UNIVERSITI MALAYA

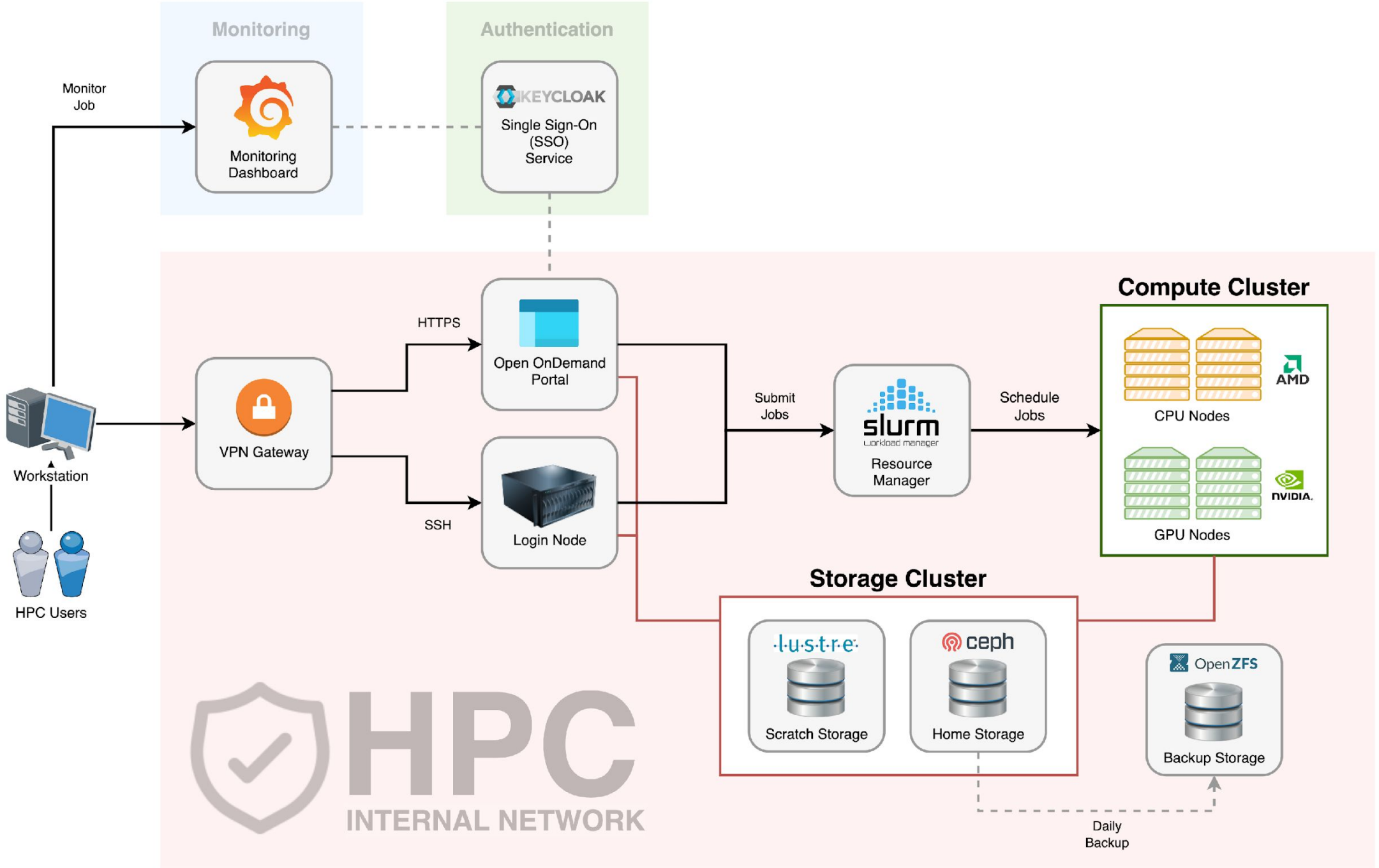
DICC

Basic Usage of HPC

Session Outcome

- Type of storages and differences
- Understand the components in UMHPC
- Understand the SLURM job parameters
- Understand how to submit a job
- How to check the log files

