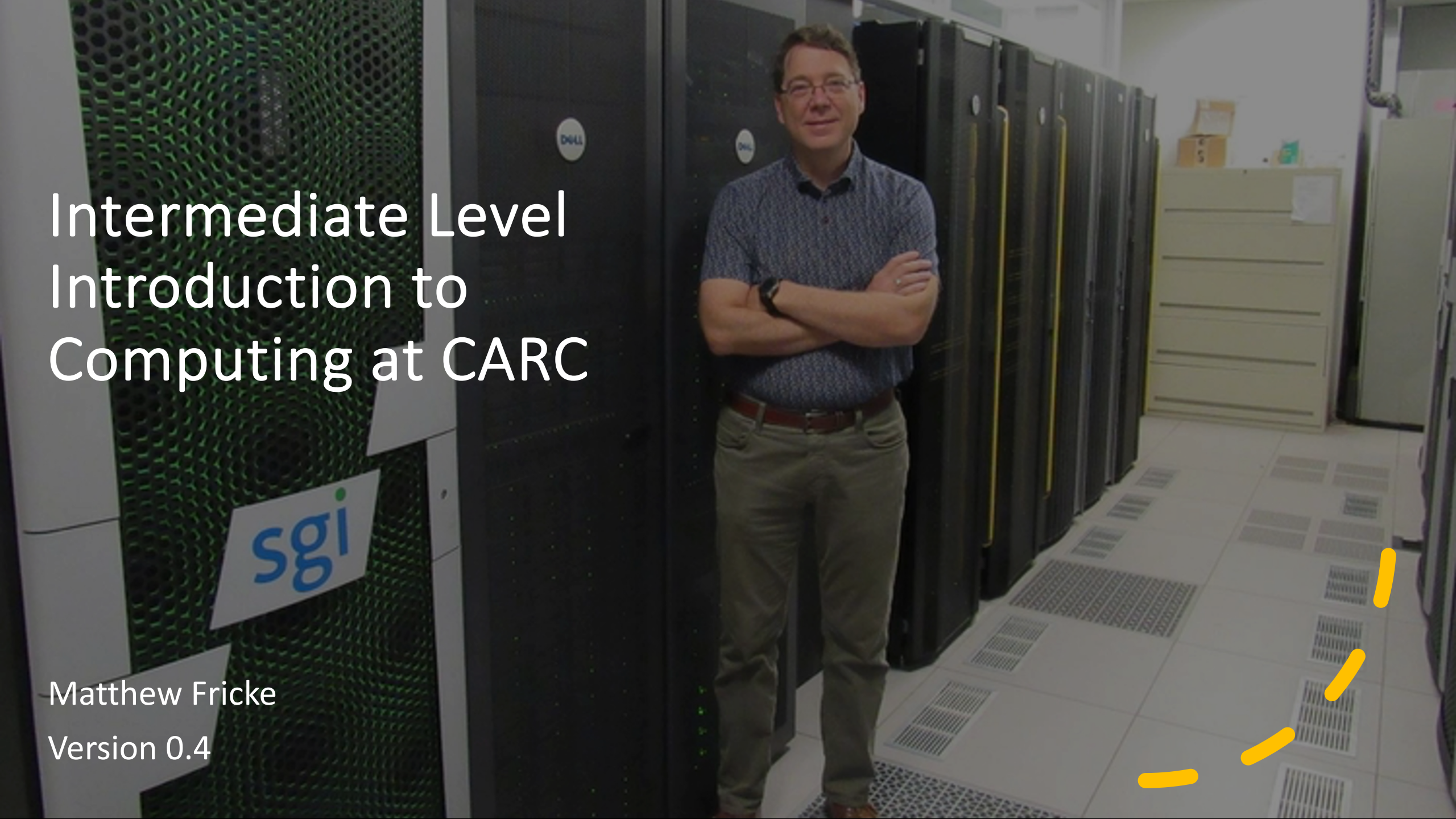


Intermediate Level Introduction to Computing at CARC

Matthew Fricke

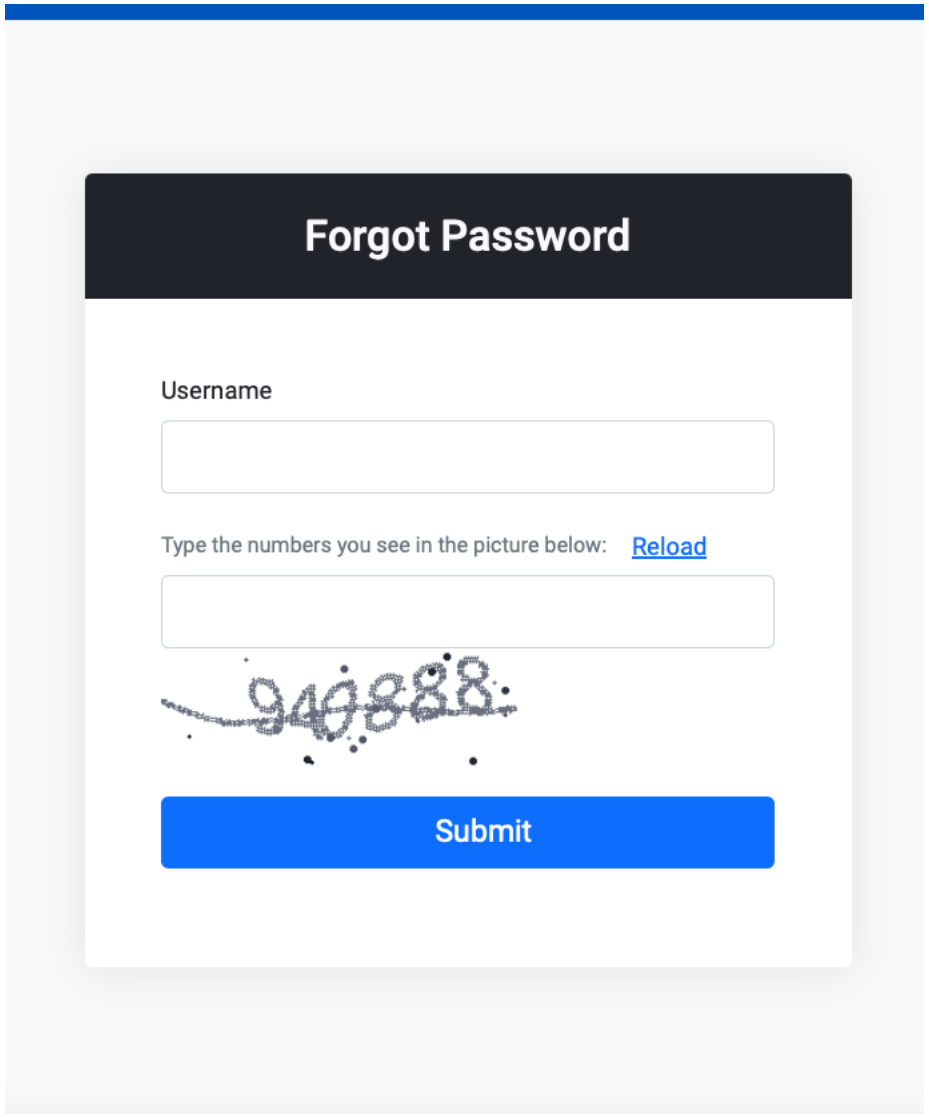
Version 0.4

Goals

- 1) SLURM scheduler literacy
- 2) Ability to employ embarrassingly parallel solutions
- 3) Ability to employ coupled parallel solutions

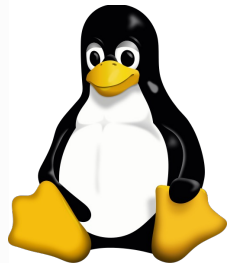
NOTE: We won't cover file transfer, storage systems, module system, conda, PBS. (These are all covered in depth in the video tutorials)

If you don’t know your CARC password go to:
https://mokey.alliance.unm.edu/auth/forgotpw



Logging into Hopper


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


On windows use PowerShell to get to
the command line.


