CARC Intro to Parallel Processing 1 hr version

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Version 0.1

Goals

- 1) SLURM scheduler literacy
- 2) Run programs interactively and in batch mode
- 3) MPI parallelism

- We wont cover file transfer, storage systems, module system, conda, PBS. (These are all covered in depth in the video tutorials)

Agenda

- Login and change password
- HPC Schedulers
- SLURM
- with MPI

We will have one 15 minute break. Opportunity to see the machine room.

Logging into Hopper

First login to the Linux **workstation** in front of you. “Welcome2CARC”

Use your CARC username and password.

We can help you login if you have trouble. Just raise your hand.

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…

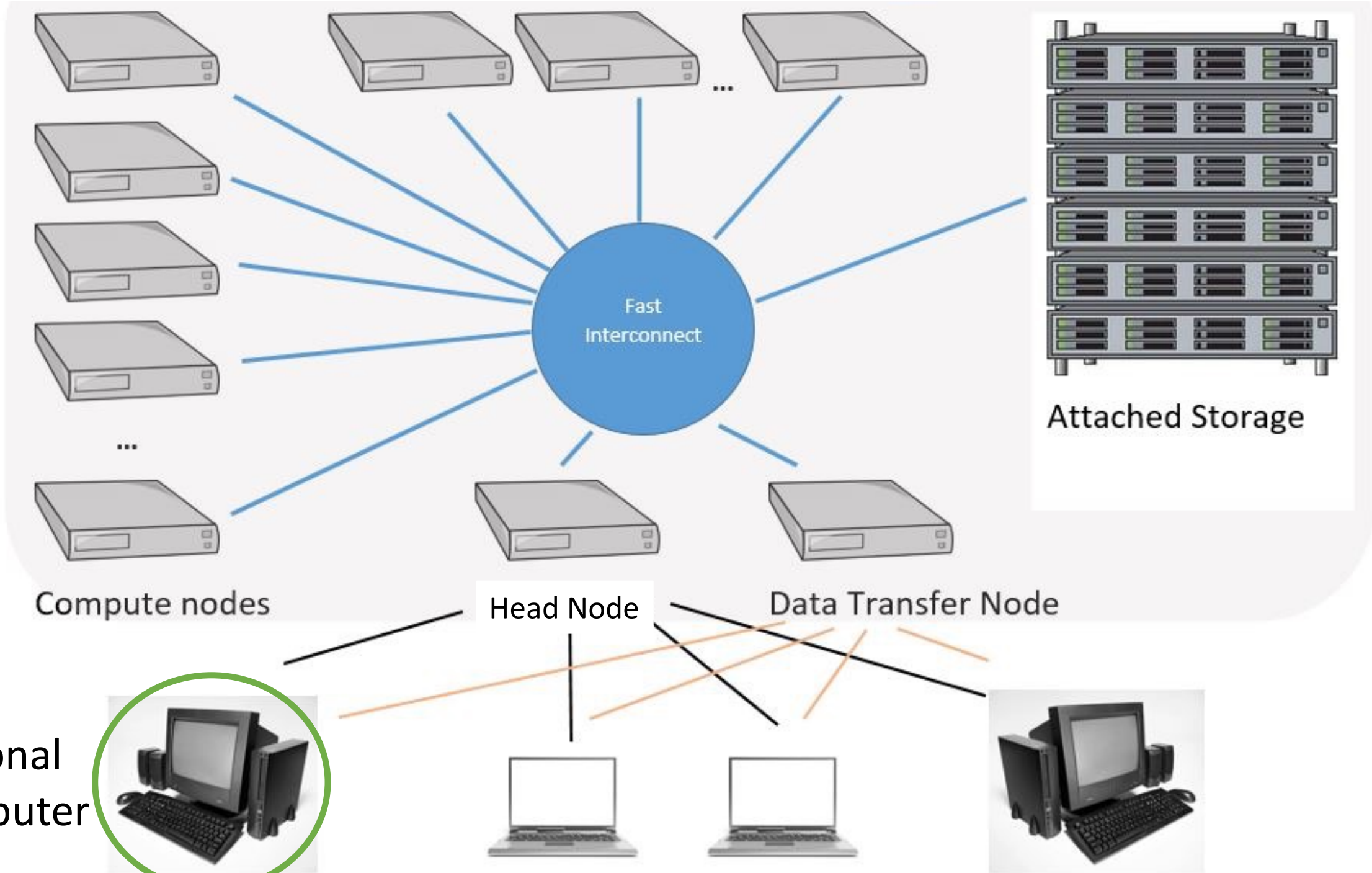
Don’t let me move on until you are able to login.