What is HPC


Monitoring
Authentication
Monitor Job
Monitoring Dashboard
KEYCLOAK
Single Sign-On (SSO) Service
HTTPS
Open OnDemand Portal
VPN Gateway
SSH
Login Node
Workstation
HPC Users
Submit Jobs
slurm
workload manager
Resource Manager
Schedule Jobs
Compute Cluster
CPU Nodes
AMD
GPU Nodes
NVIDIA
Storage Cluster
lustre
Scratch Storage
ceph
Home Storage
OpenZFS
Backup Storage
Daily Backup
HPC
INTERNAL NETWORK

Login Node

- The stuffs that users usually will do in here:
  - Transfer and manage files
  - Submit jobs
  - Check error and output logs
  - Monitor jobs
- Things to avoid:
  - Execute CPU or memory intensive scripts
  - Compile application
  - Extract large archive file

Storage Cluster

	Home Directory	Lustre Directory
File System	CephFS	Lustre
Directory	/home	/lustre
Storage Type	Persistent	Non-persistent
Storage Clean Up	No	Files that have not been accessed for 60 days
Quota	100 GB per user	Unlimited
Capacity	74 TB	230 TB
Backup	Daily	No
Group Directory	No	Yes

Compute Node

- Also referred as worker node.
- Some of the compute nodes have GPU.
- Your job will be executing in compute node(s).
- You do not have direct access to compute node unless you have submitted a job.

When Do You Need HPC?

- Your job will be running for very long period.
- Your job can utilize multiple CPU cores for parallelism.
- You need to repeat the same calculation with many different inputs.
- Your can utilize more powerful GPU(s).
- Your job consume very large amount of memory.

Basic Requirement to Access HPC

- A personal computing device
- Internet
- User account with HPC access
- OpenVPN and DICC OpenVPN profile

Account & Limits

- Every fresh user in DICC who wish to use HPC must request HPC access in DICC service desk.
- Every fresh HPC user will have limit resources access.

Resource	Limited Account	Unlocked Account
CPU	4	450
Memory	16 GB	2 TB
GPU	1	Unlimited
Wall Time	1 hour	7 days
QoS	limited	short, normal, long
Accessible Partition	cpu-opteron, gpu-k10, gpu-k40c	All partition

