Introduction to Kamiak

Training Workshop

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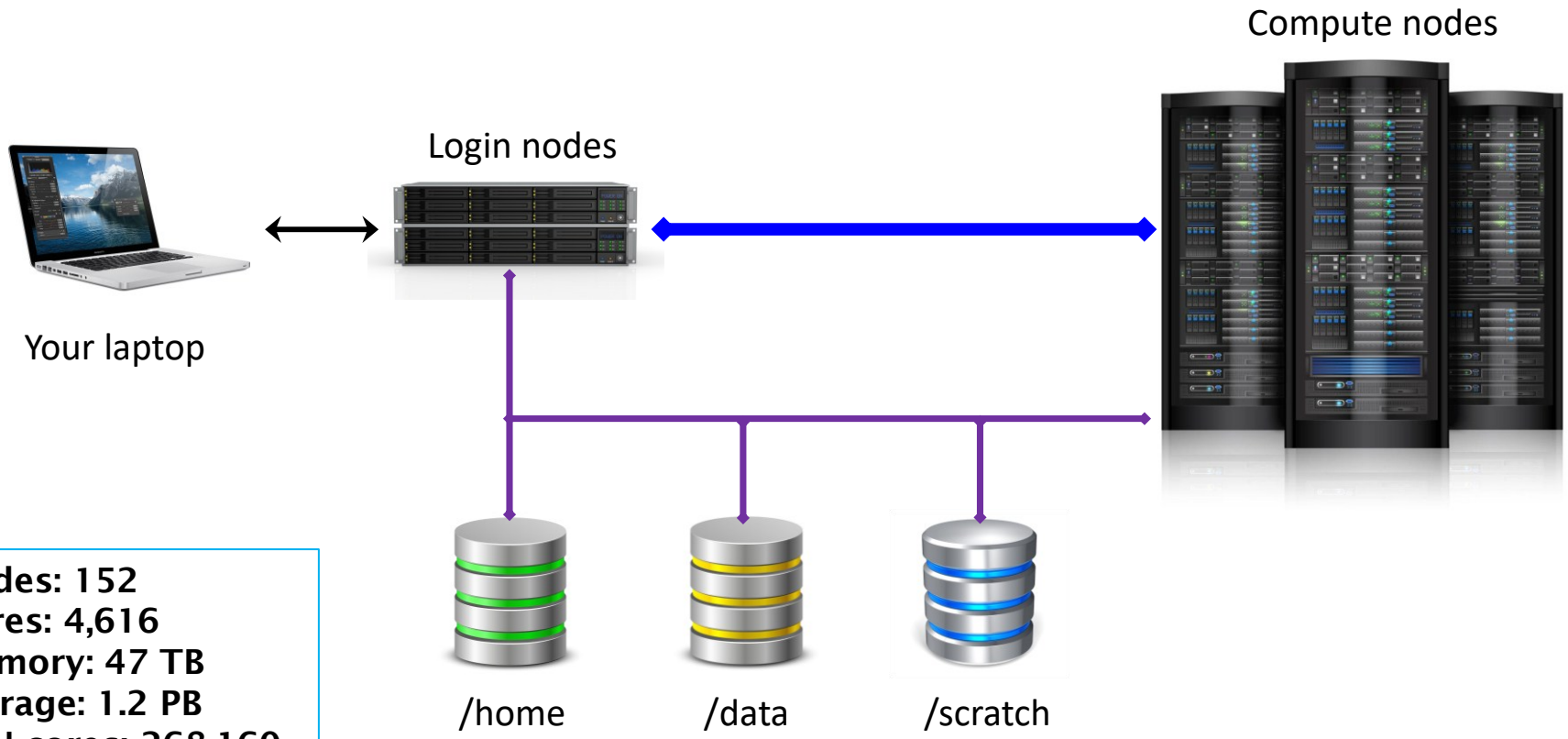
hpc.wsu.edu/training	***Documents***
hpc.wsu.edu/training/slides	***These slides***
hpc.wsu.edu/cheat-sheet	***Cheat Sheet***

