

CHEM567: Topics in Physical Chemistry

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Version 0.1



Goals

- 1) SLURM scheduler literacy
- 2) Ability to employ embarrassingly parallel solutions
- 3) Ability to employ coupled parallel solutions.
- We wont cover file transfer, storage systems, module system, conda, PBS. (These are all covered in depth in the video tutorials)

Agenda

- HPC and Parallelism
- HPC Schedulers
- SLURM
- Embarrassingly Parallel
SLURM Arrays
- GNU Parallel
- Coupled Parallelism
- MPIwith MPI



We will have one 15 minute break. Opportunity to see the machine room.
Tuesday, February 2, 20XX

Sample Footer Text

Logging into Hopper



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

Use your CARC username and password.

Kevin, Slava, and Jose can help you login if you have trouble.

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."

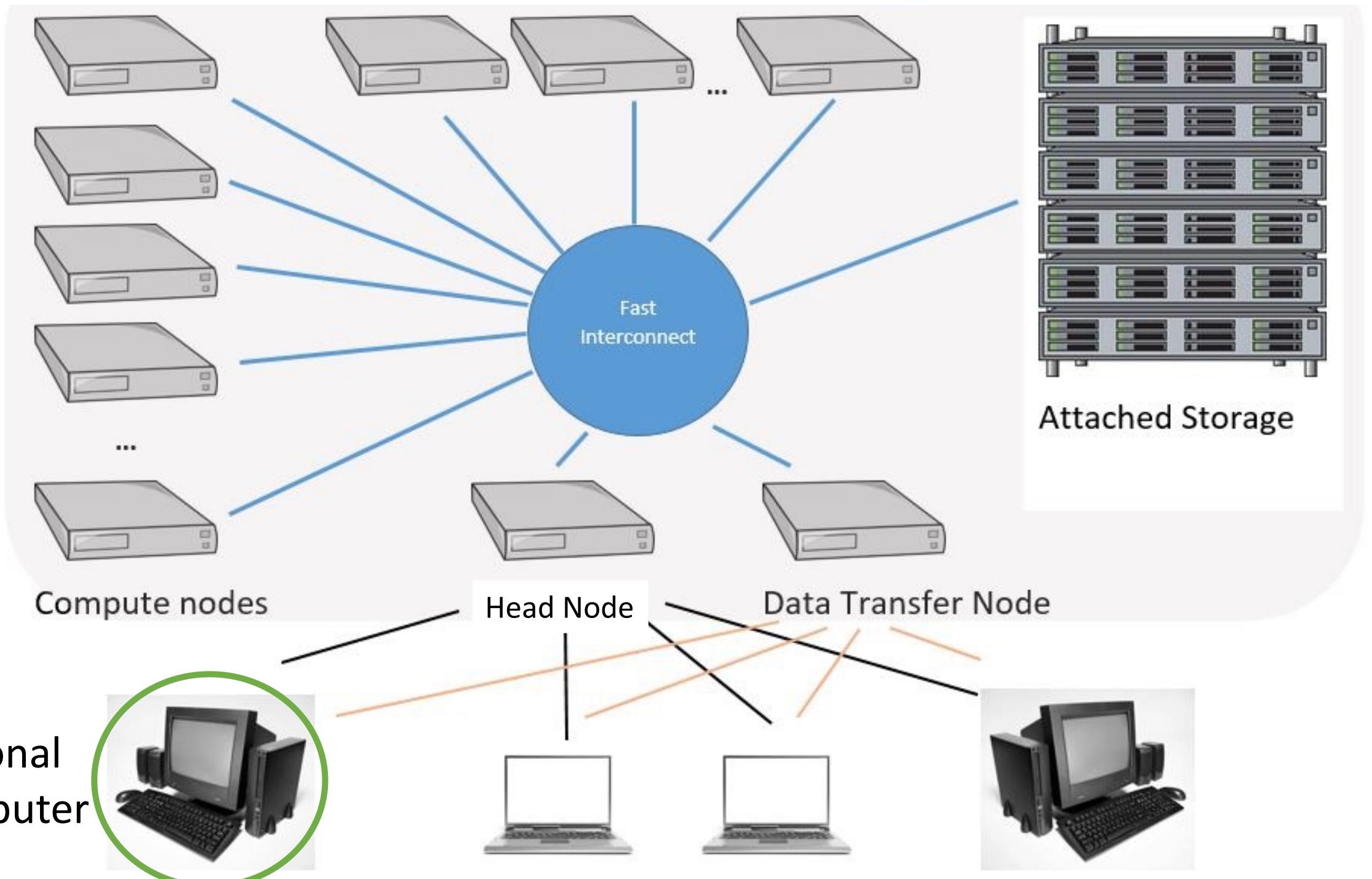
Please send citations to publications@carc.unm.edu.