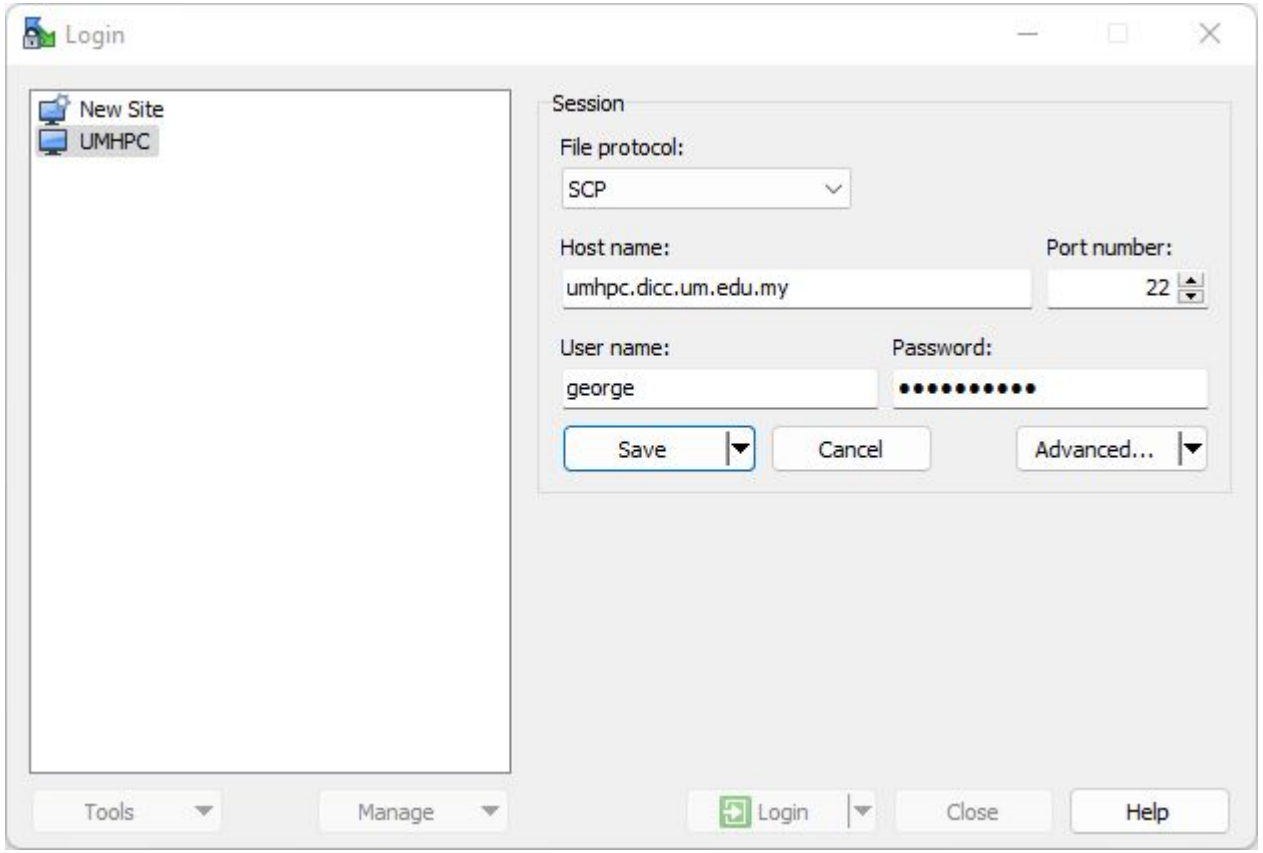
How to Submit A Job?

Things to Know

- File Transfer
- Application & Modules
- Job Parameter
- Job Submission
- Post-Job Submission

Transferring Files (Windows)

- For Windows user, we recommend user to use WinSCP:
  - Protocol: SCP
  - Port: 22
  - Host name: umhpc.dicc.um.edu.my



Transferring Files (Linux)

- For Linux and MacOS, you can use **scp** command in your terminal/console:
  - To transfer file into UMHPC:
    - **`$ scp /path/to/filename username@umhpc.dicc.um.edu.my:/path/to/destination`**
  - To transfer folder into UMHPC:
    - **`$ scp -r /path/to/directory username@umhpc.dicc.um.edu.my:/path/to/destination`**
- Alternatively, you can use **FileZilla** as your FTP/SCP client to transfer your files between UMHPC and your local workstation.

Hands On

- Create a folder, **my_first_job** in your local machine.
- Create an empty text file, **tutorial.sh**
- Transfer the folder into **UMHPC**.

Things to Know

- File Transfer
- Application & Modules
- Job Parameter
- Job Submission
- Post-Job Submission

Application & Modules

- Most of the application/module or system library are NOT available in login node.

Function	Login Node	Compute node
List all applications in all compute nodes	`node-modules`	-
List all application in current instance	`module avail`	`module avail`
Load a specific application	`module load`	`module load`
List all the loaded application/module	`module list`	`module list`
Unload a loaded module	`module unload`	`module unload`

Hands On

- Verify the presence of miniconda using the command:
  - **`conda --version`**
- Check the available module installed in login node.
- Load miniconda module.
- List all the module(s) had been loaded currently.
- Verify again the presence of miniconda using the command:
  - **`conda --version`**
- Unload all the modules.
- List out all the module installed in compute nodes.

Answer

```
$ conda --version
$ module avail
$ module load miniconda/conda-22.11.1
$ module list
$ conda --version
$ module purge
$ node-modules
```

Things to Know

- Application & Modules
- File Transfer
- Job Parameter
- Job Submission
- Post-Job Submission

Job Parameters

- Job parameters determine what kind of resources you want.

