gpu.cu
│   │       ├── vecadd_mpi_cpu
│   │       ├── vecadd_mpi_cpu.c
│   │       ├── vecaddmpi_cpu.sh
│   │       └── vecadd_mpi_gpu.c
│   ├── data
│   │   ├── H2O.gjf
│   │   └── step_sizes.txt
│   └── slurm
│       ├── calc_pi_array.sh
│       ├── calc_pi_mpi.sh
│       ├── calc_pi_parallel.sh
│       ├── calc_pi_serial.sh
│       ├── gaussian.sh
│       ├── hostname_mpi.sh
│       ├── vecadd_hopper.sh
│       ├── vecadd_xena.sh
│       ├── workshop_example2.sh
│       ├── workshop_example3.sh
│       └── workshop_example.sh
└── README.md
```

**Run tree to see how the workshops directories are organized…**

```
[vanilla@hopper ~]$ tree workshops
workshops/
├── intro_workshop
│   ├── code
│   │   ├── calcPiMPI.py
│   │   ├── calcPiSerial.py
│   │   └── vecadd
│   │       ├── Makefile
│   │       ├── vecadd_gpu.cu
│   │       ├── vecadd_mpi_cpu
│   │       ├── vecadd_mpi_cpu.c
│   │       ├── vecaddmpi_cpu.sh
│   │       └── vecadd_mpi_gpu.c
│   ├── data
│   │   ├── H2O.gjf
│   │   └── step_sizes.txt
│   └── slurm
│       ├── calc_pi_array.sh
│       ├── calc_pi_mpi.sh
│       ├── calc_pi_parallel.sh
│       ├── calc_pi_serial.sh
│       ├── gaussian.sh
│       ├── hostname_mpi.sh
│       ├── vecadd_hopper.sh
│       ├── vecadd_xena.sh
│       ├── workshop_example2.sh
│       ├── workshop_example3.sh
│       └── workshop_example.sh
└── README.md
```

**Run tree to see how the workshops directories are organized…**

**The workshop files are divided into “code”, “slurm”, and “data” directories.**

```
[vanilla@hopper intro_workshop]$ pwd
/users/vanilla/workshops/intro_workshop
[vanilla@hopper intro_workshop]$ cat slurm/workshop_example1.sh
#!/bin/bash
#SBATCH --partition debug
#SBATCH --ntasks 4
#SBATCH --time 00:05:00
#SBATCH --job-name ws_example
#SBATCH --mail-user your_username@unm.edu
#SBATCH --mail-type ALL

srun hostname
```

**Let’s take a look at the workshop_example.sh script in the slurm directory…**

```
[vanilla@hopper intro_workshop]$ sbatch slurm/workshop_example1.sh
sbatch: Account not specified in script or ~/.default_slurm_account, using latest project
Submitted batch job 5252
[vanilla@hopper intro_workshop]$
```

**We submit our slurm shell script with the sbatch command.**