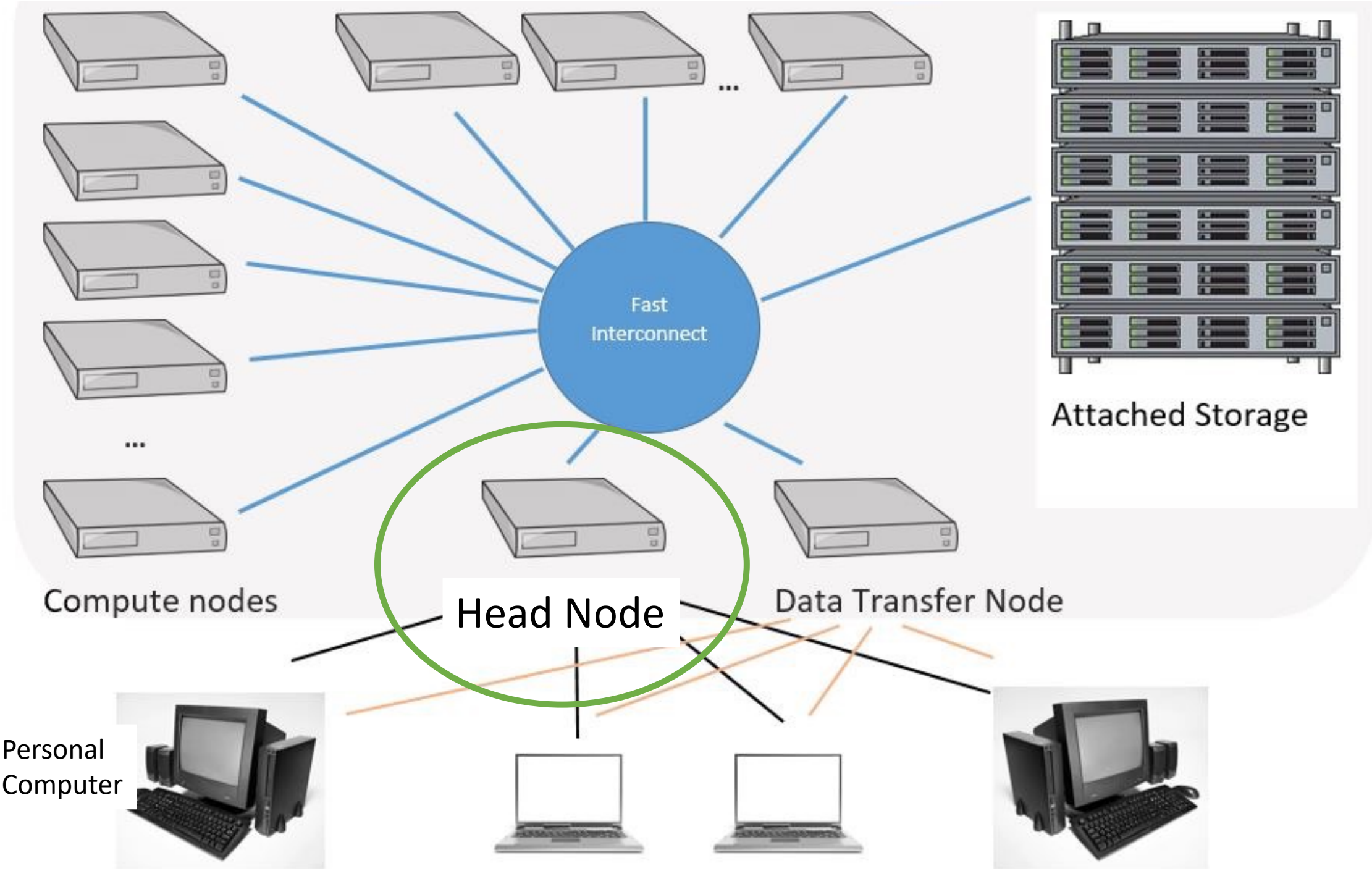
Logging into Hopper

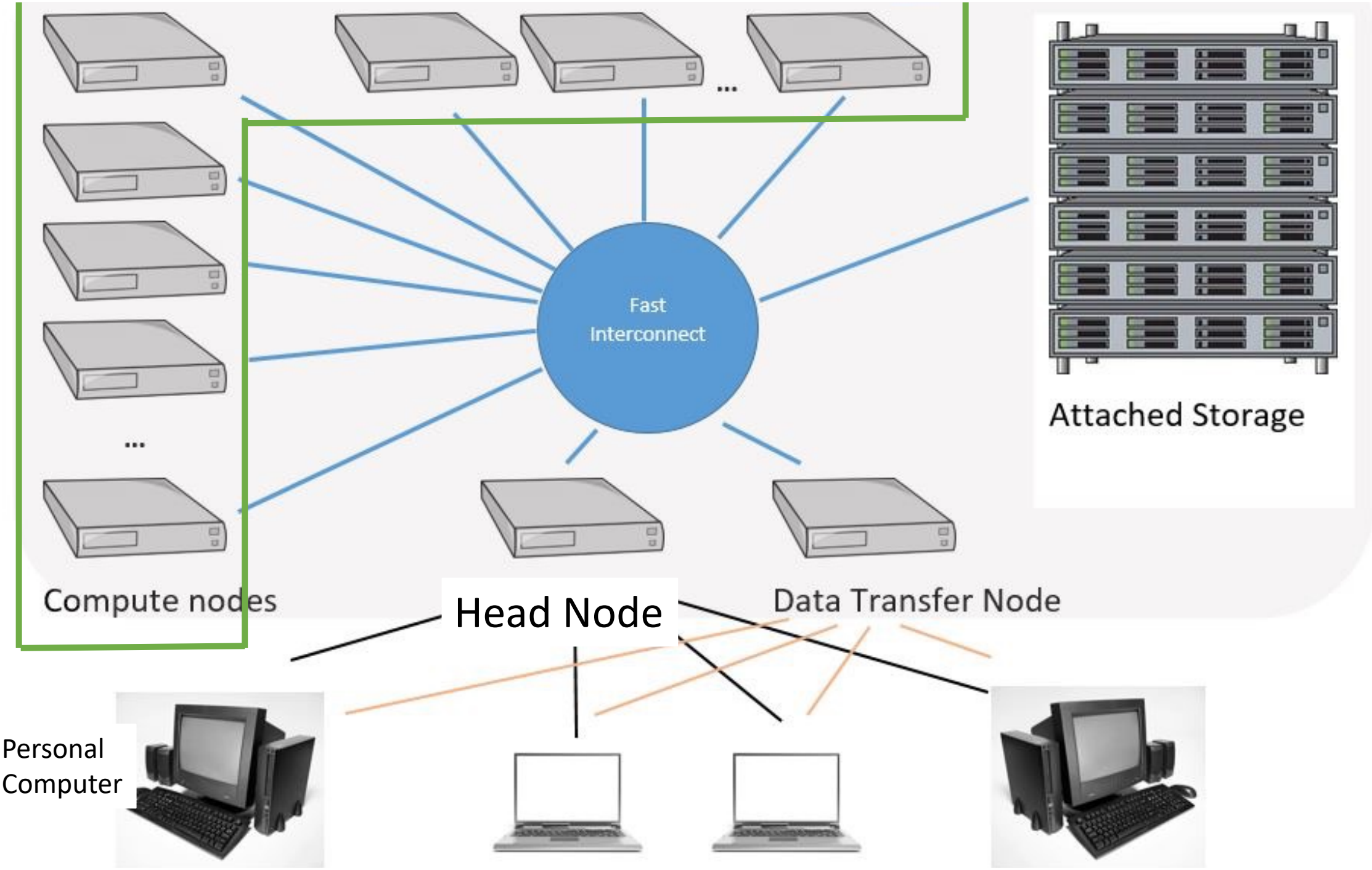
```
Welcome to Hopper

  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:~ $
```

```
[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 ~]$ 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
```


Fast
Interconnect
Attached Storage
Compute nodes
Head Node
Data Transfer Node
Personal
Computer


Fast
Interconnect
Attached Storage
Compute nodes
Head Node
Data Transfer Node
Personal
Computer


Fast
Interconnect
Attached Storage
Compute nodes
Head Node
Data Transfer Node
Personal
Computer

Technology, IT etc.

SLURM

means

Simple Linux Utility for Resource Management


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

```
[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]
```

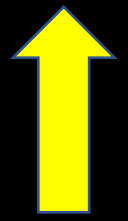
The debug queues are intended for testing your programs.

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]
```

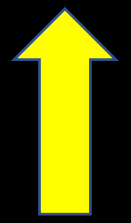
Name

```
[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.