Parameter	Description	Example
--partition, -p	Specify the partition to run job.	--partition=cpu-opteron
--ntasks, -n	Specify the number of CPUs/cores required.	--ntasks=4
--mem	Specify the amount of memory needed per node.	--mem=16G
--nodes, -N	Specify the number of compute nodes.	--nodes=1
--job-name, -J	Specify the name of the job.	--job-name=job01
--gpus, -G	Specify the number and the type of GPU card needed.	--gpus=1 or --gpus=titanxp:1
--qos, -q	Specify the QoS for the job	--qos=normal
--output, -o	Specify the filename for output log.	--output=/home/user/george/output.log
--error, -e	Specify the filename for error log.	--error=/home/user/george/error.log
--hint	Enable/Disable hyper-threading	--hint=nomultithread

Resources

- Resources summary can be displayed by using the command:
  - **`cluster-info`**

Partition	Node	Cores	Threads	Mem (GB)	GPU	
cpu-epyc	cpu12	48	2	234		
	cpu13	48	2	234		
	cpu14	48	2	234		
	cpu15	48	2	234		
cpu-opteron	cpu01	64	1	234		
	cpu03	64	1	234		
	cpu04	64	1	234		
	cpu05	64	1	234		
	cpu07	64	1	234		
	cpu08	64	1	234		
	cpu09	64	1	234		
	cpu10	64	1	234		
	cpu11	64	1	218		
gpu-k10	gpu01	16	2	39	k10:	8
	gpu03	16	2	54	k10:	8
gpu-k40c	gpu04	16	2	54	k40c:	2
gpu-titan	gpu02	16	2	117	titanx:	1
					titanxp:	2
gpu-v100s	gpu05	32	2	171	v100s:	2

Partition

- Currently, there are 6 partitions available in DICC:
  - **`cpu-opteron`** (default) – 1800 MHz
  - **`cpu-epyc`** – 3200 MHz
  - **`gpu-k10`** – 745 MHz
  - **`gpu-k40c`** – 876 MHz
  - **`gpu-titan`**
    - **`Titan X`** – 1089 MHz
    - **`Titan Xp`** – 1582 MHz
  - **`gpu-v100s`** – 1597 MHz
- Do not submit CPU only job into GPU partition!

QoS

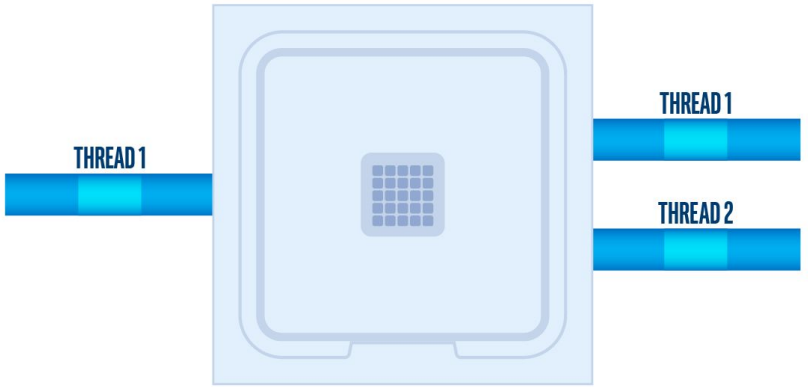
- QoS determine the maximum walltime of a job.
- Every job have its own unique priority.
  - **`sprio`** command can be used to check job priority in the queue currently.

QoS	Maximum Wall time	Priority Boost
Short	1 hour	+10,000
Normal (default)	1 day	-
Long	7 days	-