```
[vanilla@hopper intro_workshop]$ sbatch slurm/workshop_example1.sh
sbatch: Account not specified in script or ~/.default_slurm_account, using latest project
Submitted batch job 5252
[vanilla@hopper intro_workshop]$
```

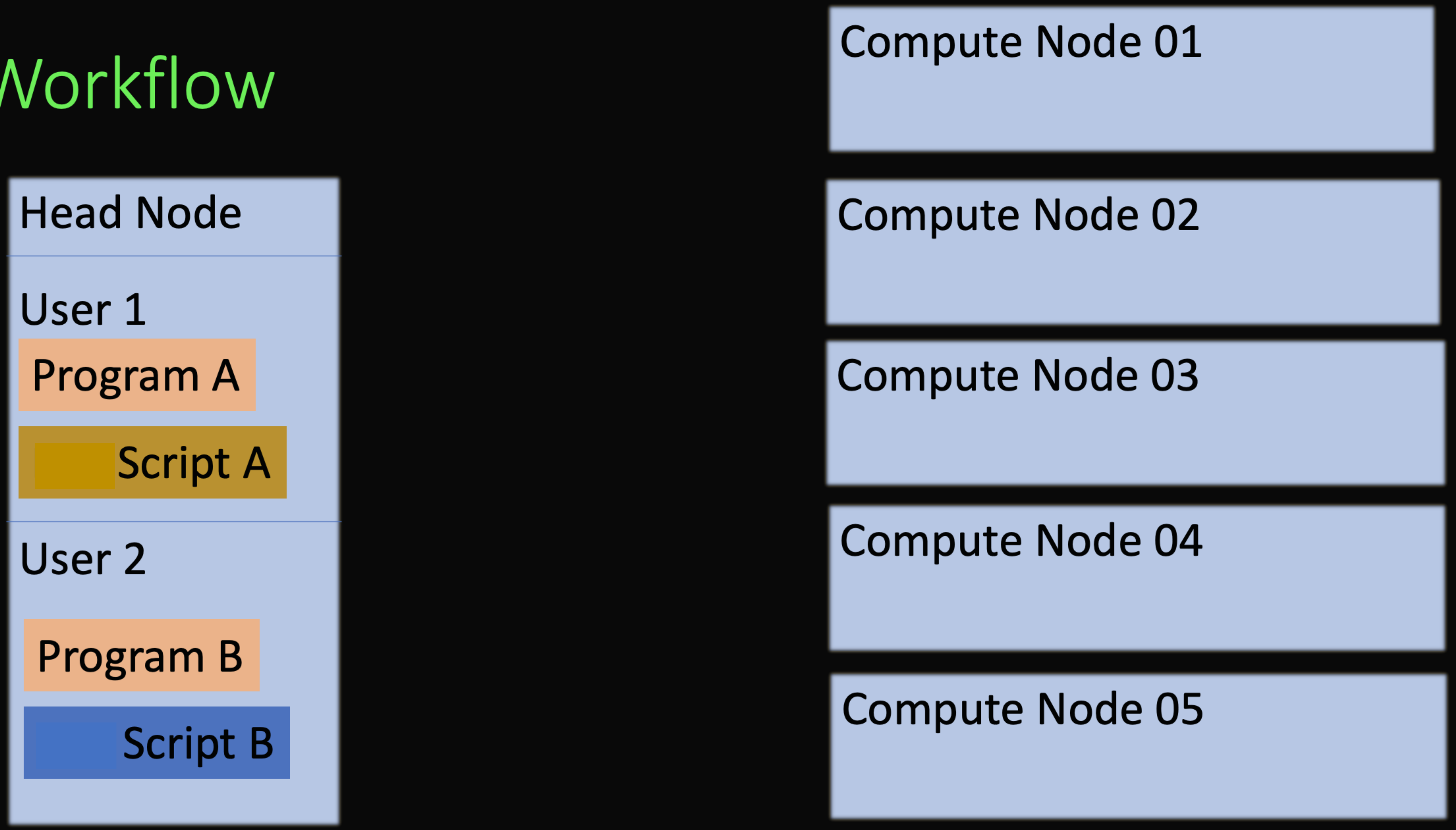
**We submit our slurm shell script with the sbatch command.**

**Notice that the only output we get is a job id.**

**This indicates that the script was successfully sent to the scheduler.