What you will learn today

- What is Kamiak
- How to run jobs on Kamiak
  - Submit batch jobs
  - Interactive compute session
  - Types of jobs
- Exercises
  - Transferring files to and from Kamiak
  - Logging into Kamiak
  - Running batch jobs
  - Running an interactive compute session
  - Running job arrays
  - Running gpu jobs
  - Using scratch storage
  - Using snapshots

What is Kamiak

- A **cluster** of computers called **nodes**, connected by a high-speed network
- Each computer is like your laptop, but with more cores and memory
- Applications can run in **parallel** over many cores and across multiple nodes
- **Speeds up** solving large problems

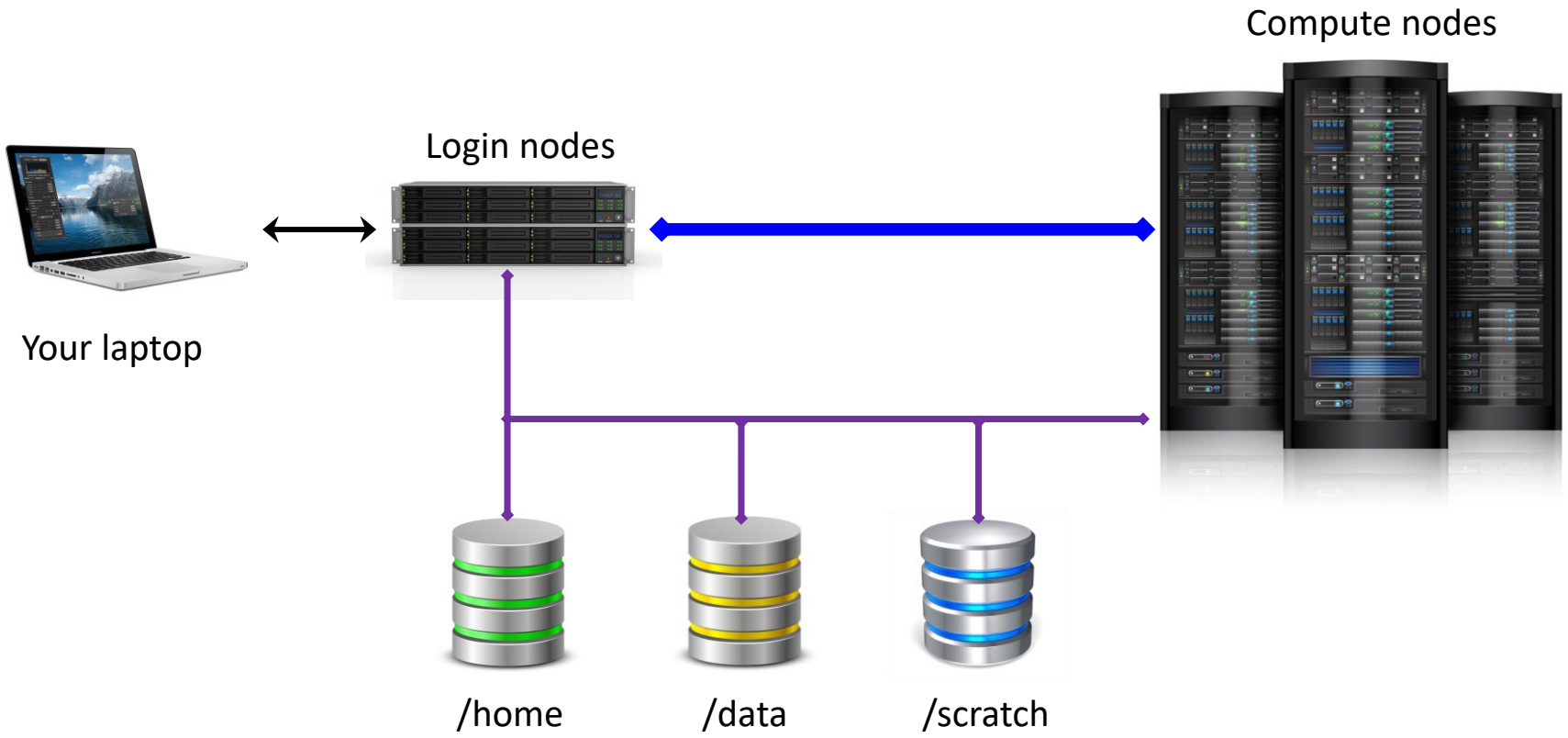


Nodes: 152
Cores: 4,616
Memory: 47 TB
Storage: 1.2 PB
GPU cores: 268,160

Kamiak Storage

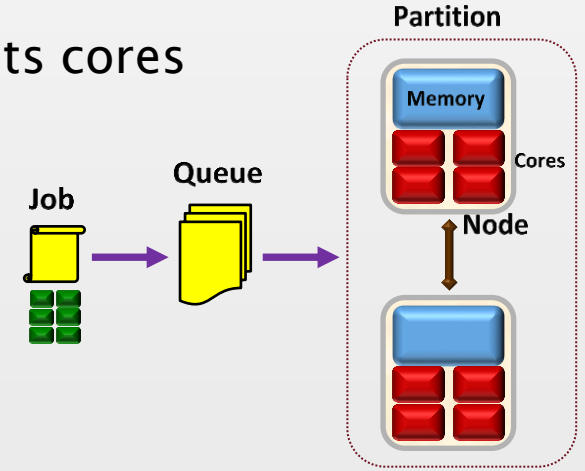
- Kamiak has 3 types of storage available to users

/home/*your.name*	100GB per user
/data/lab/*pi.labname*	500GB per faculty lab group
	Extra storage is available for rent from the CIRC service center
/scratch	Temporary storage, 2-week lifetime, 10TB limit per user



Running Jobs on Kamiak

- **Nodes** are grouped into **partitions**, each owned by a faculty or college
- All nodes also belong to a shared **kamiak** partition, available to all users
- You submit a **job** to a partition asking for **nodes**, **tasks,** and **cores**
- Job gets added to a partition's **queue** to wait until resources are available
- **Slurm** job scheduler decides ***who goes first***, ***who gets what***, ***who gets bumped***