JOBID	PARTITION	PRIORITY	SITE	AGE	FAIRSHARE	QOS
52551	gpu-v100s	19122	0	18122	1000	0
52584	gpu-v100s	18526	0	17926	600	0
52777	gpu-v100s	15713	0	13914	1800	0
52922	gpu-titan	11868	0	10668	1200	0
52965	gpu-titan	10319	0	9119	1200	0
53178	gpu-v100s	3399	0	2800	600	0
53201	cpu-opter	1691	0	1291	400	0
53209	gpu-titan	2883	0	1083	1800	0
53220	gpu-v100s	2541	0	741	1800	0
53226	gpu-v100s	2533	0	733	1800	0
53235	cpu-opter	1802	0	202	1600	0
53237	cpu-opter	1801	0	202	1600	0
53238	cpu-opter	1801	0	201	1600	0
53241	gpu-k10	959	0	159	800	0
53257	cpu-epyc	1436	0	37	1400	0
53258	cpu-epyc	1436	0	37	1400	0
53263	cpu-opter	1416	0	16	1400	0
53264	cpu-opter	1416	0	16	1400	0
53265	cpu-opter	1416	0	16	1400	0
53266	cpu-opter	1415	0	16	1400	0
53267	cpu-opter	1415	0	16	1400	0
53270	cpu-opter	3403	0	3	3400	0

Hyper-Threading

- It is highly recommended to include the **`--hint`** parameter in the submission script.
- In most of the scenario, disabling hyper-threading will yield better performance.
- To disable hyper-threading,
  - **`--hint=nomultithread`**



Recommendations

- Always start small and scale larger when your are confident on how much you have understood your job.

CPU	Memory (GB)	QoS	Usage
4	16	short	Troubleshooting & debug
16	50	normal	Standard quick job
16	50	long	Standard small job
24 for EPYC 32 for Opteron	100	long	Standard medium job
48 for EPYC 64 for OPTERON	200	long	Standard large job

Things to Know

- Application & Modules
- File Transfer
- Job Parameter
- Job Submission
- Post-Job Submission

Job Submission

Batch Mode	Interactive Mode
Use **submission script** to execute.	Enter the node to execute.
Job continue to execute even if you have lost connection or your session terminated.	Job terminated on connection lost/terminated session.
Cannot make changes during the execution.	Able to make interactive input during the execution.
Usually done by using the command: **`sbatch`**	**`salloc`** to allocate resources. **`srun`** to join allocated resources and run calculation.
Execute until the maximum walltime.	
Must go through queue for resources allocation.	

Batch Mode

- When to use Batch Mode:
  - You have unstable network connection.
  - The application take a long time to complete.
  - No input needed during the process of calculation.
  - You need to run same calculation/simulation multiple times with different input files.
- This method is the recommended and standard way of running a job in HPC environment.
- Requirements:
  - Job script
  - Job parameters
  - Commands to execute
  - Input files

Example of Batch Script

```
#!/bin/bash -l

#SBATCH --partition=cpu-epyc
#SBATCH --job-name=job01
#SBATCH --nodes=1
#SBATCH --ntasks=24
#SBATCH --mem=100G
#SBATCH --qos=normal

module load myModule
app -i input.file -o output.file
```

Batch Mode (cont.)

- Use **`sbatch`** command to submit the job script.
  - **`$ sbatch batch_script.sh`**
- Use **`scancel`** command to cancel and remove the submitted job from queue. (Note: Once the job is cancelled, it cannot be recovered!)
  - **`$ scancel 12345`**

Hands On

- Edit the script, tutorial.sh to fulfil the following scenario:
  - Submitting partition: cpu-opteron
  - Total number of CPU cores: 16
  - Number of nodes: 2
  - Amount of memory per node: 50G
  - Quality of service: short
  - Job name: tutorial
  - Disabled hyper-threading

```
#!/bin/bash -l

#SBATCH --partition=cpu-epyc
#SBATCH --job-name=job01
#SBATCH --nodes=1
#SBATCH --ntasks=24
#SBATCH --mem=100G
#SBATCH --qos=normal

module load myModule
app -i input.file -o output.file
```

Answer

```
#!/bin/bash -l
#SBATCH --partition=cpu-opteron
#SBATCH --nodes=2
#SBATCH --ntasks=16
#SBATCH --mem=50G
#SBATCH --qos=short
#SBATCH --job-name=tutorial
#SBATCH --output=%x.out
#SBATCH --error=%x.err
#SBATCH --hint=nomultithread
```

Interactive Mode

- When to use Interactive Mode:
  - You have to input commands or intermediate input during the application execution.
  - You are trying to compile your own application.
  - You are trying to debug or troubleshoot your calculation or compilation.
- Requirements:
  - Job parameters
  - Commands to execute

Interactive Mode (cont.)