On Mac or Linux machines run
terminal to access the command line.
```



Logging into Hopper

```
Welcome to Hopper
▶ By using CARC systems you agree to the CARC Good Neighbor Guide
▶ Tutorials and the Good Neighbor Guide are at https://goto.unm.edu/carc-start
▶ Need help? Email: help@carc.unm.edu

Last login: Sun Aug 24 18:04:03 2025 from 50.188.169.22

vanilla@hopper:~
```


ENJOY
Slurm
SODA
IT'S HIGHLY ADDICTIVE!
VOTED #1 SOFT DRINK OF THE 31ST CENTURY!
YOU WIN!
WHIMMY WHAM WHAM WOZZLE!
SLURMS McKENZIE

```
[vanilla@hopper ~]$ qgrok
partition          nodes  nodes  nodes  total  total  free   total  free   CPUs   RAM/node   time   CPU    GPU    RAM
name        jobs   free   busy   down   nodes  CPUs   CPUs   GPUs   GPUs   /node             limit  limit  limit  limit
----------  -----  -----  -----  -----  -----  -----  -----  -----  -----  -----  ---------  -----  -----  -----  -----
general     4      4      6      0      10     320    156    0      0      32     93G        2d     128    0      372G
debug       1      1      1      0      2      64     63     0      0      32     93G        4h     8      0      25G
totals:     5      5      7      0      12     384    219    0      0
```

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

partition name	jobs	nodes free	nodes busy	nodes down	total nodes	total CPUs	free CPUs	total GPUs	free GPUs	CPUs /node	RAM/node	time limit	CPU limit	GPU limit	RAM limit
general	4	4	6	0	10	320	156	0	0	32	93G	2d	128	0	372G
debug	1	1	1	0	2	64	63	0	0	32	93G	4h	8	0	25G
condo	29	30	25	0	55	1760	1060	37	8	32	94G-1.5T	2d	512	4	1.5T
bugs	0	0	2	0	2	64	0	0	0	32	93G	1w	64	0	
pcnc	0	0	2	0	2	64	0	0	0	32	93G	1w	64	0	
pathogen	0	1	0	0	1	32	32	0	0	32	93G	1w	32	0	
tc	8	1	9	0	10	320	104	0	0	32	93G-1.5T	1w	320	0	
gold	0	2	0	0	2	64	64	0	0	32	93G	1w	64	0	
fishgen	1	0	1	0	1	32	12	0	0	32	377G	1w	32	0	
neuro-hsc	0	14	0	0	14	448	448	0	0	32	93G	1w	448	0	
pna	0	1	0	0	1	32	32	0	0	32	93G	1w	32	0	
geodef	0	4	0	0	4	128	128	0	0	32	504G	1w	128	0	
cup-ecs	0	0	2	0	2	64	0	13	8	32	188G	1w	64	13	
tid	0	0	1	0	1	32	0	2	0	32	188G	1w	32	2	
biocomp	0	1	0	0	1	32	32	1	0	32	188G	1w	32	1	
chakra	0	0	1	0	1	32	0	1	0	32	188G	1w	32	1	
quark	0	3	7	0	10	320	112	20	0	32	377G	1w3d	320	20	
toadpole	0	1	0	0	1	32	32	0	0	32	94G	1w	32	0	
insar	0	2	0	0	2	64	64	0	0	32	504G	1w	64	0	
totals:	34	35	32	0	67	2144	1279	37	8						

```
[vanilla@hopper ~]$ qgrok
partition          nodes   nodes   nodes   total   total   free    total   free    CPUs    RAM/node    time    CPU     GPU     RAM
name        jobs   free    busy    down    nodes   CPUs    CPUs    GPUs    GPUs    /node               limit   limit   limit   limit
----------  -----  -----   -----   -----   -----   -----   -----   -----   -----   -----   ---------   -----   -----   -----   -----
general     4      4       6       0       10      320     156     0       0       32      93G         2d      128     0       372G
debug       1      1       1       0       2       64      63      0       0       32      93G         4h      8       0       25G
condo       29     30      25      0       55      1760    1060    37      8       32      94G-1.5T    2d      512     4       1.5T
bugs        0      0       2       0       2       64      0       0       0       32      93G         1w      64      0
pcnc        0      0       2       0       2       64      0       0       0       32      93G         1w      64      0
pathogen    0      1       0       0       1       32      32      0       0       32      93G         1w      32      0
tc          8      1       9       0       10      320     104     0       0       32      93G-1.5T    1w      320     0
gold        0      2       0       0       2
fishgen     1      0       1       0       1
neuro-hsc   0      14      0       0       1
pna         0      1       0       0       1
geodef      0      4       0       0       4
cup-ecs     0      0       2       0       2
tid         0      0       1       0       1
biocomp     0      1       0       0       1
chakra      0      0       1       0       1
quark       0      3       7       0       1
toadpole    0      1       0       0       1
insar       0      2       0       0       2
totals:     34     35      32      0       (
```

Open partitions for use by everyone with a CARC account.

Purchased by the Office for the Vice President for Research.

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

partition name	jobs	nodes free	nodes busy	nodes down	total nodes	total CPUs	free CPUs	total GPUs	free GPUs	CPUs /node	RAM/node	time limit	CPU limit	GPU limit	RAM limit
general	4	4	6	0	10	320	156	0	0	32	93G	2d	128	0	372G
debug	1	1	1	0	2	64	63	0	0	32	93G	4h	8	0	25G
condo	29	30	25	0	55	1760	1060	37	8	32	94G-1.5T	2d	512	4	1.5T
bugs	0	0	2	0	2	64	0	0	0	32	93G	1w	64	0	
pcnc	0	0	2	0	2	64	0	0	0	32	93G	1w	64	0	
pathogen	0	1	0	0	1	32	32	0	0	32	93G	1w	32	0	
tc	8	1	9	0	10	320	104	0	0	32	93G-1.5T	1w	320	0	
gold	0	2	0	0	2	64	64	0	0	32	93G	1w	64	0	
fishgen	1	0	1	0	1	32	12	0	0	32	377G	1w	32	0	
neuro-hsc	0	14	0	0	14	448	448	0	0	32	93G	1w	448	0	
pna	0	1	0	0	1	32	32	0	0	32	93G	1w	32	0	
geodef	0	4	0	0	4	128	128	0	0	32	504G	1w	128	0	
cup-ecs	0	0	2	0	2	64	0	13	8	32	188G	1w	64	13	
tid	0	0	1	0	1	32	0	2	0	32	188G	1w	32	2	
biocomp	0	1	0	0	1	32	32	1	0	32	188G	1w	32	1	
chakra	0	0	1	0	1	32	0	1	0	32	188G	1w	32	1	
quark	0	3	7	0	10	320	112	20	0	32	377G	1w3d	320	20	
toadpole	0	1	0	0	1	32	32	0	0	32	94G	1w	32	0	
insar	0	2	0	0	2	64	64	0	0	32	504G	1w	64	0	
totals:	34	35	32	0	67	2144	1279	37	8						

```
[vanilla@hopper ~]$ qgrok
partition          nodes  nodes  nodes  total  total  free   total  free   CPUs   RAM/node    time   CPU    GPU    RAM
name        jobs   free   busy   down   nodes  CPUs   CPUs   GPUs   GPUs   /node              limit  limit  limit  limit
----------  -----  -----  -----  -----  -----  -----  -----  -----  -----  -----  ---------  -----  -----  -----  -----
general     4      4      6      0      10     320    156    0      0      32     93G        2d     128    0      372G
debug       1      1      1      0      2      64     63     0      0      32     93G        4h     8      0      25G
condo       29     30     25     0      55     1760   1060   37     8      32     94G-1.5T   2d     512    4      1.5T
bugs        0      0      2      0      2      64     0      0      0      32     93G        1w     64     0
pcnc        0      0      2      0      2      64     0      0      0      32     93G        1w     64     0
pathogen    0      1      0      0      1      32     32     0      0      32     93G        1w     32     0
tc          8      1      9      0      10     320    104    0      0      32     93G-1.5T   1w     320    0
gold        0      2      0      0      2
fishgen     1      0      1      0      1
neuro-hsc   0      14     0      0      1
pna         0      1      0      0      1
geodef      0      4      0      0      4
cup-ecs     0      0      2      0      2
tid         0      0      1      0      1
biocomp     0      1      0      0      1
chakra      0      0      1      0      1
quark       0      3      7      0      1
toadpole    0      1      0      0      1
insar       0      2      0      0      2
totals:     34     35     32     0      0
```

Private partitions

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

```
[vanilla@hopper ~]$ qgrok
partition          nodes   nodes   nodes   total   total   free    total   free    CPUs    RAM/node    time    CPU     GPU     RAM
name        jobs   free    busy    down    nodes   CPUs    CPUs    GPUs    GPUs    /node               limit   limit   limit   limit
----------  -----  -----   -----   -----   -----   -----   -----   -----   -----   -----   ---------   -----   -----   -----   -----
general     4      4       6       0       10      320     156     0       0       32      93G         2d      128     0       372G
debug       1      1       1       0       2       64      63      0       0       32      93G         4h      8       0       25G
condo       29     30      25      0       55      1760    1060    37      8       32      94G-1.5T    2d      512     4       1.5T
bugs        0      0       2       0       2       64      0       0       0       32      93G         1w      64      0
pcnc        0      0       2       0       2       64      0       0       0       32      93G         1w      64      0
pathogen    0      1       0       0       1       32      32      0       0       32      93G         1w      32      0
tc          8      1       9       0       10      320     104     0       0       32      93G-1.5T    1w      320     0
gold        0      2       0       0       2
fishgen     1      0       1       0       1
neuro-hsc   0      14      0       0       14
pna         0      1       0       0       1
geodef      0      4       0       0       4
cup-ecs     0      0       2       0       2
tid         0      0       1       0       1
biocomp     0      1       0       0       1
chakra      0      0       1       0       1
quark       0      3       7       0       10
toadpole    0      1       0       0       1
insar       0      2       0       0       2
totals:     34     35      32      0       67
```

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 ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      1    mix hopper011
debug        up    4:00:00      1   idle hopper012
```

sinfo reports information about partitions

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      1    mix hopper011
debug        up    4:00:00      1   idle hopper012
```

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      1    mix hopper011
debug        up    4:00:00      1   idle hopper012
```

