HPC and cluster computing ~~best~~ practices

https://github.com/Whitford/ctbp-techtalks

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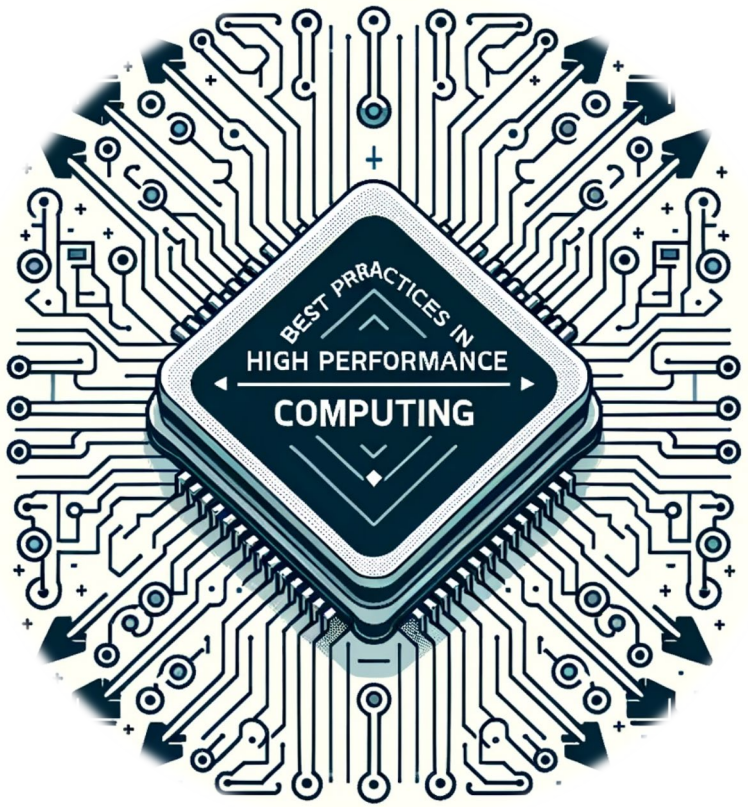
Outline

- HPC - 5W and 1H
  - What, Who, Where, When, Why, and How
- Software Stack
- Accessing the Cluster
  - Vscode and GitHub Desktop
- Slurm – Job Management
  - Run a few examples
    - Job array, Job dependency



HPC – High-Performance Computing

W1 - What is HPC?