- To start an interactive session, first, you will need to allocate the resources you need then join the session interactively.
- To allocate resource for interactive session:
  - **`$ salloc –p cpu-opteron –N 1 –n 4 --mem=16G --qos=normal`**
- To join the allocated session interactively:
  - **`$ srun --jobid=12345 --pty bash –l`**
- To exit the interactive session, enter exit in terminal twice to leave and relinquish the allocated resources.

Example of Interactive Mode

```
[user@umhpc ~]$ salloc -p cpu-opteron -N 1 -n 4 --mem=16G --qos=normal
salloc: Pending job allocation 12345
salloc: job 12345 queued and waiting for resources
salloc: job 12345 has been allocated resources
salloc: Granted job allocation 12345
salloc: Waiting for resource configuration
salloc: Nodes cpu01 are ready for job
[user@umhpc ~]$ srun --jobid=12345 --pty bash -l
[user@cpu01 ~]$ exit
logout
[user@umhpc ~]$ exit
salloc: Relinquishing job allocation 12345
```

Things to Know

- Application & Modules
- File Transfer
- Job Parameter
- Job Submission
- Post-Job Submission

Job State

- You can check your own job(s) state with the command:
  - **`$ squeue -u <username>`**
- The common job state and the descriptions:

Job State	Description
PD / PENDING	Pending for resource scheduling.
R / RUNNING	The job is currently running.
RQ / REQUEUED	The job has been requeued.
CG / COMPLETING	The job has done execute and is now completing itself.
S / SUSPENDED	The job has been suspended.

```
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
53199  cpu-epyc  PNaInPS           R   15:23:07      1 cpu15
53195  cpu-epyc PNaSnAsS           R 1-06:26:03      1 cpu12
53189  cpu-epyc     TaSe           R 2-06:23:33      1 cpu13
53235 cpu-opter mk_STAR_          PD       0:00      1 (Resources)
53237 cpu-opter H5N1_2_c          PD       0:00      1 (Priority)
53238 cpu-opter H1N1_cuf          PD       0:00      1 (Priority)
53201 cpu-opter    ONb-S          PD       0:00      1 (Priority)
53193 cpu-opter molecule           R 1-11:22:32      1 cpu04
53236 cpu-opter H5N1_1_c           R    3:52:08      1 cpu01
53136 cpu-opter       aa           R 3-05:39:24      1 cpu05
53137 cpu-opter       ss           R 3-05:39:24      1 cpu07
53138 cpu-opter       dd           R 3-05:39:24      1 cpu08
53139 cpu-opter       ff           R 3-05:39:24      1 cpu09
53140 cpu-opter       zz           R 3-05:39:24      1 cpu10
53249 cpu-opter interact           R      58:15      1 cpu01
53200 cpu-opter     ONbC           R 1-06:00:45      1 cpu11
53196 cpu-opter      C-S           R 1-06:37:24      1 cpu03
53241   gpu-k10  triplet          PD       0:00      1 (Resources)
53041   gpu-k10 02_prod_           R   12:32:19      1 gpu01
53240   gpu-k10  triplet           R    2:54:39      1 gpu03
52922 gpu-titan  06_prod          PD       0:00      1 (Resources)
52965 gpu-titan  05_prod          PD       0:00      1 (Priority)
53209 gpu-titan    jbmbq          PD       0:00      1 (Priority)
52773 gpu-titan     jxbb          PD       0:00      1 (job requeued in held state)
52921 gpu-titan  04_prod           R    1:30:05      1 gpu02
53115 gpu-titan Jupyter            R    6:20:15      1 gpu02
52551 gpu-v100s    rerun          PD       0:00      1 (Resources)
52584 gpu-v100s Jupyter           PD       0:00      1 (Priority)
52777 gpu-v100s       jq          PD       0:00      1 (Priority)
53178 gpu-v100s Jupyter           PD       0:00      1 (Priority)
53220 gpu-v100s     hxbb          PD       0:00      1 (Priority)
53226 gpu-v100s     bq11          PD       0:00      1 (Priority)
52498 gpu-v100s Jupyter            R    6:10:48      1 gpu05
```