Name

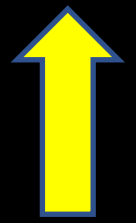
```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      1    mix hopper011
debug        up    4:00:00      1   idle hopper012
```

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      1    mix hopper011
debug        up    4:00:00      1   idle hopper012
```

There are two nodes in this partition.

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      1    mix hopper011
debug        up    4:00:00      1   idle hopper012
```



The state of the nodes in the partition

```
[vanilla@hopper ~]$ sinfo --partition debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    4:00:00      1    mix hopper011
debug        up    4:00:00      1   idle hopper012
```

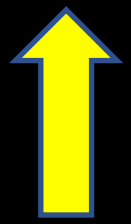
The name of the nodes in the partition

```
[vanilla@hopper ~]$ sinfo --partition general
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
general*     up 2-00:00:00      5  alloc hopper[001-009]
general*     up 2-00:00:00      4   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

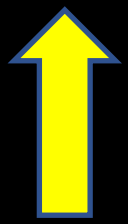
```
sinfo(1)                                                    Slurm
Commands                                                    sinfo(1)

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)
                                                       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)
             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 ~]$ 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
hopper012
hopper012
You have not be                                    se
the -G option i
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
hopper012
hopper012
You have not be                                    se
the -G option i
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 be                                    se
the -G option i
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                                    se
the -G option in
hopper011
Hopper011
```

This command is getting pretty long.

We can use salloc to avoid asking for the same resources every time we use srun.

```
[vanilla@hopper ~]$ salloc --partition debug --nodes 2
--ntasks-per-node 2
salloc: Account not specified in script or
~/.default_slurm_account, using latest project
salloc: Granted job allocation 5251
salloc: Waiting for resource configuration
salloc: Nodes hopper[011-012] are ready for job
[vanilla@hopper ~]$
```

This command is getting pretty long.

We can use salloc to avoid asking for the same resources every time we use srun.

```
[vanilla@hopper ~]$ srun hostname
hopper012
hopper012
hopper011
You have not been allocated GPUs. To request GPUs, use
the -G option in your submission script.
hopper011
[vanilla@hopper ~]$ srun hostname
hopper012
hopper011
hopper012
hopper011
[vanilla@hopper ~]$
```

Now we can use srun over and over without having to ask for a new hardware allocation each time.

```
[vanilla@hopper ~]$ exit
exit
salloc: Relinquishing job allocation 5251
```

Always type exit when you are done with the hardware.
Running salloc inside an allocation gets very confusing.

BREAK

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]$
```

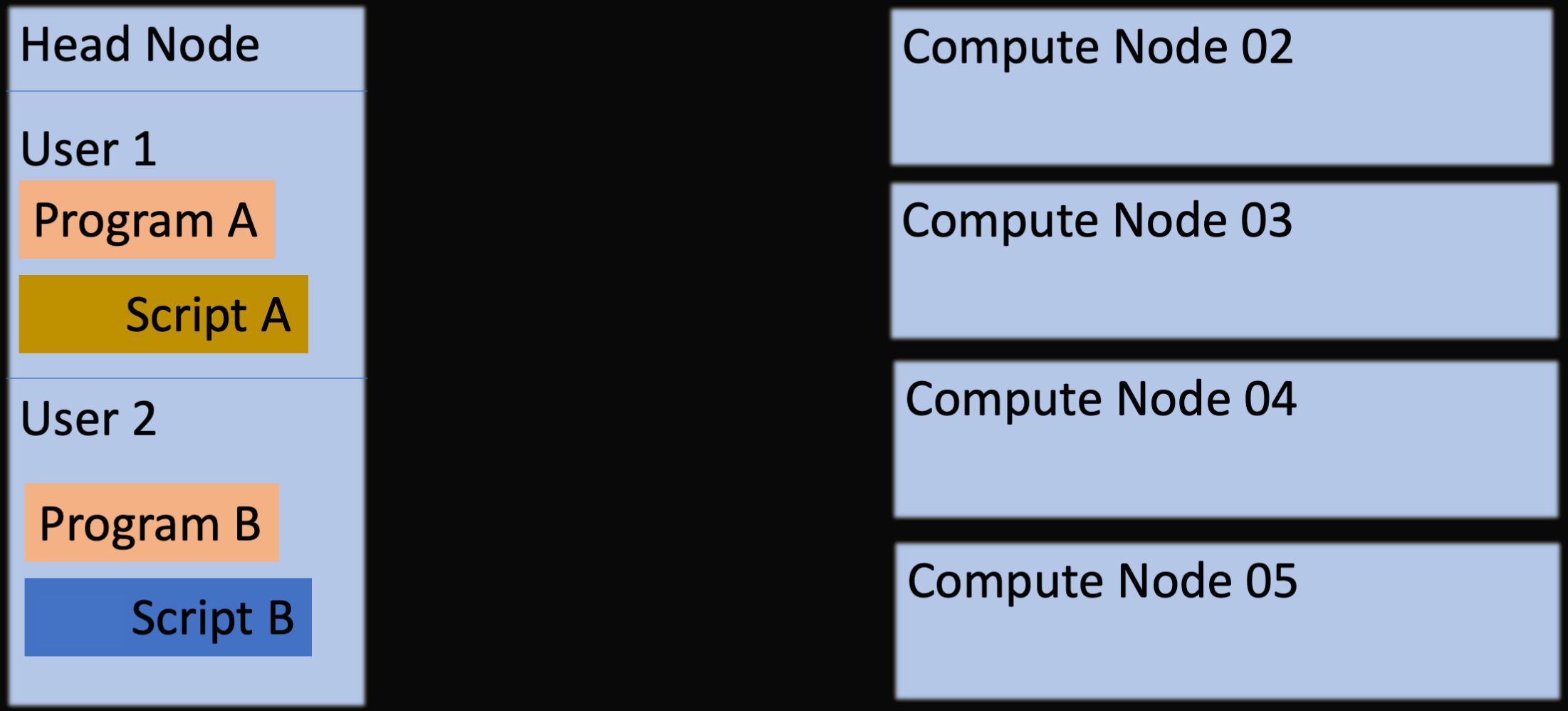
We submit our slurm shell script with the sbatch command.

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

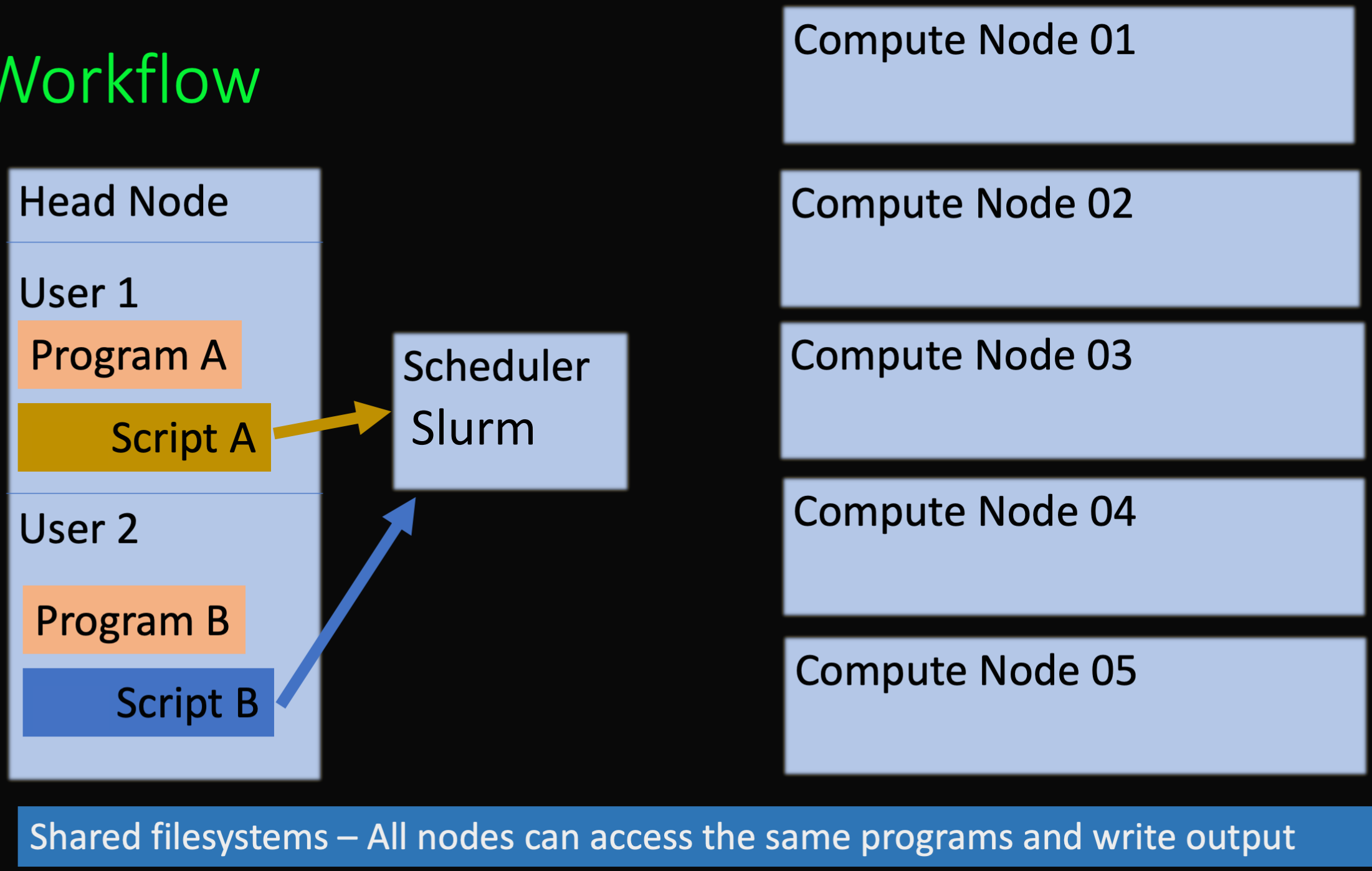
This indicates that the script was successfully sent to the scheduler.