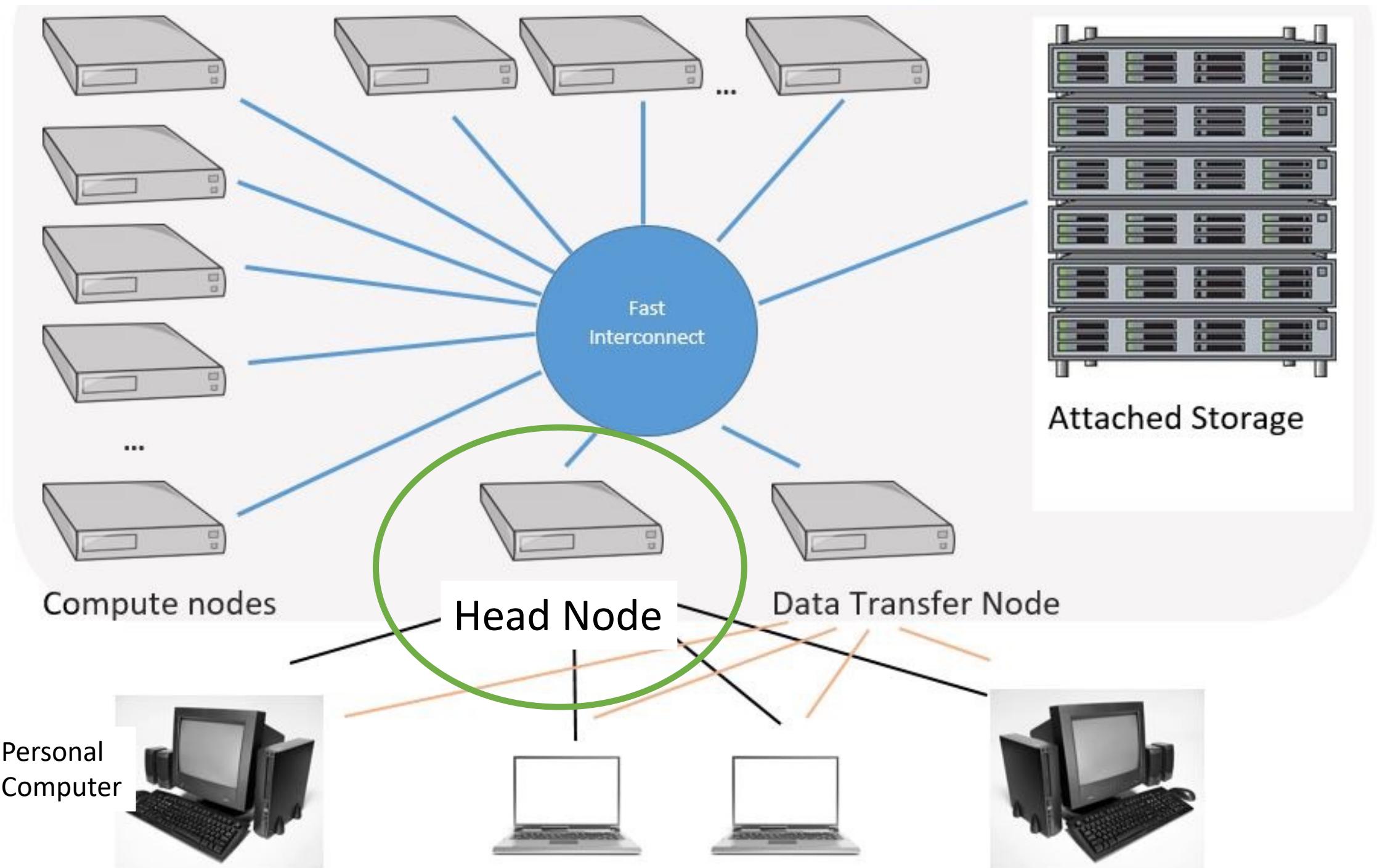
There are three types of slurm partitions on Hopper:

