Introduction to Kamiak
Training Workshop

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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
  - 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 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.
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

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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
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
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`
Submitting Batch Jobs to Kamiak

- **Create/edit a job script**
  
  ```bash
  cat myJob.sh
  ```

- **Submit the job script to the job queue**
  
  ```bash
  sbatch myJob.sh
  # To test: sbatch --test-only myJob.sh
  ```

- **View the job queue**
  
  ```bash
  squeue -u your.name
  squeue -j jobNumber
  # Shows pending and running jobs
  ```

- **See output**
  
  ```bash
  cat myJob*.out
  ```

- **Cancel the job**
  
  ```bash
  scancel jobNumber
  ```

- **View past and active jobs**
  
  ```bash
  sacct -u your.name
  scontrol show job jobNumber
  # Past job history
  # Job details
  ```
#!/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
srun python3 helloWorld.py -w       # Load software module from Kamiak repository
                                    # 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
  ```
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

kamiak$ idev -N 1 --ntasks=1 -cpus-per-task=2 -t 360
Idев 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

# Shows available apps for loaded compiler

cn32$ module avail

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)

# 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

ekamiak$
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
#!/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"
#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)

# Bash script

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

module load cuda
srun nvidia-smi

echo "Completed job on node $HOSTNAME"
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 -l $myscratch/*`

Snapshots

• *Three days of read-only backups of home and data folders*
  
  `ls /home/.snapshots`
  `ls /home/.snapshots/daily.*/your.name`
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
hpc.wsu.edu/cheat-sheet
hpc.wsu.edu/training/slides

Support & Zoom Help Desk Hours
User’s Guide / Kamiak Cheat Sheet
These slides
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/
• 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