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

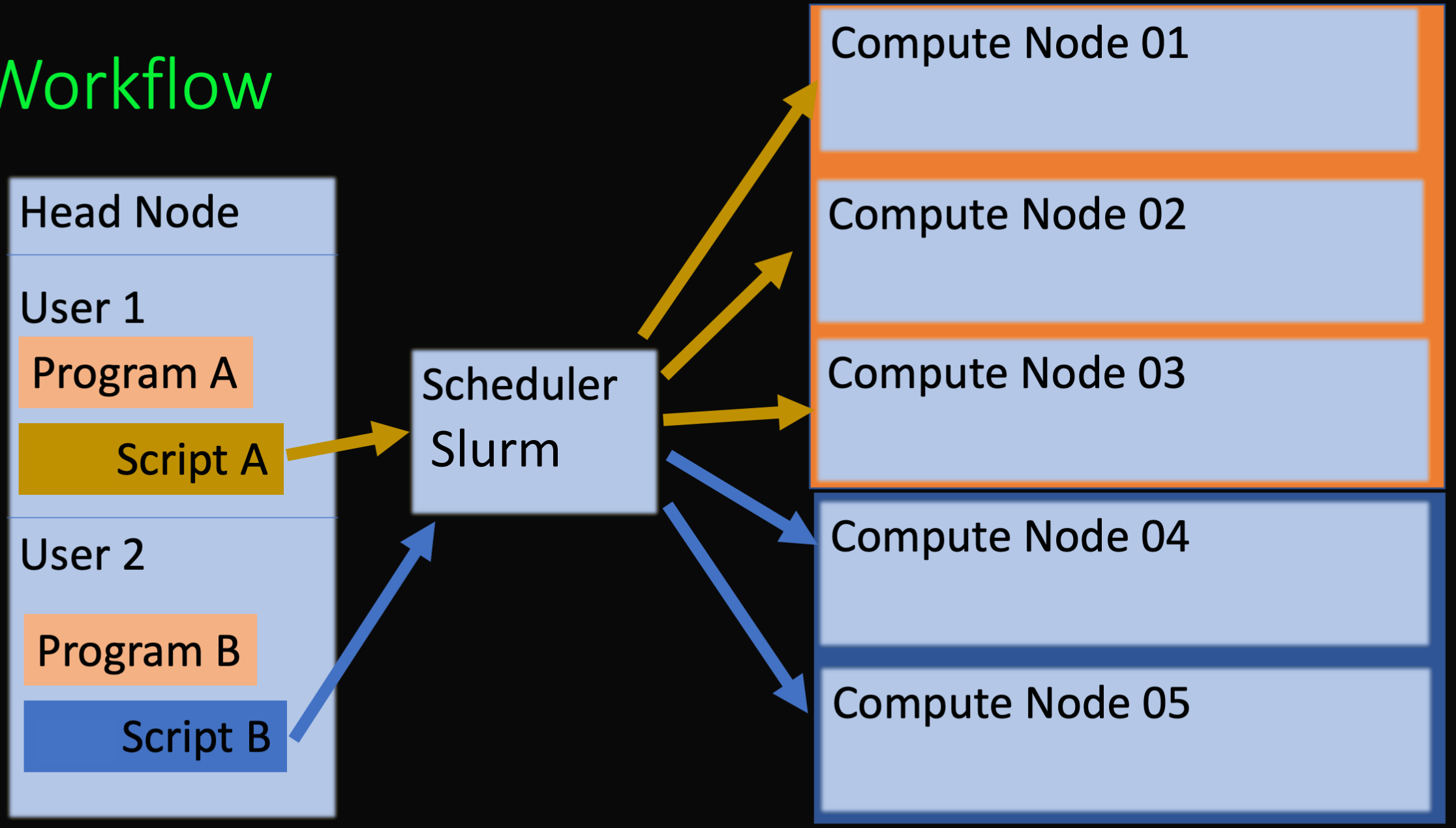
Workflow


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

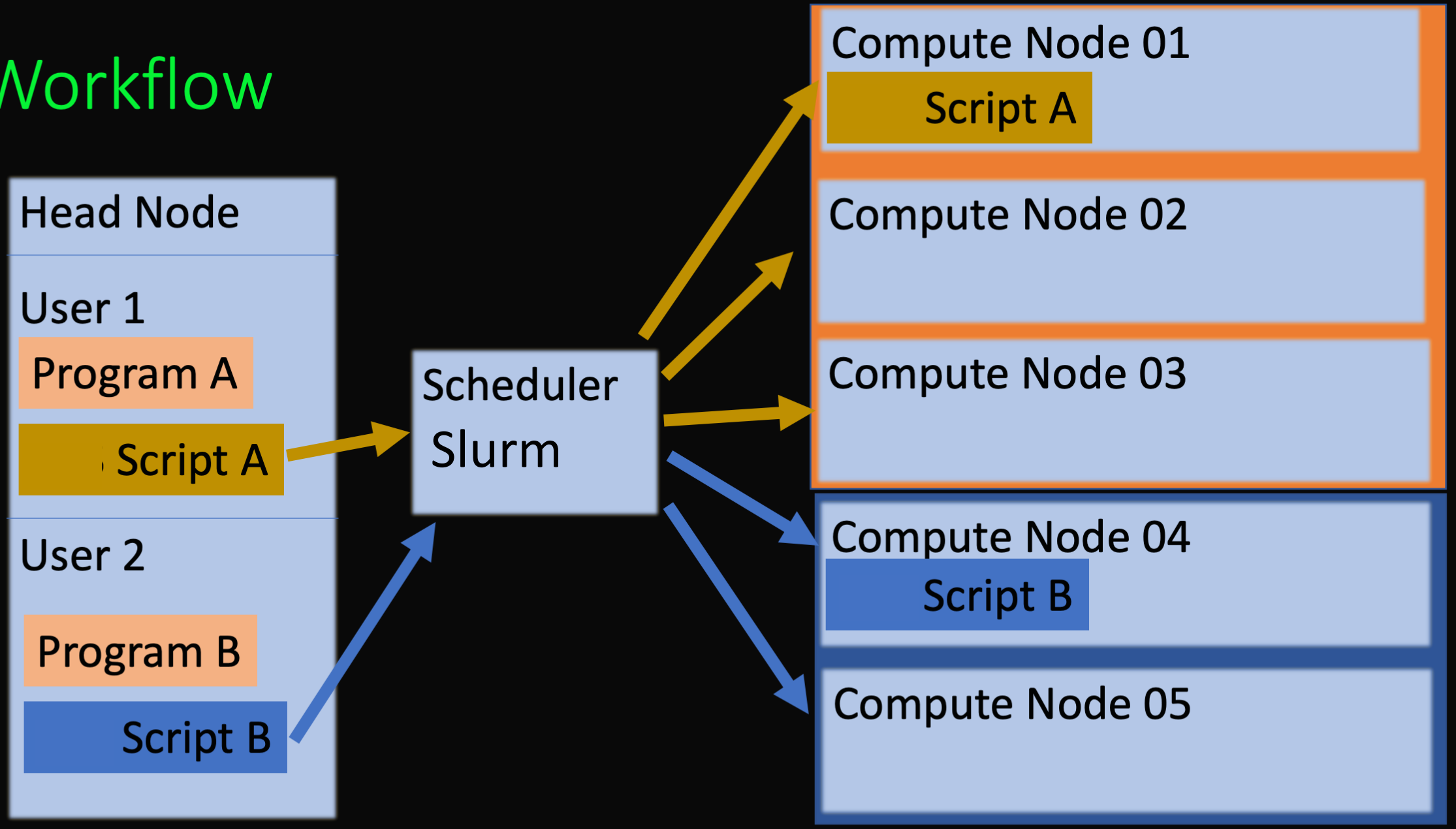

Head Node
User 1
Program A
Script A
User 2
Program B
Script B
Scheduler
Slurm
Compute Node 01
Compute Node 02
Compute Node 03
Compute Node 04
Compute Node 05
Shared filesystems – All nodes can access the same programs and write output