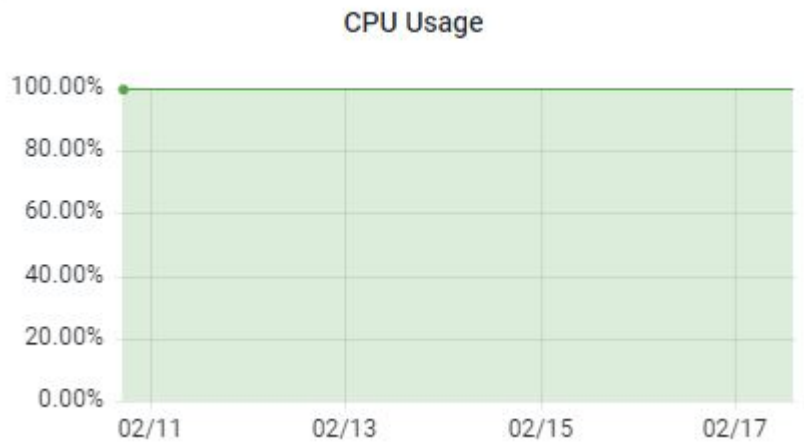
Job State (cont.)

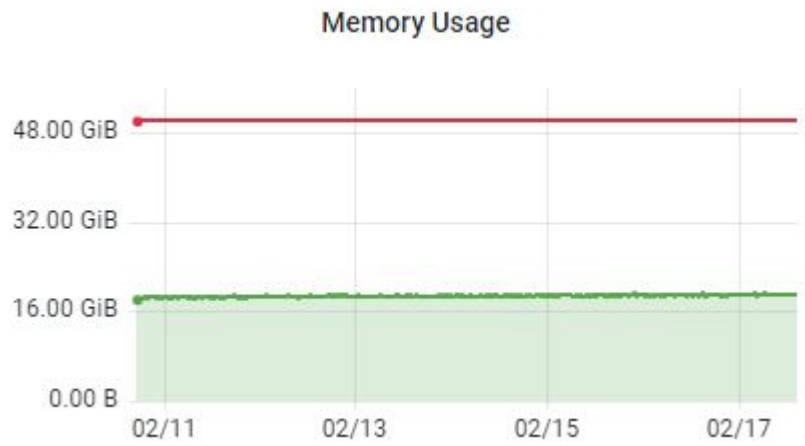
- If your job(s) is not in queue anymore, here are the possible scenario:
  - Your job(s) is/are completed. Check your output log for result.
  - Your job(s) is/are failed. Check your error log for error message.
- You can use **`sacct`** command to review the exit state of those jobs.
  - **`$ sacct --starttime=2023-01-01 --endtime=2023-01-31`**

```
[          @umhpc: ~] $ sacct
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
57721              amber   cpu-epyc       free         24    PENDING      0:0
58374         gromacs_k+   gpu-k40c       free          4    PENDING      0:0
58375         gromacs_k+   gpu-k40c       free          8    PENDING      0:0
58376         gromacs_k+   gpu-k40c       free         12    PENDING      0:0
58377         gromacs_k+   gpu-k40c       free         16    PENDING      0:0
58378         gromacs_k+   gpu-k40c       free          4    PENDING      0:0
58379         gromacs_k+   gpu-k40c       free          8    PENDING      0:0
58380         gromacs_k+   gpu-k40c       free         12    PENDING      0:0
58381         gromacs_k+   gpu-k40c       free         16    PENDING      0:0
58382         gromacs_t+  gpu-titan       free          4    PENDING      0:0
58383         gromacs_t+  gpu-titan       free          8    PENDING      0:0
58384         gromacs_t+  gpu-titan       free         16    PENDING      0:0
58385         gromacs_t+  gpu-titan       free         12    PENDING      0:0
58386         gromacs_t+  gpu-titan       free          4    PENDING      0:0
58387         gromacs_t+  gpu-titan       free          8    PENDING      0:0
58388         gromacs_t+  gpu-titan       free         12    PENDING      0:0
58389         gromacs_t+  gpu-titan       free         16    PENDING      0:0
58390              amber   cpu-epyc       free         24    PENDING      0:0
58395         gromacs_v+  gpu-v100s       free         20  COMPLETED      0:0
58395.batch        batch                 free         20  COMPLETED      0:0
58395.extern      extern                 free         20  COMPLETED      0:0
58396         gromacs_v+  gpu-v100s       free         24  COMPLETED      0:0
58396.batch        batch                 free         24  COMPLETED      0:0
58396.extern      extern                 free         24  COMPLETED      0:0
58397         gromacs_v+  gpu-v100s       free         28  COMPLETED      0:0
58397.batch        batch                 free         28  COMPLETED      0:0
58397.extern      extern                 free         28  COMPLETED      0:0
58398         gromacs_v+  gpu-v100s       free         32  COMPLETED      0:0
58398.batch        batch                 free         32  COMPLETED      0:0
58398.extern      extern                 free         32  COMPLETED      0:0
```

