HPC User Environment 2

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Outlines

- **HPC User Environment 1**

  1. Intro to HPC
  2. Getting started
  3. Into the cluster
  4. Software environment (modules)

- **HPC User Environment 2**

  1. Basic concepts
  2. Preparing my job
  3. Submitting my job
  4. Managing my jobs

Outlines

- **HPC User Environment 2**

1. Basic concepts
    1) Previously on HPC User Environment 1…
    2) Job & Job schedulers
2. Preparing my job
    1) Basic principles
    2) Job duration (wall time)
    3) Number of nodes & cores
    4) Partitions and job queues
3. Submitting my job
    1) Interactive job
    2) Batch job
4. Managing my jobs
    1) Useful commands
    2) Monitoring job health

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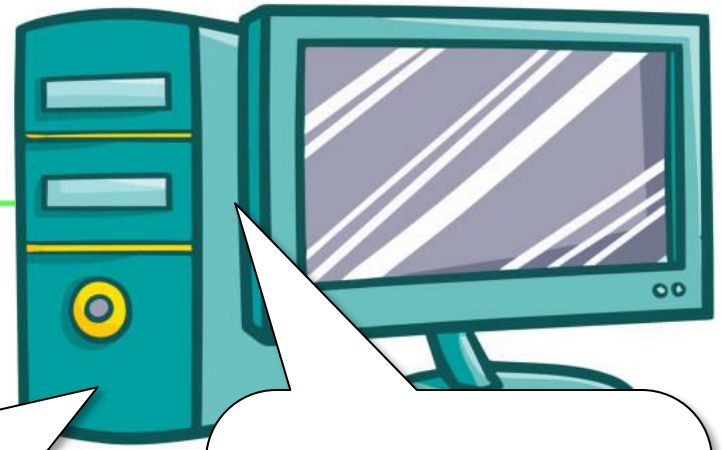
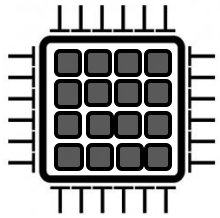
1) Previously on HPC User Environment 1…

Run my code on my machine as long as I would like to and until it is finished.

You do not share your resources with other people at home. That is your personal machine.

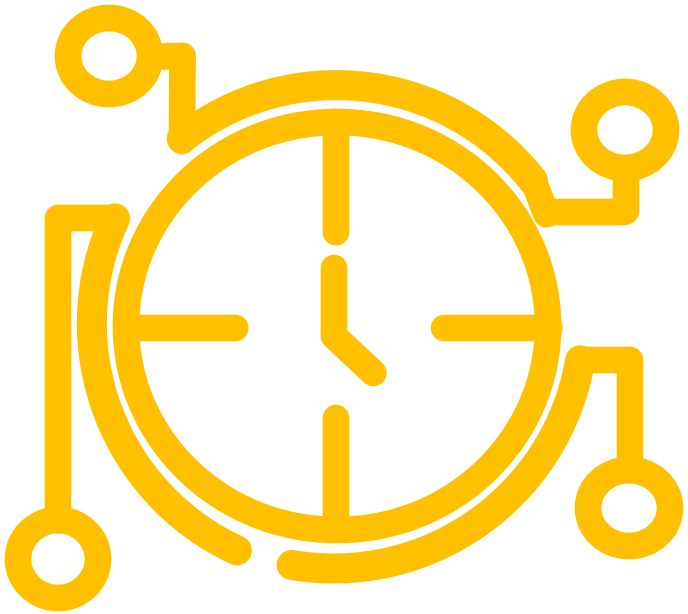


You can also install any software packages you want without restrictions using your root credentials with package management tools like yum, dnf, apt-get, etc.



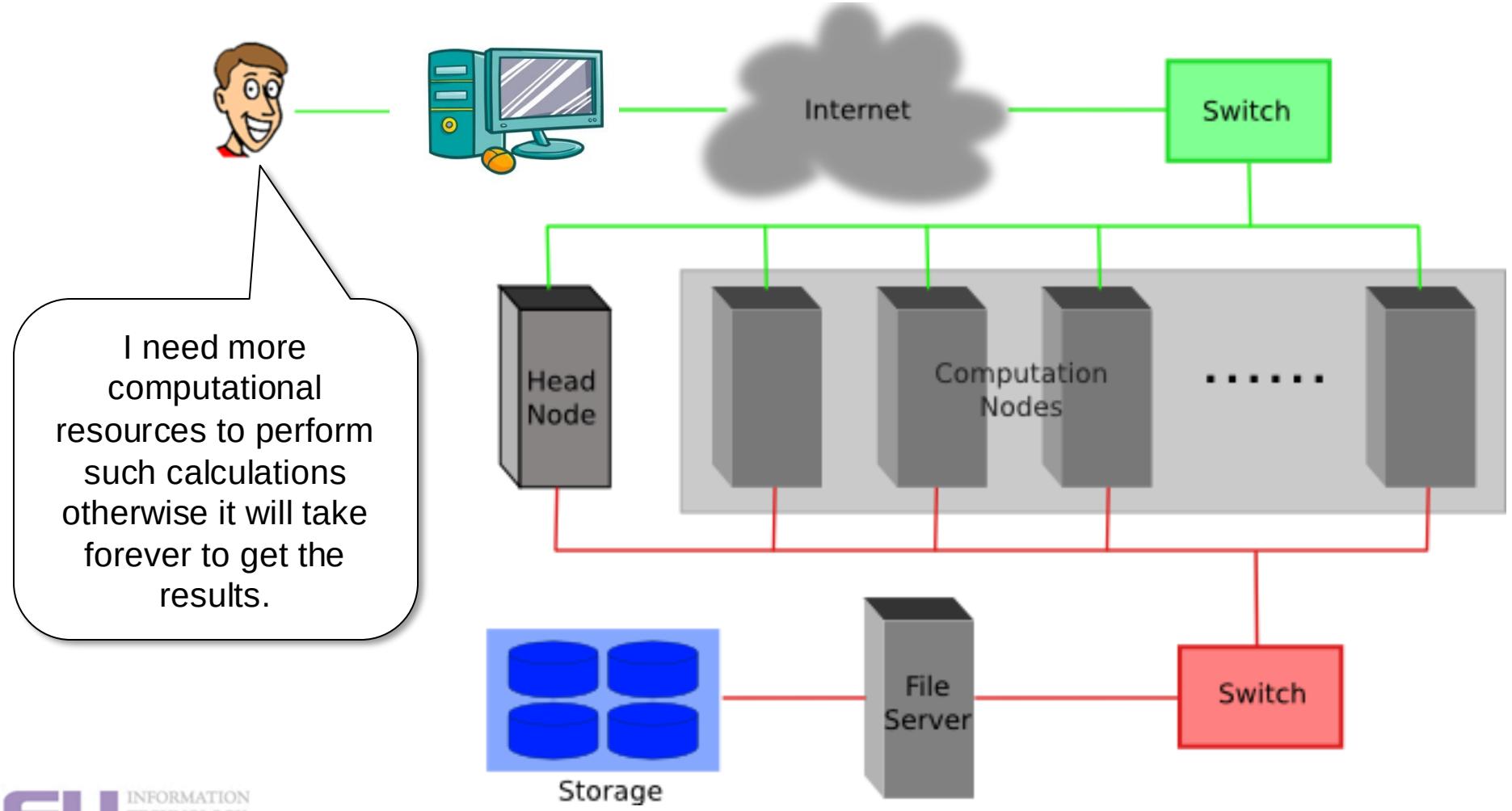
Multicore processor

Intel ® Core™ i7 ~ 4.0 GHz



You will be limited by the clock speed of your personal machine and a number of available cores.

1) Previously on HPC User Environment 1…



How do I connect, request resources, and run heavy calculations on the cluster?

What should I do about that?

1) Previously on HPC User Environment 1…

Two essential components to run jobs on LONI or LSU clusters:

1) Account

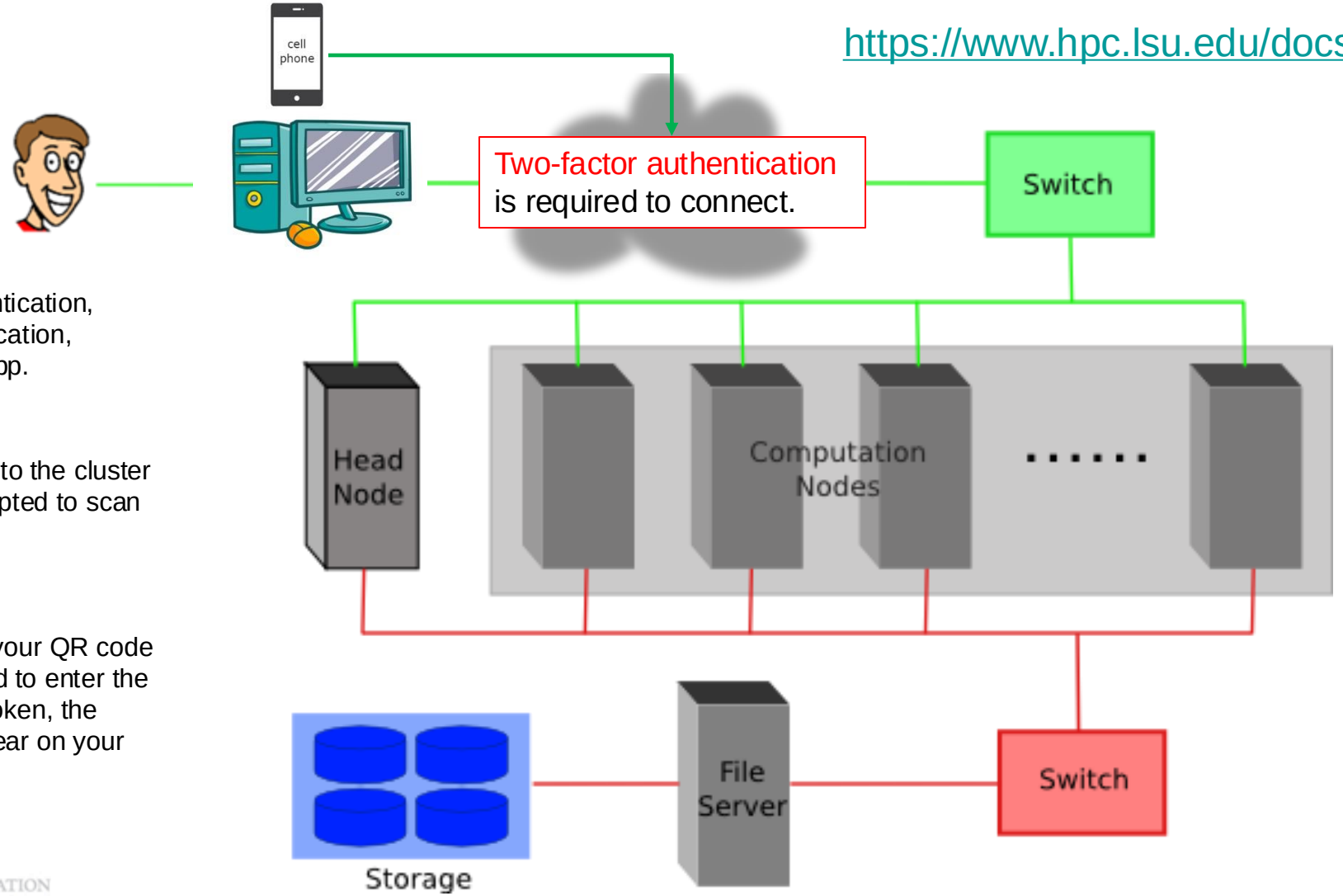
An individual who is authorized to access a computing cluster based on their affiliation, credentials, and permissions.