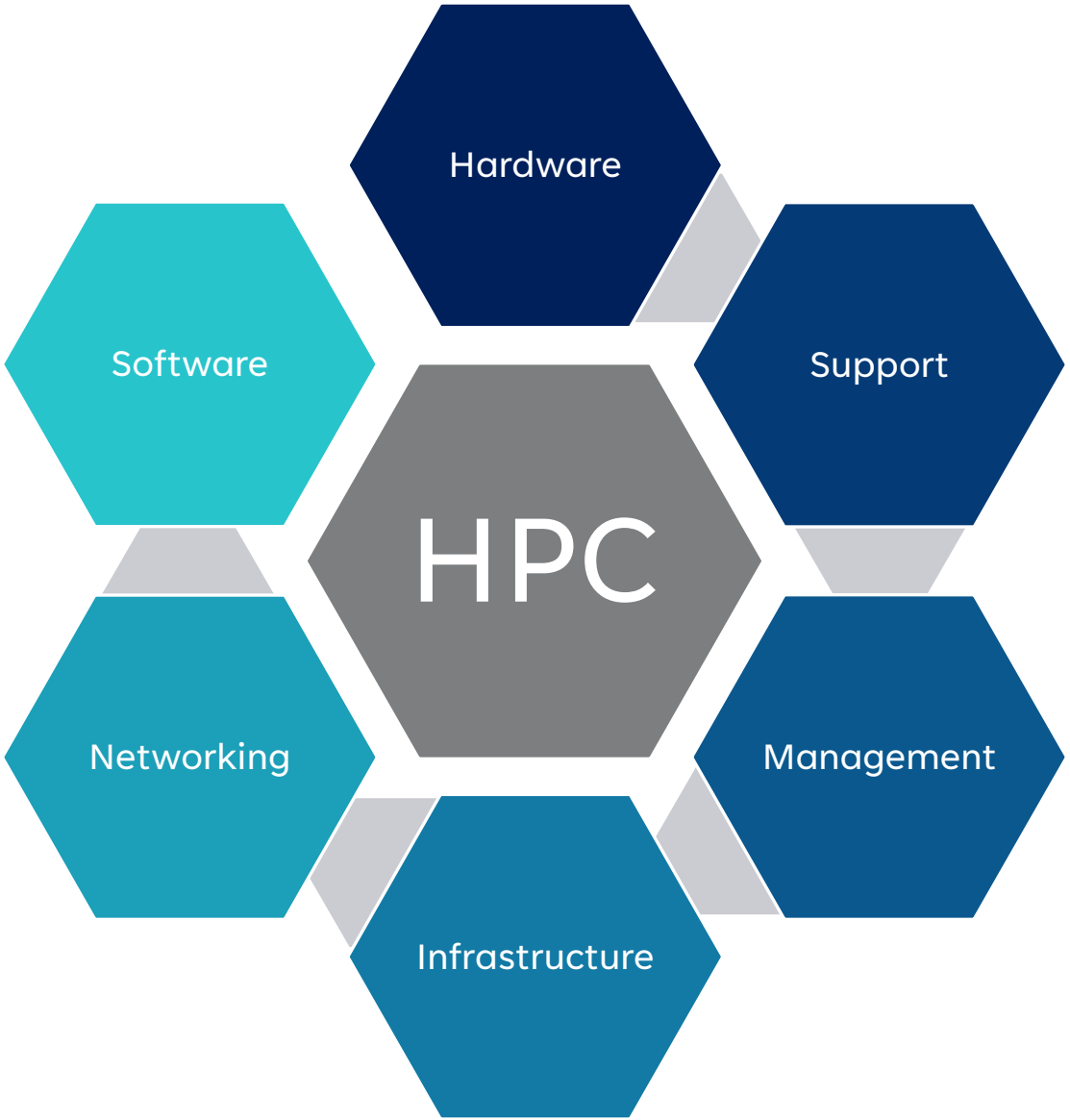
High-Performance Computing involves the usage of supercomputers/clusters and parallel processing techniques for solving complex computational problems at high speeds.

