Introduction to Kamiak Training Workshop

Alan Love, CIRC Director
Peter Mills, Deputy Director
Rohit Dhariwal, Computational Scientist
Roy Obenchain, HPC Systems Administrator
Will Aoki, HPC Systems Administrator
Tim Neumann, Program Coordinator

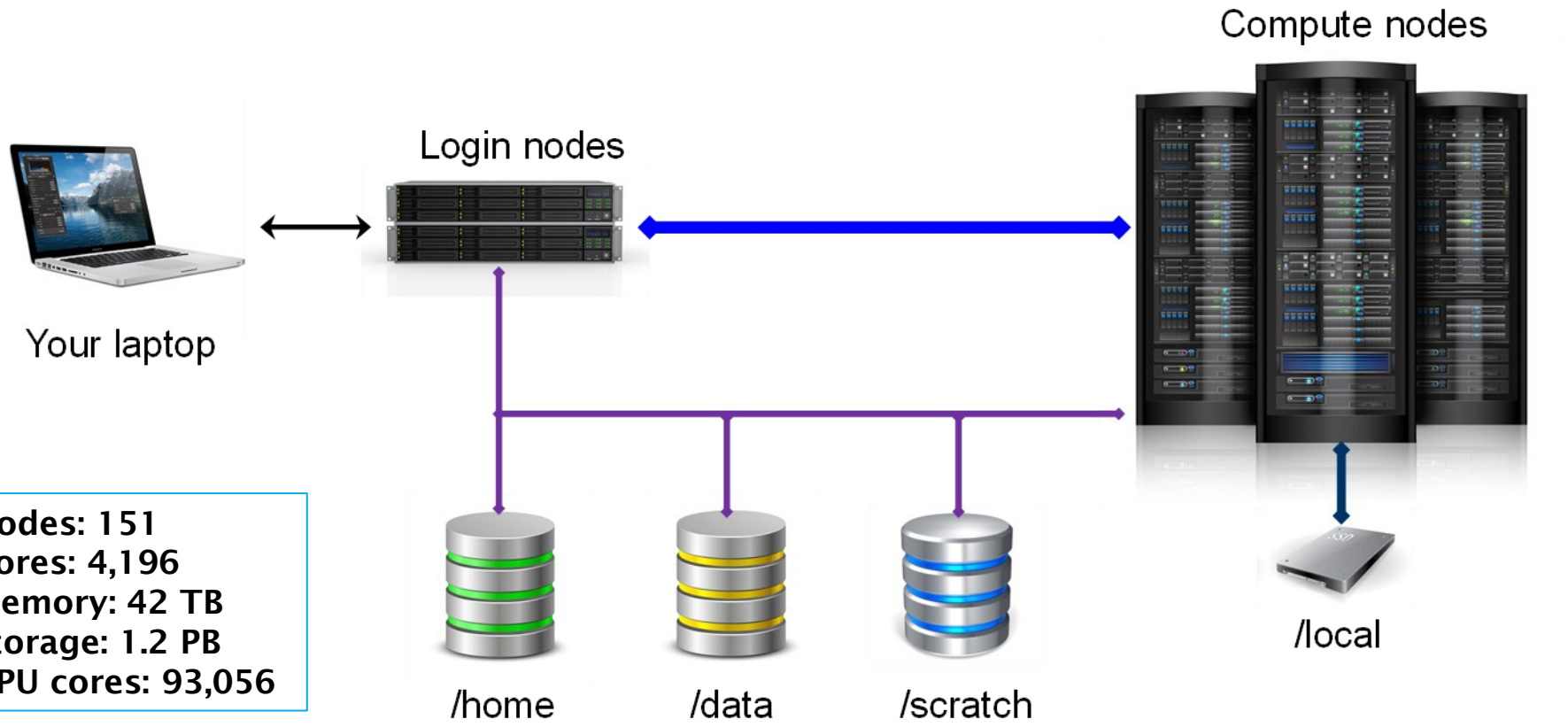
hpc.wsu.edu/training	***Documents***
hpc.wsu.edu/training/slides	***These slides***
hpc.wsu.edu/cheat-sheet	***Cheat Sheet***

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
  - 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

