

# Introduction to Kamiak Training Workshop

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*These slides*  
*Handout*  
*Cheat Sheet*



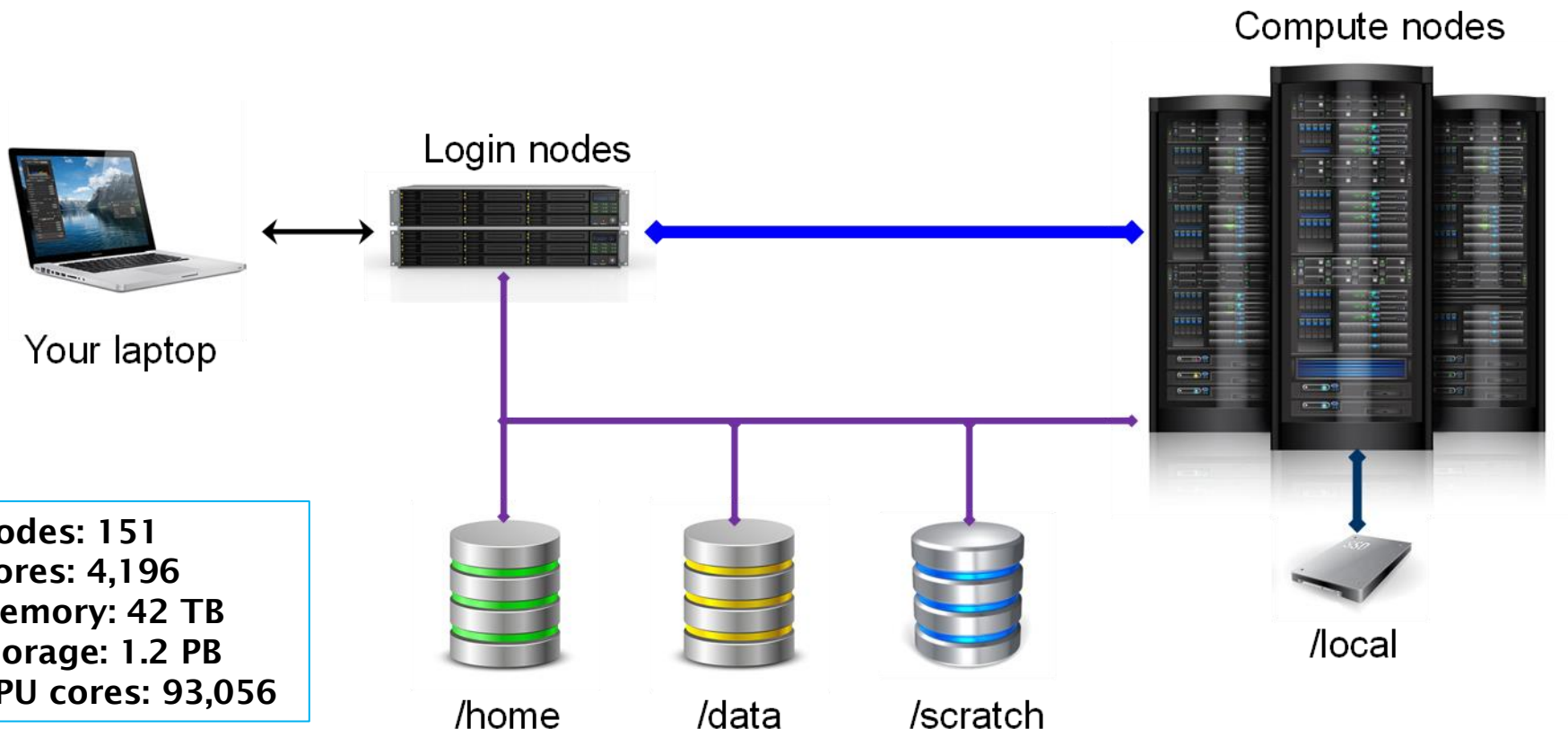
# What you will learn today

- What is Kamiak
- How to run jobs on Kamiak
  - Submit batch jobs
  - Interactive compute session
  - Types of jobs
- Exercises
  - Logging into Kamiak
  - Transferring files to and from 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: 151  
Cores: 4,196  
Memory: 42 TB  
Storage: 1.2 PB  
GPU cores: 93,056