**

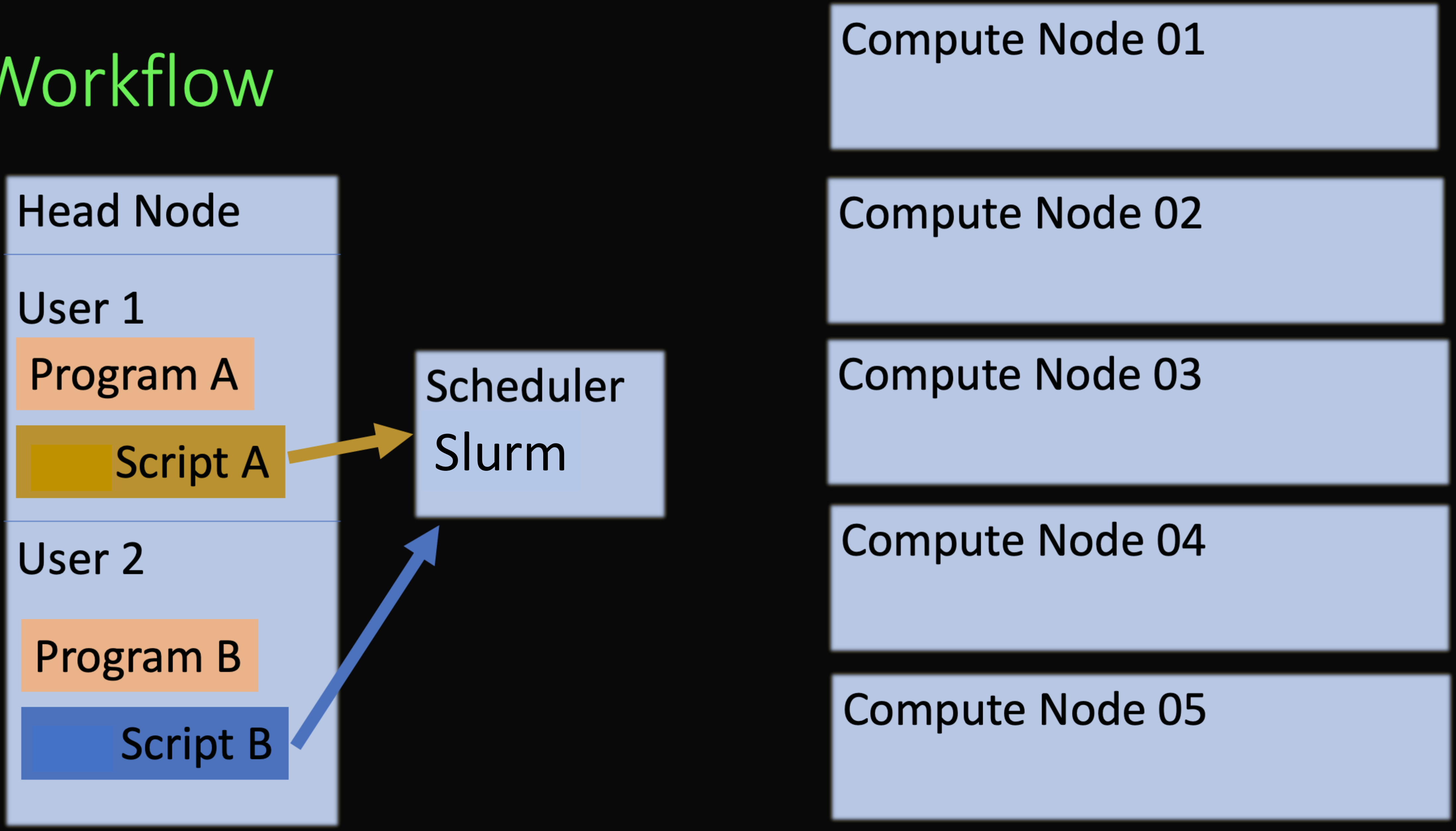
**The commands in the script will run as soon as the hardware requested is available.**

## Workflow



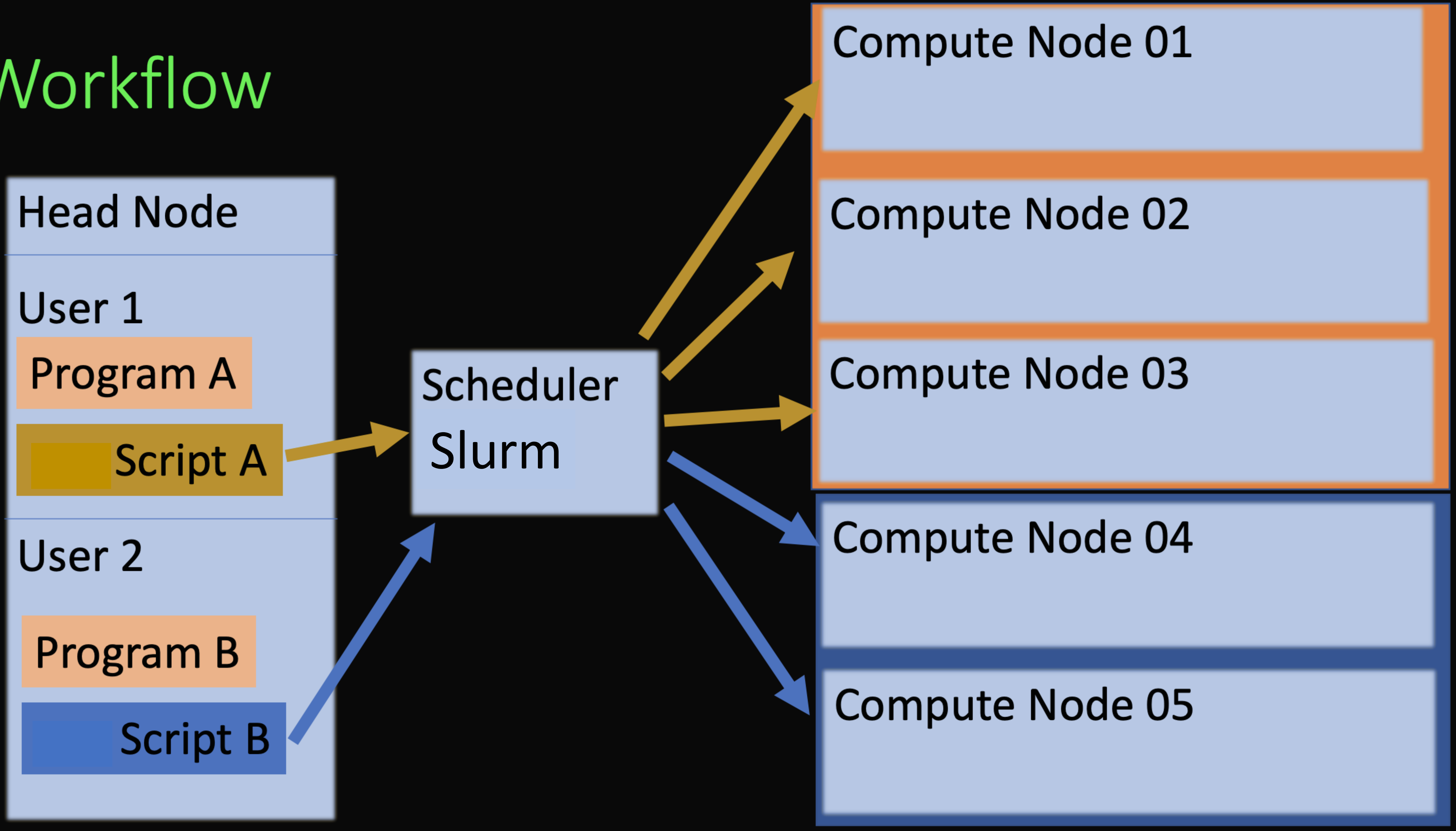
Shared filesystems – All nodes can access the same programs and write output

# Workflow



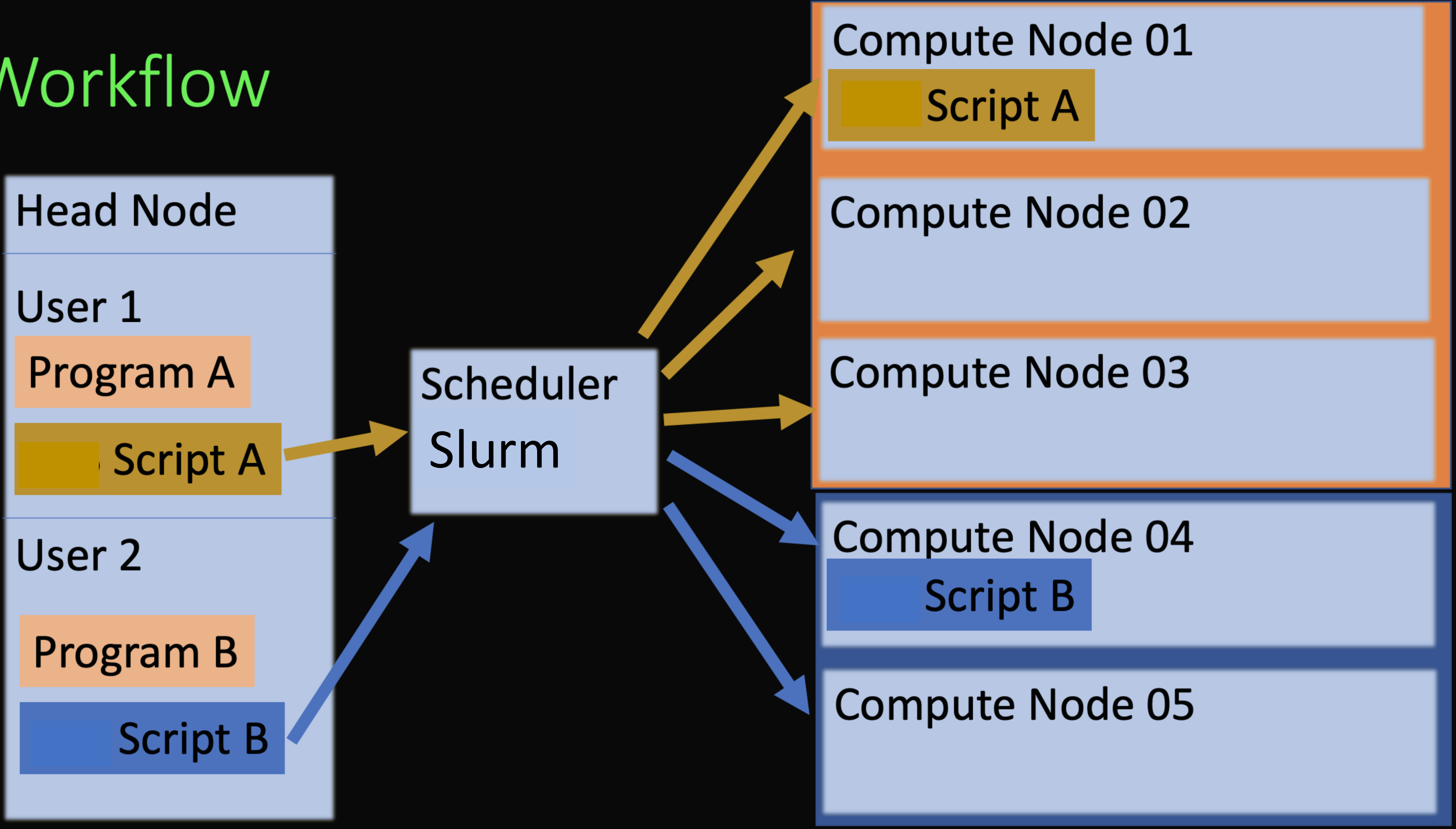
Shared filesystems – All nodes can access the same programs and write output