- Investors have priority access to the nodes they own
- Will **preempt** job in backfill if investor's job needs its cores
- Applications only run in parallel if built to do so
- Resource requirements differ for each app



How to Run Jobs on Kamiak

There are two ways to run jobs on Kamiak

- **sbatch** *myJob.sh* ***Batch job submission***
  - Says which partition to submit to (default is kamiak)
  - Says what resources your job needs (cpu's/cores, memory, GPU's)
  - Says what program to run
- **idev** ***Interactive session on compute node***
  - Puts you on a compute node
  - Just type in commands and see them executed

Do not run applications or installs on the login nodes, use sbatch or idev instead to run them on a compute node

Types of Jobs

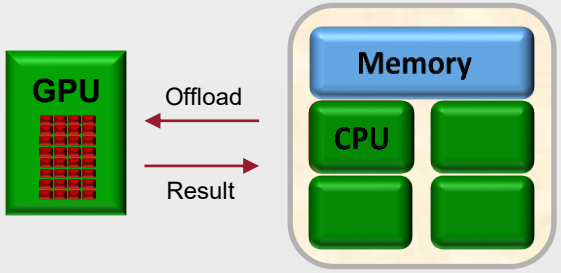
- **Single node**
  - Single program instance
  - Multithreading over multiple cores
  - Threads share memory

```
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=10
export OMP_NUM_THREADS=
$SLURM_CPUS_PER_TASK
```

- **Multiple nodes**
  - Each task is a program instance
  - Tasks do not share memory
  - Communicate by message-passing

```
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=10
```

- **GPU (Graphics Processing Unit)**
  - Thousands of tiny pixel cores, and matrix processors
  - Offloads kernel function to run over many data points
  - Requires CUDA, OpenACC




```
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=1
#SBATCH --gres=gpu:tesla:1
```