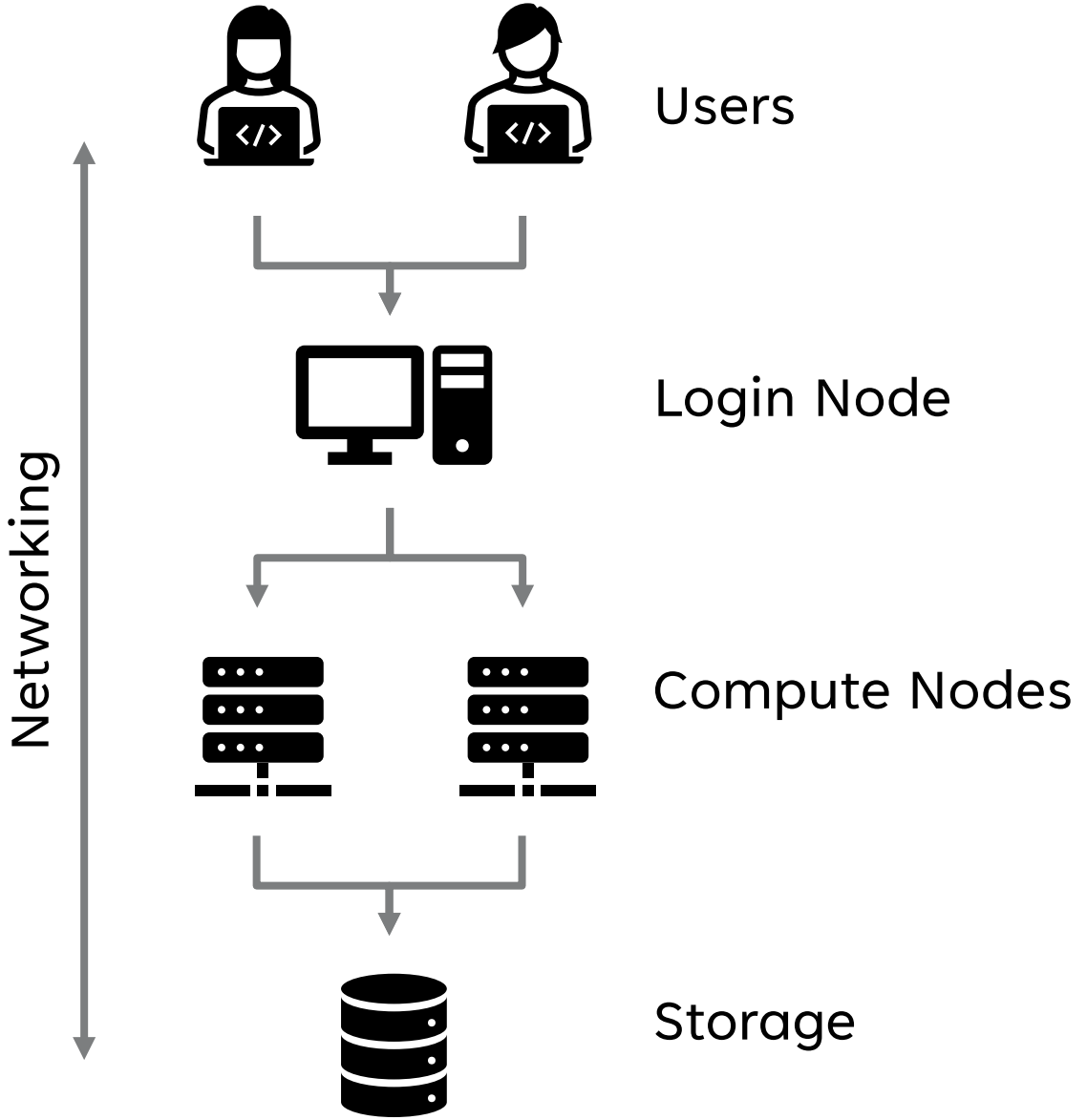
HPC – High-Performance Computing

H1 – How does HPC work?

HPC systems use parallel processing, where multiple processors work simultaneously to perform computations quickly. They also utilize advanced networking, high-speed storage systems, and optimized software to handle large datasets and perform complex simulations.

HPC – High-Performance Computing





HPC Software Stack

- **Operating Systems:** Predominantly, HPC clusters run on **Linux**.
- **Schedulers and Resource Managers:** Most commons are **Slurm** and Torque/PBS. Manages the job queue and ensuring equitable and efficient resource distribution.
- **Parallelization Tools: MPI** handles inter-node communication, and **OpenMP** takes care of intra-node parallelism.

Recipe: Running a Job in the HPC Cluster Soup

- 1 Laptop, preferably lightweight, with a fresh sprinkle of SSH installed
- 1 Stable internet access, preferably high-speed.
- 1 Large Cluster, ripe and ready for computation
- A pinch of patience (sometimes more, depending on the queue)
- 1 Job script, marinated in correct syntax
- A dash of debugging skills (just in case)
- Optional: 1 cup of coffee or tea for those longer jobs

Accessing the Cluster – NOTS (Night Owls Time-Sharing)

Terminal (Rice Network or VPN)

```
ssh -Y (your_login_name)@nots.rice.edu
```

Gateway Access First

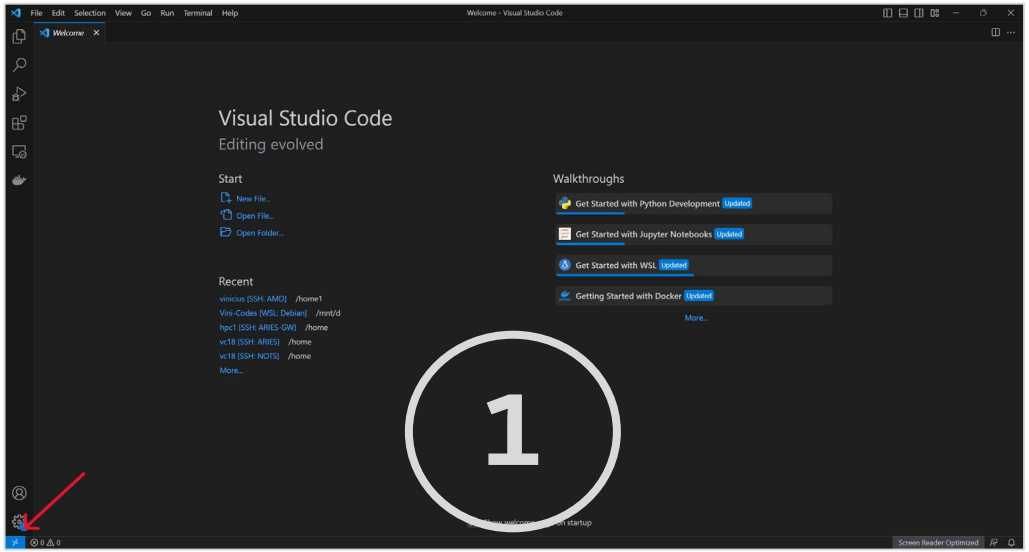
```
ssh -Y (your_login_name)@gw.crc.rice.edu
```