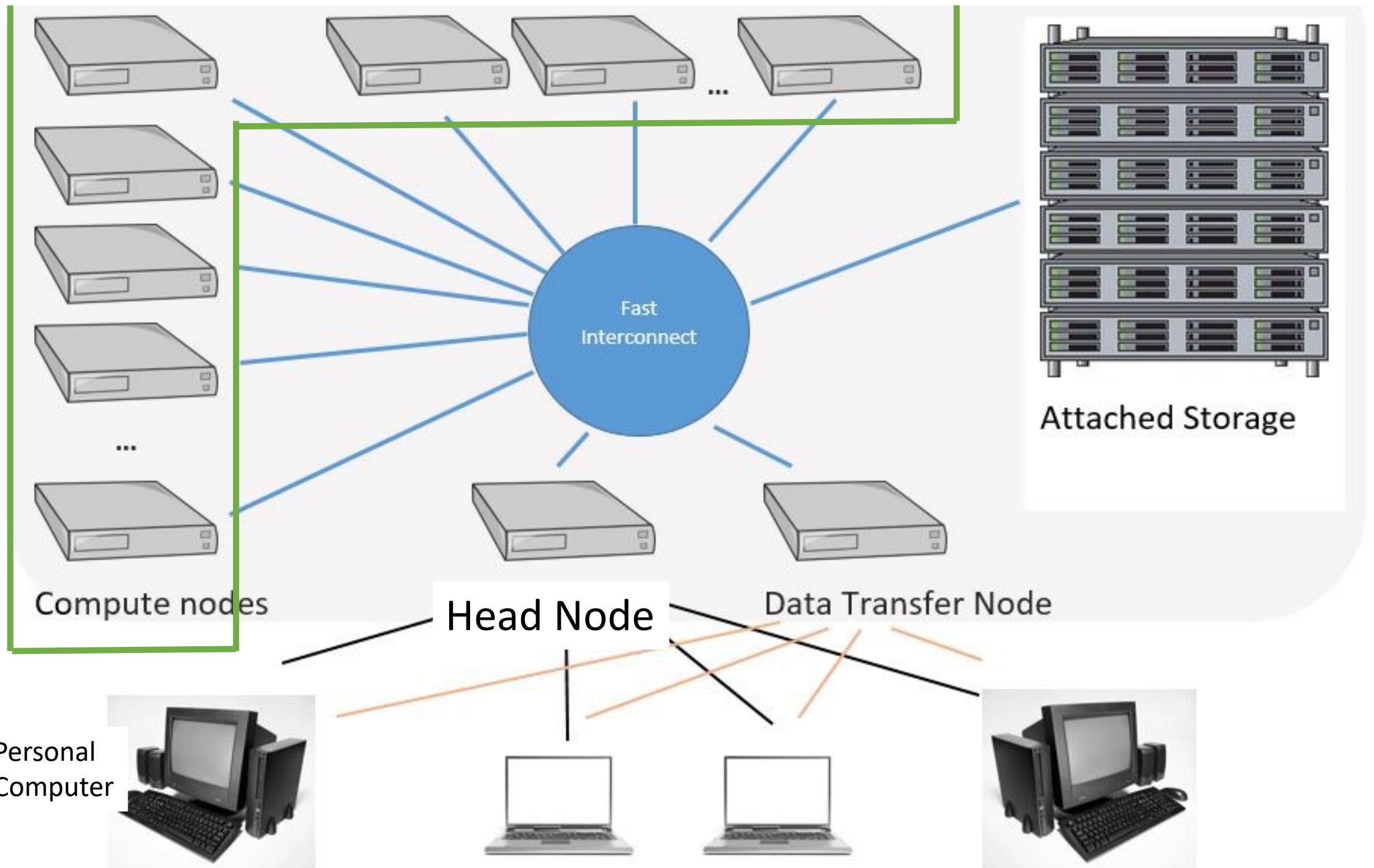
- 1) General - this partition is accessible by all CARC users.
- 2) Condo - preemptable scavenger queue available to all condo users. Your job must use checkpointing to use this queue or you will lose any work you have done if it is preempted by the partition's owner.
- 3) Named partitions - these partitions 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:~ \$









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!



SLURM MCKENZIE

```
[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
totals:	1	9	0	7	10	320	0

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Welcome to the Center for Advanced Research Computing

The UNM Center for Advanced Research Computing is the hub of computational research at UNM and one of the largest computing centers in the State of New Mexico. It is an interdisciplinary community that uses computational resources to create new research insights. The goal is to lead and grow the computational research community at UNM.

Get started at CARC

Create a help ticket

CARC systems information
CARC infrastructure
Resource limits 
Storage and backup
Export control
JupyterHub cluster links
System status and downtime
System Usage by Principal Investigator years

CARC launches new condo cluster

Hopper Configuration

Queue:	General	Debug	Condo	Private
Number of Processors	64	8	192	Determined by queue owner
Number of Nodes	2	2	6	
Processors per Node	32	8	32	
Walltime(H:M:S)	48:00:00	04:00:00	48:00:00	

```
[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)
Commands

Slurm
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



WARNING !!



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 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	2 (QOSMaxCpuPerUserLimit)
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)

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
```

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
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
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
```

```
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 been  
the -G option in  
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 assigned to a project.  
the -G option is required.  
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  
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.

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