## Workflow



Shared filesystems – All nodes can access the same programs and write output

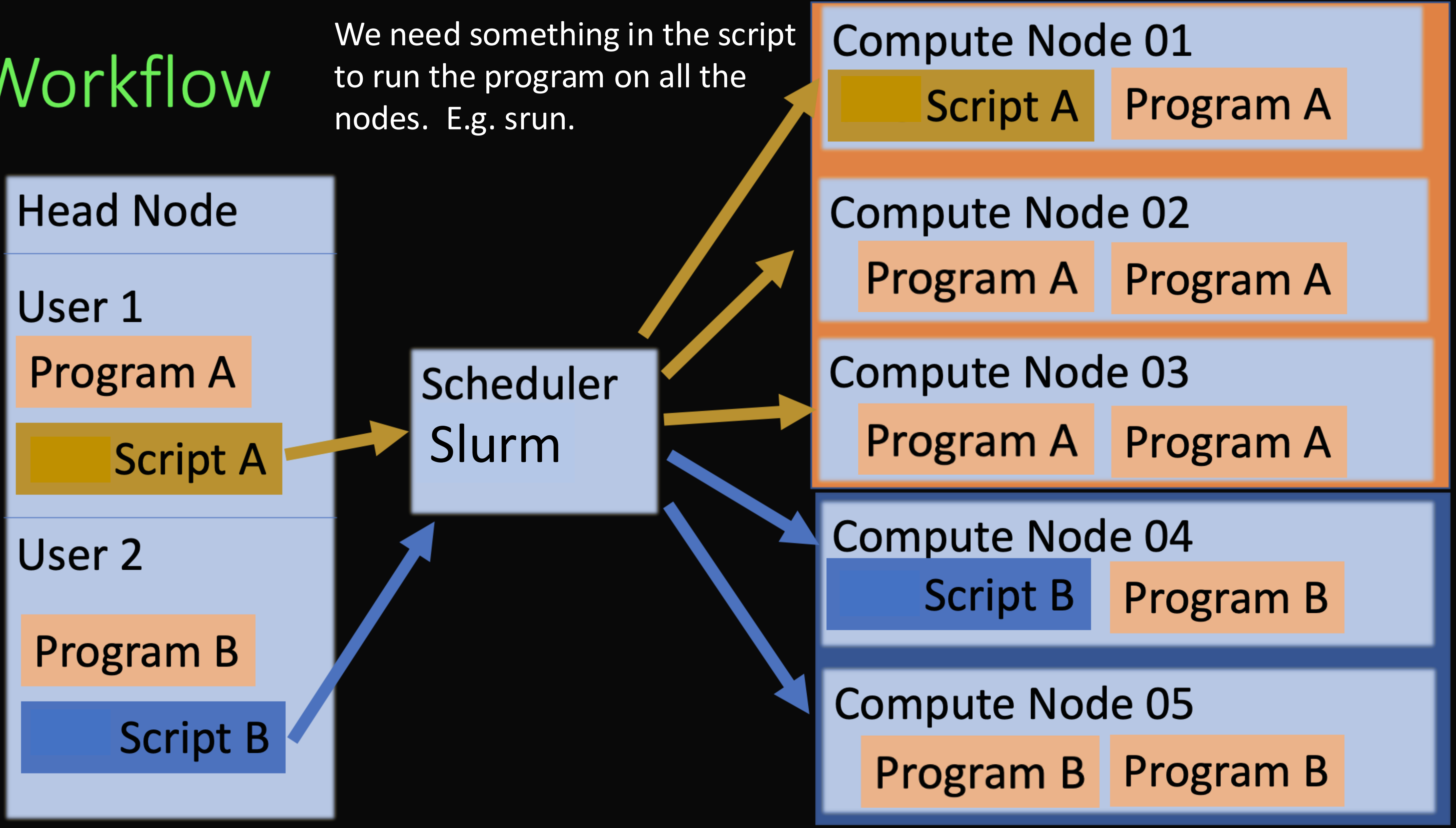
# Workflow



Shared filesystems – All nodes can access the same programs and write output

## Workflow

We need something in the script to run the program on all the nodes. E.g. srun.



Shared filesystems – All nodes can access the same programs and write output