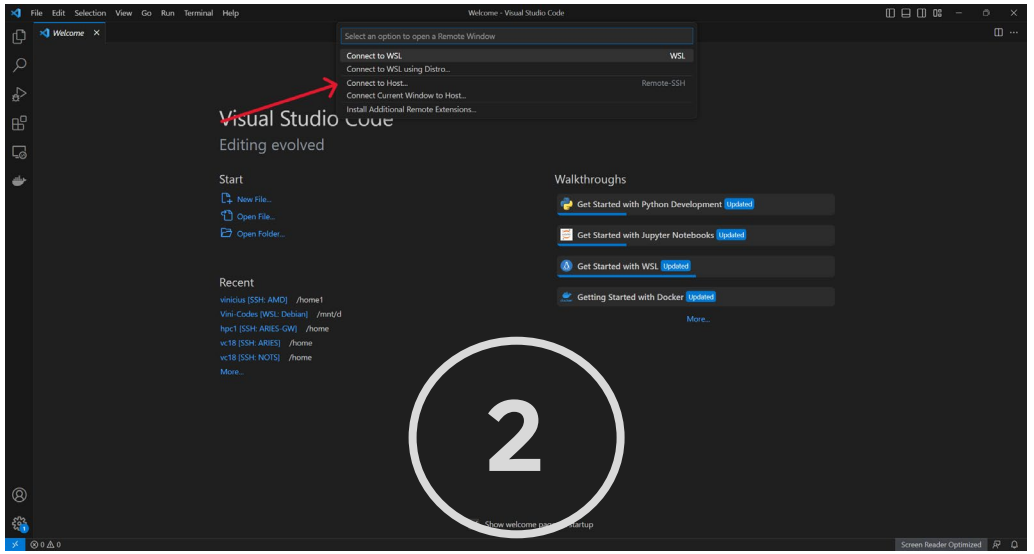
Accessing the Cluster – NOTS (Night Owls Time-Sharing)