See samples in: /opt/apps/samples/advanced

Follow along

Transferring Files to and from Kamiak

Make sure you are on your laptop, not logged into Kamiak

- ***Open a terminal window***

  Terminal >> New Window (for Windows, Start >> Ubuntu)

- ***Copy from Kamiak to your laptop***

  scp -r *your.name*@kamiak.wsu.edu:/opt/apps/samples/tests ~/

  ↑ *Recursive, copies all files* ↑ *From Kamiak* ↑ *To laptop*

  ls -l -R tests

- ***Copy from your laptop to Kamiak***

  scp -r tests *your.name*@kamiak.wsu.edu:~/

  ↑ *From my laptop* ↑ *To my home folder on Kamiak*

- ***Synchronize folder contents (copies changed or added files, does not delete)***

  rsync -ravx tests/ *your.name*@kamiak.wsu.edu:~/tests

  ↑ *All files* ↑ *From laptop* ↑ *To Kamiak*

Follow along

Logging Into Kamiak

- ***Open a terminal window***

  Terminal >> New Window (for Windows, Start >> Ubuntu)

- ***Log into Kamiak***

  ssh *your.name*@kamiak.wsu.edu **# To logout: exit**

- ***One-time setup only for this training***

  source /opt/apps/samples/training/training_only_setup.sh

  cd training

Follow along

Submitting Batch Jobs to Kamiak

- ***Create/edit a job script***

  cat myJob.sh

- ***Submit the job script to the job queue***

  sbatch myJob.sh **# To test: sbatch --test-only myJob.sh**

- ***View the job queue***

  squeue -u *your.name* **# Shows pending and running jobs**

  squeue -j *jobNumber*

- ***See output***

  cat myJob*.out

- ***Cancel the job***

  scancel *jobNumber*

- ***View past and active jobs***

  sacct -u *your.name* **# Past job history**

  scontrol show job *jobNumber* **# Job details**

Batch Job Script

Output

```
kamiak$ cat myJob.sh
#!/bin/bash
#SBATCH --partition=kamiak        # Partition/Queue to use
#SBATCH --job-name=myJob          # Job name
#SBATCH --output=%x_%j.out        # Output file (stdout)
#SBATCH --error=%x_%j.err         # Error file (stderr)
#SBATCH --mail-type=ALL           # Email notification: BEGIN,END,FAIL,ALL
#SBATCH --mail-user=your.name@wsu.edu     # Email address for notifications
#SBATCH --time=7-00:00:00         # Wall clock time limit Days-HH:MM:SS

#SBATCH --nodes=1                 # Number of nodes (min-max)   Where (layout)
#SBATCH --ntasks-per-node=1       # Number of tasks per node (processes)
#SBATCH --cpus-per-task=2         # Number of cores per task (threads) What


echo "I am job $SLURM_JOBID running on nodes $SLURM_JOB_NODELIST"

module load python3               # Load software module from Kamiak repository
srun python3 helloWorld.py -w     # Each task runs this program (total 1 times)
                                  # Each srun is a job step, and spawns -ntasks

echo "Completed job on node $HOSTNAME"
```

Viewing Information about the Cluster

- ***What partitions and nodes are available***

  sinfo -a | more **# Availability (alloc, idle, mix)**

- ***View all running and queued jobs***

  squeue -a | more **# Queued jobs for all partitions**

- ***View node details***

  scontrol show node cn93 **# Amount of memory, cpus, GPUs**

Follow along

Interactive Jobs

- ***Create interactive session on a compute node***

```
idev  -N 1 --ntasks=1 --cpus-per-task=2 -t 360
```

Same options as **sbatch**
Can **ssh** to node if have job on it

- ***Module commands to set up app environment***

```
module avail                          # Shows available apps for loaded compiler
module avail python3
module help python3/3.9.5             # See app-specific instructions,
                                      #          resources differ for each app
module load python3/3.9.5             # Loads specific version (recommended)
module list                           # See loaded modules
```

- ***Run the app (use srun for multiple nodes, runs program once for each task)***

```
python3 -i
        print ("Hello World!")
        exit()
srun -I python3 helloWorld.py     # Use srun -I to avoid hanging if no resources
exit
```