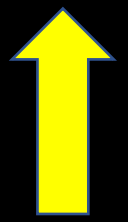
```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      2   idle hopper[011-012]
```

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 ~]$ 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.
```

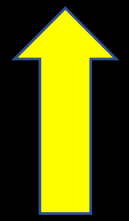
[vanilla@hopper ~]$ sinfo --all

```
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
```

Never run computations on the head node

Always use compute nodes

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



Tell slurm to run a program on a debug 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       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)
              4319   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4320   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4321   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4322   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4323   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4324   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4325   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4326   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4328   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4329   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4330   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4331   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4332   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4333   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4334   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4335   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4336   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
              4337   general      PRE erowland PD       0:00      2 (QOSMaxCpuPerUserLimit)
```

```
[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
```

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.

```
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)
```

```
[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)
                                                                 2 (QOSMaxCpuPerUserLimit)
             4337   general      PRE erowland PD       0:00      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
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 ~]$ 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…

Change directory into ~/workshops/intro_workshop

```
[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 = 3.142425985001098709 40, (Diff=0.0008333314113055934 1)
(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.

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 ~]$ 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
```

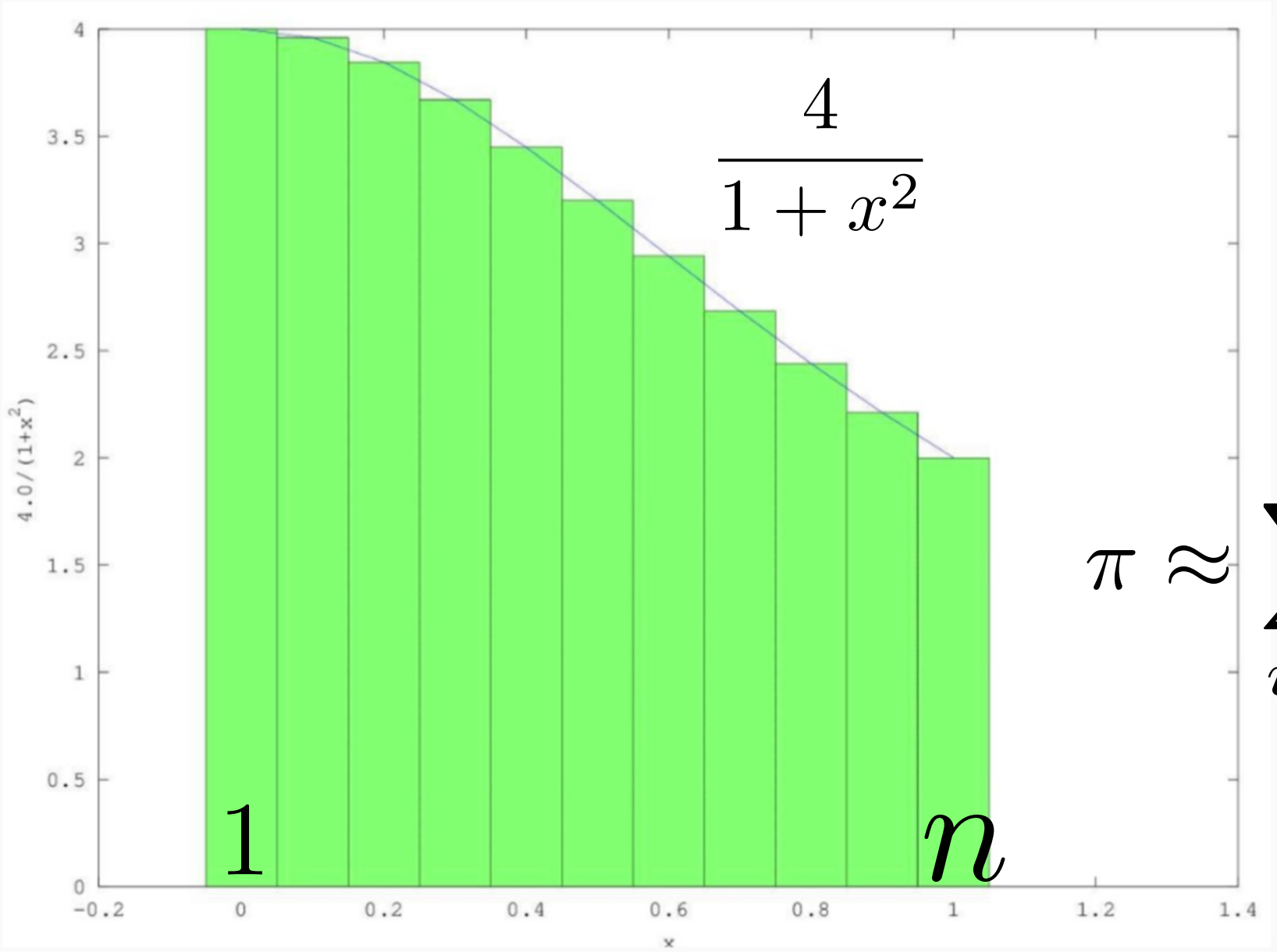
Run tree to see how the workshops directories are organized…

```
[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.

Serial Program to Calculate π



$$\frac{4}{1+x^2}$$

$$w = \frac{1}{n}$$

$$\pi \approx \sum_{i=0}^{n} \frac{4}{1+(i+\frac{w}{2})^2}$$

```
# A program that calculates pi using the area under a curve
# The program checks the value of pi calculated against the
# value provided by numpy
import time
import sys
import numpy as np # Value of PI to compare to


def Pi(num_steps): #Function to calculate pi
      step = 1.0 / num_steps
      sum = 0
        for i in range(num_steps):
                  x = (i + 0.5) * step
                  sum = sum + 4.0 / (1.0 + x * x)
         pi = step * sum
         return pi
```

```
# Check that the caller gave us the number of steps to use
if len(sys.argv) != 2:
        print("Usage: ", sys.argv[0], " <number of steps>")
        sys.exit(1)

num_steps = int(sys.argv[1],10);

# Call function to calculate pi
start = time.time() #Start timing
pi = Pi(num_steps)
end = time.time() # End timing

# Print our estimation of pi, the difference from numpy's value,
and how long it took
print("Pi = %.20f, (Diff=%.20f) (calculated in %f secs with %d
steps)" %(pi, pi-np.pi, end - start, num_steps))
sys.exit(0)
```

```
[vanilla@hopper ~]$ 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 ~]$ cat slurm/calc_pi_serial.sh

#!/bin/bash
#SBATCH --partition debug
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module load miniconda3
source activate numpy

cd $SLURM_SUBMIT_DIR
python code/calcPiSerial.py 1000000000
```