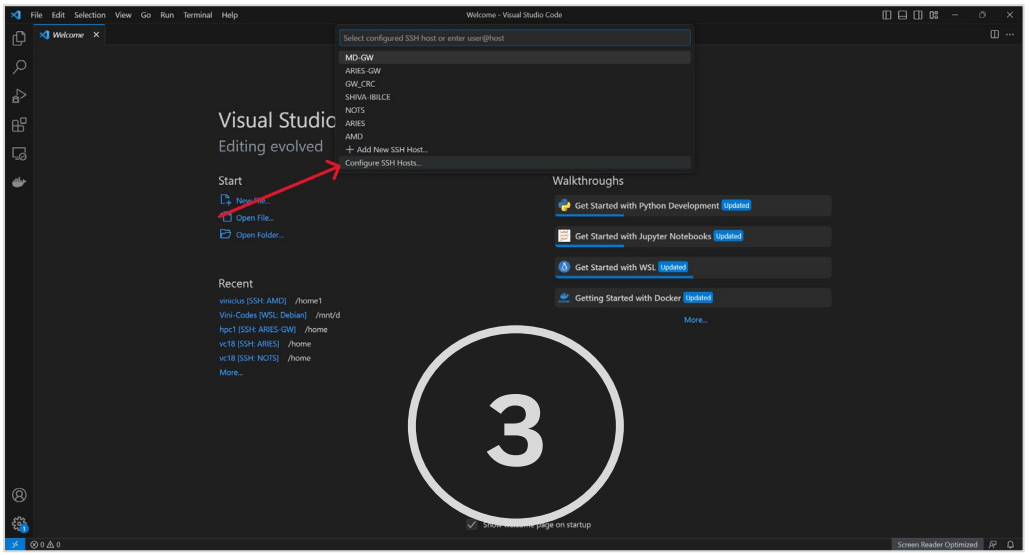
VScode – Visual Studio Code

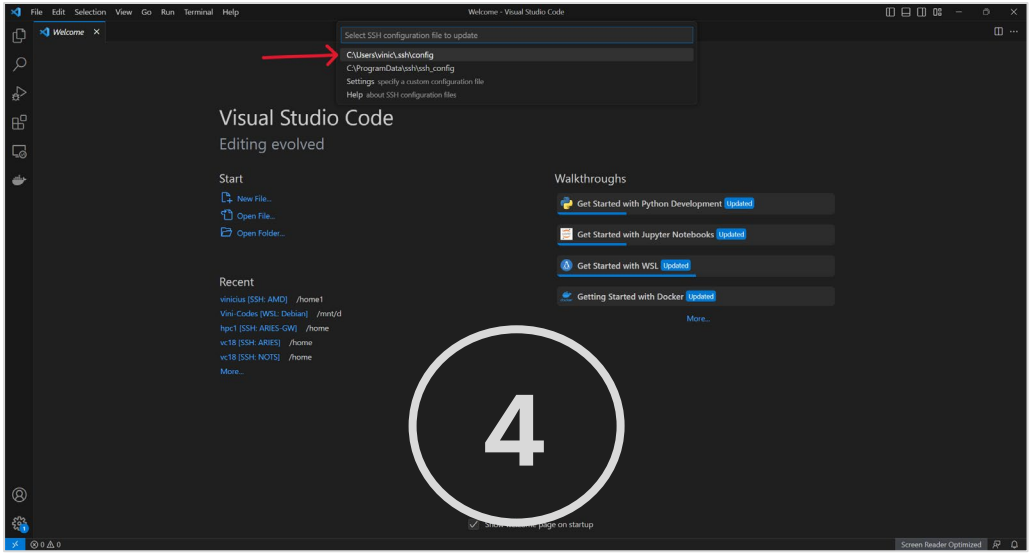
- **Download at:** https://code.visualstudio.com
- **Install the Remote - SSH Extension**: Go to Extensions and search for “Remote - SSH” and install it.
- **Connect to Your Cluster:** Press Ctrl+Shift+P, type “Remote-SSH: Connect to Host...”, and then enter ssh –AY username@cluster-address.

VScode – Visual Studio Code – Cluster access









VScode – Config file Example

```
Host GW_CRC
  User vc18
  HostName gw.crc.rice.edu
  ForwardAgent yes
  IdentityFile C:\\Users\\vinic\\.ssh\\id_rsa

Host NOTS
  HostName nots.rice.edu
  User vc18
  Port 22
  ForwardAgent yes
  ProxyJump GW_CRC
  IdentityFile C:\\Users\\vinic\\.ssh\\id_rsa

Host ARIES
  HostName aries.rice.edu
  User vc18
  ForwardAgent yes
  ProxyJump GW_CRC
  Port 22
  IdentityFile C:\\Users\\vinic\\.ssh\\id_rsa
```

GitHub Desktop – Download Files

GitHub Desktop

- **Download at:** https://desktop.github.com
- **Clone the Repository**: https://github.com/Whitford/ctbp-techtalks
  - Go to the green button “ <> Code” -> Open with GitHub Desktop
- **Transfer Data to the Cluster:** Copy & Paste the folder **Intro_HPC** to home folder in cluster

Some useful command lines

```
sacctmgr show associations user=username

sinfo -p ctbp-onuchic

squeue -p ctbp-onuchic

quota –s

module avail

module spider Anaconda3/2022.10
```

Running Our First Job

```
#!/bin/bash
#SBATCH --job-name=job_1
#SBATCH --account=ctbp-onuchic
#SBATCH --partition=ctbp-onuchic
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --time=00:05:00
#SBATCH --mem-per-cpu=100M
#SBATCH -e slurm-%j-%x.err
#SBATCH -o slurm-%j-%x.out

echo "Job ID: $SLURM_JOB_ID"
echo "Hostname: $(hostname)"
echo "Memory Usage: $(free -h)"
echo "Node: $SLURM_NODELIST"
echo "CPUs: $SLURM_CPUS_ON_NODE"
echo "Threads: $(nproc --all)"
echo "Number of Nodes: $SLURM_NNODES"
echo "Number of Tasks: $SLURM_NTASKS"
echo "Cores/CPUs per Node: $SLURM_CPUS_ON_NODE"
echo "Runtime Duration: $(($SECONDS / 60)) minutes and $(($SECONDS % 60)) seconds."
```