```

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_example.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
```

hostname

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

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

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.

We submit our slurm shell script with the sbatch command.

Workflow

Head Node

User 1

Program A

Script A

User 2

Program B

Script B

Compute Node 01

Compute Node 02

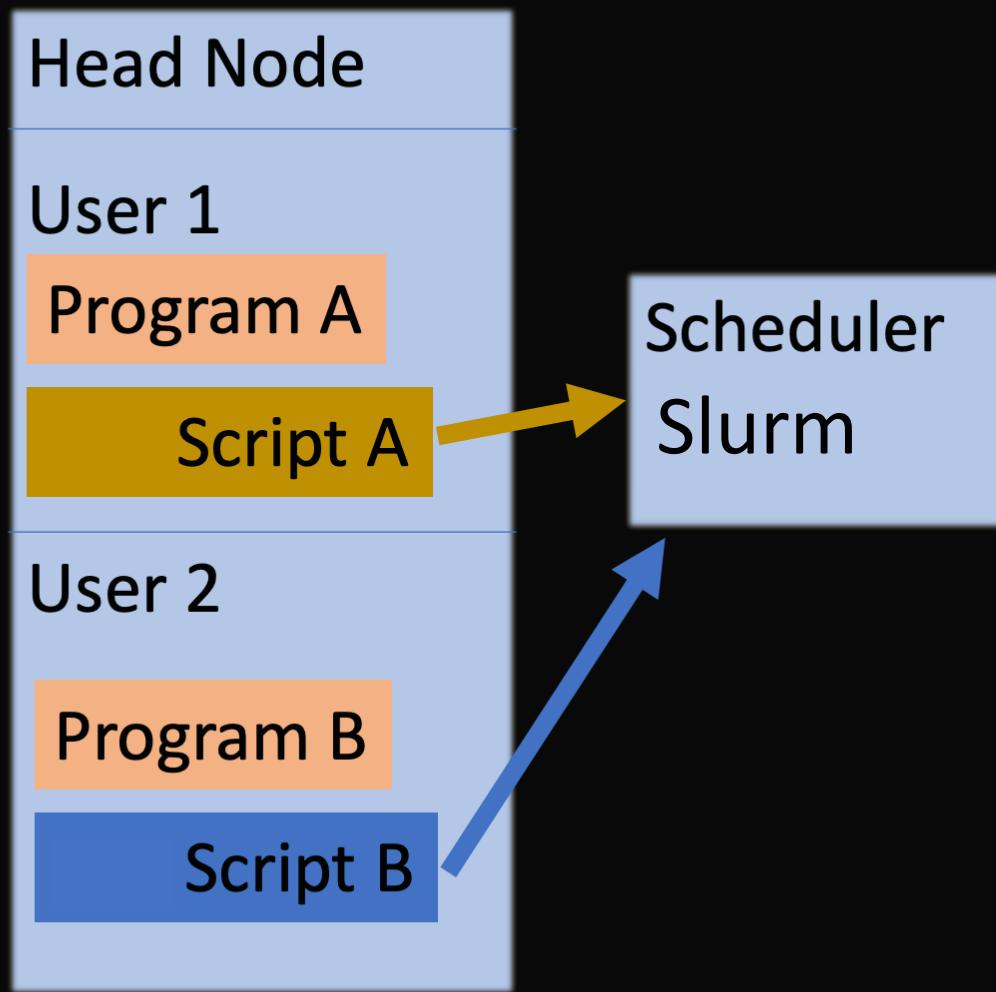
Compute Node 03

Compute Node 04

Compute Node 05

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

Workflow



Compute Node 01

Compute Node 02