2) Allocation

http://www.hpc.lsu.edu/links.php

1) Previously on HPC User Environment 1…

https://www.hpc.lsu.edu/docs/systems/twofa.php



Step 1:
Microsoft Authentication, Google Authentication, or Mobile Due app.

Step 2:
While you log in to the cluster you will be prompted to scan your QR code.

Step 3:
Once you scan your QR code you will be asked to enter the Authentication token, the number will appear on your app.

Step 4:
If you did not scan the QR code the first time, you should be able to log in to the cluster in another way.

If nothing works, you can send a ticket to the LONI Systems Support team and ask for help.

sys-help@loni.org

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   2) Job and Job Scheduler
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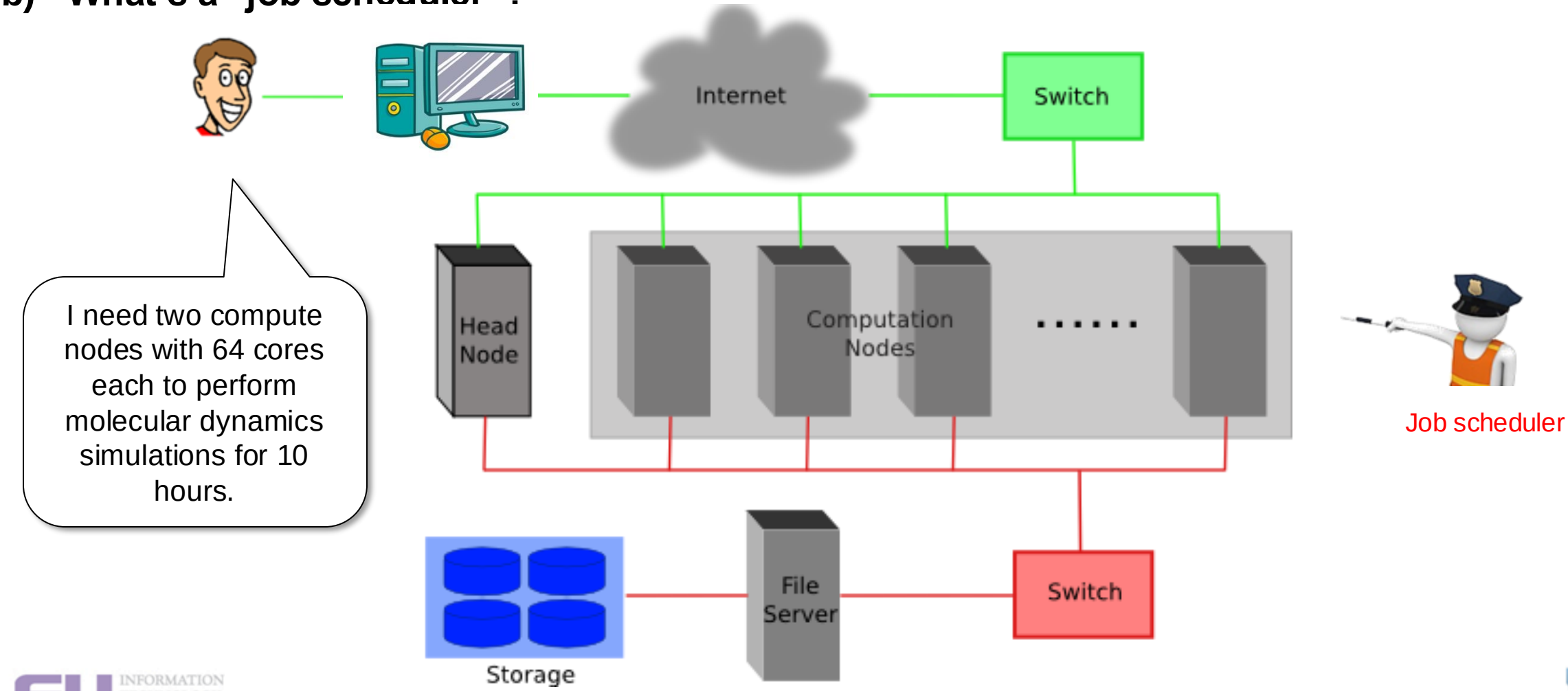
2) Job

a) The job is a computational task submitted to a cluster for execution.

- **Job script:** It can be a file that contains all the instructions and parameters needed to execute the job written in the shell scripting language. It specifies **the resource requirements** and **the commands**.
  - **Resource requirements**: You should define the computational resources needed, such as the partition type, the number of nodes, the number of cores, the amount of memory, and the computational time limit, to execute your job using Slurm directives such as **#SBATCH . . .**
  - **Commands:** After the Slurm directives, you can add any commands to execute your job.
- **SUs** are deducted from allocations based on the actual usage of each job.
  - Example:
    - My allocation balance: 50,000 SU
    - Running a job: 128 cores * 10 hours = 1280 SU
    - Balance after the job is completed: 48,720 SU

1 SU Unit = 1 CORE / hour

b) What's a "job scheduler"?

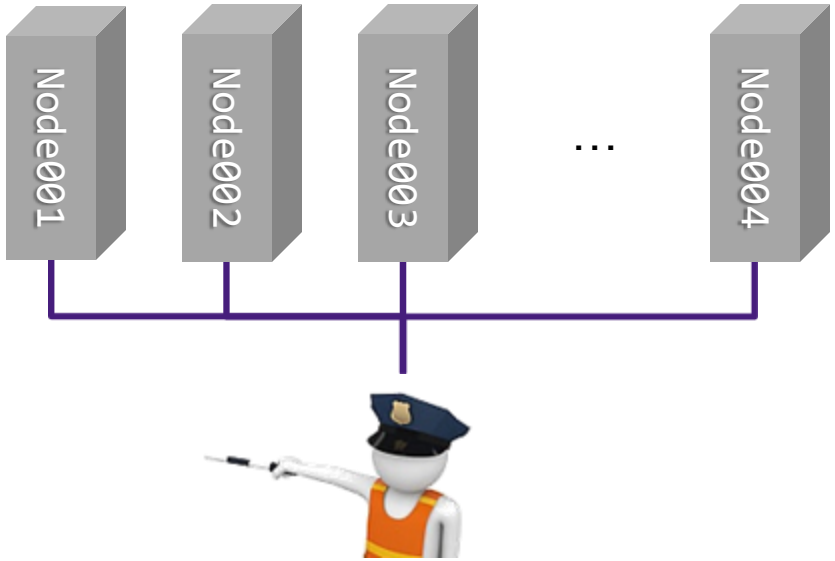


2) Job Scheduler

b) What's a "job scheduler"?

Allocation of resources: queue management and allocation of the resources based on job requirements.

Priority scheduling: assigns priority to jobs based on required computational resources and job duration. It also checks for fair resource distribution.



Monitoring and reporting: monitoring of the job progress, resource usage, and job status.

Fault tolerance and recovery: supports job checkpointing and recovery. It also handles job rescheduling when a compute node fails.

Command line tools: provide users with the tool submission, monitoring, and management.

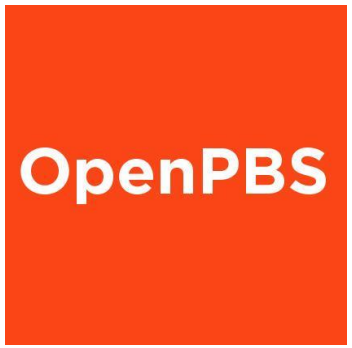
Online Web tools: support web-based interfaces for easier job scheduling and management, such as **Open OnDemand** https://ondemand.qbd.loni.org

b) What's a "job scheduler"?

https://www.ibm.com/docs/en/spectrum-lsf/10.1.0

LSF (Load Sharing Facility)

SLURM (Simple Linux Utility for Resource Management)



https://github.com/openpbs/openpbs

PBS (Portable Batch System)

https://slurm.schedmd.com/documentation.html

b) What's a "job scheduler"?

Workload manager	LSU HPC	LONI
slurm workload manager	Deep Bayou SuperMike III SMIC	QB3 (QBC) QB4 (QBD)

2) Job & Job Scheduler

Job	Job Scheduler
• Computational task: data processing … • Resources: CPU cores, RAM memory … • Execution environment: modules … • Input/Output: input files/output files • A job script might be submitted by a user to the job scheduler for execution.	• Allocation of resources: Nodes, CPUs, memory … • Priority scheduling: assigns priority to jobs … • Monitoring and reporting: the job progress • Fault tolerance and recovery: checkpointing … • Command line tools: job management • Online web tools: job management using OOD

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1) Basic principles

Large enough	Small enough
• To successfully complete your job	• To ensure quick turnaround • Not to waste resources for other users

1) Basic principles

Available HPC Resources	Description
• Time:	• Job run time / wall time
• Compute resources:	• Nodes, CPU cores, threads
• Memory:	• RAM, per-core memory, total memory
• Partition or queue:	• Appropriate queues
• Software:	• Modules or specific software (containers)

… and other resources such as storage, networking, and other special hardware.

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#SBATCH --time=DD-**HH**:**MM**:**SS**

2) Job duration (wall time)

- **SuperMike3**

Partition Name	Max Walltime	Max Jobs (per user)	Max Nodes (per user)	Allowed Cores per Node
single	168	32	96	1– 64
checkpt	72	32	96	64
workq	72	32	96	64
bigmem	72	–	4	64
gpu	72	8	4	32/64
gpu4	72	8	4	16/32/48/64

http://www.hpc.lsu.edu/docs/guides.php?system=SuperMike3

2) Job duration (wall time)

- **FAQ**

Q	A
• What if my command is still running when the wall time runs out?	• Job is **terminated**. Any running process will be **killed.**
• What if all my commands in the job finished before the wall time runs out?	• Job **exits** successfully when all commands finished.
• If my job exits before requested wall time, how many SUs will I be charged?	• You will be charged based on your **actual time used** (if less than requested).
• In that case, why don't I just request maximum wall time every time?	• Your queuing time might be quite long.