```
[vanilla@hopper intro_workshop]$ ls
code  data  pbs  slurm  slurm-5252.out
```

The hostname command is very fast so everyone's job should finish in a few seconds.

When it is finished you will have a new file named slurm-{your job id}.out.

```
[vanilla@hopper intro_workshop]$ ls
code  data  pbs  slurm  slurm-5252.out
```

**When it is finished you will have a new file named slurm-{your job id}.out.**

```
[vanilla@hopper intro_workshop]$ cat slurm-5252.out
hopper011
```

```
[vanilla@hopper intro_workshop]$ module load miniconda3
[vanilla@hopper intro_workshop]$ conda create -n numpy numpy
```

Wait a while – introduce yourselves to your neighbor…

Conda allows you to install software into your home directory. In this case we need the numerical python libraries for calcPiSerial.py

**Let's experiment with a program that does slightly more than print the hostname.**

```
[vanilla@hopper intro_workshop]$source activate numpy
[vanilla@hopper intro_workshop]$srun --partition debug python code/calcPiSerial.py 10
srun: Using account 2016199 from ~/.default_slurm_account
You have not been allocated GPUs. To request GPUs, use the -G option in your submission
script.
Pi = 3.14242598500109870940, (Diff=0.00083333141130559341) (calculated in 0.000005 secs
with 10 steps)
```

**Activate the numpy environment and**
**Run calcPiSerial.py on a compute node.**

**For our example program the more steps it takes the more accurate it is, but the longer it takes.**

```
[vanilla@hopper intro_workshop]$ cat slurm/calc_pi_serial.sh
#!/bin/bash
#SBATCH --partition debug
#SBATCH --ntasks 1
#SBATCH --time 00:05:00
#SBATCH --job-name calc_pi_serial
#SBATCH --mail-user your_username@unm.edu
#SBATCH --mail-type ALL

module load miniconda3
source activate numpy

cd $SLURM_SUBMIT_DIR
python code/calcPiSerial.py 1000000000
[vanilla@hopper intro_workshop]$
```

```
[vanilla@hopper intro_workshop]$ source deactivate
[vanilla@hopper intro_workshop]$ sbatch slurm/calc_pi_serial.sh
 sbatch: Using account 2016199 from ~/.default_slurm_account
Submitted batch job 5263
vanilla@hopper:~/workshops/intro_workshop$ squeue --me
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
5263     debug calc_pi_  vanilla  R       0:44      1 hopper011
```

**Edit slurm/calc_pi_serial.sh.**
**Change the email address to your address and submit the script.**

**Then enter squeue --me to see the job status.**

**Take a look at the job output.**

## Install the tools we need

- Tensorflow – Machine Learning from Google
- Scikit-learn – Open Source (was a Google summer intern project)
- Ipykernel – So we can use our python libraries in a Jupyter Notebook
- Matplotlib and Seaborn – For plotting and graphics
- Pandas – Data Science
- Numpy – Numerical libraries

And lots of other things will be installed…

```
[vanilla@hopper intro_workshop]$ conda create --name
machine_learning matplotlib ipykernel scikit-learn
seaborn tensorflow-gpu=2.4.1 tqdm --channel defaults
<snip>
  zipp               pkgs/main/linux-64::zipp-3.17.0-py39h06a4308_0
  zlib               pkgs/main/linux-64::zlib-1.2.13-h5eee18b_1
  zstd               pkgs/main/linux-64::zstd-1.5.5-hc292b87_2

Proceed ([y]/n)?
```

Don’t forget to enter “y” here

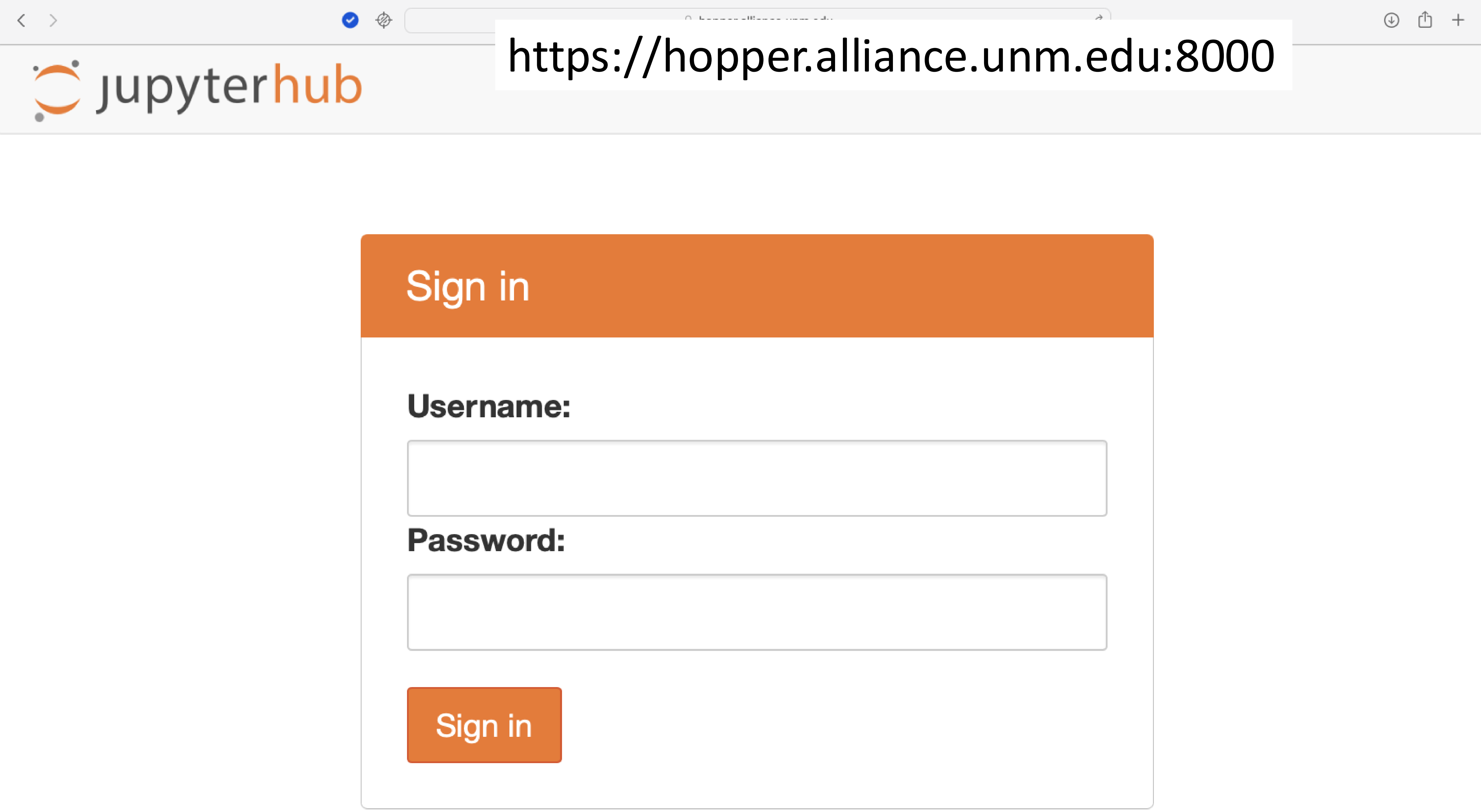
## Using conda environments

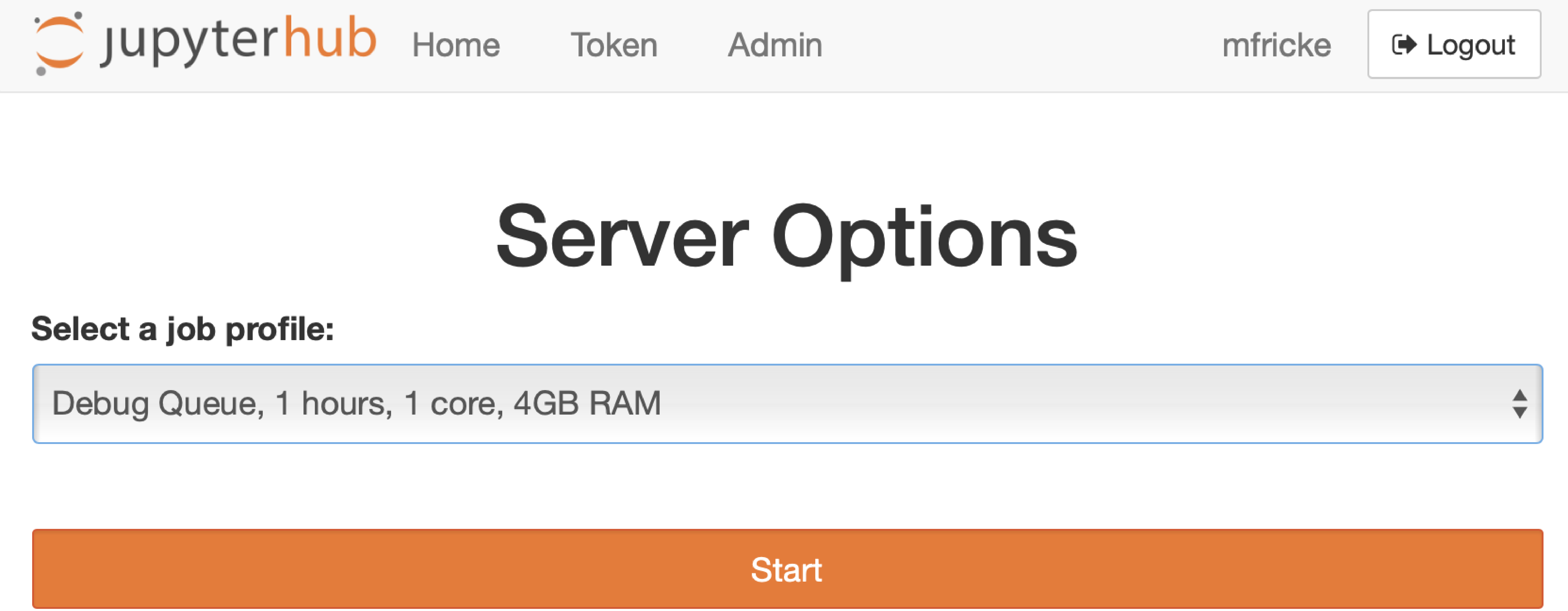
- Conda create
- Conda delete
- conda info --envs

Conda activate {env name}