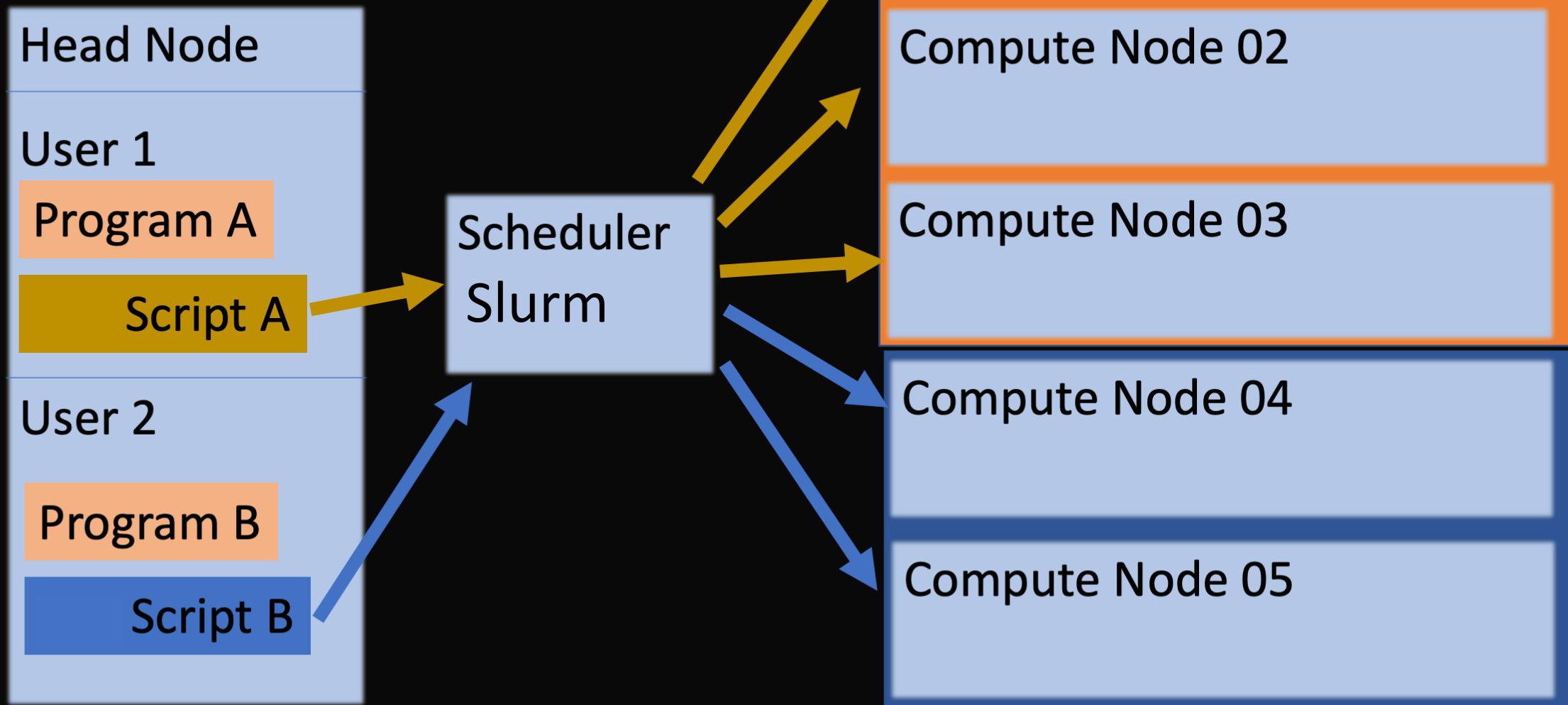
Compute Node 03

Compute Node 04

Compute Node 05

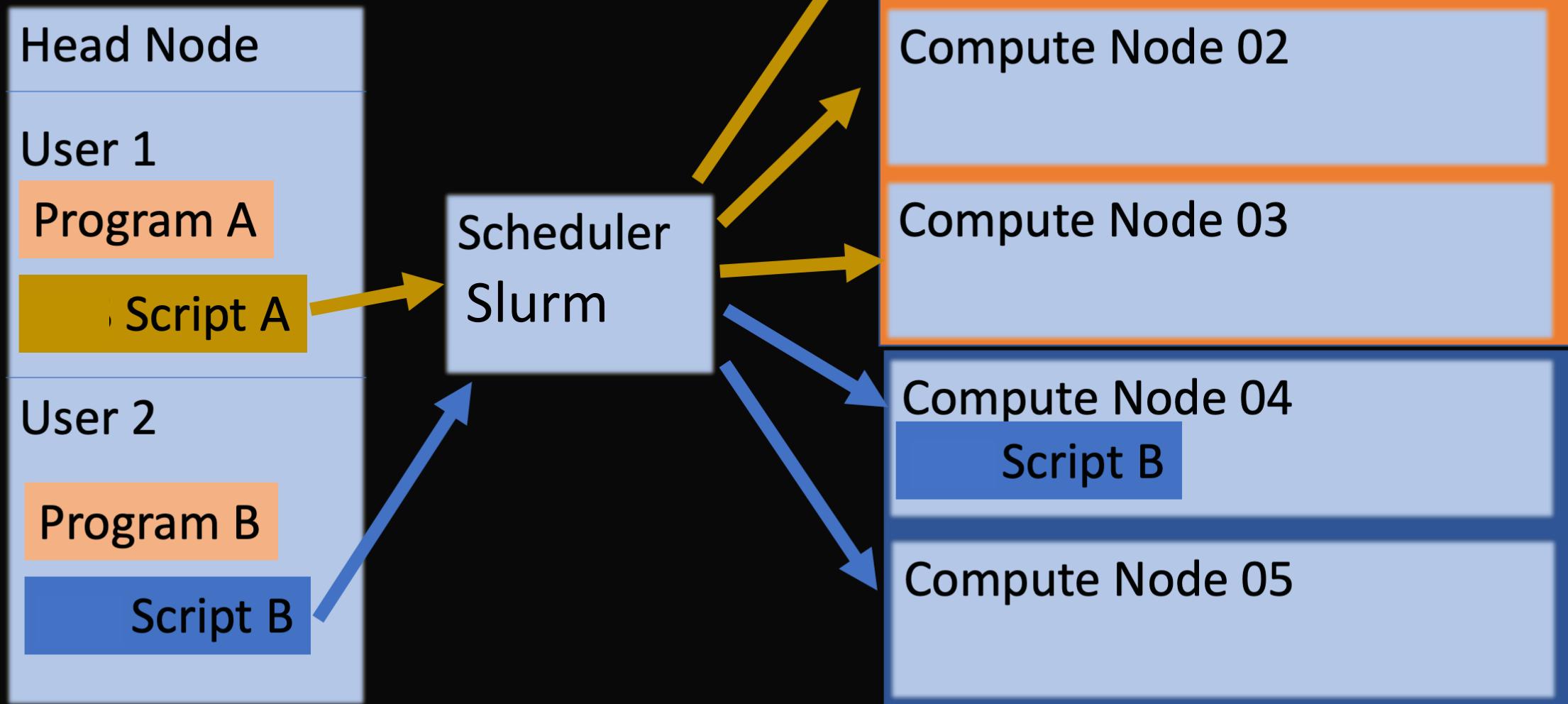
Shared filesystems – All nodes can access the same programs and write output

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.

Head Node

User 1

Program A

Script A

User 2

Program B

Script B

Scheduler
Slurm

Compute Node 01

Script A

Program A

Compute Node 02

Program A

Program A

Compute Node 03

Program A

Program A

Compute Node 04

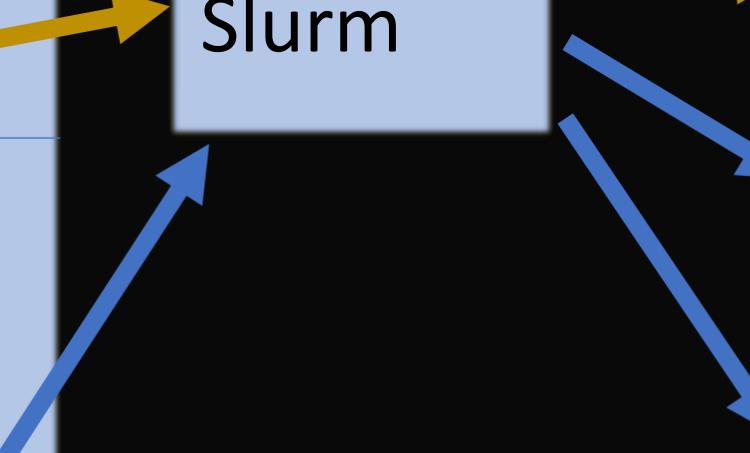
Script B

Program B

Compute Node 05

Program B

Program B



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]$ 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
```