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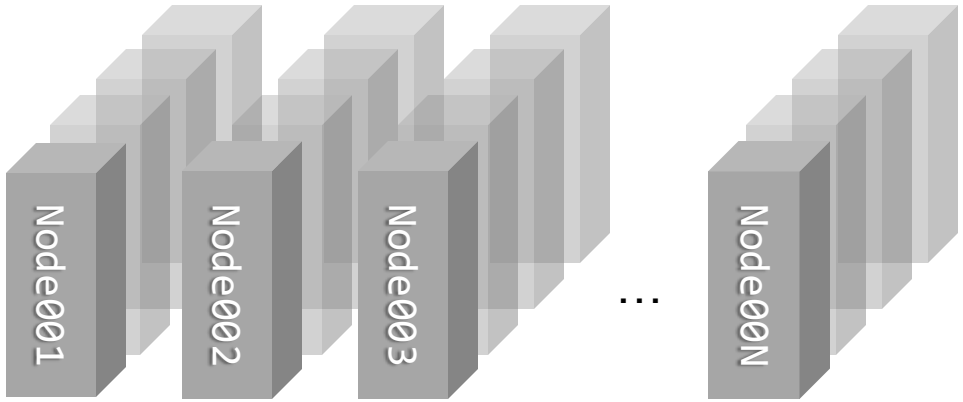

3) Number of nodes & cores

- **Previously in HPC User Environment 1 …**

SuperMIC	
Hostname	smic.hpc.lsu.edu
Peak Performance/TFlops	925
Compute nodes	360
Processor/node	2 10-core
Processor Speed	2.8 GHz
Processor Type	Intel Xeon 64bit
Nodes with Accelerators	360
Accelerator Type	Xeon Phi 7120P
OS	RHEL v6
Vendor	
Memory per node	64 GB
Detailed Cluster Description	
User Guide	
Available Software	

Deep Bayou	
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
Processor Speed	2.4 GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
Accelerator Type	2 x NVIDIA Volta V100S
OS	RHEL v7
Vendor	Dell
Memory per node	192 GB
Detailed Cluster Description	
User Guide	
Available Software	

SuperMike III	
Hostname	mike.hpc.lsu.edu
Peak Performance/TFlops	1,285
Compute nodes	183
Processor/node	2 32-core
Processor Speed	2.6GHz
Processor Type	Intel Xeon Ice Lake
Nodes with Accelerators	8
Accelerator Type	4 NVIDIA A100
OS	RHEL v8
Vendor	Dell
Memory per node	256/2048 GB
Detailed Cluster Description	
User Guide	
Available Software	

https://www.hpc.lsu.edu/resources/hpc/index.php#lsuhpc

3) Number of nodes & cores

[username@host ~]$ ssh –X username@host
(username@host) Password:
(username@host) TOPT Authenticator Token:

```
################################################################################
Send questions and comments to the email ticket system at sys-help@loni.org.
################################################################################

QB-4 at LONI (Open for general use)

# 02-May-2024

QB-4 is a 4.3 PetaFlop peak performance cluster with 35,008 CPU cores and
144 NVIDIA A100 GPUs, comprised of 547 compute nodes connected by 200 Gbps
Infiniband fabric.


Node Specs:
compute CPUs=64 SocketsPerBoard=2 CoresPerSocket=32 ThreadsPerCore=1 RealMemory=256000 DefMemPerCPU=3920 MB
bigmem  CPUs=64 SocketsPerBoard=2 CoresPerSocket=32 ThreadsPerCore=1 RealMemory=2063000 DefMemPerCPU=32100 MB
gpu2    Gres=gpu:2 CPUs=64 SocketsPerBoard=2 CoresPerSocket=32 ThreadsPerCore=1 RealMemory=514000 DefMemPerGPU=254000 MB
gpu4    Gres=gpu:4 CPUs=64 SocketsPerBoard=2 CoresPerSocket=32 ThreadsPerCore=1 RealMemory=514000 DefMemPerGPU=127000 MB
```

3) Number of nodes & cores

[username@qbd1]$ scontrol show partition

PartitionName=workq
AllowGroups=ALL AllowAccounts=ALL AllowQos=ALL
AllocNodes=ALL Default=NO QoS=normal
DefaultTime=12:00:00 DisableRootJobs=YES ExclusiveUser=NO GraceTime=0 Hidden=NO
MaxNodes=UNLIMITED **MaxTime=3-00:00:00** MinNodes=0 LLN=NO **MaxCPUsPerNode=64**
MaxCPUsPerSocket=UNLIMITED
Nodes=qbd[001-480]
PriorityJobFactor=1 PriorityTier=1 RootOnly=NO ReqResv=NO OverSubscribe=EXCLUSIVE
OverTimeLimit=NONE PreemptMode=OFF
State=UP TotalCPUs=30720 TotalNodes=480 SelectTypeParameters=NONE
JobDefaults=(null)
DefMemPerCPU=3920 **MaxMemPerCPU=4000**
TRES=cpu=30720,mem=120000G,node=480,billing=30720
TRESBillingWeights=CPU=1

3) Number of nodes & cores

- **FAQ**

Q	A
• My code runs slow. Can I request more nodes / cores to make it faster?	• Not quite! Your code most likely is **NOT** using multiple nodes / cores, if: - You **do not know** if it is using multiple nodes / cores - You **did not tell** it to use multiple nodes / cores - You are **not familiar** with names like “MPI” / “OpenMP” • **Underutilization** is THE most common warning received on our clusters
• How many nodes / cores should I request?	• In short: We can’t answer that • Each code / job is different. You must test to determine

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4) Partitions and job queues

[username@host ~]$ sinfo

```
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
single*      up 7-00:00:00      1 drain* qbd422
single*      up 7-00:00:00      1  down* qbd041
single*      up 7-00:00:00    163  alloc qbd[056-080,088-091,191-299,431-455]
single*      up 7-00:00:00    315   idle qbd[001-040,042-055,081-087,092-190,300-421,423-430,456-480]
checkpt      up 3-00:00:00      1 drain* qbd422
checkpt      up 3-00:00:00      1  down* qbd041
checkpt      up 3-00:00:00    163  alloc qbd[056-080,088-091,191-299,431-455]
checkpt      up 3-00:00:00    315   idle qbd[001-040,042-055,081-087,092-190,300-421,423-430,456-480]
workq        up 3-00:00:00      1 drain* qbd422
workq        up 3-00:00:00      1  down* qbd041
workq        up 3-00:00:00    163  alloc qbd[056-080,088-091,191-299,431-455]
workq        up 3-00:00:00    315   idle qbd[001-040,042-055,081-087,092-190,300-421,423-430,456-480]
bigmem       up 3-00:00:00      1  alloc qbd482
bigmem       up 3-00:00:00      4   idle qbd[481,483-485]
gpu2         up 3-00:00:00     52   idle qbd[486-511,517-542]
gpu4         up 3-00:00:00      3    mix qbd[543-545]
gpu4         up 3-00:00:00      6   idle qbd[512-516,546]
gpu-small    up 3-00:00:00      1   idle qbd547
```

4) Partitions and job queues

[username@host ~]$ sinfo --states=idle

```
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
single*      up 7-00:00:00    105   idle mike[002-003,005,...,155-158]
checkpt      up 3-00:00:00    105   idle mike[002-003,005,...,155-158]
workq        up 3-00:00:00    105   idle mike[002-003,005,...,155-158]
bigmem       up 3-00:00:00      1   idle mike175
gpu          up 3-00:00:00      2   idle mike[182-183]
gpu4         up 3-00:00:00      2   idle mike[182-183]
```

4) Partitions and job queues

b) Available partitions/queues

i. workq / checkpt

Purpose		• General purposes • Most likely your **default** queue • Difference: **non-preemptible** (workq) vs. **preemptible** (checkpt)
Name		• All clusters: **workq** / **checkpt**
Resource availability	**Nodes**	• **Entire** node(s) • Up to a maximum
	Cores	• **All** cores on the node(s)
	Memory	• **All** memory on the node(s)
Max duration		• **72** hours (3 days)

4) Partitions and job queues

b) Available partitions/queues

ii. single

Purpose		• Only need a **portion** of one node
Names		• All clusters: **single**
Resource availability	**Nodes**	• **Portion** of one node: 1/2/4/8/16/32/64
	Cores	• **1** ~ **all** cores
	Memory	• A **portion**, **proportional** to the number of requested cores
Max duration		• **168** hours (7 days)

[QB-4]

- **Total**: 64 cores, 256 GB memory
  → 4 GB / core
- **Request**: 10 cores
  → 40 GB memory

b) Available partitions/queues

iii. bigmem

Purpose		• Need **large memory** (larger than regular computing nodes have)
Names		• All clusters: **bigmem**
Resource availability	**Nodes**	• **Entire** node(s)
	Cores	• **All** cores on the node
	Memory	• **All** memory on the node
Max duration		• **72** hours (3 days)

4) Partitions and job queues

b) Available partitions/queues

iv. GPU

gpuX :
X = [Number of GPUs on one node]

Purpose		• Need **GPU**	
Name		• QB-3: **gpu2**	• SMIC: **gpu2** • Deep Bayou: **gpu2**, **gpu4** • SuperMike 3: **gpu4** • QB-4: **gpu2**, **gpu4**
Resource availability	**Nodes**	• **Entire** node(s)	• **Portion** or **entire** node(s)
	Cores	• **All** cores on the node(s)	• **Portion** or **all** on the node
	Memory	• **All** memory on the node(s)	• **Portion** or **all** on the node
	GPU	• **All** GPUs on the node(s)	• **1** ~ **all** GPU on the node(
Max duration		• **72** hours (3 days)	

[QB-4 / gpu4]

- **Total**: 64 cores, 4 GPUs
  → 16 cores / GPU
- **Request**: 3 GPUs
  → 48 cores

4) Partitions and job queues

c) Available partitions/queues by clusters (LSU HPC)

Cluster	Partition/Queue	Cores per node (ppn)	Max running jobs	Max nodes per user
SuperMIC (smic.hpc.lsu.edu)	workq	20	45 (*global*)	86
	checkpt			
	single	1 ~ 20		
	gpu2	18,36		2
	bigmem	28		3
DeepBayou (db1.hpc.lsu.edu)	gpu2	24,48	-	8
	gpu4	12,24,36,48		2
SuperMike-III (mike.hpc.lsu.edu)	workq	64	32 (*global*)	96
	checkpt			
	single	1 ~ 64		
	gpu4	16,32,48,64		4
	bigmem	64		4