Workflow



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

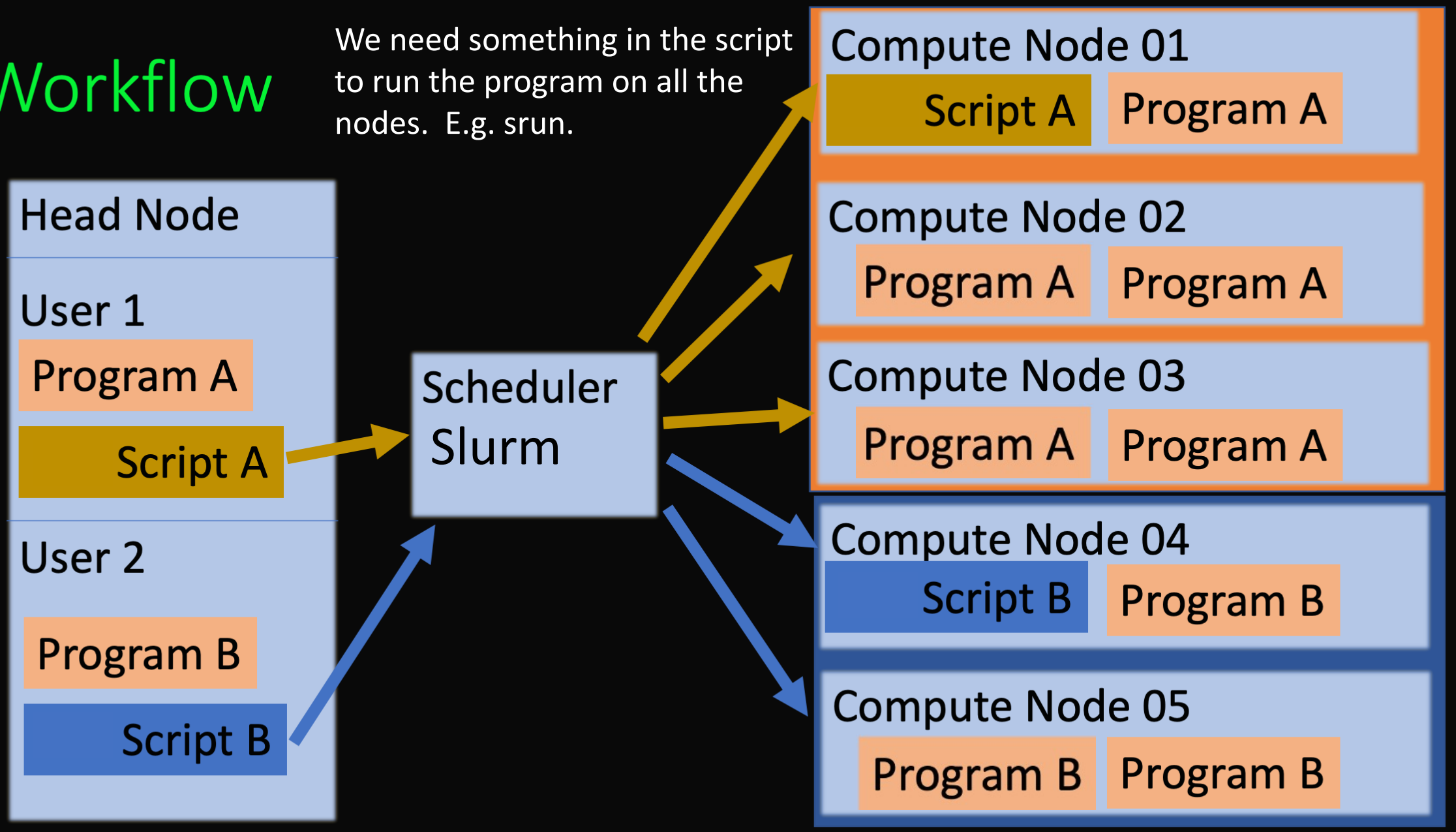
Workflow



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

```
[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
```

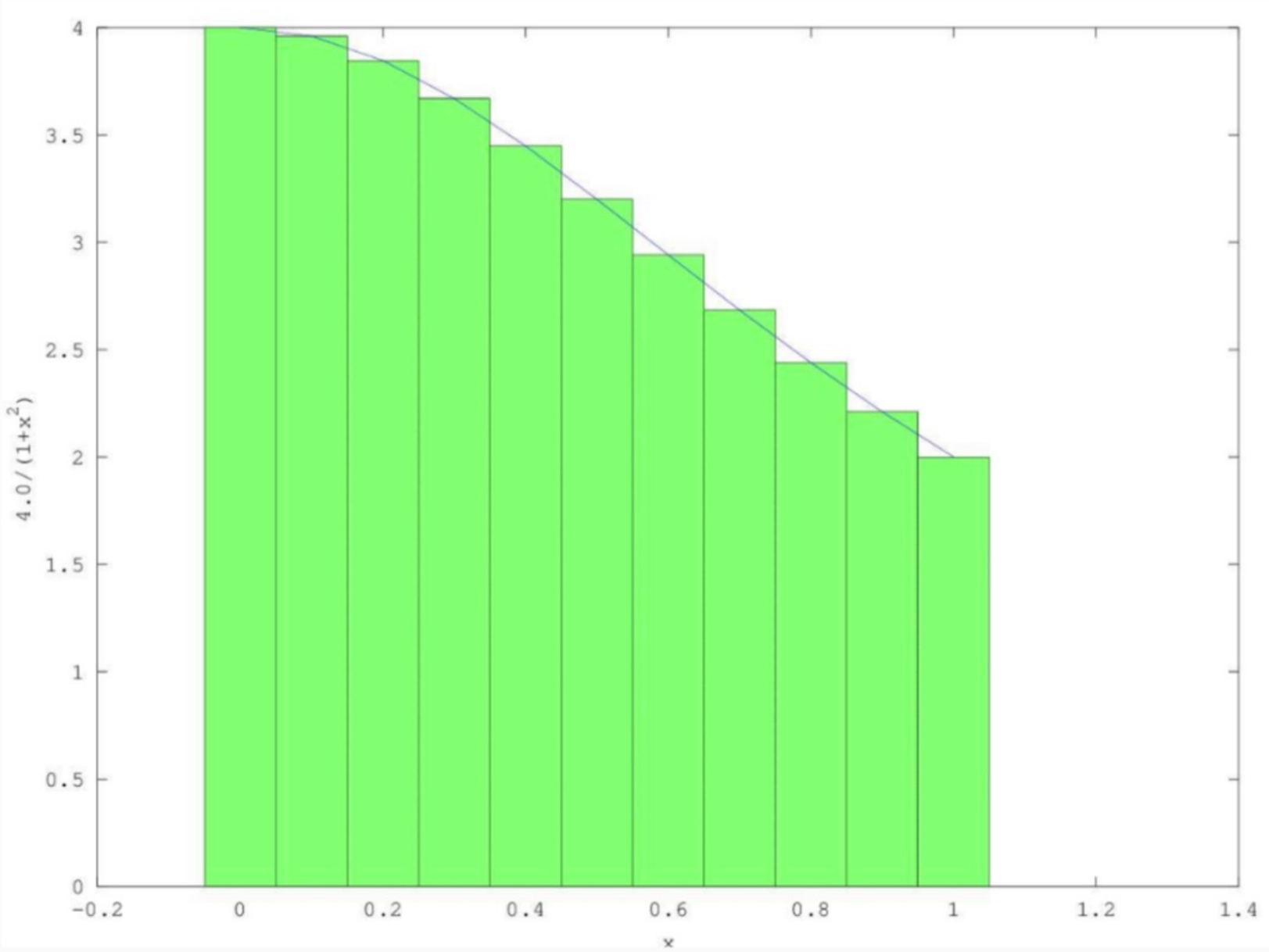

```
[vanilla@hopper intro_workshop]$ cat slurm-5252.out
hopper011
```

```
[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
What do you see?
```