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

If you don't have a favorite linux text editor, then nano is simple.

```
[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
```

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

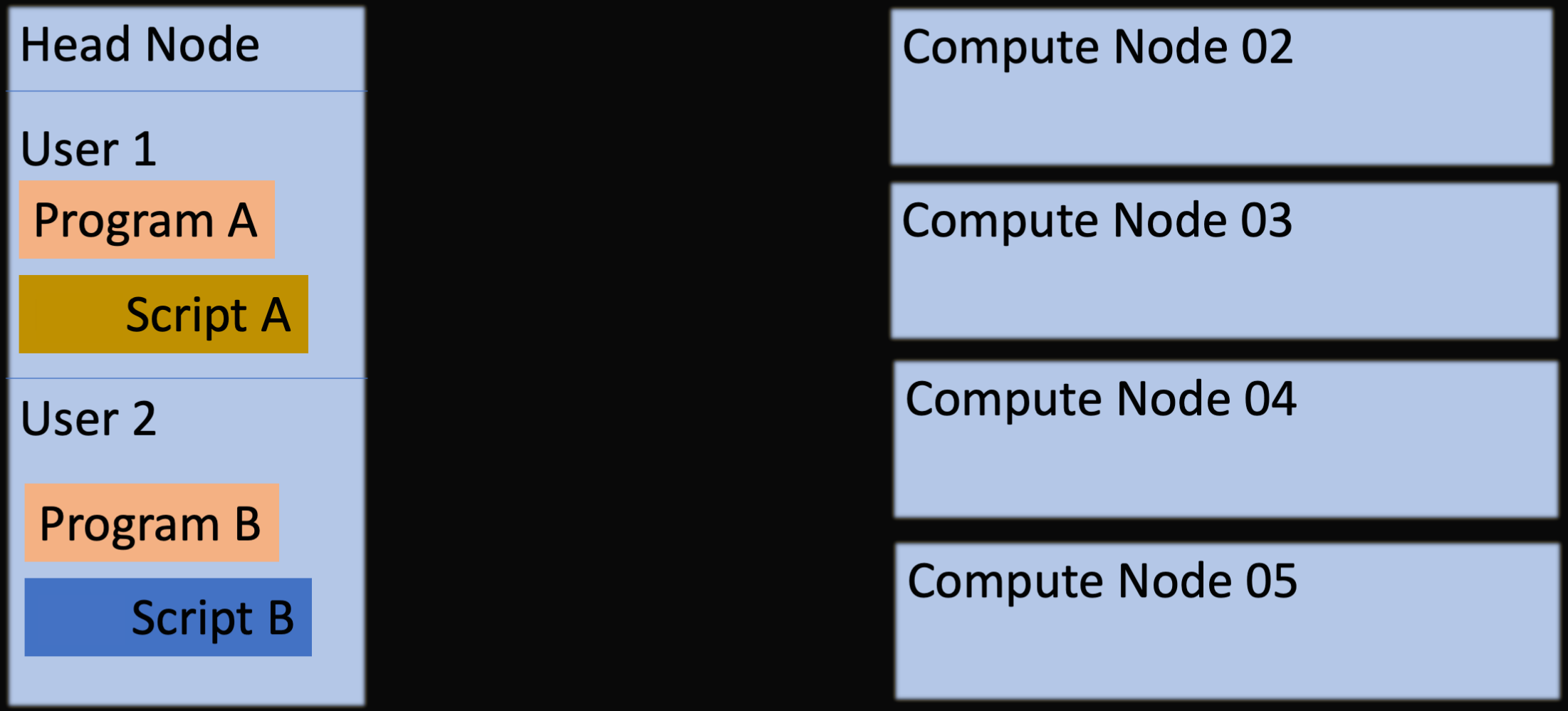
Take a look at the job output.

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

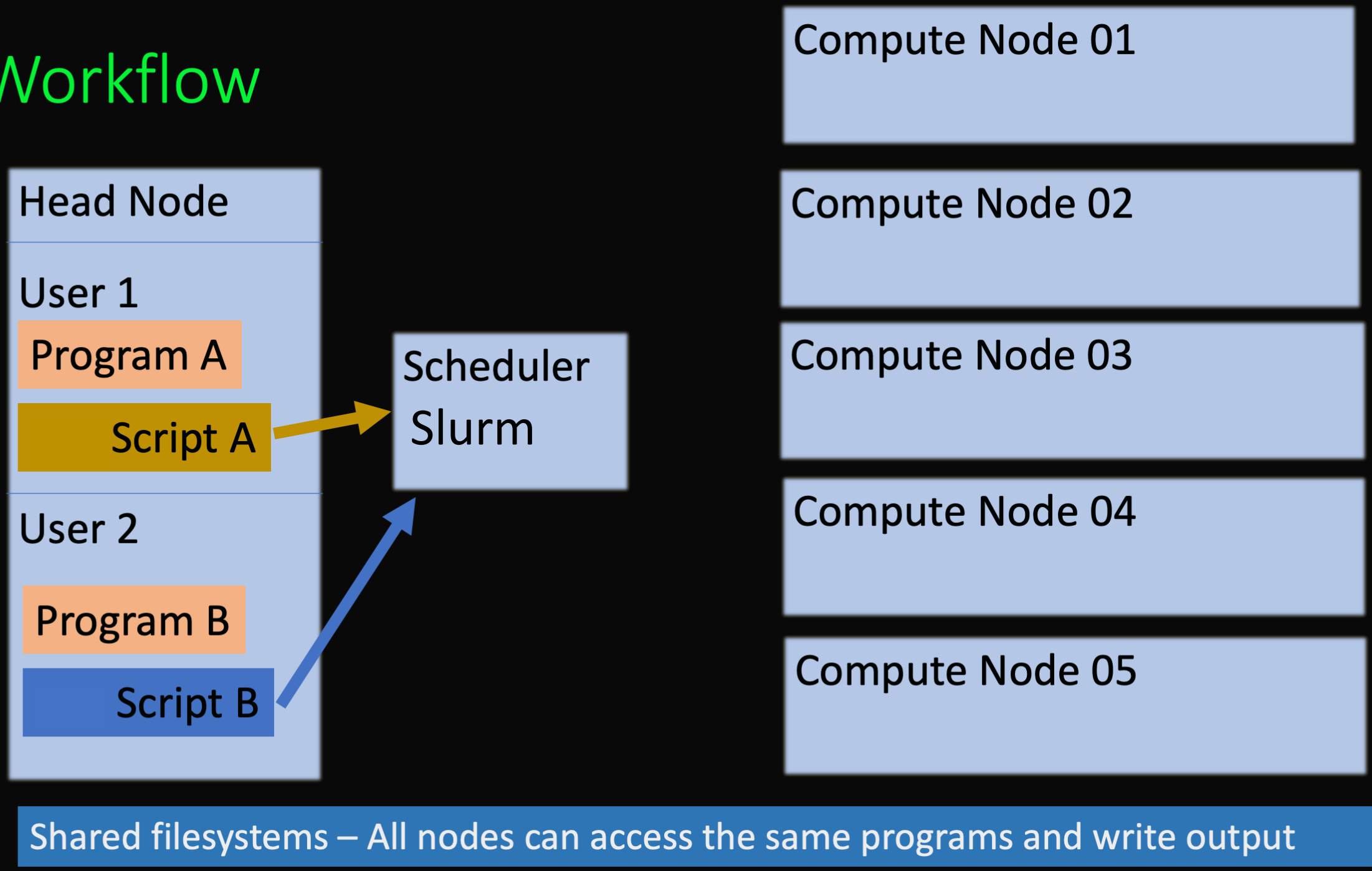
When it is finished you will have a new file named slurm-{your job id}.out.