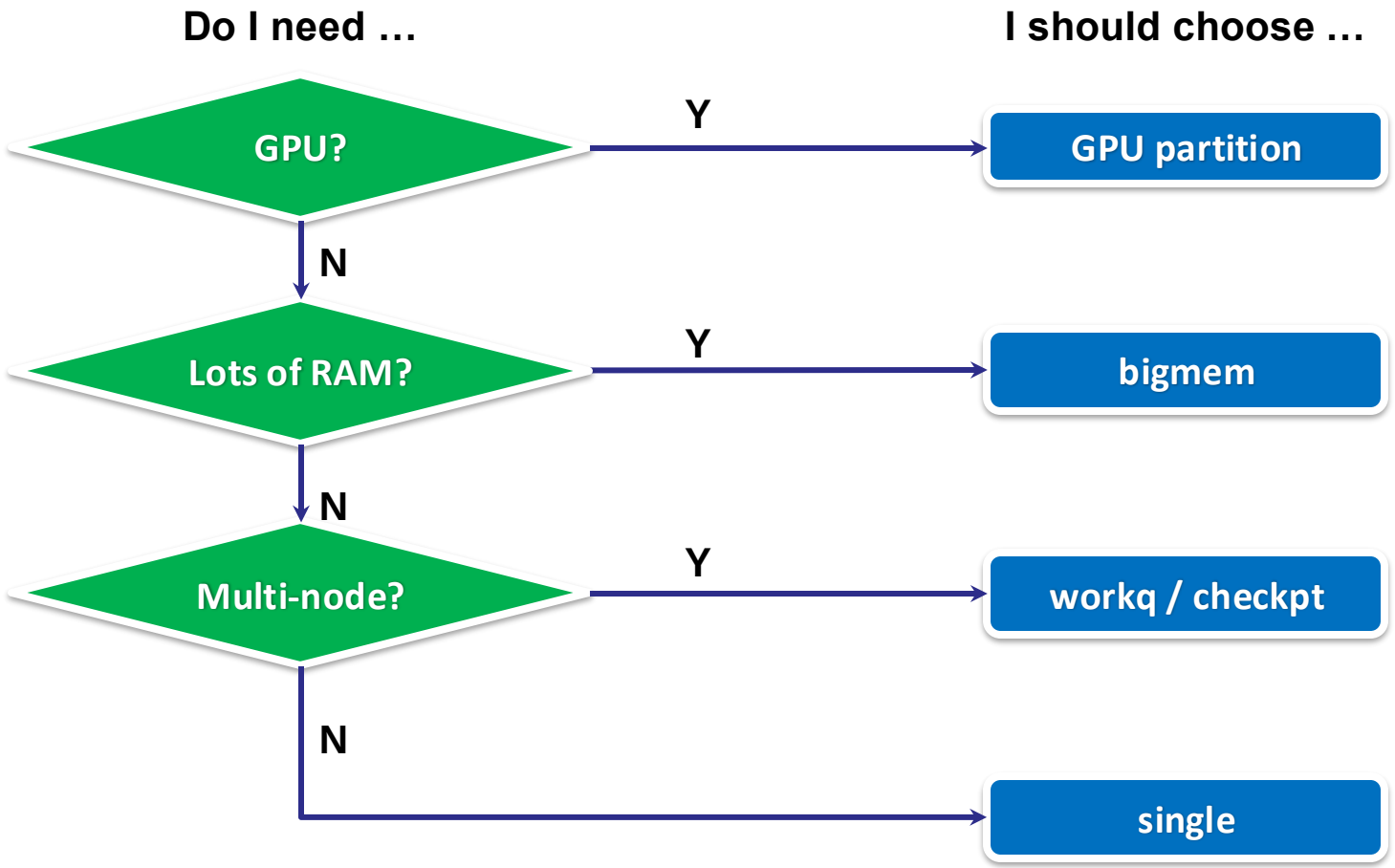
4) Partitions and job queues

c) Available partitions/queues by clusters (LONI)

Cluster	Partition/Queue	Cores per node (ppn)	Max running jobs	Max nodes per user
QB-3	workq	48	32 (*global*)	48
	checkpt			
	single	1 ~ 48		
	gpu2	48		4
	bigmem	48		2
QB-4	workq	64	32 (*global*)	96
	checkpt			
	single	1 ~ 64		
	gpu2	32,64		4
	gpu4	16,32,48,64		4
	bigmem	64		5

4) Partitions and job queues

d) Choose your partition/queue



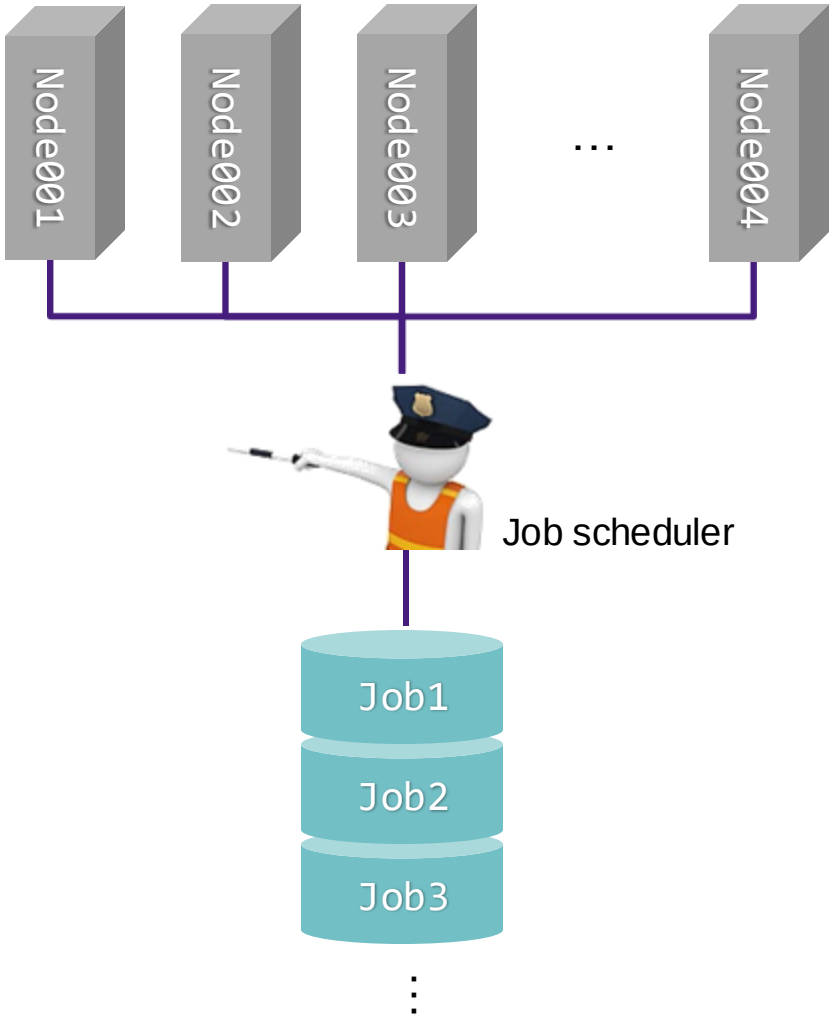
4) Partitions and job queues

d) Choose your partition/queue

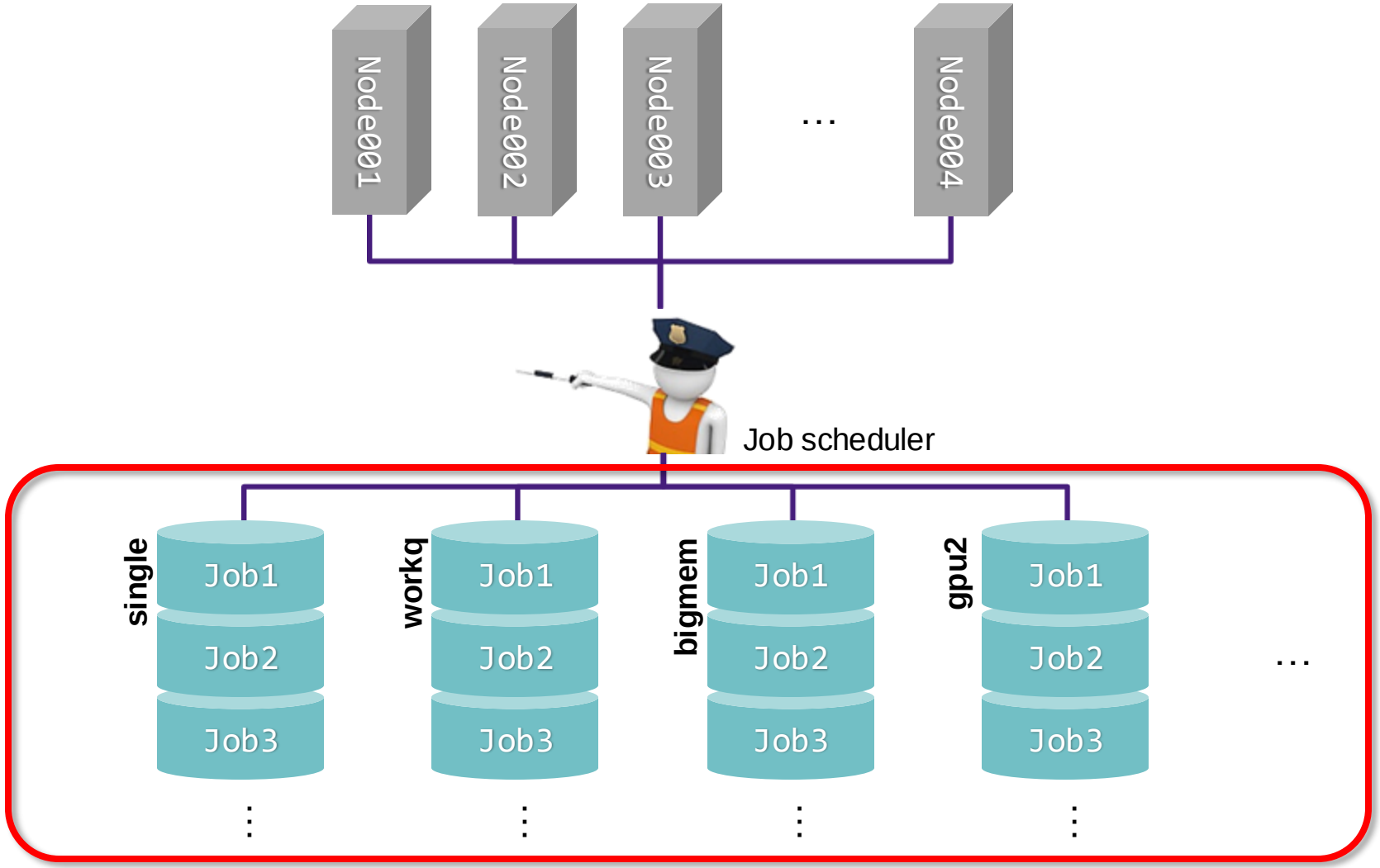
Test

My job	Queue choice? (include number of nodes / cores)
• **SMIC** • MPI code, needs 100 CPU cores - Hint: SMIC has 20 cores / node	**workq** / **checkpt** (5 nodes, 20 cores per node)
• **SuperMike 3** • Uses 3 GPUs to train a neural network - Hint: SuperMike 3 has 64 cores / node, 4 GPUs / node → 16 cores / GPU	**gpu4** (1 node, 48 cores per node)
• **QB-3** • Single-core serial code • Needs to store and process 30 GB data in RAM - Hint: QB-3 has 192 GB RAM / node, 4 GB RAM / core	**single** (1 node, 8 cores per node)