Do not run applications or installs on the login nodes, use sbatch or idev instead to run them on a compute node

Interactive Jobs

Output

```
kamiak$ idev -N 1 --ntasks=1 -cpus-per-task=2 -t 360
Idev interactively runs commands on a compute node.
See 'man salloc' for idev options to reserve a job allocation.
To use a GPU within idev: use 'srun yourCommand', e.g. 'srun python -i'.
To use X11 forwarding from a compute node:
  Use 'ssh -Y' or more secure 'ssh -X' to log into Kamiak.
  Within idev, use 'srun --x11' to launch a task with a user interface.
Recommend using 'srun -I' to launch a task without hanging.
Default time is 60 minutes.  Use '-t yourMinutes' to override.
salloc: Granted job allocation 1160832
Allocated nodes: cn32
                                  # Module commands set up app environment
cn32$ module avail                # Shows available apps for loaded compiler

cn32$ module help python3/3.9.5   # See any app-specific instructions
                                  #      (Resources differ for each app)
cn32$ module load python3/3.9.5   # Loads specific version (recommended)

cn32$ module list                 # See loaded modules
Currently Loaded Modules:
 1) intel/20.2   2) StdEnv   3) python3/3.9.5
```

Interactive Jobs

Output

```
cn32$ python3 -i
Python 3.9.5 (default, Jun  2 2021, 10:10:20)
[GCC 7.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> print ("Hello World!")
Hello World!
>>> exit()

cn32$ srun -I python3 helloWorld.py
Hello World! from cn32

cn32$ exit
exit
salloc: Relinquishing job allocation 1160832

kamiak$
```

Use srun -I to avoid hanging if resources are not available

Follow along

Job Arrays

- *Placeholder to create instances of a job as resources become available*
  #SBATCH --array=1-3 # Creates 3 job instances, one for each index 1,2,3
- *Each instance is an individual job with the same resources*
- *Can use the index* **$SLURM_ARRAY_TASK_ID** *in many ways*
- *The below job splits data into 3 files: data_1.txt, data_2.txt, data_3.txt*

```
cat  jobArray.sh
sbatch  jobArray.sh
squeue -u your.name
cat myJobArray*.out
scancel  jobNumber
```

Use job arrays instead of submitting hundreds of individual jobs

Job Array Script

Output

```
kamiak$ $ cat jobArray.sh
#!/bin/bash
#SBATCH --partition=kamiak        # Partition/Queue to use
#SBATCH --job-name=myJobArray     # Job name
#SBATCH --output=%x_%A_%a.out     # Output filename, jobname_jobid_index.out
#SBATCH --error=%x_%A_%a.err      # Error filename, jobname_jobid_index.err
#SBATCH --time=7-00:00:00         # Wall clock time limit Days-HH:MM:SS
#SBATCH --mail-type=ALL           # Email notification: BEGIN,END,FAIL,ALL
#SBATCH --mail-user=your.name@wsu.edu  # Email address for notifications
#SBATCH --array=1-3:1             # Indices of job instances, in steps of 1

#SBATCH --nodes=1                 # Number of nodes (min-max)
#SBATCH --ntasks-per-node=1       # Number of tasks per node (processes)
#SBATCH --cpus-per-task=1         # Number of cores per task (threads)
#SBATCH --mem-per-cpu=8G          # Memory per core (gigabytes)

# Placeholder to create instances of a job as resources become available
# Creates 3 job instances, one for each index 1,2,3 ($SLURM_ARRAY_TASK_ID)
# Each instance is an individual job with the above resources
# Can use the index (in $SLURM_ARRAY_TASK_ID) in many ways
# Below the index splits data into 3 files: data_1.txt, data_2.txt, data_3.txt

echo "Starting job array $SLURM_ARRAY_TASK_ID on host $HOSTNAME"

module load python3
srun python3 helloWorld.py -w "inputs/data_${SLURM_ARRAY_TASK_ID}.txt"

echo "Completed job array $SLURM_ARRAY_TASK_ID on host $HOSTNAME"
```