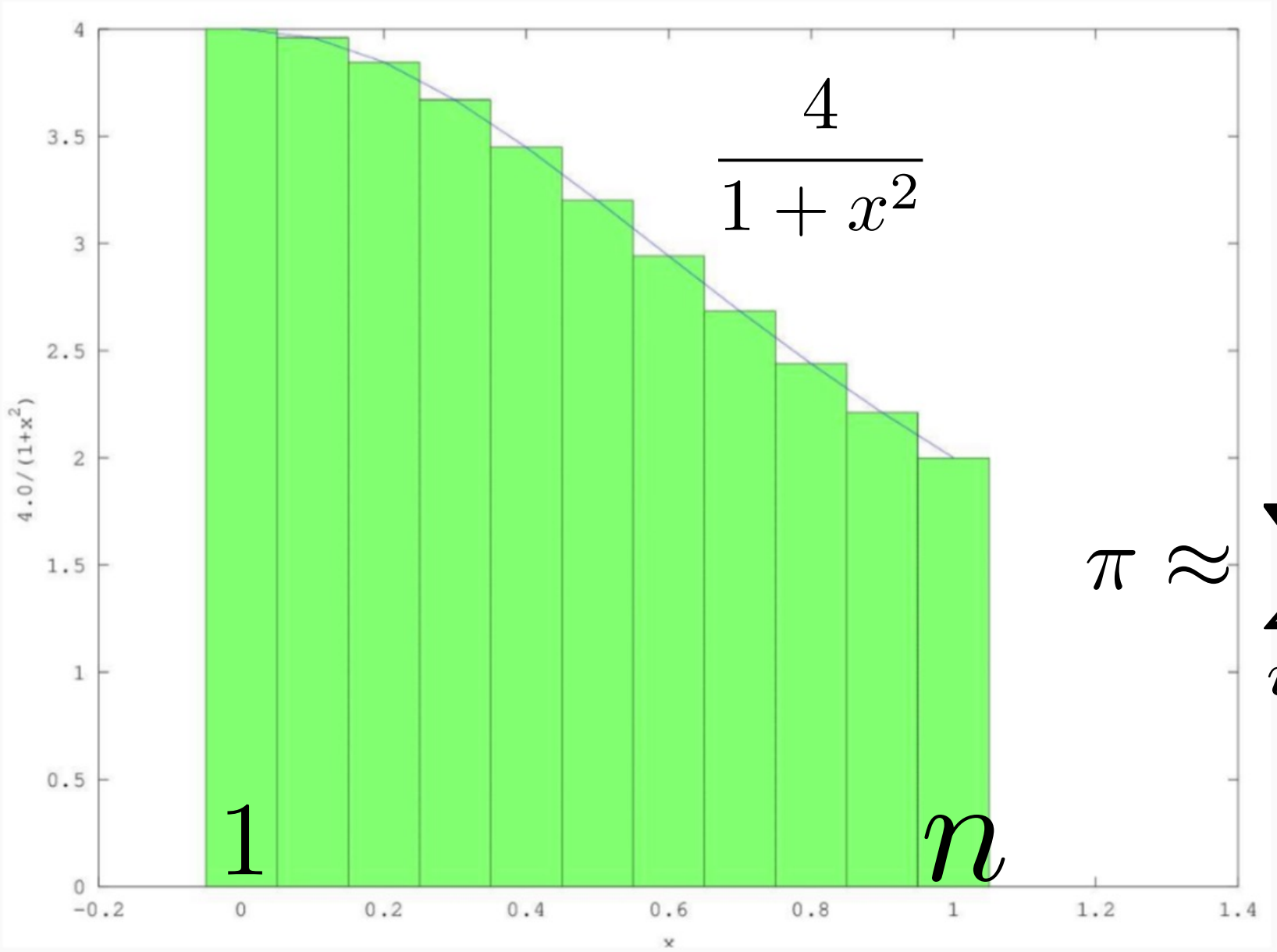
Serial Program to Calculate π



$$\int \frac{4}{1+x^2} = \pi$$

$$\Sigma_{i=1}^{N} \frac{4}{1+\left(\frac{i+\frac{1}{2}}{N}\right)^2} \approx \pi$$

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 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.

```
[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.

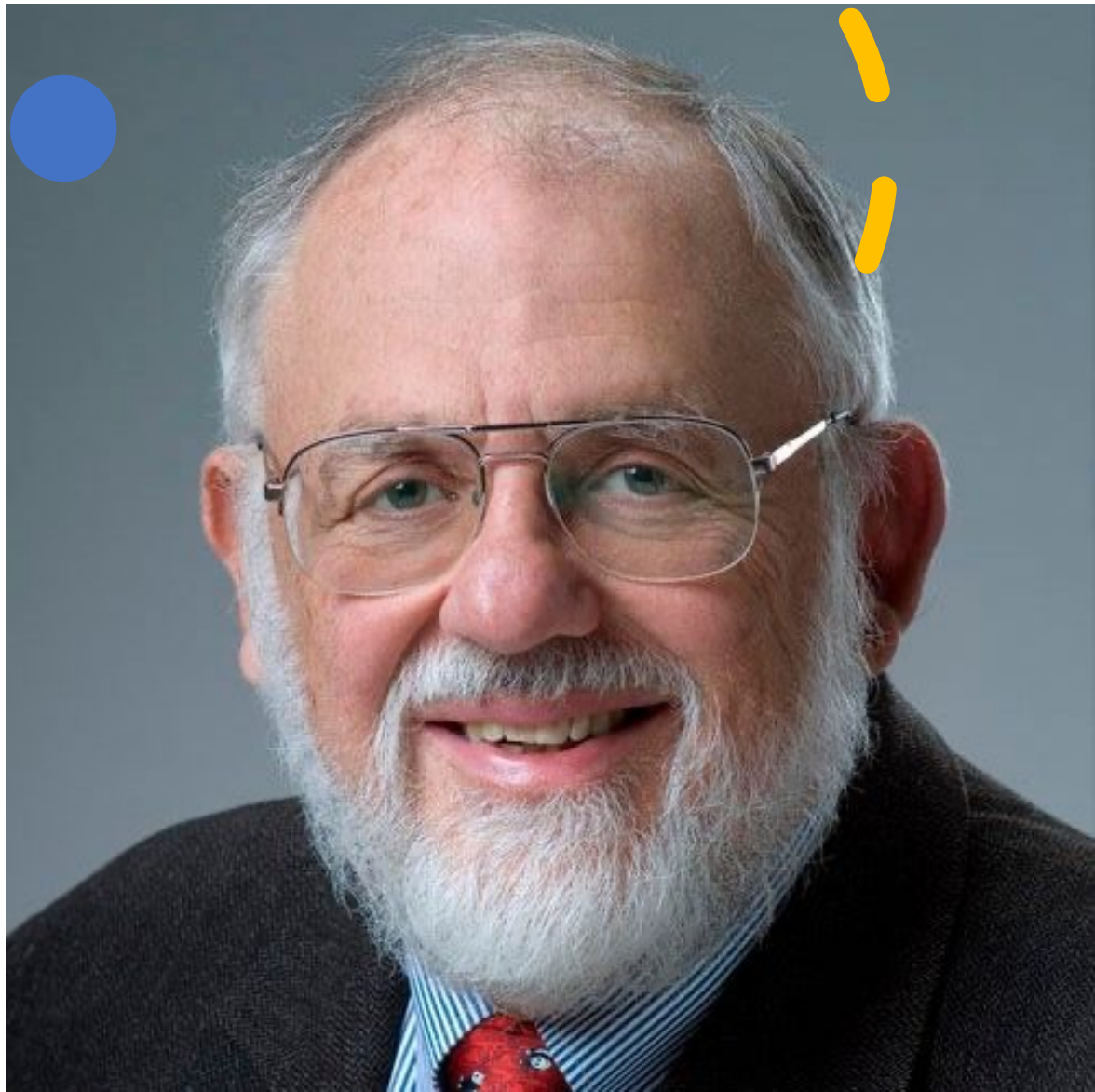
Take a look at the job output.

Parallelism – Embarrassingly Parallel

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

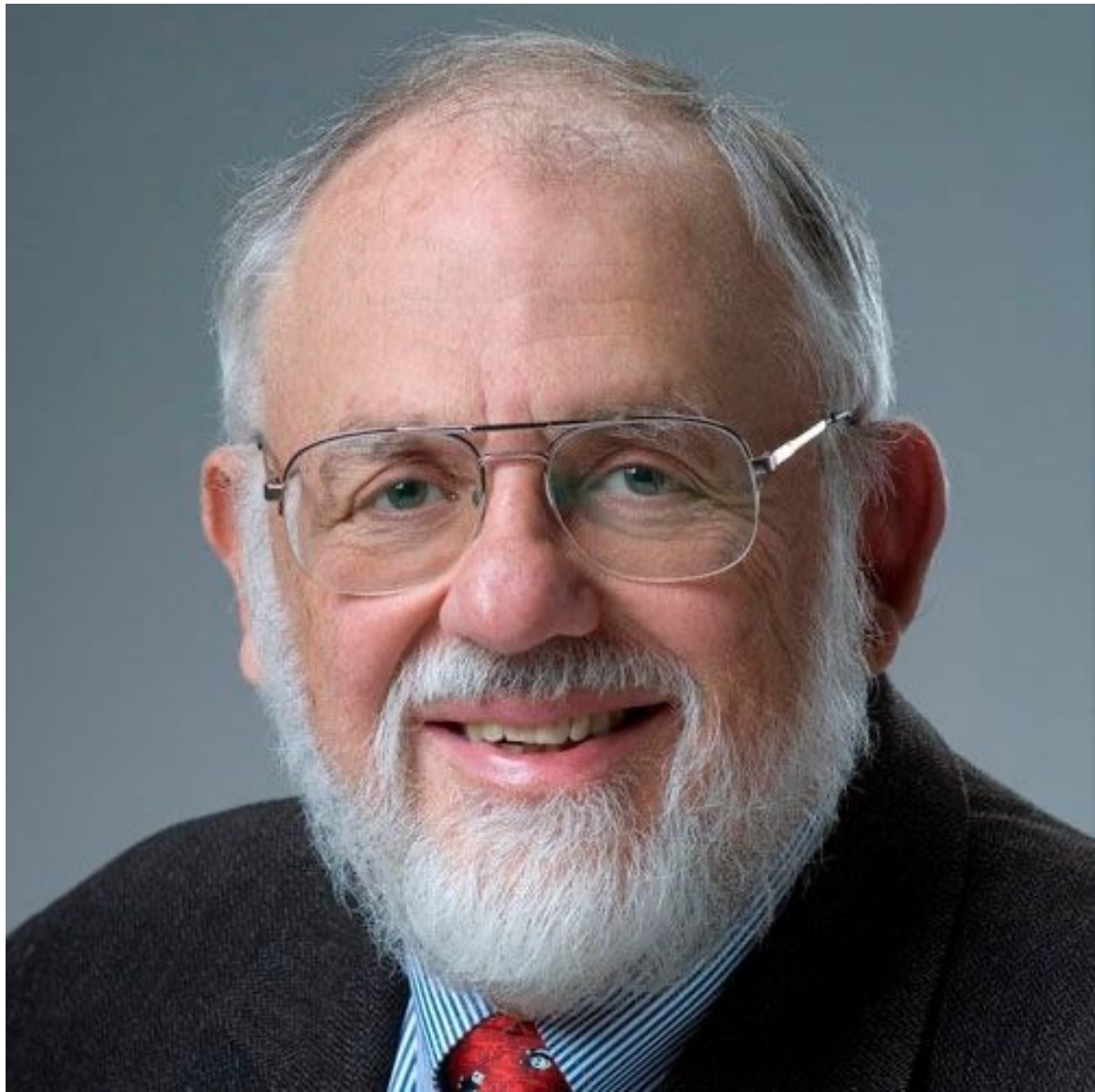
- The most common example is that you have a program that runs in serial and takes some input file, processes it, and produces some output.

- The problem is that you have 1,000 of the input files and want to run your program on each one.



Parallelism – Embarrassingly Parallel

This is ”embarrassing” because all you have to do is run 1,000 copies of your program on 1,000 CPUs each with a different input file and you are done.



SLURM ARRAYS

- One way to run the 1,000 copies of your program on 1,000 different inputs would be to write 1,000 slurm scripts each specifying a different input to your program and then sbatch submit them all. (this would work but there are better ways).

- SLURM arrays are used to schedule a lot of jobs with one slurm script.