4) Partitions and job queues



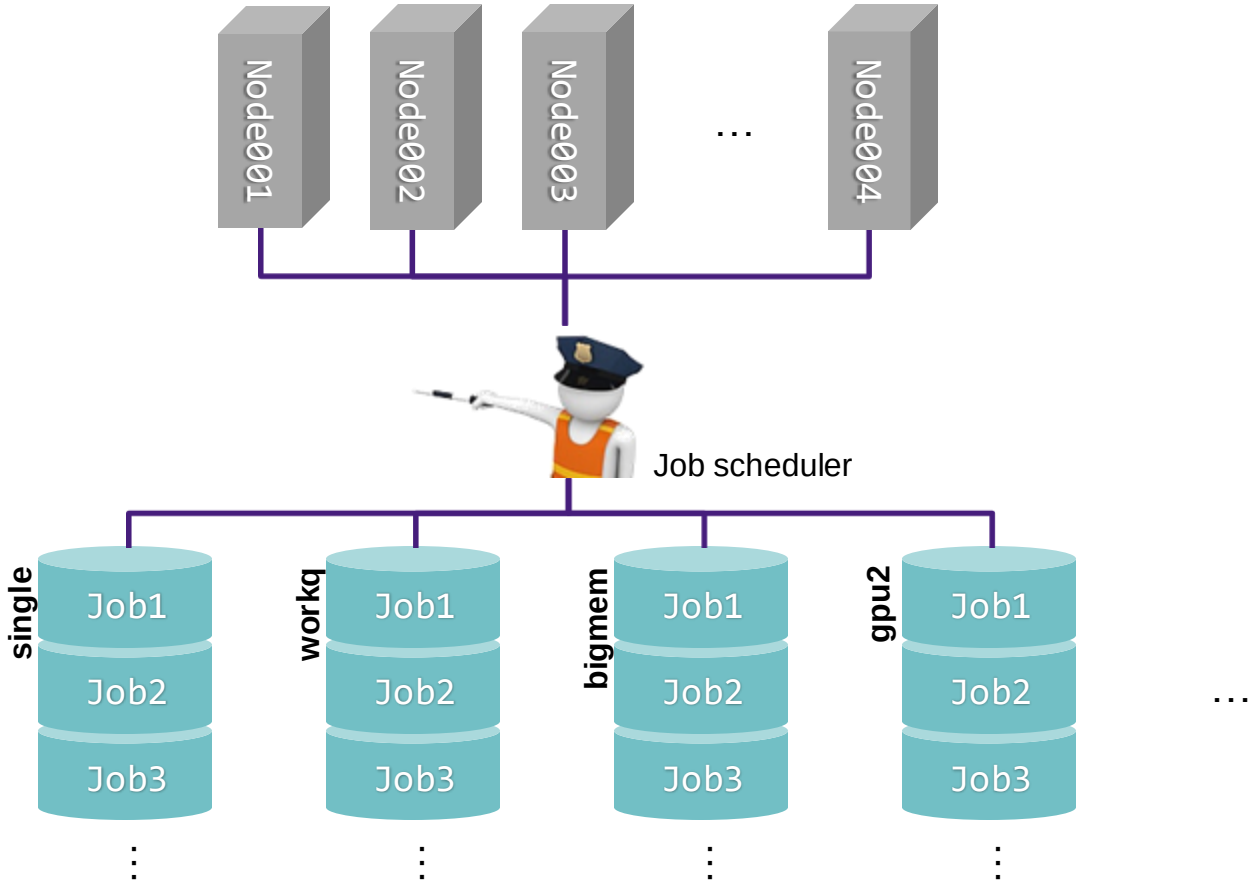
4) Partitions and job queues



4) Partitions and job queues

a) Definition

- Lines where jobs are waiting to be executed
- Must pick one queue
- Goal: Use the resources efficiently



4) Partitions and job queues

[username@host ~]$ squeue

```
JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
50878    bigmem submit-p  username1   RUNNING 2-06:28:02 3-00:00:00      1 qbd482
51761   checkpt CuFe_Fit  username2   RUNNING       1:29 1-00:00:00      1 qbd081
51257   checkpt GOM1km_e  username3   RUNNING 1-17:35:43 3-00:00:00     25 qbd[275-299]
51731      gpu4 submit-1  username6   RUNNING    2:55:23 3-00:00:00      1 qbd544
50873     workq   qbd.sh  username8   RUNNING 2-07:06:42 3-00:00:00     84 qbd[191-274]
```

[username@host ~]$ squeue -u $USER

```
JOBID    PARTITION  NAME          USER    ST  TIME_LIMIT  TIME      CPUS  NODES  NODELIST(REASON)
51740    gpu4       submit-1-4.sh username6  R  3-00:00:00  2:40:00    16   1      qbd545
51731    gpu4       submit-1-4.sh username6  R  3-00:00:00  2:57:14    16   1      qbd544
```

[username@host ~]$ squeue -j 158426

```
JOBID    PARTITION  NAME          USER    ST  TIME_LIMIT  TIME      CPUS  NODES  NODELIST(REASON)
158426   workq      Test          username5  R  5:00        0:17      64   1      qbd096
```

[username@host ~]$ squeue --me

```
JOBID    PARTITION  NAME          USER    ST  TIME_LIMIT  TIME      CPUS  NODES  NODELIST(REASON)
158426   workq      Test          username5  R  5:00        0:17      64   1      qbd096
```

Summary

1. **Basic concepts**
   a) How job works on clusters
   b) Job scheduler and how it works
2. **Preparing my job**
   a) Basic principles
      - "**large enough**" and "**small enough**"
   b) Information you need to tell job scheduler:
      - Time duration
      - Number of nodes & cores
      - Job partition

End of the first section

Let’s have a 5-minute break!

Outlines

- **HPC User Environment 2**

1. Basic concepts
   1) Previously on HPC User Environment 1…
   2) Job & Job schedulers
2. Preparing my job
   1) Basic principles
   2) Job duration (wall time)
   3) Number of nodes & cores
   4) Job queues
3. Submitting my job
   1) Interactive job
   2) Batch job
4. Managing my jobs
   1) Useful commands
   2) Monitoring job health

3. Submitting a job

- **Two types of jobs:**

1) Interactive job

- Runs **in terminal** (just like using a local machine)
- **Can interact** with the job while running

2) Batch job

- Submit to server and runs **by itself**, until finished or error
- **Cannot interact** with the job while running

3. Submitting a job

- **Two types of jobs:**

	1) Interactive job	2) Batch job
Pros	• Can interact and monitor with job in real time	• Submit and leave it • Repeatable for complicated jobs
Cons	• Waiting for human intervention is the opposite of “high performance”	• Cannot edit or interact with job while running
Ideal for	• Debugging, testing, and compiling	• Production

Outlines

- **HPC User Environment 2**

1. Basic concepts
   1) Previously on HPC User Environment 1…
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3. Submitting my job
   1) Interactive job
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4. Managing my jobs
   1) Useful commands
   2) Monitoring job health

1) Interactive job

a) Starting an interactive job (bare minimum)

salloc [options]

1) Interactive job

a) Starting an interactive job (bare minimum)

```
salloc
    -A <allocation name>
    -t   <D-HH:MM:SS>
    -p  <partition name>
    -N  <number of nodes>
    -n  <number of tasks/cores>
```

Allocation name

1) Interactive job

a) Starting an interactive job (bare minimum)

salloc

-A <allocation name>

-t <D-HH:MM:SS>

-p <partition name>

-N <number of nodes>

-n <number of tasks/cores>

Job duration

1) Interactive job

a) Starting an interactive job (bare minimum)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p  <partition name>
-N  <number of nodes>
-n  <number of tasks/cores>
```

Job queue

1) Interactive job

a) Starting an interactive job (bare minimum)

salloc

-A <allocation name>

-t <D-HH:MM:SS>

-p <partition name>

-N <number of nodes>

-n <number of tasks/cores>

Number of nodes

1) Interactive job

a) Starting an interactive job (bare minimum)

salloc
-A <allocation name>
-t <D-HH:MM:SS>
-p <partition name>
-N <number of nodes>
-n <number of tasks/cores>

Total number of cores

1) Interactive job

a) Starting an interactive job (bare minimum)

```
[username@host ~]$ salloc -A loni_loniadmin1 -p workq –N 1 –n64 --time=01:00:00
```

```
salloc: Pending job allocation 51814
salloc: lua: Submitted job 51814
salloc: job 51814 queued and waiting for resources
salloc: job 51814 has been allocated resources
salloc: Granted job allocation 51814
salloc: Waiting for resource configuration
salloc: Nodes qbd085 are ready for job
```

1) Interactive job

a) Starting an interactive job (bare minimum)

```
[username@host ~]$ salloc -A loni_loniadmin1 -p workq –N 1 –n64 --time=01:00:00
```

```
salloc: Pending job allocation 51814
salloc: lua: Submitted job 51814
salloc: job 51814 queued and waiting for resources
salloc: job 51814 has been allocated resources
salloc: Granted job allocation 51814
salloc: Waiting for resource configuration
salloc: Nodes qbd085 are ready for job
```

1) Interactive job

a) Starting an interactive job (bare minimum)

```
[username@qbd1 ~]$ salloc -A loni_loniadmin1 -p workq -N1 -n 64 --time=12:00:00
```

```
[username@qbd085 ~]$
```

Successfully started: on a computing node (**3-digit** number)

1) Interactive job

a) Starting an interactive job (bare minimum)

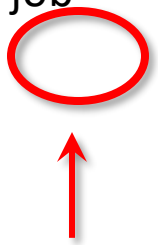
```
[username@qbd1 Tests]$ salloc --account=loni_loniadmin1 --partition=workq --nodes=1 --ntasks=64 --time=12:00:00 --job-name=training --mail-user=username@lsu.edu
--mail-type=BEGIN,END
salloc: Pending job allocation 51860
salloc: lua: Submitted job 51860
salloc: job 51860 queued and waiting for resources
salloc: job 51860 has been allocated resources
salloc: Granted job allocation 51860
salloc: Nodes qbd083 are ready for job
[username@qbd083 Tests]$
```

Job starts in **where the job was submitted**

1) Interactive job

a) Starting an interactive job (bare minimum)

```
[username@qbd1 Tests]$ salloc --account=loni_loniadmin1 --partition=workq --nodes=1 --ntasks=64 --time=12:00:00 --job-name=training --mail-user=username@lsu.edu
--mail-type=BEGIN,END
salloc: Pending job allocation 51860
salloc: lua: Submitted job 51860
salloc: job 51860 queued and waiting for resources
salloc: job 51860 has been allocated resources
salloc: Granted job allocation 51860
salloc: Nodes qbd083 are ready for job
[username@qbd083 Tests]$
```



Once a job starts, **type and run commands** as you normally do.

b) Starting an MPI / OpenMP hybrid job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p  <partition name>
-N  <number of nodes>
-n  <number of tasks/cores>
```

Number of total cores

1) Interactive job

b) Starting an MPI / OpenMP hybrid job (For those who use it)

salloc

-A <allocation name>

-t <D-HH:MM:SS>

-p <queue name>

-N <number of nodes>

-n <number of tasks/cores>

-c < number of cores per process>

<# of TOTAL cores>

= <n> * <c>

1) Interactive job

b) Starting an MPI / OpenMP hybrid job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p   workq
-N  2
-n  32
-c  4
```

[QB-4 / workq]

- **64** / node
- **2** nodes → **128** cores
- **32** processes
- **4** cores / process

b) Starting an MPI / OpenMP hybrid job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p   workq
-N   2
-n   32
-c   4
```

[QB-4 / workq]

- **64** / node
- **2** nodes → **128** cores
- **32** processes
- **4** cores / process

1) Interactive job

b) Starting an MPI / OpenMP hybrid job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p   workq
-N   2
-n   32
-c   4
```

[QB-4 / workq]

- **64** / node
- **2** nodes → **128** cores
- **32** processes
- **4** cores / process

1) Interactive job

b) Starting an MPI / OpenMP hybrid job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p   workq
-N   2
-n   32
-c   4
```