Running Our First Job

```
sbatch script_job_1.sh
```

```
Job ID: 7053026
Hostname: bc6u11n6
Memory Usage:               total        used        free      shared  buff/cache   available
Mem:            31G        804M         28G         98M        1.8G         29G
Swap:            0B          0B          0B
Node: bc6u11n6
CPUs: 2
Threads: 32
Number of Nodes: 1
Number of Tasks: 1
Cores/CPUs per Node: 2
Runtime Duration: 0 minutes and 0 seconds.
```

Job Monitoring

```
sbatch script_job_2.sh
```

```
squeue -u username
```

```
(base) [vc18@nlogin3 Workshop_Nov_2023]$ squeue -u vc18
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           7054057 ctbp-onuc    job_2     vc18  R       0:06      1 bc6u11n6
```

Job Monitoring

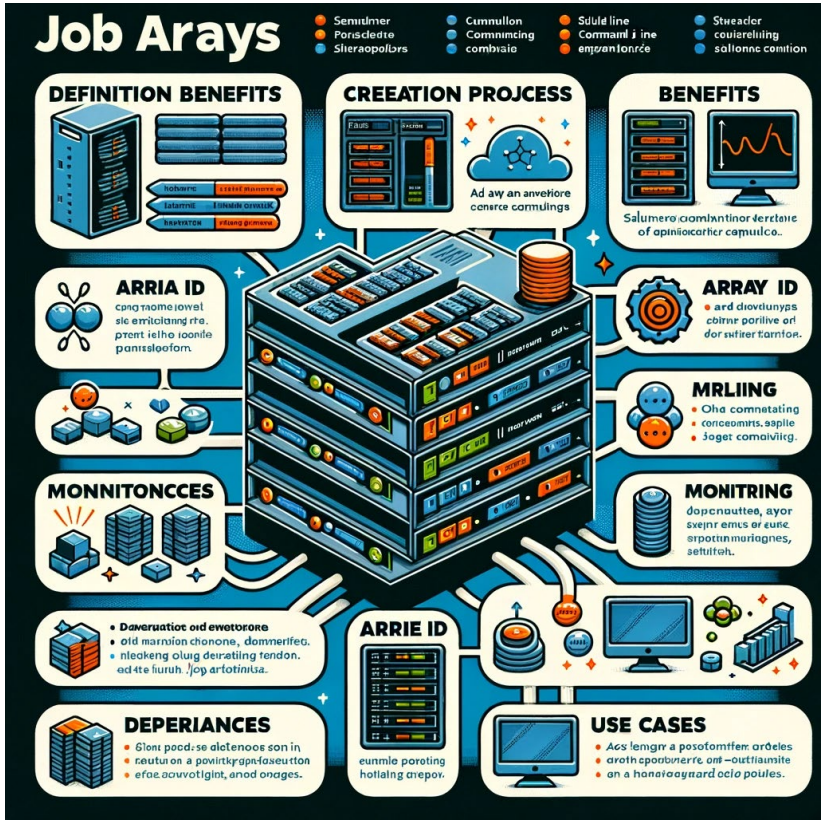
```
scancel job_ID
```

```
scancel 7054057

(base) [vc18@nlogin3 Workshop_Nov_2023]$ cat slurm-7054057-job_2.err
slurmstepd: error: *** JOB 7054057 ON bc6u11n6 CANCELLED AT 2023-10-30T13:45:10 ***
```

Job Array

What is Job Array?

- A job array allows the submission of many similar jobs using a single script.
- Each job in the array is assigned a unique "array ID", which can be used within the script to vary the behavior of individual tasks.



Job Array

```
#!/bin/bash
#SBATCH --job-name=job_3_array
#SBATCH --account=ctbp-onuchic
#SBATCH --partition=ctbp-onuchic
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --time=00:10:00
#SBATCH --mem-per-cpu=100M
#SBATCH -e slurm-%A_%a-%x.err
#SBATCH -o slurm-%A_%a-%x.out
#SBATCH --array=1-8

echo "Array Task ID: $SLURM_ARRAY_TASK_ID"
echo "Job ID: $SLURM_JOB_ID"
echo "Hostname: $(hostname)"
echo "Memory Usage: $(free -h)"
echo "Node: $SLURM_NODELIST"
echo "CPUs: $SLURM_CPUS_ON_NODE"
echo "Threads: $(nproc --all)"
echo "Number of Nodes: $SLURM_NNODES"
echo "Number of Tasks: $SLURM_NTASKS"
echo "Cores/CPUs per Node: $SLURM_CPUS_ON_NODE"
sleep 240 # time in seconds
echo "Runtime Duration: $(($SECONDS / 60)) minutes and $(($SECONDS % 60)) seconds."
```