# Kamiak Storage

- Kamiak has 4 types of storage available to users

`/home/your.name`

100GB per user

`/data/lab/pi.labname`

500GB per PI lab (e.g., `/data/clark`)

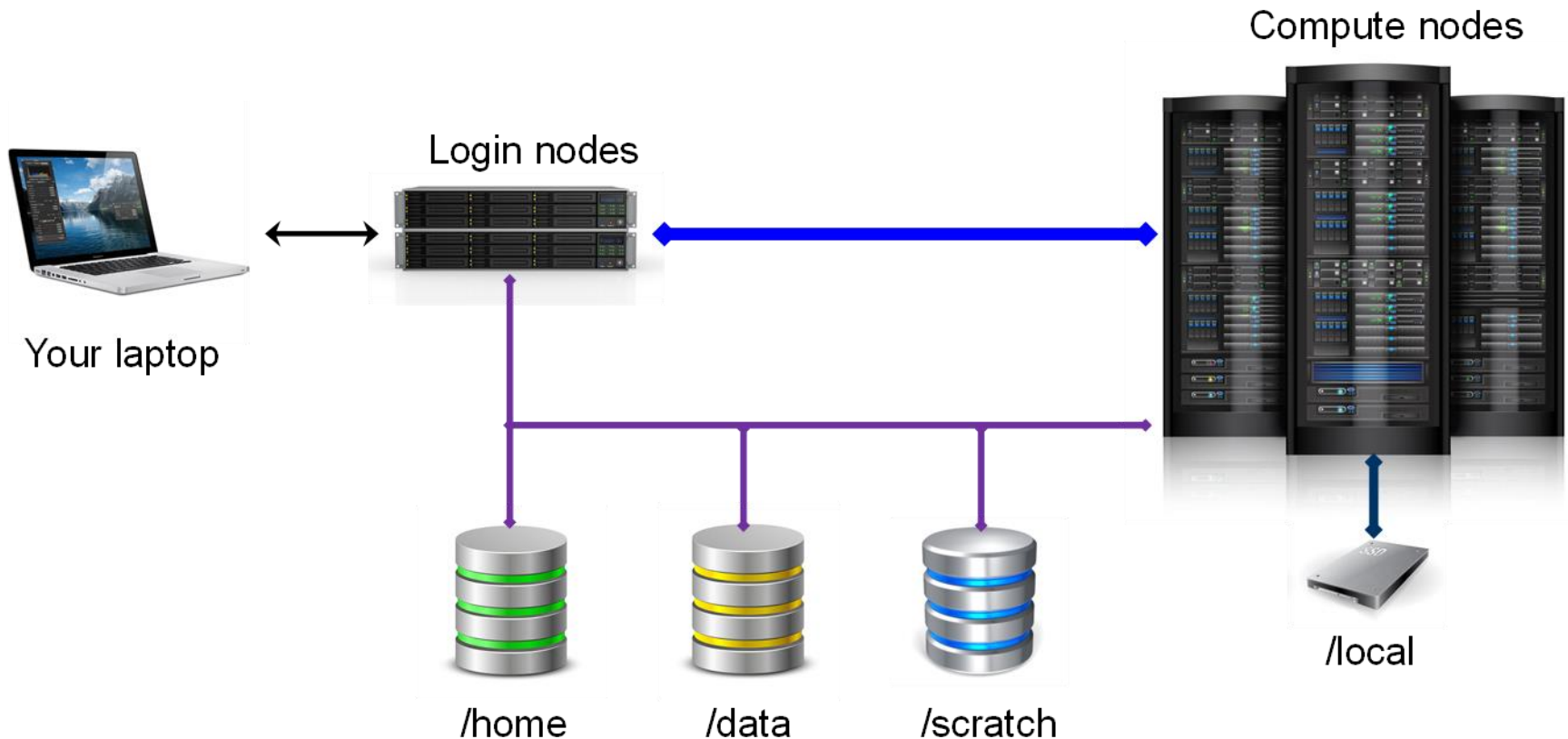
*Extra storage is available for rent from CIRC service center*