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

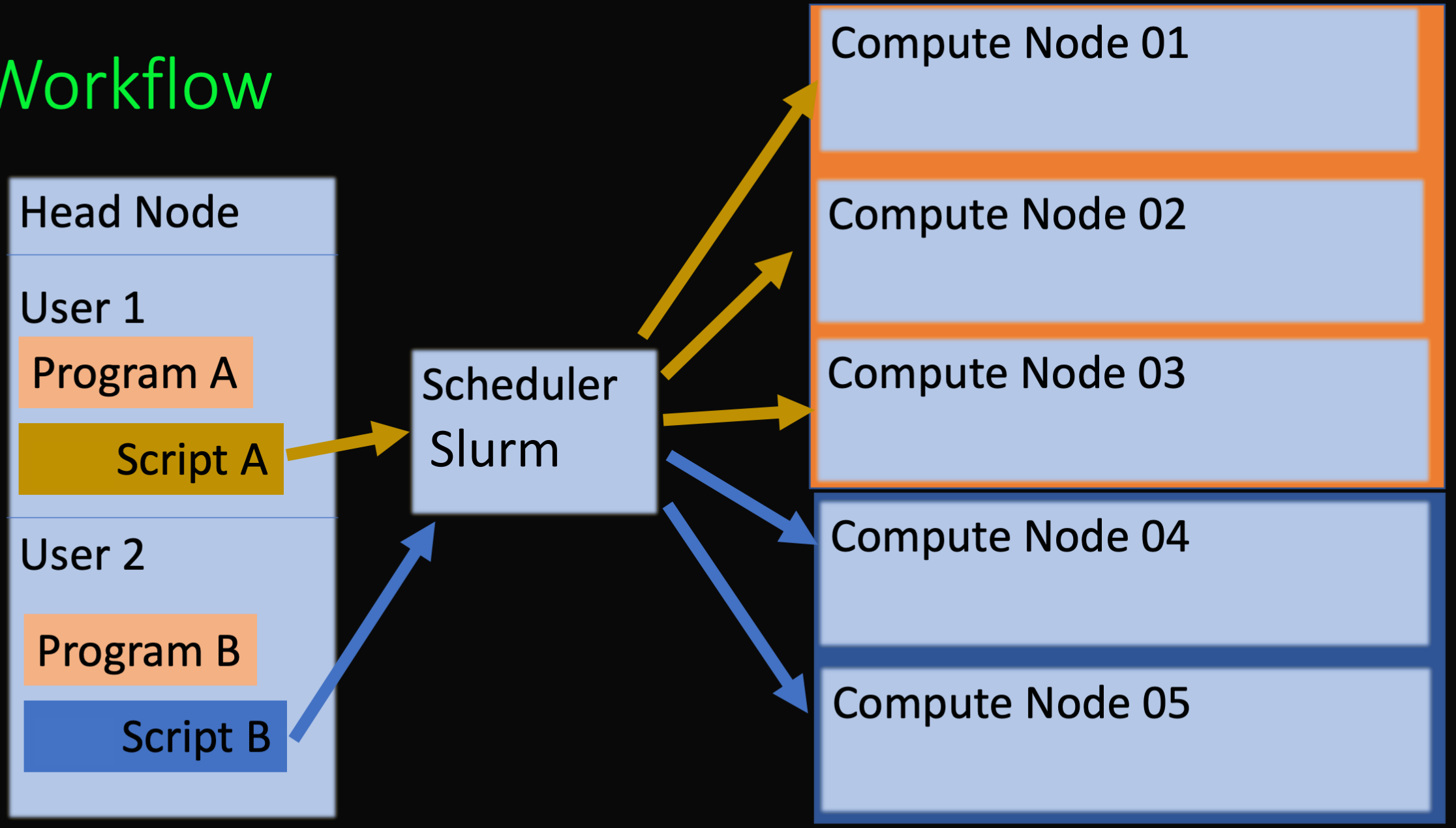
Workflow


Head Node
User 1
Program A
Script A
User 2
Program B
Script B
Compute Node 01
Compute Node 02
Compute Node 03
Compute Node 04
Compute Node 05
Shared filesystems – All nodes can access the same programs and write output