```
conda create --name machine_learning matplotlib
ipykernel scikit-learn seaborn tensorflow-
gpu=2.4.1 tqdm --channel defaults
```

https://hopper.alliance.unm.edu:8000




jupyterhub Home Token Admin mfricke Logout

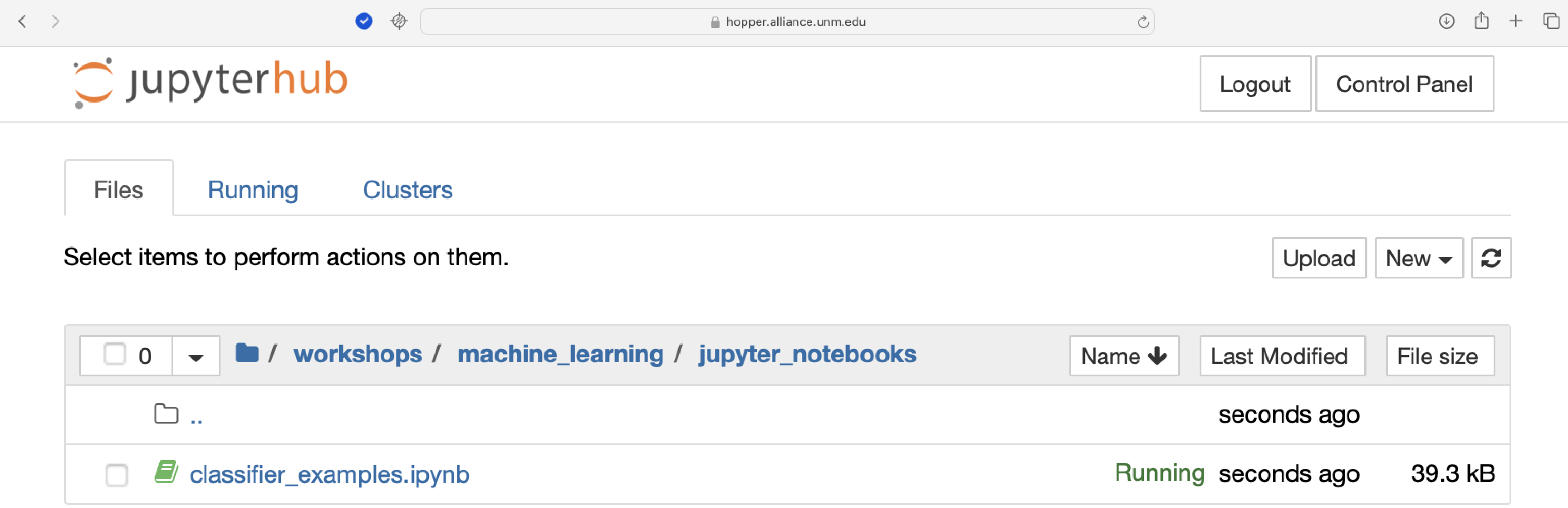
Server Options

Select a job profile:

Debug Queue, 1 hours, 1 core, 4GB RAM

Start

You might not see this the first time.

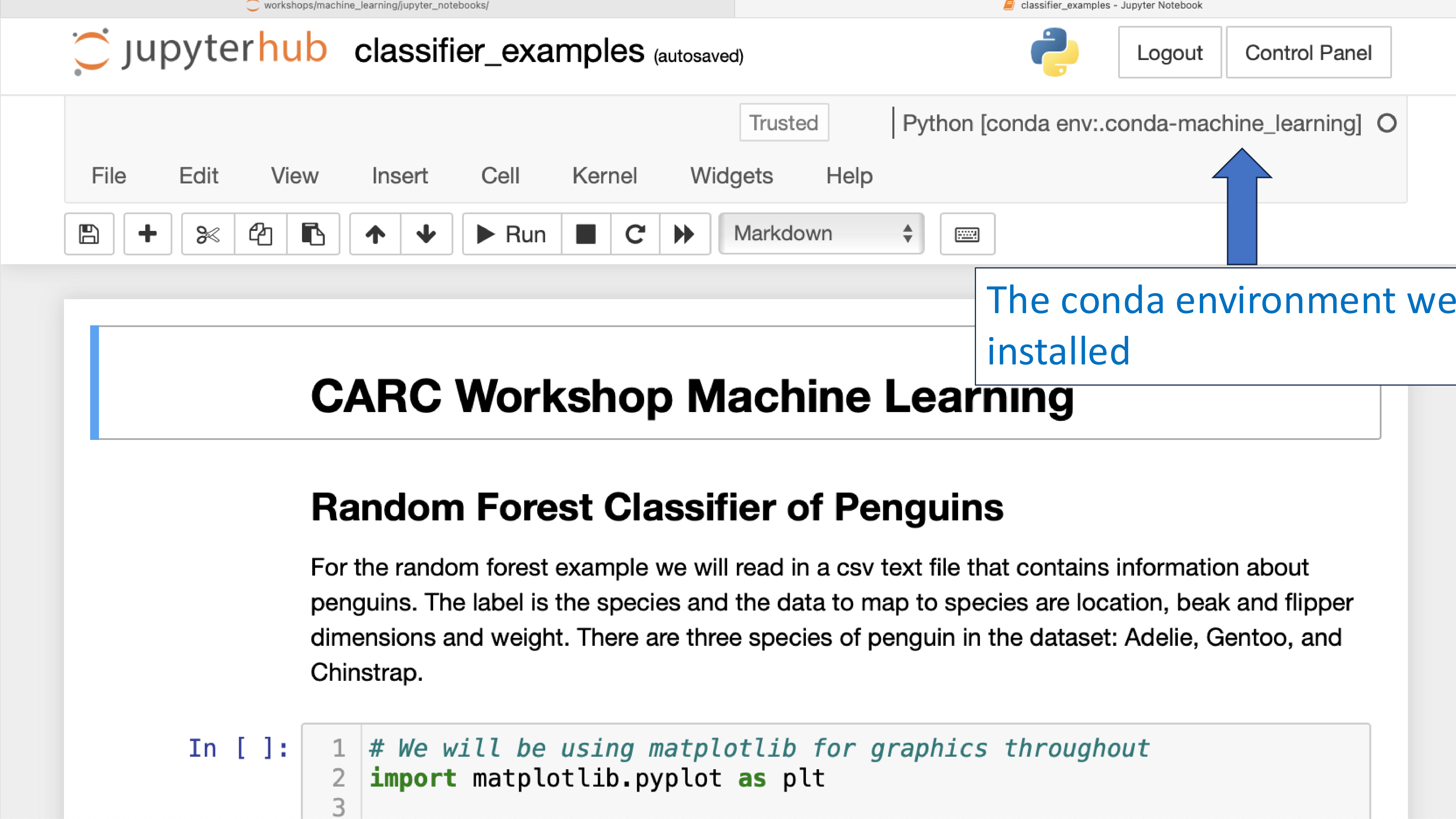

hopper.alliance.unm.edu

Select items to perform actions on them.

/ workshops / machine_learning / jupyter_notebooks

| | | | |
|---|---|---|---|
| .. | | seconds ago | |
| classifier_examples.ipynb | Running | seconds ago | 39.3 kB |

Jupyter Notebook