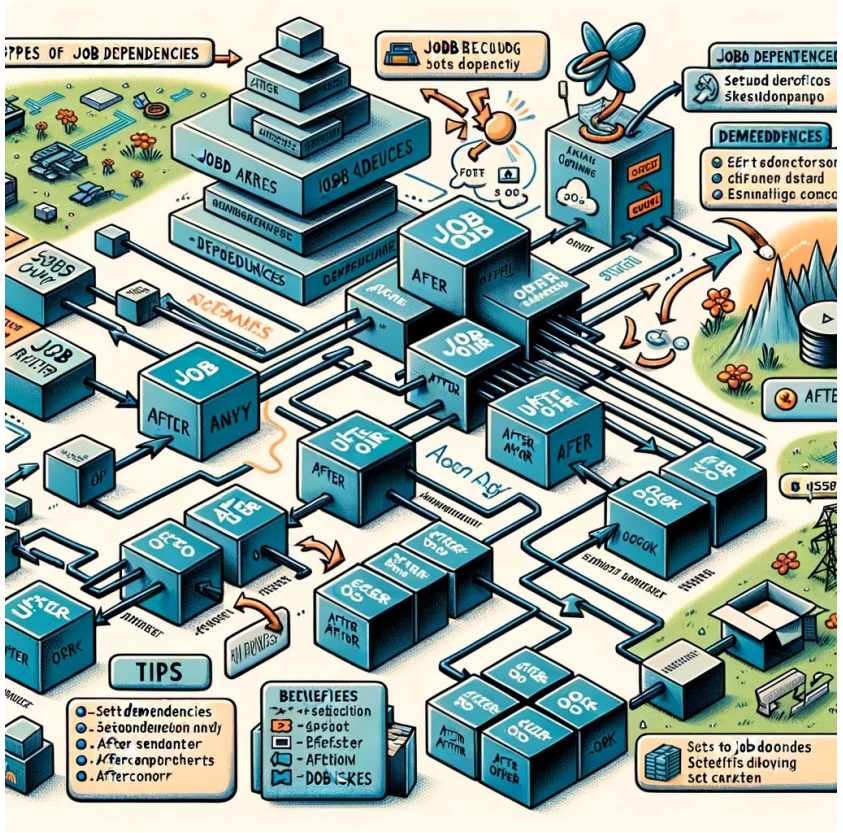
Job Array

```
sbatch script_job_3_array.sh

Submitted batch job 7054274

(base) [vc18@nlogin3 Workshop_Nov_2023]$ squeue -u vc18
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
     7054274_[1-8] ctbp-onuc job_3_ar     vc18 PD       0:00      1 (Priority)

(base) [vc18@nlogin3 Workshop_Nov_2023]$ squeue -u vc18
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
         7054274_1 ctbp-onuc job_3_ar     vc18  R       0:36      1 bc6u15n1
         7054274_2 ctbp-onuc job_3_ar     vc18  R       0:36      1 bc6u15n1
         7054274_3 ctbp-onuc job_3_ar     vc18  R       0:36      1 bc6u15n1
         7054274_4 ctbp-onuc job_3_ar     vc18  R       0:36      1 bc6u15n1
         7054274_5 ctbp-onuc job_3_ar     vc18  R       0:36      1 bc6u15n1
         7054274_6 ctbp-onuc job_3_ar     vc18  R       0:36      1 bc6u15n1
         7054274_7 ctbp-onuc job_3_ar     vc18  R       0:36      1 bc6u15n1
         7054274_8 ctbp-onuc job_3_ar     vc18  R       0:36      1 bc6u15n1
```

Job Dependency

What is Job Dependency?

- Allows you to define conditions under which a job will start based on the state of one or more other jobs.
- Useful for workflows, where tasks need to be executed in a specific order or condition.