Workflow

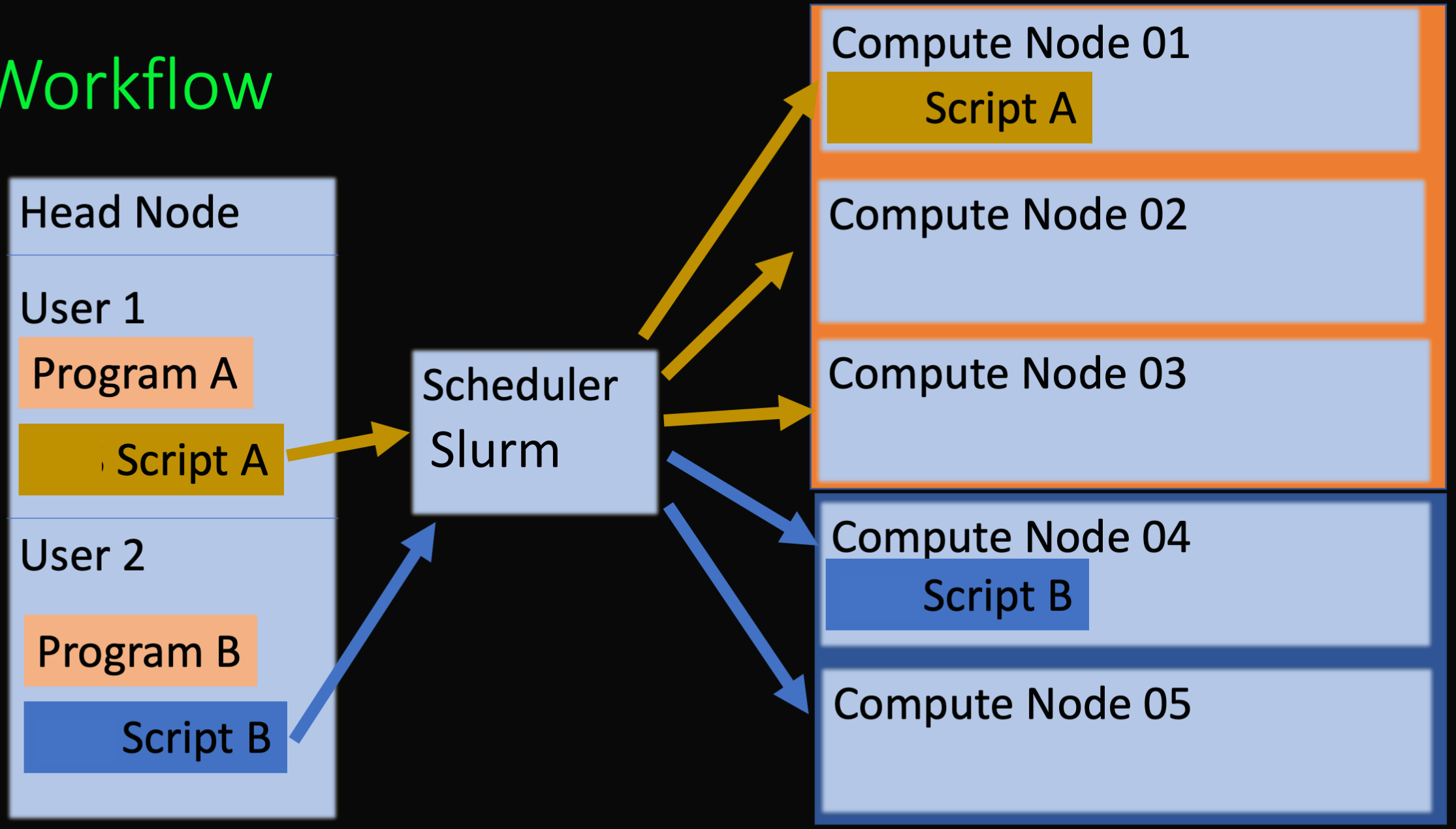

Head Node
User 1
Program A
Script A
User 2
Program B
Script B
Scheduler
Slurm
Compute Node 01
Compute Node 02
Compute Node 03
Compute Node 04
Compute Node 05
Shared filesystems – All nodes can access the same programs and write output

Workflow



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

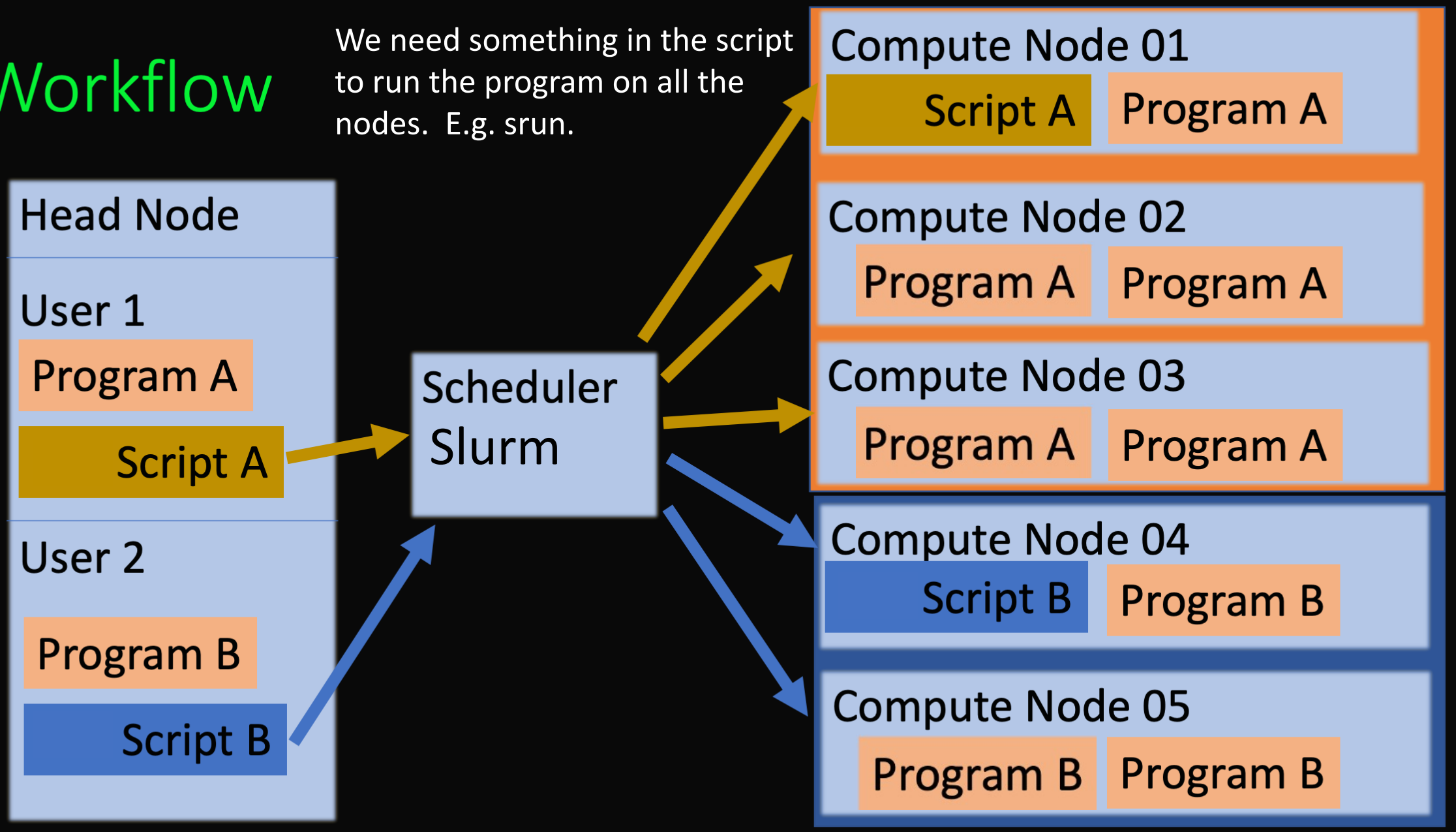
Workflow



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.