`/scratch`

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

`/local`

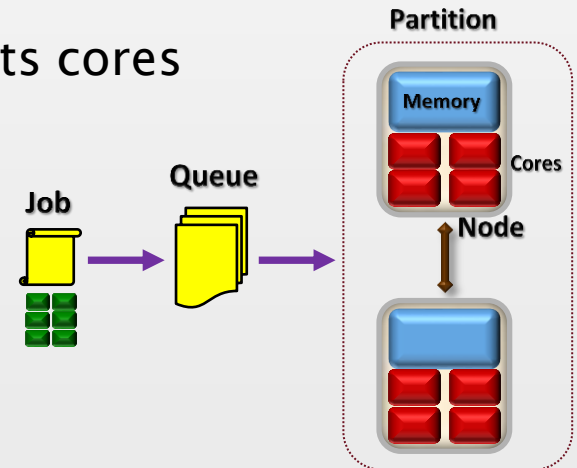
Temporary storage on node, 2-week lifetime, ~400GB





# 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 compute or compile jobs on login nodes, use **sbatch** or **idev** instead



# 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
```

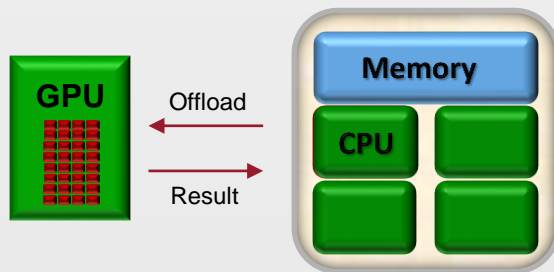
- **Multiple nodes**

- 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>

# Introduction 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  
exit
```

### Transferring Files to and from Kamiak

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

#### **Copy from Kamiak to your laptop**

```
scp -r your.name@kamiak.wsu.edu:/opt/apps/samples/training .  
    ↑ Recursive, copies all files      ↑ From Kamiak      ↑ To current folder  
ls -l training
```

#### **Copy from your laptop to Kamiak**

```
scp -r training your.name@kamiak.wsu.edu:~/  
    ↑ From my laptop      ↑ To my home directory on Kamiak
```

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

```
rsync -ravx training/ your.name@kamiak.wsu.edu:~/training  
    ↑ All files  ↑ From laptop      ↑ To Kamiak
```

### Submitting Batch Jobs to Kamiak

#### **Log back into Kamiak**

```
ssh your.name@kamiak.wsu.edu
```

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

```
cd training  
source training_only_setup.sh
```

#### **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

## **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

## **Interactive Jobs**

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

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

### **Module commands set up app environment**

`module avail` # Shows available apps for loaded compiler  
`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

**Do not run compute jobs on the login nodes**

**Run the app (use srun only 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 resources not available
exit
```

## Job Arrays

**Placeholder to create instances of a job as resources become available**

```
#SBATCH --array=1-5 # Creates 5 job instances, one for each index 1,2,3,4,5
```

**Each instance is an individual job with the same resources (index is \$SLURM\_ARRAY\_TASK\_ID)**

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

*Use job arrays instead of submitting hundreds of individual jobs*

## Using Scratch Storage

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

```
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 -l $myscratch/*
```

## Snapshots

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

```
ls /home/.snapshots
ls /home/.snapshots/daily.2022-03-21_0000/your.name
ls /data/.snapshots/daily.2022-03-21_0000
```

## 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	

## Getting Help

<a href="http://hpc.wsu.edu">hpc.wsu.edu</a>	<b><i>Support &amp; Zoom Help Desk Hours</i></b>
<a href="http://hpc.wsu.edu/cheat-sheet">hpc.wsu.edu/cheat-sheet</a>	<b><i>User's Guide / Kamiak Cheat Sheet</i></b>
<a href="http://hpc.wsu.edu/training/slides">hpc.wsu.edu/training/slides</a>	
<a href="http://hpc.wsu.edu/training/follow-along">hpc.wsu.edu/training/follow-along</a>	



# 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 compute jobs 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/](http://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=myJob_%j.out  # Output file (stdout)
#SBATCH --error=myJob_%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=output/myJobArray_%A_%a.out  # Output filename, jobid_index
#SBATCH --error=output/myJobArray_%A_%a.err  # Error filename, jobid_index
#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=0-2:1              # Number of jobs, 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)

# Runs this job 3 times, with index SLURM_ARRAY_TASK_ID as 0,1,2
# Split your data into 3 files, name them data_0.txt, data_1.txt, data_2.txt
# Each job array step is scheduled as an individual job
# Each job array step is allocated the above resources (cores, memory)

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"
```