GPU Job Script

Output

```
kamiak$ cat gpuJob.sh
#!/bin/bash
#SBATCH --partition=kamiak        # Partition/Queue to use
#SBATCH --job-name=gpuJob         # Job name
#SBATCH --output=%x_%j.out        # Output file (stdout)
#SBATCH --error=%x_%j.err         # Error file (stderr)
#SBATCH --mail-type=ALL           # Email notification: BEGIN,END,FAIL,ALL
#SBATCH --mail-user=your.name@wsu.edu     # Email address for notifications
#SBATCH --time=7-00:00:00         # Wall clock time limit Days-HH:MM:SS

#SBATCH --nodes=1                 # Number of nodes (min-max)   Where (layout)
#SBATCH --ntasks-per-node=1       # Number of tasks per node (processes)
#SBATCH --cpus-per-task=2         # Number of cores per task (threads) What
#SBATCH --gres=gpu:tesla:1        # Gpu's per node (up to 4)

echo "I am job $SLURM_JOBID running on nodes $SLURM_JOB_NODELIST"

module load cuda
srun nvidia-smi

echo "Completed job on node $HOSTNAME"
```

Follow along

Using Scratch Storage

- ***Create a scratch directory that expires in two weeks***

```
mkworkspace
export myscratch="$(mkworkspace)"      # Can use inside or outside a job script
echo $myscratch
```

- ***List your scratch allocations***

```
lsworkspace
```

- ***Can optionally delete contents when done***

```
rm -r -I $myscratch/*
```

Snapshots

- ***Three days of read-only backups of home and data folders***

```
ls /home/.snapshots
ls /home/.snapshots/daily.*/your.name
```

Follow along

Using Available Software on Kamiak

```
module avail                        # Available modules compatible with compiler
module load python3/3.9.5           # Load specific version (recommended)
module list                         # See loaded modules
module avail python3                # See available python3 modules
module load python3                 # Load latest version
module unload python3               # Unload a module
module spider                       # See all modules
module whatis anaconda3             # See what a module does
module help anaconda3               # See help for a module
which python3                       # See that python is in your path
printenv PATH                       # See effects of loading modules
printenv LD_LIBRARY_PATH
```

Getting Help

hpc.wsu.edu	***Support & Zoom Help Desk Hours***
hpc.wsu.edu/cheat-sheet	***User's Guide / Kamiak Cheat Sheet***
hpc.wsu.edu/training/slides	***These slides***

Being a Good User

Kamiak is a shared cluster for all of WSU and your access to it is a privilege. Its resources are finite and care must be taken to ensure its continued usefulness for yourself and the research community.

Do

- Cite Kamiak in your work
- Report issues via Kamiak's Service Desk
- Abide by Kamiak's End User License Agreement and WSU policies
- Use accurate resource requirements (CPU, time, memory)

Don't

- Do not run applications or installs on a login node, use **sbatch** or **idev** to run on a compute node
- Do not submit thousands of jobs – use **job arrays**
- Do not give your password to anyone, ever

Purchasing Nodes and Renting Extra Storage

- All users have access to the backfill queue, /home and /scratch storage, and any /data/lab storage made available by their PI
- If you need more → **have your PI become an investor**
- Submit a service request to purchase nodes or rent extra storage
  - *Nodes are permanently owned by the investor with a 5-year warranty*
  - *Storage can be rented annually in units of 512GB per year*
- Standard compute nodes
  - *64-cores Intel Xeon Gold, 512GB memory*
  - *Optional Nvidia A100 GPU's*
  - *Optional large-memory, 1-2TB*
- For price quotes, please submit a service request
  For detailed node descriptions, please see
  hpc.wsu.edu/kamiak-hpc/becoming-an-investor/

The End

- We will be sending out a survey to get your feedback about this training event
- Other training sessions are planned throughout the year – let us know in the survey what topics would be of interest
- Other ways to learn more and participate in Kamiak governance:
  - CIRC Advisory Committee - share your ideas with its members
  - WSU HPC club - 4 nodes purchased through Tech Fee grant