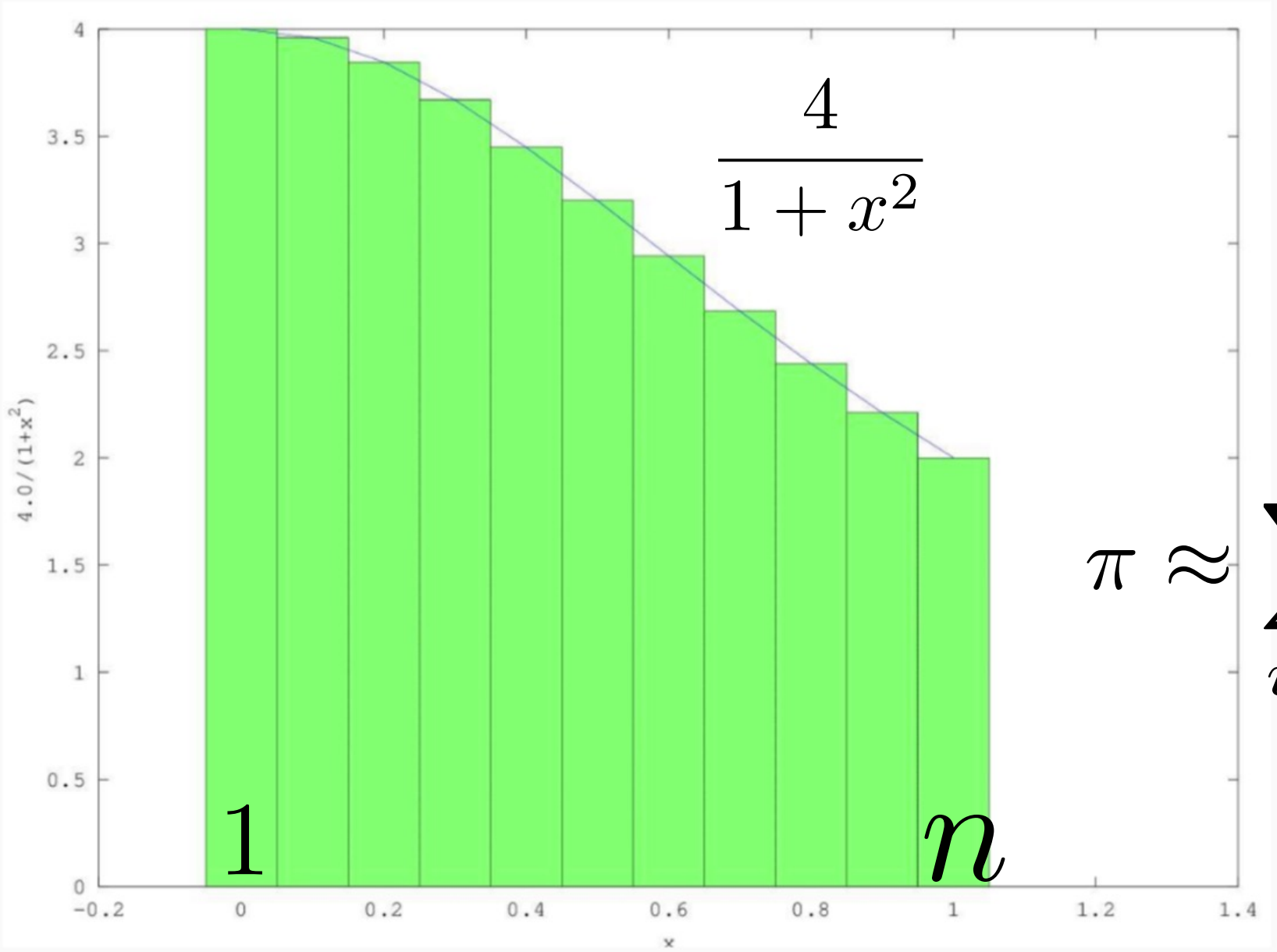
Shared filesystems – All nodes can access the same programs and write output

Parallelism – Coupled Parallelism

- Coupled problems are those where the CPUs need to work together to solve a problem by communicating with each other.
- Many commercial and research programs designed to run on HPC systems like CARC use a library called the message passing interface (MPI) to do this.

- We have written an MPI version of our python pi calculator to demonstrate.

Serial Program to Calculate π



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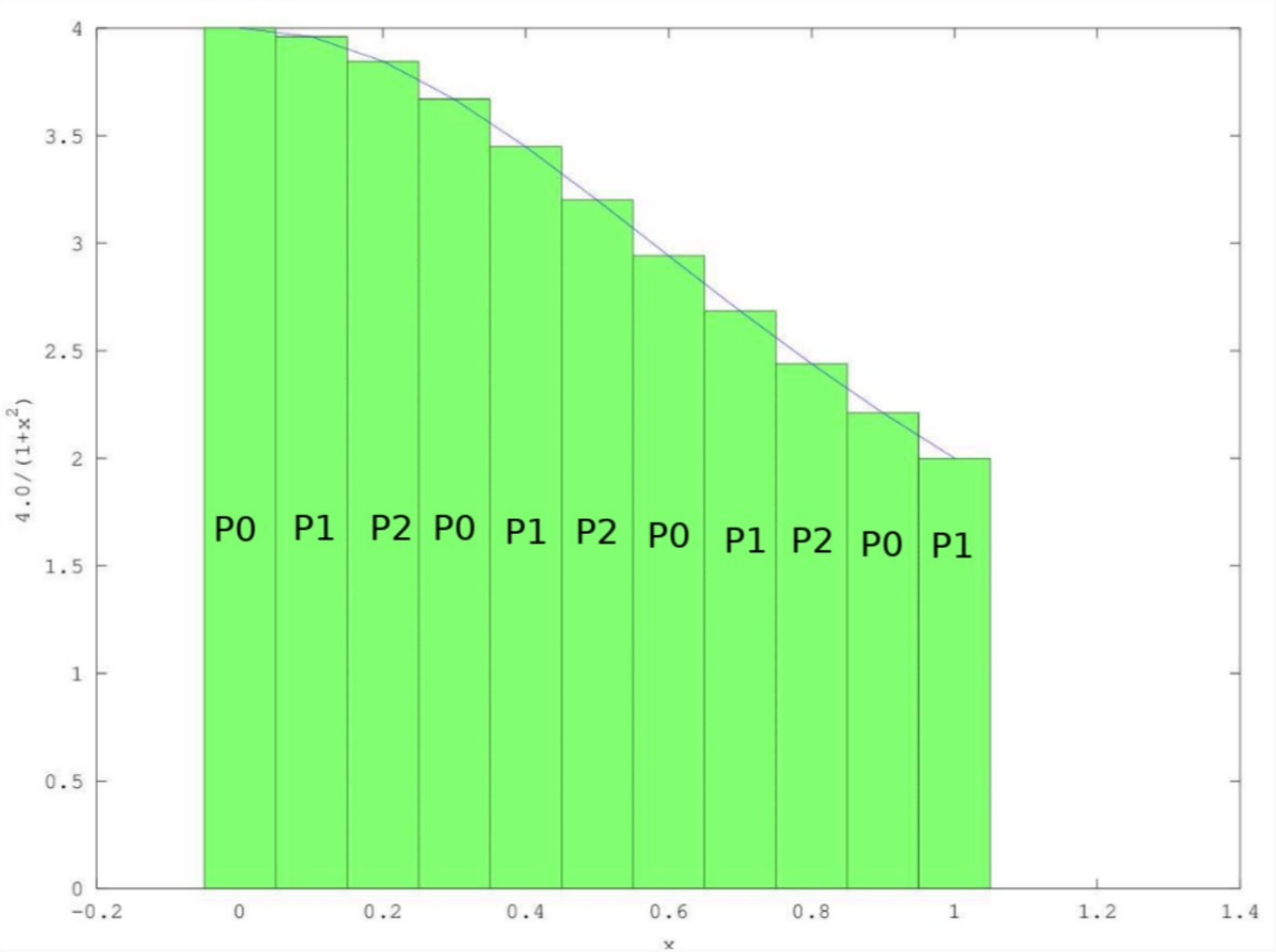
Parallel Program to Calculate π



