

Introduction to Kamiak Training Workshop

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hpc.wsu.edu/training

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Documents

These slides

Cheat Sheet



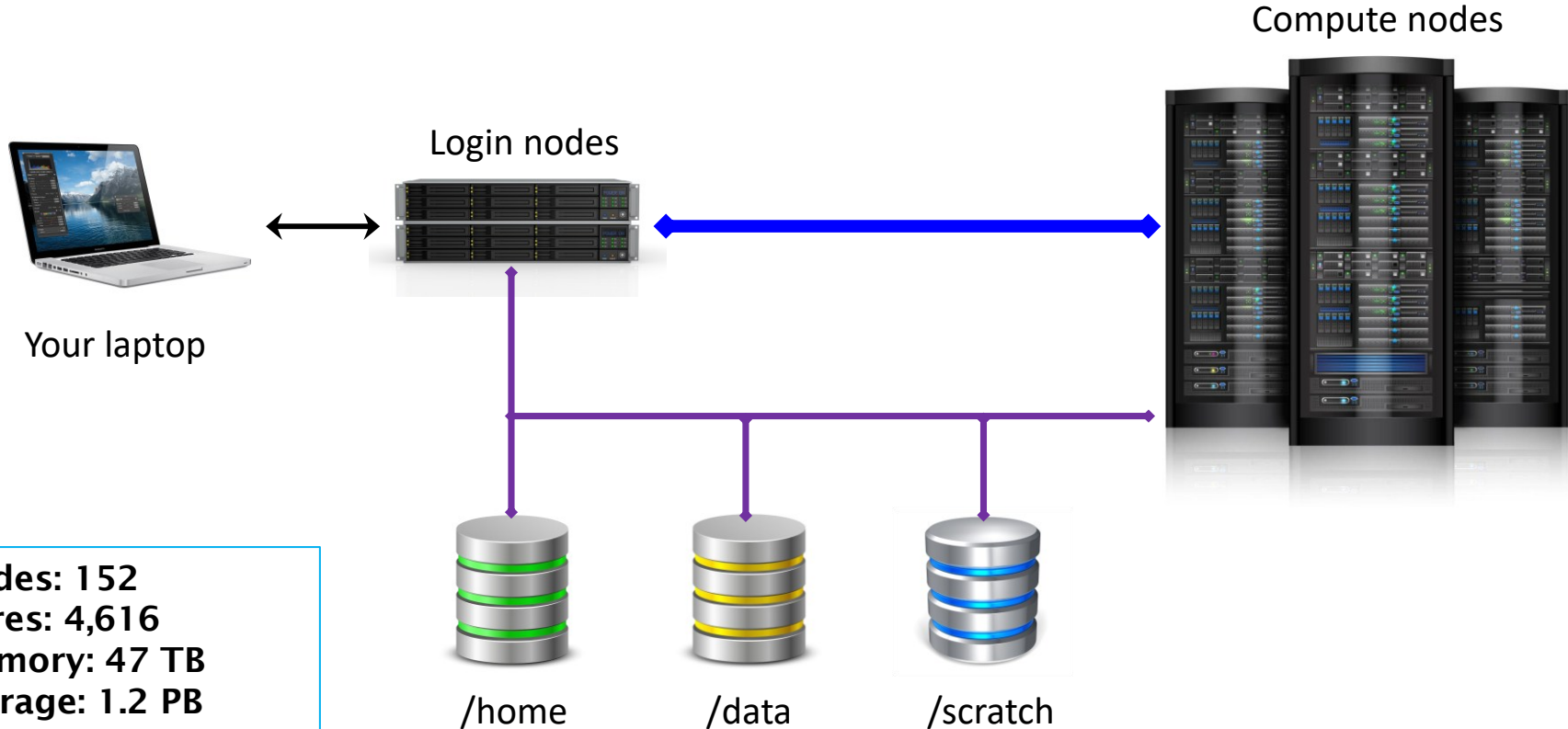
What you will learn today

- 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
 - 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