workshops/machine_learning/jupyter_notebooks/
classifier_examples - Jupyter Notebook
jupyterhub
classifier_examples (autosaved)
Logout
Control Panel
Trusted
Python [conda env:.conda-machine_learning]
File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Run
Markdown

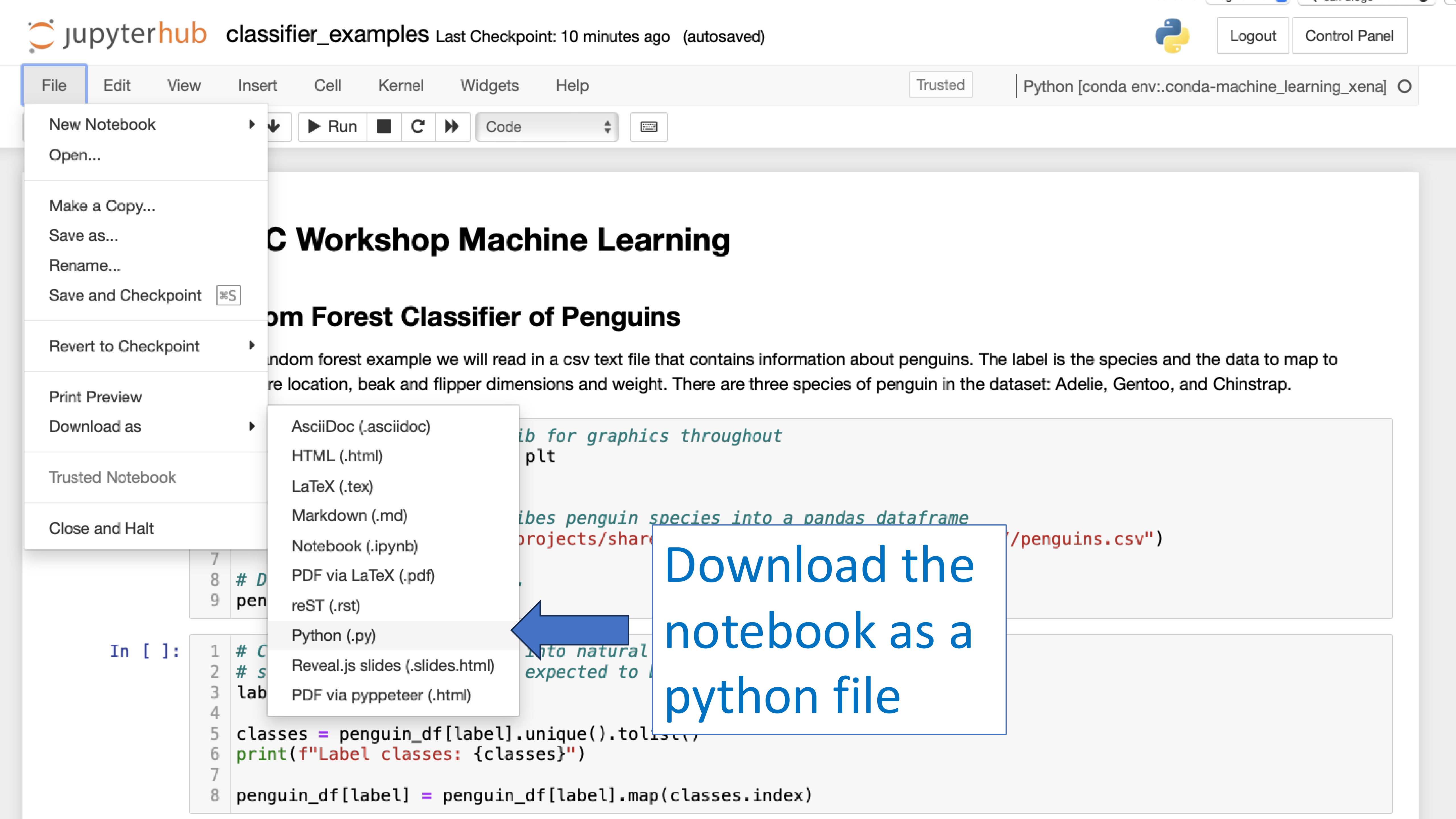
The conda environment we installed

# CARC Workshop Machine Learning

## Random Forest Classifier of Penguins

For the random forest example we will read in a csv text file that contains information about penguins. The label is the species and the data to map to species are location, beak and flipper dimensions and weight. There are three species of penguin in the dataset: Adelie, Gentoo, and Chinstrap.