```
[vanilla@hopper intro_workshop]$ nano slurm/calc_pi_array.sh
#!/bin/bash
#SBATCH --partition debug
#SBATCH --ntasks 1
#SBATCH --time 00:05:00
#SBATCH --job-name calc_pi_array
#SBATCH --mail-user your_username@unm.edu
#SBATCH --mail-type ALL
#SBATCH --array=1-12%3

echo "$HOSTNAME - $SLURM_ARRAY_TASK_ID"

module load miniconda3
source activate numpy

NUM_STEPS="${SLURM_ARRAY_TASK_ID}0000"
echo "Calculating pi with $NUM_STEPS..."
cd $SLURM_SUBMIT_DIR
python code/calcPiSerial.py $NUM_STEPS
```

Requires some annoying bash scripting.

$something means get the value of the variable "something"

--array says

1) **run 12 separate jobs**
2) **Store the count of the job in the variable SLURM_ARRAY_TASK_ID**

```
[vanilla@hopper intro_workshop]$ cat slurm/calc_pi_array.sh
#!/bin/bash
#SBATCH --partition debug
#SBATCH --ntasks 1
#SBATCH --cpus-per-task 3
#SBATCH --time 00:05:00
#SBATCH --job-name calc_pi_array
#SBATCH --mail-user your_username@unm.edu
#SBATCH --mail-type ALL
#SBATCH --array=1-12%3

echo "$HOSTNAME - $SLURM_ARRAY_TASK_ID"

module load miniconda3
source activate numpy

NUM_STEPS="${SLURM_ARRAY_TASK_ID}0000"
echo "Calculating pi with $NUM_STEPS..."
cd $SLURM_SUBMIT_DIR
python code/calcPiSerial.py $NUM_STEPS
```

```
[vanilla@hopper intro_workshop]$ sbatch slurm/calc_pi_array.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
```

Submit the array script.
Then enter squeue --me to see the job status.
Take a look at the job output. (How many output files do you have?)

JOB arrays are OK or very simple inputs like programs that take a single file as input. But even passing in a value takes some annoying variable manipulation.

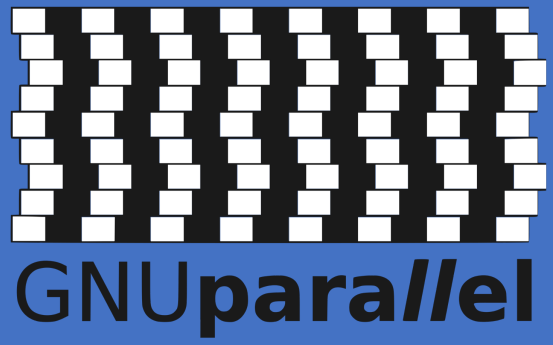
GNU Parallel is much more sophisticated it can take inputs in all sorts of ways. We will look at just 3 ways.

To access GNU parallel enter **module load parallel**

Let's experiment with parallel interactively…

***NOTE: we don't use srun to run parallel.**

GNU Parallel



Has been around for a very long time and has lots and lots of great features.

But basically it creates a job for every input it receives. The inputs can be specified in the command, read from a file, or be the output of another program.

It also remembers which jobs have finished and which still need to be run. So when you run out of time and resubmit it will automatically pick up where it left off.

```
[vanilla@hopper intro_workshop]$ salloc --partition debug --ntasks 2
salloc: Using account 2016199 from ~/.default_slurm_account
salloc: Granted job allocation 5275
salloc: Waiting for resource configuration
salloc: Nodes hopper011 are ready for job

$ LANG=C
$ parallel python code/calcPiSerial.py ::: 10 20 30 40

Pi = 3.14180098689309428295, (Diff=0.00020833330330116695)
(calculated in 0.000006 secs with 20 steps)
Pi = 3.14164473692265744376, (Diff=0.00005208333286432776)
(calculated in 0.000008 secs with 40 steps)
Pi = 3.14242598500109870940, (Diff=0.00083333141130559341)
(calculated in 0.000006 secs with 10 steps)
Pi = 3.14168524617974842528, (Diff=0.00009259258995530928)
(calculated in 0.000012 secs with 30 steps)
```

```
[vanilla@hopper intro_workshop]$ seq 10 10 100
10
20
30
40
50
60
70
80
90
100
```

GNU Parallel can read the output of other programs and use them as inputs to your program.
Here a copy of calc pi is run for each row in the output of seq

```
[vanilla@hopper intro_workshop]$ seq 10 10 100 | parallel python code/calcPiSerial.py
Pi = 3.141800986893094282 95, (Diff=0.00020833330330116695) (calculated in 0.000007
secs with 20 steps)
Pi = 3.142425985001098709 40, (Diff=0.00083333141130559341) (calculated in 0.000006
secs with 10 steps)
Pi = 3.141685246179748425 28, (Diff=0.00009259258995530928) (calculated in 0.000007
secs with 30 steps)
etc
```

```
[vanilla@hopper intro_workshop]$ find -name *.sh
./slurm/calc_pi_array.sh
./slurm/calc_pi_mpi.sh
./slurm/calc_pi_parallel.sh
./slurm/calc_pi_serial.sh
./slurm/gaussian.sh
./slurm/hostname_mpi.sh
etc

$ find -name *.sh | parallel wc -l
7  ./code/vecadd/vecaddmpi_cpu.sh
19 ./slurm/calc_pi_array.sh
15 ./slurm/calc_pi_mpi.sh
20 ./slurm/calc_pi_parallel.sh
14 ./slurm/calc_pi_serial.sh
16 ./slurm/gaussian.sh
15 ./slurm/hostname_mpi.sh
etc
```

A common application is to use find to produce a list of paths with some extension.

Then parallel runs some program on each path.

In this case wc -l counts the lines in a file. In some real CARC examples the input files are phylogenetic trees, graphs, neuroimages, or CT scans.

```
[vanilla@hopper intro_workshop]$ exit
exit
salloc: Relinquishing job allocation 5275
```

Don’t forget to exit your salloc allocation.

```
(numpy)[vanilla@hopper intro_workshop]$ cat slurm/calc_pi_parallel.sh
#!/bin/bash
#SBATCH --partition debug
#SBATCH --nodes 2
#SBATCH --ntasks-per-node 4
#SBATCH --time 00:05:00
#SBATCH --job-name calc_pi_parallel
#SBATCH --mail-user your_username@unm.edu
#SBATCH --mail-type ALL

module load parallel
module load miniconda3
source activate numpy

LANG=C
cd $SLURM_SUBMIT_DIR
parallel --sshloginfile $PBS_NODEFILE \
--env PATH \
--workdir $SLURM_SUBMIT_DIR \
"hostname; python code/calcPiSerial.py {}" :::: data/step_sizes.txt
```

Take a look at slurm/calc_pi_parallel.sh.

In this example parallel reads the parameters from a file and runs a copy of calcPiSerial.py on each row.