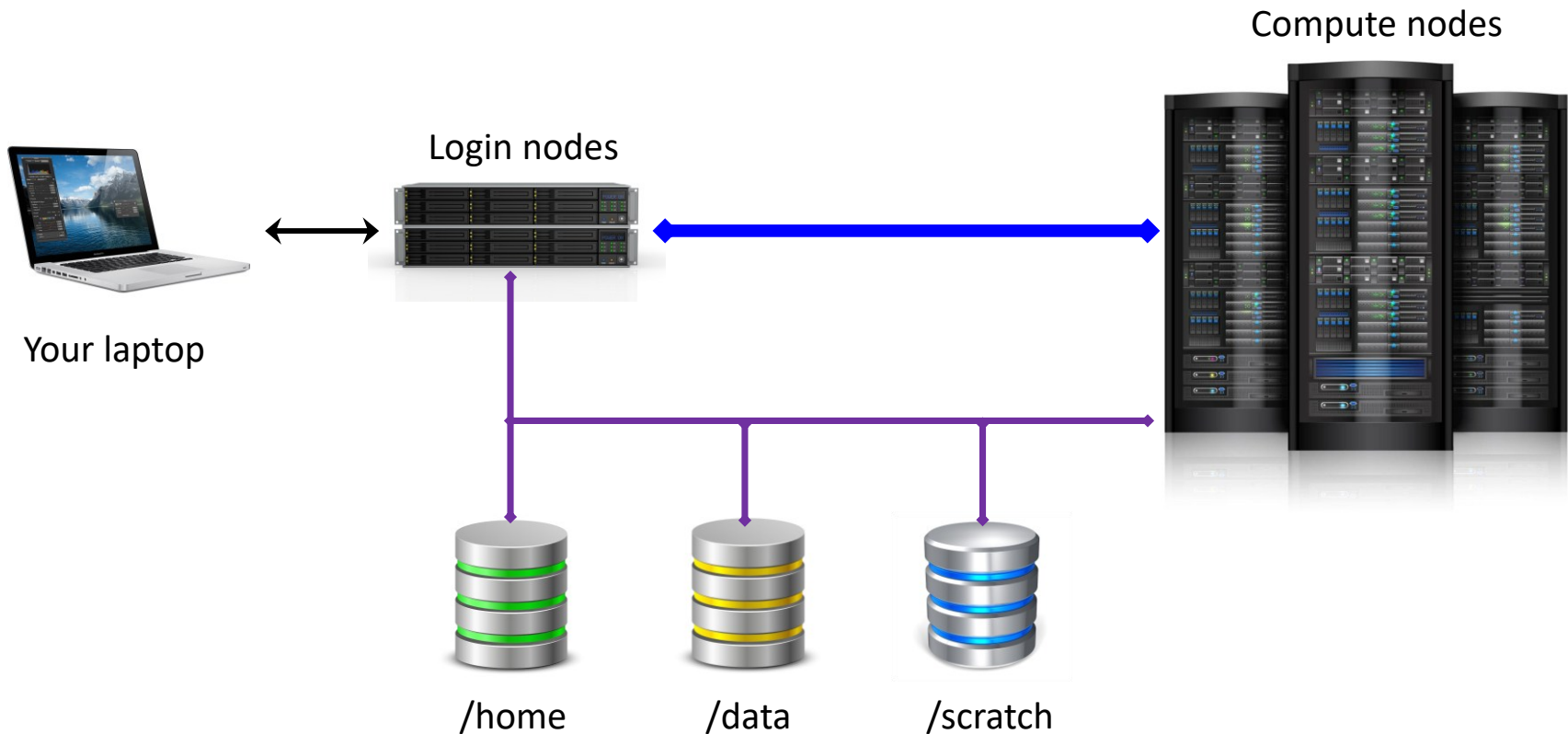
`/data/lab/pi.labname`

500GB per PI lab group

Extra storage is available for rent from the CIRC service center

`/scratch`

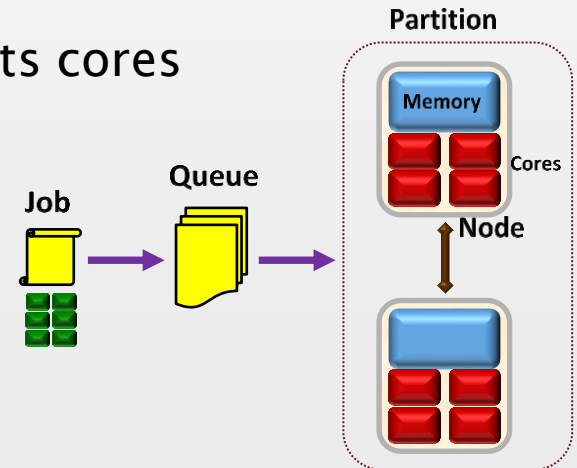
Temporary storage, 2-week lifetime, 10TB limit per user





Running Jobs on Kamiak

- **Nodes** are grouped into **partitions**, each owned by a PI or college
- All nodes also belong to 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=1
#SBATCH --cpus-per-task=10
export OMP_NUM_THREADS=
$SLURM_CPUS_PER_TASK
```

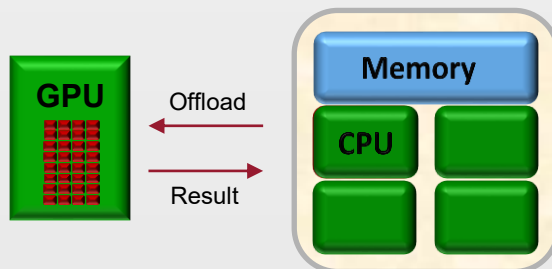
- **Multiple nodes**

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

```
#SBATCH --nodes=2
#SBATCH --ntasks=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=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
```

```
squeue -j jobNumber
```

```
# Shows pending and running jobs
```

- **See output**

```
cat myJob*.out
```

- **Cancel the job**

```
scancel jobNumber
```

- **View past and active jobs**

```
sacct -u your.name
```

```
scontrol show job jobNumber
```

```
# Past job history
```

```
# Job details
```



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
```

- **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 -l python3 helloWorld.py # Use srun -l 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



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
queue -u your.name
cat myJobArray*.out
scancel jobNumber
```

Use job arrays instead of submitting hundreds of individual jobs



Follow Along

Using Scratch Storage

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

```
mkworkspace
```

```
export myscratch="$$(mkworkspace)"
```

```
echo $myscratch
```

Can use inside or outside a job script

- **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 (<i>recommended</i>)
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	



Follow Along

Getting Help

hpc.wsu.edu

hpc.wsu.edu/cheat-sheet

hpc.wsu.edu/training/slides

Support & Zoom Help Desk Hours

User's Guide / Kamiak Cheat Sheet

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



Batch Job Script

Follow along

```
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 (max)
#SBATCH --ntasks=1           # Number of tasks (processes) What (cpus)
#SBATCH --cpus-per-task=2    # Number of cores per task (threads)

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"
```



- **idev** creates an interactive session on a compute node
 - Same options as **sbatch**
 - Can also **ssh** to a compute node if you have a job allocated on it

```
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
```

```
cn32$ module avail # Module commands set up app environment  
# 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
```



```
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 -l** to avoid hanging
if resources are not available



Job Array Script

Follow along

```
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 (max)
#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"
```