[QB-4 / workq]

- **64** / node
- **2** nodes → **128** cores
- **32** processes
- **4** cores / process

c) Starting a GPU job (For those who use it)

salloc

-A <allocation name>

-t <D-HH:MM:SS>

-p <partition name>

-N <number of nodes>

-n <number of tasks/cores>

1) Interactive job

c) Starting a GPU job (For those who use it)

salloc

-A <allocation name>

-t <D-HH:MM:SS>

-p <partition name>

-N <number of nodes>

-n <number of tasks/cores>

- - gres=gpu:1 < number of GPUs per node>

Number of GPUs **per node**

c) Starting a GPU job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p   gpu 4
-N   1
-n   16
- - gres=gpu:1
```

[QB-4 / gpu4]

- **64** cores, **4** GPUs → **16** cores / GPU
- **1** nodes (only need ¼)
- **16** cores (¼ of total)
- **1** GPU (¼ of total)

c) Starting a GPU job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p  gpu 4
-N  1
-n  16
- - gres=gpu:1
```

[QB-4 / gpu4]

- **64** cores, **4** GPUs → **16** cores / GPU
- **1** nodes (only need ¼)
- **16** cores (¼ of total)
- **1** GPU (¼ of total)

1) Interactive job

c) Starting a GPU job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p  gpu 4
-N  1
-n  16
- - gres=gpu:1
```

[QB-4 / gpu4]

- **64** cores, **4** GPUs → **16** cores / GPU
- **1** nodes (only need ¼)
- **16** cores (¼ of total)
- **1** GPU (¼ of total)

c) Starting a GPU job (For those who use it)

```
salloc
-A <allocation name>
-t   <D-HH:MM:SS>
-p  gpu 4
-N  1
-n  16
- - gres=gpu:1
```

[QB-4 / gpu4]

- **64** cores, **4** GPUs → **16** cores / GPU
- **1** nodes (only need ¼)
- **16** cores (¼ of total)
- **1** GPU (¼ of total)

d) Other useful flags

Flag		Description	
`--x11`		Enable x11 forwarding for GUI (exclusive to interactive job)	
`-J`		Job name	
`--dependency=afterok:[jobid]`		Dependent job (starts after another job finishes)	
`--mail-type`	`FAIL`	Send email when …	Job aborts / fails
	`BEGIN`		Job begins
	`END`		Job ends
`--mail-user`		Email address (will check against registered institutional email)	

[1] http://www.hpc.lsu.edu/docs/slurm.php

1) Interactive job

The default partition/queue

single

1) Interactive job

d) Other useful flags

[username@host ~]$ salloc **-A** loni_loniadmin1 **-p** workq **-N**1 **-n**64 **–t** 12:00:00

[username@host ~]$ salloc **-A** loni_loniadmin1 **-p** workq **–t** 1-00:00:00

[username@host ~]$ salloc **--account**=loni_loniadmin1 **--partition**=workq **--nodes**=1 **--ntasks**=64 **--time**=1-00:00:00 **--job-name**=training **--mail-user**=user@mail.address **--mail-type**=BEGIN,END

[1] http://www.hpc.lsu.edu/docs/slurm.php

1) Interactive job

e) Running an interactive job

– After job started:

Serial (Single-thread)	Parallel (MPI)

• **Run commands as you normally do**
 	
`$ <Executable> [options]`
	• **Method 1 (Recommended)**
	
	`$ srun -N[..] -n[..] -c[..] <mpi_executable> [options]`
	
	• **Method 2**
	
	`$ module load <desired MPI>`
	`$ export OMP_NUM_THREADS=[..]`
	`$ mpirun -np [..] <mpi_executable> [options]`

Outlines

- **HPC User Environment 2**

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2) Batch job

- **What do you need?**

1. A **batch file** (containing job parameters and bash scripts)

2. Submit this batch file with the **submission command <sbatch>**

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH --gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END
```

[Header]

Job parameters

[Body]

Commands to run after job starts

```
module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END
```

[Header]
Job parameters

```
module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Info for interpreter

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

GPU partition/queue

2) Batch job

a) Batch file

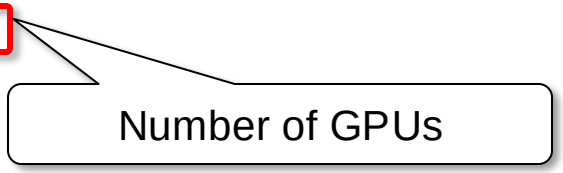
```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```



2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Number of nodes (N)

Number of processes (n)

and the number of cores per process (c)

a) Batch file

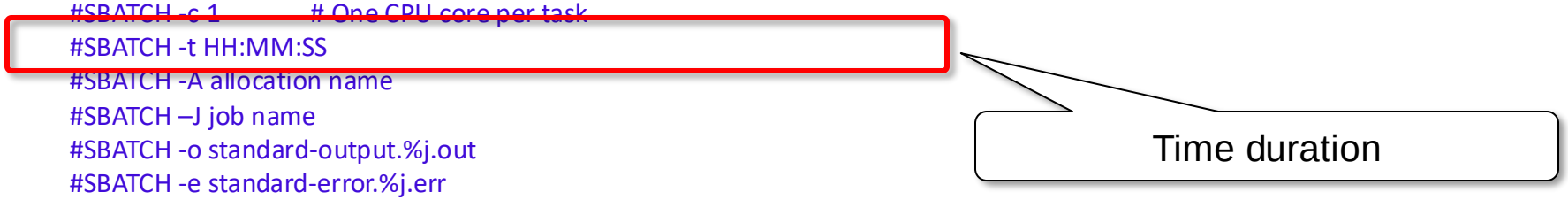
```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```



2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Standard error and output

a) Batch file

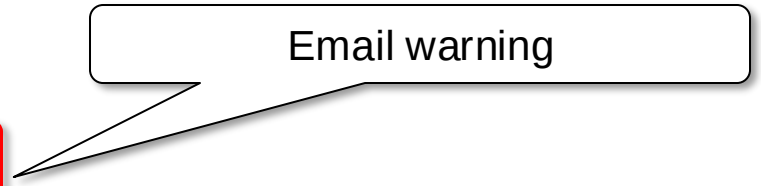
```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END

module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```



2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation name
#SBATCH –J job name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END

module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Loading some modules to the environment

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
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#SBATCH -A allocation name
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#SBATCH -o standard-output.%j.out
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module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Setting up the number of OpenMP threads for the job

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
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#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Switching to the submit directory

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation-name
#SBATCH –J job-name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Executing the command lmp_mpi

2) Batch job

a) Batch file

```
#!/bin/bash
#SBATCH -p gpu4
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32          # Total number of MPI tasks
#SBATCH -c 1           # One CPU core per task
#SBATCH -t HH:MM:SS
#SBATCH -A allocation-name
#SBATCH –J job-name
#SBATCH -o standard-output.%j.out
#SBATCH -e standard-error.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END


module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=1 # One core per task

echo “Current working directory: $SLURM_SUBMIT_DIR”
cd  $SLURM_SUBMIT_DIR

time srun –N 1 –n 32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Leave one space after the command line to avoid error

a) Batch file

Flag		Description	
`-o`		Standard output file (exclusive to batch job)	
`-e`		Standard error file (exclusive to batch job)	
`-J`		Job name	
`--dependency=afterok:[jobid]`		Dependent job (starts after another job finishes)	
`--mail-type`	`FAIL`	Send email when …	Job aborts / fails
	`BEGIN`		Job begins
	`END`		Job ends
`--mail-user`		Email address (will check against registered institutional email)	

[1] http://www.hpc.lsu.edu/docs/slurm.php

b) Submit

```
sbatch batch-script.sh
```

Outlines

- **HPC User Environment 2**

1. Basic concepts
   1) Previously on HPC User Environment 1…
   2) Job & Job schedulers
2. Preparing my job
   1) Basic principles
   2) Job duration (wall time)
   3) Number of nodes & cores
   4) Partitions and job queues
3. Submitting my job
   1) Interactive job
   2) Batch job
4. Managing my jobs
   1) Useful commands
   2) Monitoring job health

4. Manage jobs

- **Running jobs on HPC ≠ "Submit and done"**
  - Monitoring and managing jobs are part of the work

Outlines

- **HPC User Environment 2**

1. Basic concepts
   1) Previously on HPC User Environment 1…
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   3) Number of nodes & cores
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   1) Interactive job
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   1) Useful commands
   2) Monitoring job health

1) Useful commands

Command		Description
squeue		List all jobs
	-j <Job ID>	List the job of specific ID
	-u <Username>	List all jobs belong to a specific user
	-p <partition name>	List all jobs in a particular partition/queue
	--start	Estimated start time of queuing jobs
scontrol show job <Job ID>		Show job details
scancel <Job ID>		Cancel <Job ID>

Alter jobs after submission? → NOT allowed!

[1] http://www.hpc.lsu.edu/docs/slurm.php

Outlines

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2) Monitoring job health

A job requesting n cores ≠ A job utilizing n cores

- **Goal**
  - Use the allocated resources (CPU cores, RAM, time, …) **as fully and efficiently as possible**
  - **No serious underutilizing**
  - **No serious overutilizing**

- **Things to check**
  - CPU / GPU load
  - Memory usage

2) Monitoring job health

a) Method 1: qshow <Job ID>

- Displays diagnostic information of a **running job**
- Can be run on **head node**

2) Monitoring job health

a) Method 1: qshow <Job ID>