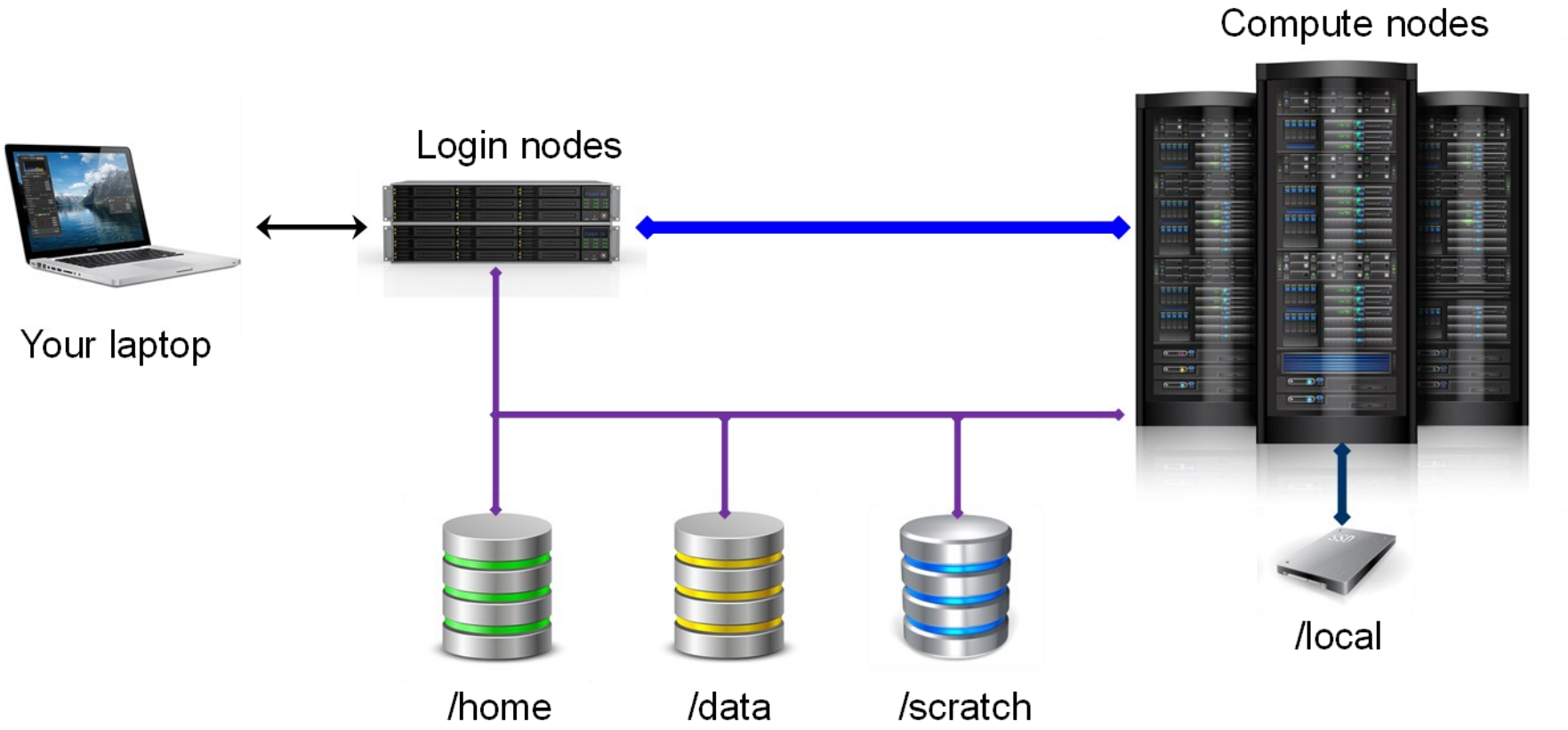


Nodes: 151
Cores: 4,196
Memory: 42 TB
Storage: 1.2 PB
GPU cores: 93,056

Kamiak Storage

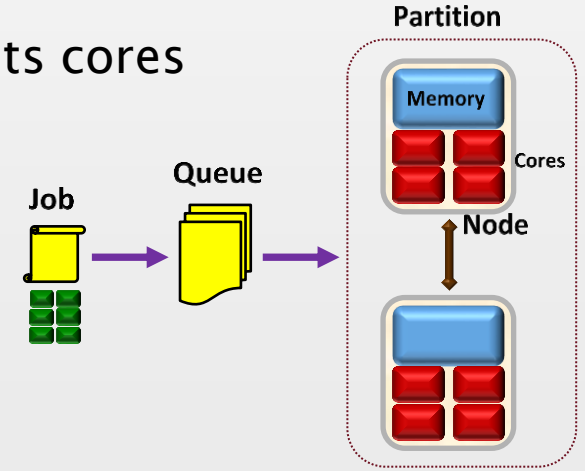
- Kamiak has 4 types of storage available to users

/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 the 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 applications or installs on the login nodes, use sbatch or idev instead to run them on a compute node

Types of Jobs

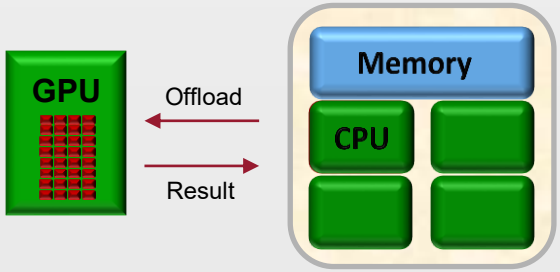
- **Single node**
  - Single program instance
  - Multithreading over multiple cores
  - Threads share memory

```
#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/scripts ~/

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

  ls -l -R scripts

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

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

  ↑ ***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**

Follow Along

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 -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

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

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
```

Follow Along

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

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"
```

Interactive Jobs

Follow along

- **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
                                  # 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

Follow along

```
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

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"
```