```
In [ ]:
# We will be using matplotlib for graphics throughout
import matplotlib.pyplot as plt

```



# C Workshop Machine Learning

## om Forest Classifier of Penguins

ndom forest example we will read in a csv text file that contains information about penguins. The label is the species and the data to map to re location, beak and flipper dimensions and weight. There are three species of penguin in the dataset: Adelie, Gentoo, and Chinstrap.

```
ib for graphics throughout
 plt

ibes penguin species into a pandas dataframe
projects/share                  /penguins.csv")

# D                              .
pen
```

In [ ]:
```
# C                    nto natural
# s                    expected to
lab

classes = penguin_df[label].unique().tolist()
print(f"Label classes: {classes}")

penguin_df[label] = penguin_df[label].map(classes.index)
```

Download the notebook as a python file

```
[vanilla@hopper machine_learning]$ sbatch slurm/ml_example_hopper.sh
sbatch: Account not specified in script or ~/.default_slurm_account, using latest project
Submitted batch job 5252

[vanilla@hopper machine_learning]$ tail –f slurm-{job ID}.out
```

```
32 by 32 by 3
[1]
Train data size:  50000
Train target size:  50000
Train data size:  26032
Train data size:  26032
100%|██████████| 50000/50000 [01:09<00:00, 723.6
 25%|██        | 6431/26032 [00:08<00:26, 726.59
```

**We can monitor the output live**

```
[vanilla@xena machine_learning]$ tail -f slurm-687248.out
<snip>
665/665 [==============================] - 3s 4ms/step - loss: 0.2996 - accuracy: 0.9135 - val_loss: 0.4952 - Epoch 00014:
val_accuracy improved from 0.86947 to 0.87267, saving model to checkpoints_best_cnn/checkpoint.weights.h5
Epoch 15/30
665/665 [==============================] - 3s 4ms/step - loss: 0.2996 - accuracy: 0.9135 - val_loss: 0.4952 - val_accuracy:
0.8727
[1587 5711 3958 2686 2723 2270 2499 1981 1039 1578]
[[1528   30   32   22    6    9   46   24   12   35]
 [  68 4617   86   75   81   19   14  105   26    8]
 [  21   38 3815   71   51   19    8   67   33   26]
 [  30   78  113 2236   23  129   25   40   74  134]
 [  27   93   47   52 2183   22   24   20   27   28]
 [  10   13   31  110   21 2021  106   13   20   39]
 [  54   29   12   35   40   91 1632    8   55   21]
 [   8   74   67   18    5   15    6 1812    4   10]
 [  42   17   26   68   24   54  155    6 1212   56]
 [  56   17   50   30   11   49   15   28   33 1306]]
[1844 5006 4279 2717 2445 2428 2031 2123 1496 1663]
```

**We can monitor the output live**

## You have learned

- how to run programs using the SLURM scheduler
- the difference between interactive and batch jobs
- how to check the status of your jobs
- how to select debug vs general SLURM partitions
- how to ask for the hardware resources you need
- you ran machine learning classifiers interactively with Jupyerhub and in batch mode