```
(base) [jasonli3@mike4 ~]$ qshow 38581
PBS job: 38581, nodes: 1
Hostname  Days Load CPU U# (User:Process:VirtualMemory:Memory:Hours)
mike145    278 64.12 6033 68 yxan:lmp_mik+:524M:104M:13.5 yxan:lmp_mik+:524M:104M:13.5 yxan:lmp_mik+:533M:107M:13.5 yxan:lmp_mik+:748M:128M:13.5
yxan:lmp_mik+:738M:124M:13.5 yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:587M:109M:13.5 yxan:lmp_mik+:743M:128M:13.5 yxan:lmp_mik+:696M:118M:13.5
yxan:lmp_mik+:528M:101M:13.5 yxan:lmp_mik+:578M:108M:13.5 yxan:lmp_mik+:528M:105M:13.5 yxan:lmp_mik+:528M:106M:13.5 yxan:lmp_mik+:520M:105M:13.5
yxan:lmp_mik+:561M:106M:13.5 yxan:lmp_mik+:583M:109M:13.5 yxan:lmp_mik+:520M:103M:13.5 yxan:lmp_mik+:524M:103M:13.5 yxan:lmp_mik+:738M:125M:13.5
yxan:lmp_mik+:709M:119M:13.5 yxan:lmp_mik+:524M:103M:13.5 yxan:lmp_mik+:574M:107M:13.5 yxan:lmp_mik+:697M:121M:13.5 yxan:lmp_mik+:658M:115M:13.5
yxan:lmp_mik+:528M:102M:13.5 yxan:lmp_mik+:557M:108M:13.5 yxan:lmp_mik+:524M:105M:13.5 yxan:lmp_mik+:524M:105M:13.5 yxan:lmp_mik+:515M:102M:13.5
yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:567M:108M:13.5 yxan:lmp_mik+:566M:108M:13.5 yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:536M:105M:13.5
yxan:lmp_mik+:519M:104M:13.5 yxan:lmp_mik+:528M:103M:13.5 yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:524M:104M:13.5 yxan:lmp_mik+:524M:104M:13.5
yxan:lmp_mik+:528M:104M:13.5 yxan:lmp_mik+:516M:101M:13.5 yxan:lmp_mik+:515M:101M:13.5 yxan:lmp_mik+:515M:104M:13.5 yxan:lmp_mik+:520M:101M:13.5
yxan:lmp_mik+:524M:103M:13.5 yxan:lmp_mik+:520M:101M:13.5 yxan:lmp_mik+:515M:103M:13.5 yxan:lmp_mik+:516M:102M:13.5 yxan:lmp_mik+:587M:110M:13.5
yxan:lmp_mik+:558M:108M:13.5 yxan:lmp_mik+:524M:102M:13.5 yxan:lmp_mik+:537M:103M:13.5 yxan:lmp_mik+:572M:109M:13.5 yxan:lmp_mik+:549M:104M:13.5
yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:528M:104M:13.5 yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:515M:103M:13.5 yxan:lmp_mik+:515M:103M:13.5
yxan:lmp_mik+:520M:105M:13.5 yxan:lmp_mik+:528M:105M:13.5 yxan:lmp_mik+:515M:103M:13.5 yxan:lmp_mik+:515M:104M:13.5 yxan:lmp_mik+:515M:104M:13.5
yxan:slurm_s+:12M:3M yxan:srun:324M:8M yxan:srun:53M:1M
PBS_job=38581 user=yxan allocation=hpc_lipidhpre queue=checkpt total_load=64.12 cpu_hours=866.08 wall_hours=13.21 unused_nodes=0 total_nodes=1 pp
n=64 avg_load=64.12 avg_cpu=6033% avg_mem=6852mb avg_vmem=36176mb top_proc=yxan:lmp_mik+:mike145:524M:104M:13.5hr:100% toppm=yxan:lmp_mikeCpu:mik
e145:730M:125M node_processes=68
```

What to look at …	Normal behavior …	You should be concerned if …

2) Monitoring job health

a) Method 1: qshow <Job ID>

```
(base) [jasonli3@mike4 ~]$ qshow 38581
PBS job: 38581, nodes: 1
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mike145    278 64.12 6033 68 yxan:lmp_mik+:524M:104M:13.5 yxan:lmp_mik+:524M:104M:13.5 yxan:lmp_mik+:533M:107M:13.5 yxan:lmp_mik+:748M:128M:13.5
yxan:lmp_mik+:738M:124M:13.5 yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:587M:109M:13.5 yxan:lmp_mik+:743M:128M:13.5 yxan:lmp_mik+:696M:118M:13.5
yxan:lmp_mik+:528M:101M:13.5 yxan:lmp_mik+:578M:108M:13.5 yxan:lmp_mik+:528M:105M:13.5 yxan:lmp_mik+:528M:106M:13.5 yxan:lmp_mik+:520M:105M:13.5
yxan:lmp_mik+:561M:106M:13.5 yxan:lmp_mik+:583M:109M:13.5 yxan:lmp_mik+:520M:103M:13.5 yxan:lmp_mik+:524M:103M:13.5 yxan:lmp_mik+:738M:125M:13.5
yxan:lmp_mik+:709M:119M:13.5 yxan:lmp_mik+:524M:103M:13.5 yxan:lmp_mik+:574M:107M:13.5 yxan:lmp_mik+:697M:121M:13.5 yxan:lmp_mik+:658M:115M:13.5
yxan:lmp_mik+:528M:102M:13.5 yxan:lmp_mik+:557M:108M:13.5 yxan:lmp_mik+:524M:105M:13.5 yxan:lmp_mik+:524M:105M:13.5 yxan:lmp_mik+:515M:102M:13.5
yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:567M:108M:13.5 yxan:lmp_mik+:566M:108M:13.5 yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:536M:105M:13.5
yxan:lmp_mik+:519M:104M:13.5 yxan:lmp_mik+:528M:103M:13.5 yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:524M:104M:13.5 yxan:lmp_mik+:524M:104M:13.5
yxan:lmp_mik+:528M:104M:13.5 yxan:lmp_mik+:516M:101M:13.5 yxan:lmp_mik+:515M:101M:13.5 yxan:lmp_mik+:515M:104M:13.5 yxan:lmp_mik+:520M:101M:13.5
yxan:lmp_mik+:524M:103M:13.5 yxan:lmp_mik+:520M:101M:13.5 yxan:lmp_mik+:515M:103M:13.5 yxan:lmp_mik+:516M:102M:13.5 yxan:lmp_mik+:587M:110M:13.5
yxan:lmp_mik+:558M:108M:13.5 yxan:lmp_mik+:524M:102M:13.5 yxan:lmp_mik+:537M:103M:13.5 yxan:lmp_mik+:572M:109M:13.5 yxan:lmp_mik+:549M:104M:13.5
yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:528M:104M:13.5 yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:515M:103M:13.5 yxan:lmp_mik+:515M:103M:13.5
yxan:lmp_mik+:520M:105M:13.5 yxan:lmp_mik+:528M:105M:13.5 yxan:lmp_mik+:515M:103M:13.5 yxan:lmp_mik+:515M:104M:13.5 yxan:lmp_mik+:515M:104M:13.5
yxan:slurm_s+:12M:3M yxan:srun:324M:8M yxan:srun:53M:1M
PBS job=38581 user=yxan allocation=hpc_lipidhpre queue=checkpt total_load=64.12 cpu_hours=866.08 wall_hours=13.21 unused_nodes=0 total_nodes=1 pp
n=64 avg_load=64.12 avg_cpu=6033% avg_mem=6852mb avg_vmem=36176mb top_proc=yxan:lmp_mik+:mike145:524M:104M:13.5hr:100% toppm=yxan:lmp_mikeCpu:mik
e145:730M:125M node_processes=68
```

What to look at …	Normal behavior …	You should be concerned if …
avg_load	Close to allocated number of cores on the node	Consistently too low or too high

2) Monitoring job health

a) Method 1: qshow <Job ID>

```
(base) [jasonli3@mike4 ~]$ qshow 38581
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yxan:lmp_mik+:738M:124M:13.5 yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:587M:109M:13.5 yxan:lmp_mik+:743M:128M:13.5 yxan:lmp_mik+:696M:118M:13.5
yxan:lmp_mik+:528M:101M:13.5 yxan:lmp_mik+:578M:108M:13.5 yxan:lmp_mik+:528M:105M:13.5 yxan:lmp_mik+:528M:106M:13.5 yxan:lmp_mik+:520M:105M:13.5
yxan:lmp_mik+:561M:106M:13.5 yxan:lmp_mik+:583M:109M:13.5 yxan:lmp_mik+:520M:103M:13.5 yxan:lmp_mik+:524M:103M:13.5 yxan:lmp_mik+:738M:125M:13.5
yxan:lmp_mik+:709M:119M:13.5 yxan:lmp_mik+:524M:103M:13.5 yxan:lmp_mik+:574M:107M:13.5 yxan:lmp_mik+:697M:121M:13.5 yxan:lmp_mik+:658M:115M:13.5
yxan:lmp_mik+:528M:102M:13.5 yxan:lmp_mik+:557M:108M:13.5 yxan:lmp_mik+:524M:105M:13.5 yxan:lmp_mik+:524M:105M:13.5 yxan:lmp_mik+:515M:102M:13.5
yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:567M:108M:13.5 yxan:lmp_mik+:566M:108M:13.5 yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:536M:105M:13.5
yxan:lmp_mik+:519M:104M:13.5 yxan:lmp_mik+:528M:103M:13.5 yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:524M:104M:13.5 yxan:lmp_mik+:524M:104M:13.5
yxan:lmp_mik+:528M:104M:13.5 yxan:lmp_mik+:516M:101M:13.5 yxan:lmp_mik+:515M:101M:13.5 yxan:lmp_mik+:515M:104M:13.5 yxan:lmp_mik+:520M:101M:13.5
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yxan:lmp_mik+:558M:108M:13.5 yxan:lmp_mik+:524M:102M:13.5 yxan:lmp_mik+:537M:103M:13.5 yxan:lmp_mik+:572M:109M:13.5 yxan:lmp_mik+:549M:104M:13.5
yxan:lmp_mik+:519M:103M:13.5 yxan:lmp_mik+:528M:104M:13.5 yxan:lmp_mik+:520M:104M:13.5 yxan:lmp_mik+:515M:103M:13.5 yxan:lmp_mik+:515M:103M:13.5
yxan:lmp_mik+:520M:105M:13.5 yxan:lmp_mik+:528M:105M:13.5 yxan:lmp_mik+:515M:103M:13.5 yxan:lmp_mik+:515M:104M:13.5 yxan:lmp_mik+:515M:104M:13.5
yxan:slurm_s+:12M:3M yxan:srun:324M:8M yxan:srun:53M:1M
PBS_job=38581 user=yxan allocation=hpc_lipidhpre queue=checkpt total_load=64.12 cpu_hours=866.08 wall_hours=13.21 unused_nodes=0 total_nodes=1 pp
n=64 avg_load=64.12 avg_cpu=603% avg_mem=6852mb avg_vmem=36176mb top_proc=yxan:lmp_mik+:mike145:524M:104M:13.5hr:100% toppm=yxan:lmp_mikeCpu:mik
e145:730M:125M node_processes=68
```

What to look at …	Normal behavior …	You should be concerned if …
avg_load	Close to allocated number of cores on the node	Consistently too low or too high
ave_mem	Does not exceed total allocated memory	Exceeds total allocated memory

2) Monitoring job health

b) Method 2: top

- Displays dynamic real-time view of a **computing node**
- Must run on **computing nodes** !

  * ssh to computing nodes while job running (cannot ssh if you do not have jobs on it)

2) Monitoring job health

b) Method 2: top

```
top - 02:23:58 up 278 days, 19:17,  2 users,  load average: 63.63, 39.81, 17.49
Tasks: 981 total,  65 running, 916 sleeping,   0 stopped,   0 zombie
%Cpu(s): 90.2 us,  9.2 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.5 hi,  0.0 si,  0.0 st
MiB Mem : 257004.8 total, 211261.0 free,  41926.9 used,   3816.9 buff/cache
MiB Swap:  16641.0 total,  16580.7 free,     60.2 used. 212737.8 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND
2701318 jasonli3  20   0  595668 582356   2568 R 100.0   0.2   4:08.94 TDSE_np3_e0
2701342 jasonli3  20   0  595668 581944   2616 R 100.0   0.2   4:08.90 TDSE_np3_e0
2701249 jasonli3  20   0  595668 581792   2464 R  99.7   0.2   4:08.97 TDSE_np3_e0
2701252 jasonli3  20   0  595668 514684   2520 R  99.7   0.2   4:09.00 TDSE_np3_e0
2701261 jasonli3  20   0  595668 393828   2616 R  99.7   0.1   4:08.97 TDSE_np3_e0
2701264 jasonli3  20   0  595668 581856   2532 R  99.7   0.2   4:08.92 TDSE_np3_e0
2701270 jasonli3  20   0  595668 582480   2432 R  99.7   0.2   4:08.95 TDSE_np3_e0
2701273 jasonli3  20   0  595668 581776   2448 R  99.7   0.2   4:08.81 TDSE_np3_e0
2701276 jasonli3  20   0  595668 582160   2568 R  99.7   0.2   4:08.98 TDSE_np3_e0
```

What to look at …	Normal behavior …	You should be concerned if …

2) Monitoring job health

b) Method 2: top