MPI: Message Passing Interface

When programs need to run on many processors but also communicate with one another.

Here the parallel version of calcPi needs to communicate the partial sums computed by each process so they can all be added up.

To communicate we will use the MPI library:

```
module load miniconda3
conda create –n mpi_numpy mpi mpi4py numpy
```

```
import time
import sys
import numpy as np # Value of PI to compare to

##################### SETUP MPI - START #####################
from mpi4py import MPI        #Import the MPI library
comm = MPI.COMM_WORLD         #Communication framework
root = 0                      #Root process
rank = comm.Get_rank()        #Rank of this process
num_procs = comm.Get_size()   #Total number of processes
############################## END ##############################

#Distributed function to calculate pi
def Pi(num_steps):
    step = 1.0 / num_steps
    sum = 0
    for i in range(rank, num_steps, num_procs): # Divide sum among
processes
        x = (i + 0.5) * step
        sum = sum + 4.0 / (1.0 + x * x)
    mypi = step * sum

    # Get that partial sums from all the processes, add them up, and give
to the root process
    pi = comm.reduce(mypi, MPI.SUM, root)
    return pi
```

```
#Main function
# Check that the caller gave us the number of steps to use
if len(sys.argv) != 2:
    print("Usage: ", sys.argv[0], " <number of steps>")
    sys.exit(1)

num_steps = int(sys.argv[1],10);

#Broadcast number of steps to use to the other processes
comm.bcast(num_steps, root)

# Call function to calculate pi
start = time.time() #Start timing
pi = Pi(num_steps) # Call the function that calculates pi
end = time.time() # End timing

# If we are the root process then print our estimation of pi,
# the difference from numpy's value, and how long it took
print("Pi = %.20f, (Diff=%.20f) (calculated in %f secs with %d
steps)" %(pi, pi-np.pi, end - start, num_steps))
```

```
########################## SETUP MPI - START ##########################
from mpi4py import MPI          #Import the MPI library
comm = MPI.COMM_WORLD           #Communication framework
root = 0                        #Root process
rank = comm.Get_rank()          #Rank of this process
num_procs = comm.Get_size()     #Total number of processes
################################## END ##################################
```

```
#Distributed function to calculate pi
def Pi(num_steps):
    step = 1.0 / num_steps
    sum = 0
    for i in range(rank, num_steps, num_procs): # Divide sum among processes
        x = (i + 0.5) * step
        sum = sum + 4.0 / (1.0 + x * x)
    mypi = step * sum

# Get that partial sums from all the processes, add them up,
# and give to the root process
    pi = comm.reduce(mypi, MPI.SUM, root)
    return pi
```

```
#Main function
<snip>
num_steps = int(sys.argv[1],10);

#Broadcast number of steps to use to the other processes
comm.bcast(num_steps, root)

# Call function to calculate pi
start = time.time() #Start timing
pi = Pi(num_steps) # Call the function that calculates pi
end = time.time() # End timing

# If we are the root process then print our estimation of pi,
# the difference from numpy's value, and how long it took
print("Pi = %.20f, (Diff=%.20f) (calculated in %f secs with %d steps)"
%(pi, pi-np.pi, end - start, num_steps))
```

```
#!/bin/bash
#SBATCH --partition debug
#SBATCH --nodes 2
#SBATCH --ntasks-per-node 4
#SBATCH --time 00:05:00
#SBATCH --job-name calc_pi_mpi
#SBATCH --mail-user your_username@unm.edu
#SBATCH --mail-type ALL

module load miniconda3
source activate mpi_numpy

cd $SLURM_SUBMIT_DIR
srun --mpi=pmi2 python code/calcPiMPI.py 1000000000
```

sbatch slurm/calc_pi_mpi.sh

```
srun --mpi=pmi2 python code/calcPiMPI.py 1000000000
```

srun understands MPI programs!

If you ever used mpirun or mpiexec you had to provide a lot of parameters to describe how many compute nodes you had and what their names are, etc.

But srun is part of SLURM so it already knows all that.

The only thing you have to specify is the communication library to use. In our case “pmi2”.

Experiment

Compare the time it took for the parallel MPI version of calcPi to run compared to Serial calcPi.

What is your hypothesis about the time difference?

Parallelism – Embarrassingly Parallel

- Embarrassingly parallel (Cleve Moler) are problems that are really really easy to speed up with mode CPUs.

- If you run 1000 copies of your program on 1000 CPUs then it takes 1/1000th the time.
- Problems fall on a spectrum between inherently serial and embarrassingly parallel.

Useful Slurm Commands

squeue --me --long	shows information about jobs you submitted
squeue --me --start	shows when slurm expects your job to start
scancel jobid	cancels a job
scancel --u $USER	cancels all your jobs
sacct	shows your job history
seff jobid	shows how efficiently the hardware was used