Why did it only run the program once instead of 4 times?

```
[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]$
```

Take a look at the
output file.

```
[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]$ 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
```

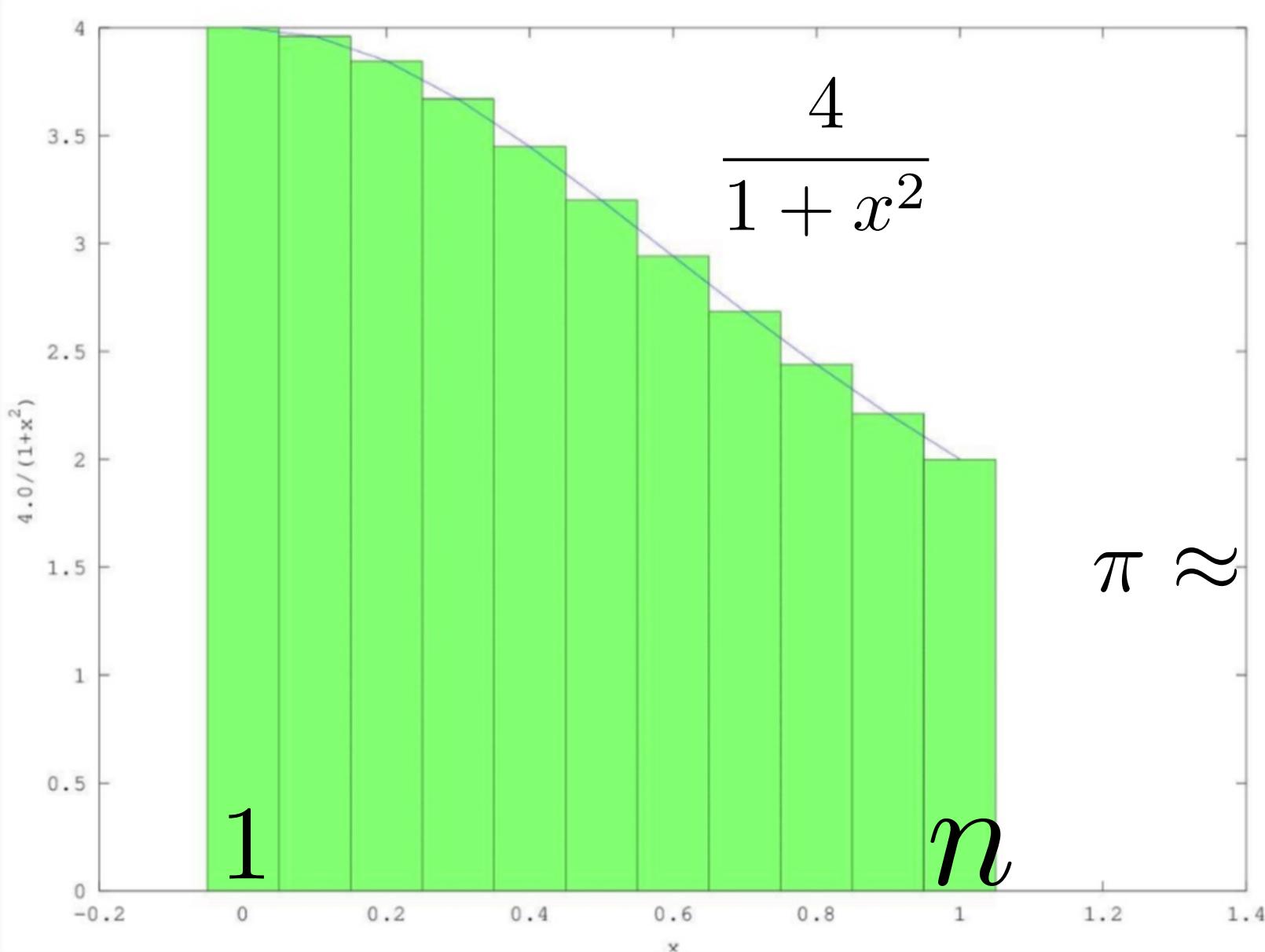
Edit `slurm/calc_pi_serial.sh`.

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.

Serial Program to Calculate π



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

```
# 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)
```

Parallelism – Embarrassingly Parallel

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

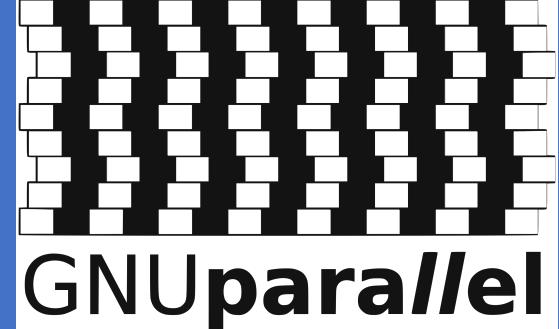


Parallelism – Embarrassingly Parallel

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.



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
```

```
$ module load parallel
$ 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 = 3.14180098689309428295, (Diff=0.00020833330330116695) (calculated in 0.000007  
secs with 20 steps)  
Pi = 3.14242598500109870940, (Diff=0.00083333141130559341) (calculated in 0.000006  
secs with 10 steps)  
Pi = 3.14168524617974842528, (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.

```
(numpy)$ seq 10 10 100 | parallel srun python code/calcPiSerial.py
```

The parallel commands we executed so far ran on the head node (don't worry it wasn't much computation).

To get parallel to use slurm and run on a compute node we have to add srun.

```
(numpy)$ seq 10 10 100 | parallel srun python code/calcPiSerial.py
```

You have not been allocated GPUs. To request GPUs, use the -G option in your submission script.