Job Dependency

```
#!/bin/bash
#SBATCH --job-name=job_4_dependency
#SBATCH --account=ctbp-onuchic
#SBATCH --partition=ctbp-onuchic
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --time=00:10:00
#SBATCH --mem-per-cpu=100M
#SBATCH -e slurm-%A_%a-%x.err
#SBATCH -o slurm-%A_%a-%x.out
#SBATCH --array=1-8
```

```
# If it's the last job in the array, submit the dependent job
if [ $SLURM_ARRAY_TASK_ID -eq 1 ]; then
    sbatch --dependency=afterany:$SLURM_ARRAY_JOB_ID script_job_5.sh
fi
```

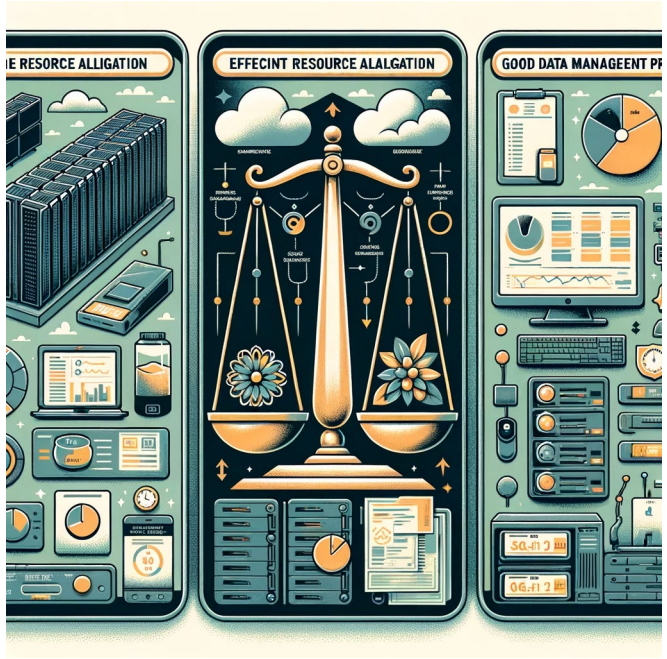
```
echo "Number of Nodes: $SLURM_NNODES"
echo "Number of Tasks: $SLURM_NTASKS"
echo "Cores/CPUs per Node: $SLURM_CPUS_ON_NODE"

sleep $TOTAL_SLEEP_TIME

echo "Runtime Duration: $(($SECONDS / 60)) minutes and $(($SECONDS % 60)) seconds."
```

Job Dependency

```
#!/bin/bash
#SBATCH --job-name=job_5_after_all_4
#SBATCH --account=ctbp-onuchic
#SBATCH --partition=ctbp-onuchic
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --time=00:10:00
#SBATCH --mem-per-cpu=100M
#SBATCH -e slurm-%j-%x.err
#SBATCH -o slurm-%j-%x.out

# Your job commands go here
echo "Running script_job_5.sh after the job array completed."
sleep 120
```

Best Practices for HPC Cluster Usage

- **Efficient Resource Allocation:** Overestimating can lead to wasteful usage of cluster resources, while underestimating can result in job failure or suboptimal performance.
- **Effective Job Monitoring and Management:** Keeping track of your jobs' status and performance is essential for catching errors early and ensuring efficient use of the cluster.
- **Practice Good Data Management:** Organize, back up, and manage your data efficiently to ensure smooth operations and avoid data loss during your computations.



BENCHMARKING

Intermediate SLURM Operations

Interactive Section and Node Allocation

```
run --pty --partition=ctbp-onuchic --account=ctbp-onuchic --ntasks=1 --mem=1G --time=00:30:00 $SHELL
```

GPU Request

```
#SBATCH --gres=gpu:1
```

OpenMP, MPI, and Hybrid Jobs

```
(base) [vc18@nlogin3 advanced_slurm_parallel]$ ls
hybrid_mpi_openmp_example.py  mpi_example.py     result_hybridJob.txt  result_openmpJob.txt  slurm_mpi.sh
interactive_command.txt       openmp_example.py  result_mpiJob.txt     slurm_hybrid.sh       slurm_openmp.sh
```

CTBP – Resources & Useful links

- https://kb.rice.edu/page.php?id=108237 (**NOTS**)
- https://wiki.rice.edu/confluence/display/CTBP/CTBP+Computing+Activities (**CTBP**)
- https://researchcomputing.rice.edu (**CRC**)
- https://slurm.schedmd.com/tutorials.html (**SLURM**)