Job Monitoring

- Make sure your job(s) is running properly.
- Ways to monitor your job(s):
  - Visit DICC OnDemand portal at https://ood.dicc.um.edu.my/ under **Jobs** > **Active Jobs** section.
  - SSH into the node executing your jobs and use **`htop`** command for CPU usage and **`nvidia-smi`** for GPU usage.
  - Check your output log and error log.
- In most scenario, Opteron will yield 100% CPU usage and the other partition will yield a maximum of 50% CPU usage.





FAQ

- Why my job is in PENDING state with the reason of “job is requeued in held state”?
  - The job is running incorrectly and causing problem to the service.
- My job was failed and the error message show “OOM error”. Why?
  - Out-of-Memory (OOM) error is due to the application tend to use more memory than allocated memory. You try to allocate more memory for that particular job.
- Why my job(s) is/are queueing in the queue for very long period?
  - Check the reason in squeue:
    - Priority: There are more jobs with higher priority than your job(s).
    - Resources: Your job(s) is/are up next once the job(s) currently running in the partition have completed.

Useful Portal

- DICC Website – https://dicc.um.edu.my
- DICC Jira Service Desk – https://jira.dicc.um.edu.my
- DICC Documentation Confluence – https://confluence.dicc.um.edu.my

Hands On

- Create a job script, **first_job.sh** in the directory, **my_first_job** to fulfil the following scenario:
  - Submit to **`cpu-opteron`** partition.
  - Allocate 4 CPUs, 8 GB memory and 1 node
  - QoS: **limited**
  - Job name: **my_first_job**
  - With output and error log specified
- Commands to be executed by the job:
  - **`echo "This is my first job in $(hostname -s)"`**
  - **`sleep 10m`**
- Submit the job as batch mode.
- Use **`squeue`** to check the job state.
- Use **`scancel`** to cancel the job.
- Use **`sacct`** to check your account history.

```
#!/bin/bash -l

#SBATCH --partition=cpu-epyc
#SBATCH --job-name=job01
#SBATCH --nodes=1
#SBATCH --ntasks=24
#SBATCH --mem=100G
#SBATCH --qos=normal

module load myModule
app -i input.file -o output.file
```

Answer

```
#!/bin/bash -l

#SBATCH --partition=cpu-opteron
#SBATCH --job-name=my_first_job
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --mem=8G
#SBATCH --output=%x.out
#SBATCH --error=%x.err
#SBATCH --qos=limited

echo “This is my first job in $(hostname -s)”
sleep 10m
```

Answer

```
[user@umhpc ~]$ sbatch first_job.sh
[user@umhpc ~]$ squeue
[user@umhpc ~]$ scancel <job_id>
[user@umhpc ~]$ sacct
```

Thank You!