Pi = 3.14180098689309428295, (Diff=0.00020833330330116695) (calculated in 0.000015 secs with 20 steps)

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 = 3.14160966039249744952, (Diff=0.00001700680270433352) (calculated in 0.000029 secs with 70 steps)

...

Pi = 3.14160098692312539370, (Diff=0.0000083333333227770) (calculated in 0.000036 secs with 100 steps)

```
[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
```

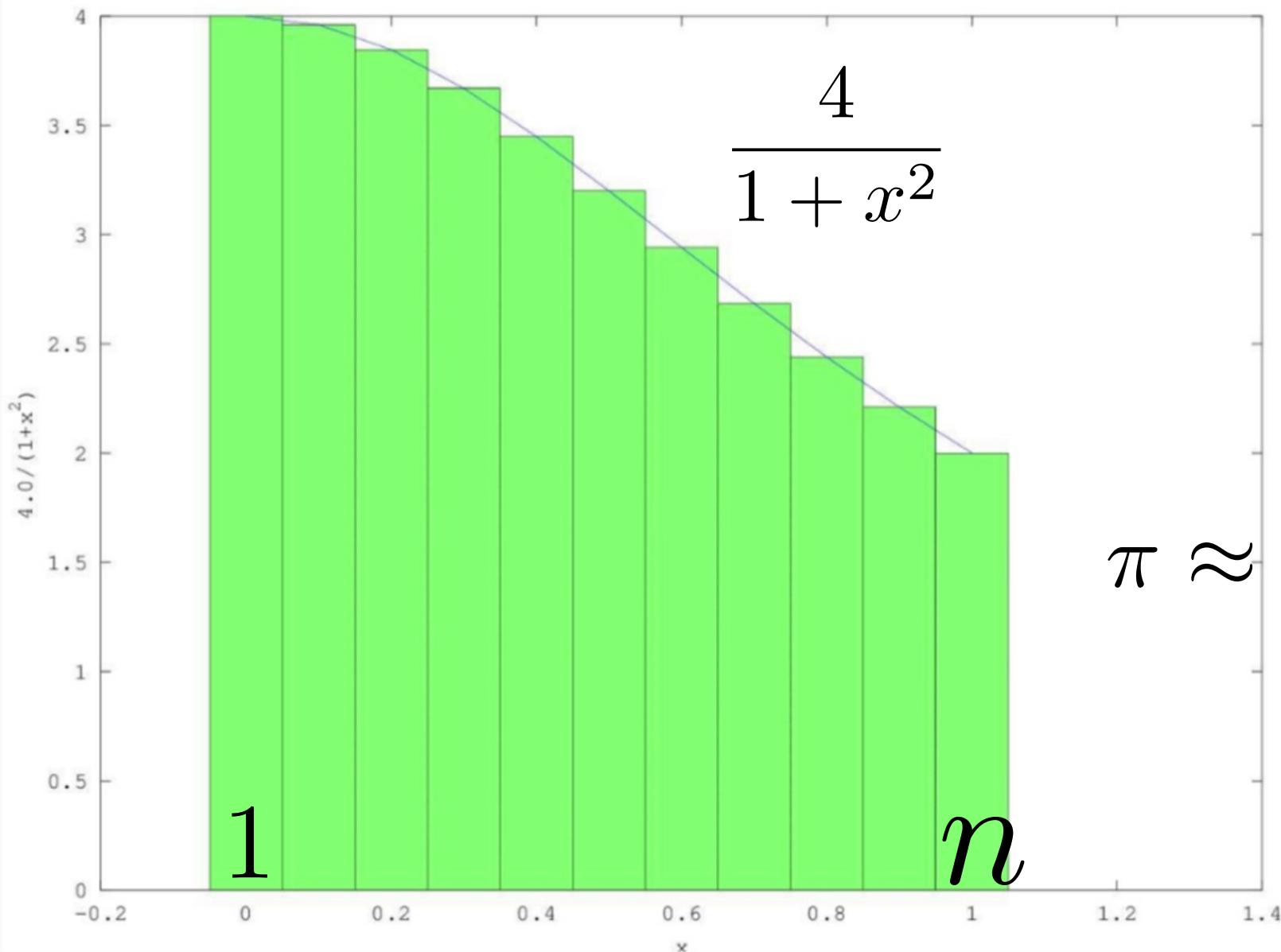
Submit the job, check it's progress with `squeue --me`, and take a look at the output.

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.