```
(numpy)$sbatch slurm/calc_pi_parallel.sh
sbatch: Using account 2016199 from ~/.default_slurm_account
Submitted batch job 5276
```

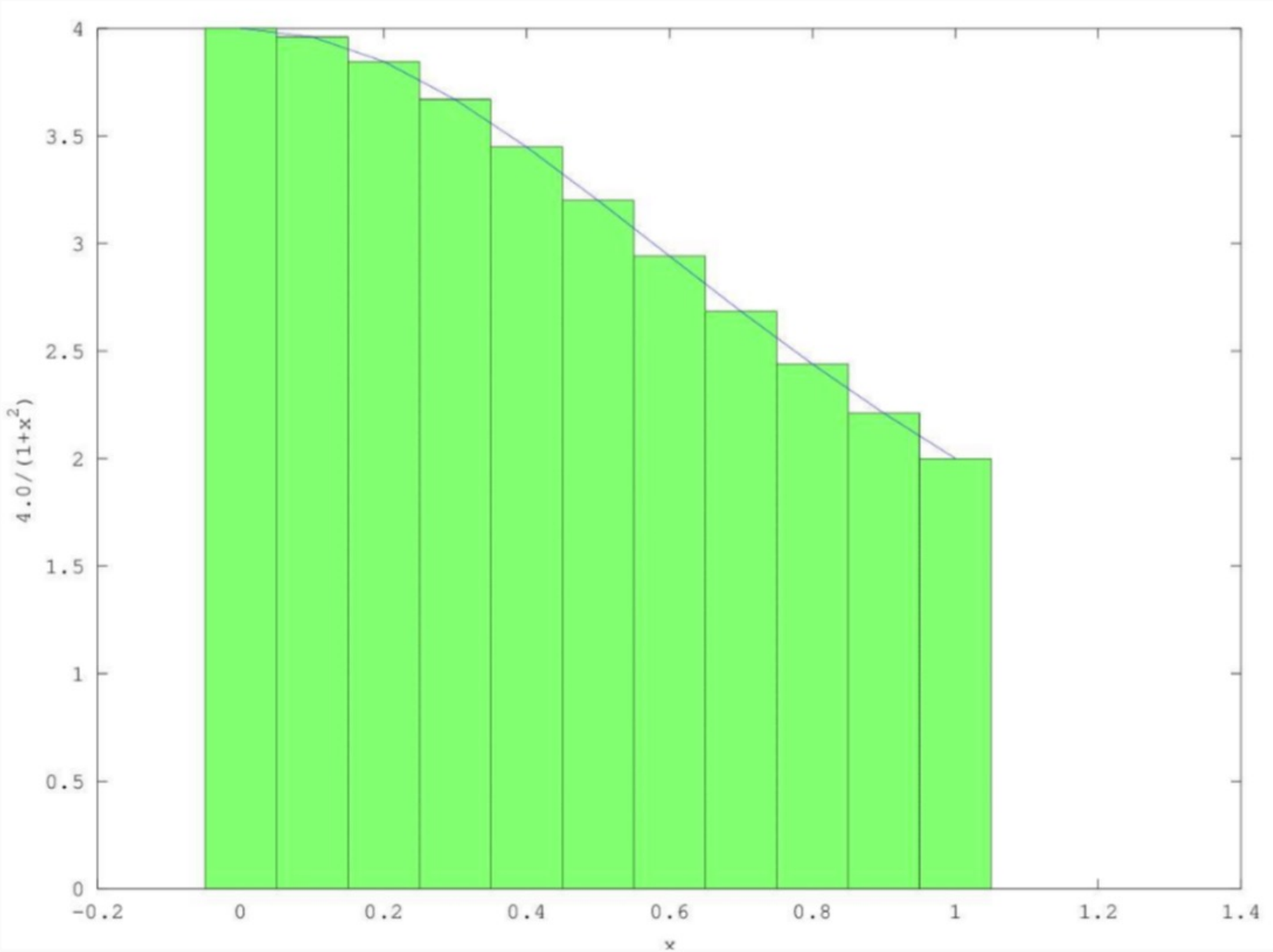
Submit the job, check it's progress with squeue --me, and take a look at the output.

Parallelism – Coupled Parallelism

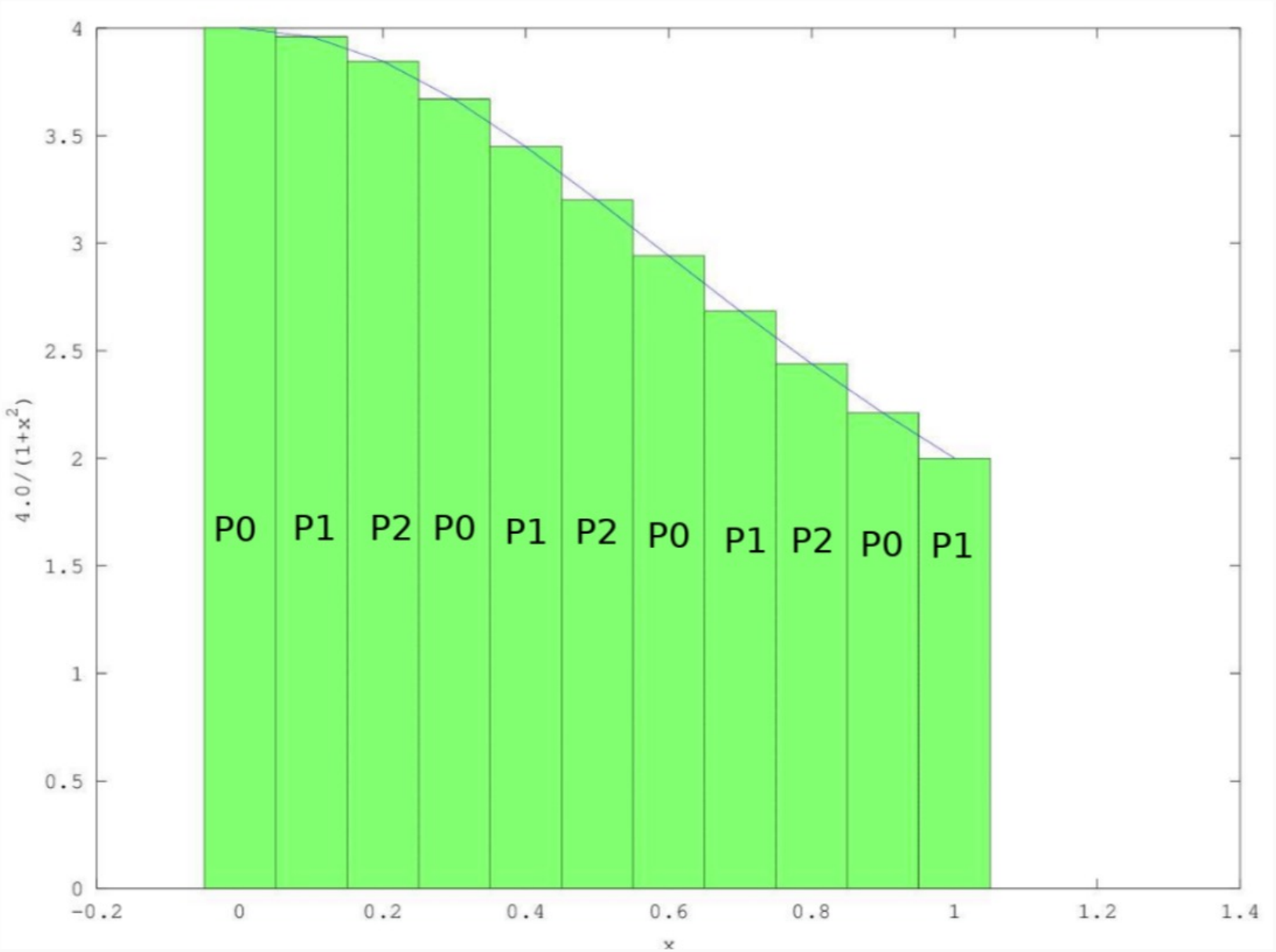
- Coupled problems are those where the CPUs need to work together to solve a problem by communicating with each other.
- Many commercial and research programs designed to run on HPC systems like CARC use a library called the message passing interface (MPI) to do this.

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

Serial Program to Calculate π



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.

Make sure you are in the ~/workshops/intro_workshops directory.
Install your mpi conda environment from file:

```
conda env create –f conda_envs/mpi_numpy.yml
```

```
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))
```

```
#!/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

Run calc_pi_mpi.sh.

Vary the number of tasks it uses.

Use squeue to monitor the state of your job,

Look at your output files.

What is the relationship between the number of tasks and how cast it calculates pi?

Section on Easley

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