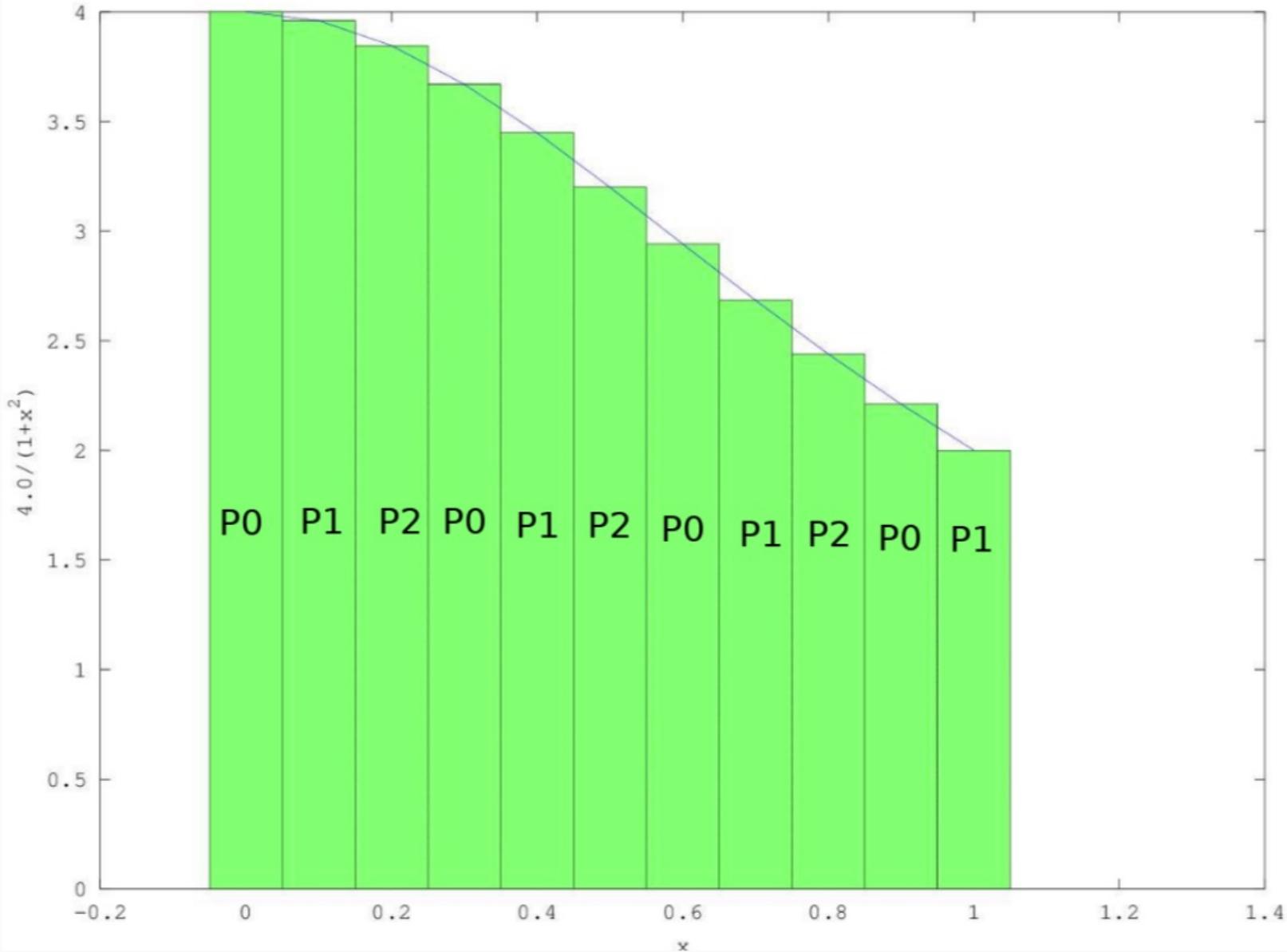


Serial Program to Calculate π



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

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 100000000
```

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?

BONUS: Example Code with MPI and CUDA

- Let's take a look at `~/workshops/intro_workshop/code/vecadd`
- The Makefile allows you to compile C code for CPU using MPI or a MPI and CUDA code.
- First though we have to provide a MPI library

```
module load openmpi
```

BONUS: Example Code with MPI and CUDA

- This code just takes two vectors and corresponding elements together to create a new array.
- This code is NOT written to be efficient – I tried to write it to make the relationship between MPI processes clear.

```
$ cd ~/workshops/intro_workshop/code/vecadd  
$ module load openmpi
```

```
$ cd ~/workshops/intro_workshop/code/vecadd  
$ module load openmpi  
$ cat Makefile
```

```
gpu:  
nvcc -arch sm_35 -c vecadd_gpu.cu -o vecadd_gpu.o  
mpic++ -c vecadd_mpi_gpu.c -o vecadd_mpi_gpu.o  
mpic++ vecadd_mpi_gpu.o vecadd_gpu.o -lcudart -o vecadd_mpi_gpu  
  
cpu:  
mpic++ vecadd_mpi_cpu.c -o vecadd_mpi_cpu  
  
clean:  
rm vecadd_mpi_gpu vecadd_mpi_cpu vecadd_mpi_gpu.o  
vecadd_mpi_cpu.o vecadd_gpu.o
```

```
$ cd ~/workshops/intro_workshop/code/vecadd  
$ module load openmpi  
$ make cpu  
mpic++ vecadd_mpi_cpu.c -o vecadd_mpi_cpu
```

```
$ cd ~/workshops/intro_workshop/code/vecadd
$ module load openmpi
$ make cpu
mpic++ vecadd_mpi_cpu.c -o vecadd_mpi_cpu
$ ls
Makefile  vecadd_gpu.cu  vecadd_mpi_cpu  vecadd_
_mpi_cpu.c  vecaddmpi_cpu.sh  vecadd_mpi_gpu.c
```

```
$ cd ~/workshops/intro_workshop/code/vecadd
$ module load openmpi
$ make cpu
mpic++ vecadd_mpi_cpu.c -o vecadd_mpi_cpu
$ ls
Makefile  vecadd_gpu.cu  vecadd_mpi_cpu  vecadd_
_mpi_cpu.c  vecaddmpi_cpu.sh  vecadd_mpi_gpu.c
$
```

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