```
top - 02:23:58 up 278 days, 19:17,  2 users,  load average: 63.63, 39.81, 17.49
Tasks: 981 total,  65 running, 916 sleeping,   0 stopped,   0 zombie
%Cpu(s): 90.2 us,  9.2 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.5 hi,  0.0 si,  0.0 st
MiB Mem : 257004.8 total, 211261.0 free,  41926.9 used,   3816.9 buff/cache
MiB Swap:  16641.0 total,  16580.7 free,     60.2 used. 212737.8 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND
2701318 jasonli3  20   0  595668 582356   2568 R 100.0   0.2   4:08.94 TDSE_np3_e0
2701342 jasonli3  20   0  595668 581944   2616 R 100.0   0.2   4:08.90 TDSE_np3_e0
2701249 jasonli3  20   0  595668 581792   2464 R  99.7   0.2   4:08.97 TDSE_np3_e0
2701252 jasonli3  20   0  595668 514684   2520 R  99.7   0.2   4:09.00 TDSE_np3_e0
2701261 jasonli3  20   0  595668 393828   2616 R  99.7   0.1   4:08.97 TDSE_np3_e0
2701264 jasonli3  20   0  595668 581856   2532 R  99.7   0.2   4:08.92 TDSE_np3_e0
2701270 jasonli3  20   0  595668 582480   2432 R  99.7   0.2   4:08.95 TDSE_np3_e0
2701273 jasonli3  20   0  595668 581776   2448 R  99.7   0.2   4:08.81 TDSE_np3_e0
2701276 jasonli3  20   0  595668 582160   2568 R  99.7   0.2   4:08.98 TDSE_np3_e0
```

What to look at …	Normal behavior …	You should be concerned if …
Load average	Close to allocated number of cores on the node	Consistently too low or too high

2) Monitoring job health

b) Method 2: top

```
top - 02:23:58 up 278 days, 19:17,  2 users,  load average: 63.63, 39.81, 17.49
Tasks: 981 total,  65 running, 916 sleeping,   0 stopped,   0 zombie
%Cpu(s): 90.2 us,  9.2 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.5 hi,  0.0 si,  0.0 st
MiB Mem : 257004.8 total, 211261.0 free,  41926.9 used,   3816.9 buff/cache
MiB Swap:  16641.0 total,  16580.7 free,     60.2 used. 212737.8 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND
2701318 jasonli3  20   0  595668 582356   2568 R 100.0   0.2   4:08.94 TDSE_np3_e0
2701342 jasonli3  20   0  595668 581944   2616 R 100.0   0.2   4:08.90 TDSE_np3_e0
2701249 jasonli3  20   0  595668 581792   2464 R  99.7   0.2   4:08.97 TDSE_np3_e0
2701252 jasonli3  20   0  595668 514684   2520 R  99.7   0.2   4:09.00 TDSE_np3_e0
2701261 jasonli3  20   0  595668 393828   2616 R  99.7   0.1   4:08.97 TDSE_np3_e0
2701264 jasonli3  20   0  595668 581856   2532 R  99.7   0.2   4:08.92 TDSE_np3_e0
2701270 jasonli3  20   0  595668 582480   2432 R  99.7   0.2   4:08.95 TDSE_np3_e0
2701273 jasonli3  20   0  595668 581776   2448 R  99.7   0.2   4:08.81 TDSE_np3_e0
2701276 jasonli3  20   0  595668 582160   2568 R  99.7   0.2   4:08.98 TDSE_np3_e0
```

What to look at …	Normal behavior …	You should be concerned if …
Load average	Close to allocated number of cores on the node	Consistently too low or too high
Memory usage (not virtual memory)	Does not exceed total allocated memory	Exceeds total allocated memory

2) Monitoring job health

c) Method 3: nvidia-smi (for GPU only)

```
(base) [jasonli3@qbc193 ~]$ nvidia-smi
Wed Feb  1 02:38:32 2023
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 510.47.03    Driver Version: 510.47.03    CUDA Version: 11.6     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  Tesla V100-PCIE...  On   | 00000000:3B:00.0 Off |                  Off |
| N/A   36C    P0    54W / 250W |   4155MiB / 32768MiB |     72%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+
|   1  Tesla V100-PCIE...  On   | 00000000:AF:00.0 Off |                  Off |
| N/A   36C    P0    52W / 250W |   4155MiB / 32768MiB |     78%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|    0   N/A  N/A    259491      C   ...che/TeraChem/bin/terachem     4147MiB |
|    1   N/A  N/A    259491      C   ...che/TeraChem/bin/terachem     4147MiB |
+-----------------------------------------------------------------------------+
```

What to look at …	Normal behavior …	You should be concerned if …

2) Monitoring job health

c) Method 3: nvidia-smi (for GPU only)

```
(base) [jasonli3@qbc193 ~]$ nvidia-smi
Wed Feb  1 02:38:32 2023
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 510.47.03    Driver Version: 510.47.03    CUDA Version: 11.6     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  Tesla V100-PCIE...  On   | 00000000:3B:00.0 Off |                  Off |
| N/A   36C    P0    54W / 250W |   4155MiB / 32768MiB |     72%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+
|   1  Tesla V100-PCIE...  On   | 00000000:AF:00.0 Off |                  Off |
| N/A   36C    P0    52W / 250W |   4155MiB / 32768MiB |     78%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|    0   N/A  N/A    259491      C   ...che/TeraChem/bin/terachem     4147MiB |
|    1   N/A  N/A    259491      C   ...che/TeraChem/bin/terachem     4147MiB |
+-----------------------------------------------------------------------------+
```

What to look at …	Normal behavior …	You should be concerned if …
GPU usage	Close to 100%	Consistently too low

2) Monitoring job health

c) Method 3: nvidia-smi (for GPU only)

```
(base) [jasonli3@qbc193 ~]$ nvidia-smi
Wed Feb  1 02:38:32 2023
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 510.47.03    Driver Version: 510.47.03    CUDA Version: 11.6     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  Tesla V100-PCIE...  On   | 00000000:3B:00.0 Off |                  Off |
| N/A   36C    P0    54W / 250W |   4155MiB / 32768MiB |     72%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+
|   1  Tesla V100-PCIE...  On   | 00000000:AF:00.0 Off |                  Off |
| N/A   36C    P0    52W / 250W |   4155MiB / 32768MiB |     78%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|    0   N/A  N/A    259491      C   ...che/TeraChem/bin/terachem     4147MiB |
|    1   N/A  N/A    259491      C   ...che/TeraChem/bin/terachem     4147MiB |
+-----------------------------------------------------------------------------+
```

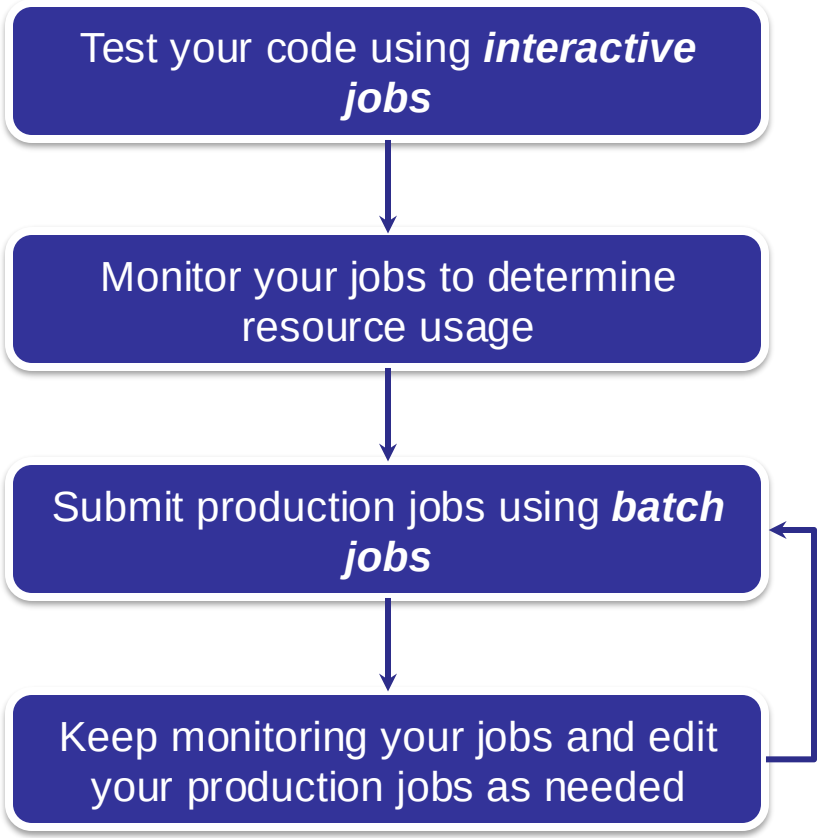
What to look at …	Normal behavior …	You should be concerned if …
GPU usage	Close to 100%	Consistently too low
Memory usage (not virtual memory)	Not used up	Used up

d) Common issues

Issue	What would happen
Exceeded memory allocation (e.g., using more memory than allocated w/ single queue)	Terminated. Receive email notice.
Exceeded ppn/core allocation (e.g., using more cores than allocated w/ single queue)	Terminated. Receive email notice.
Seriously underutilize node CPU cores / unused nodes (e.g., Requested multiple nodes but only runs on one node)	Receive email warning. (* Killed if ***completely idle*** for a long time)
Submitting to bigmem but only using little memory	Receive email warning.
Running intensive calculation on head nodes	Terminated. Receive email notice.
Submitting too many (i.e., hundreds of) single-thread jobs	Poor parallelization and bad for server. We may reach out to you to help. (Better yet, reach out to us first)

Summary

- **A typical workflow --**



Outlines

- **HPC User Environment 2**

1. Basic concepts
   1) Previously on HPC User Environment 1…
   2) Job & Job schedulers → **All calculation must be submitted as jobs**
2. Preparing my job
   1) Basic principles → **Large enough & small enough**
   2) Job duration (wall time)
   3) Number of nodes & cores
   4) Partitions and job queues
3. Submitting my job
   1) Interactive job → **Good for testing and debugging**
   2) Batch job → **Good for production**
4. Managing my jobs
   1) Useful commands
   2) Monitoring job health → **How to monitor jobs health, and how to create health jobs**

Auxiliary information

salloc -A loni_loniadmin1 -p single --nodelist=qbd042 -t 1-00:00:00

salloc -A loni_loniadmin1 -p single --nodelist=qbd042 –N1 –n64 -t 1-00:00:00

salloc -A loni_loniadmin1 -p workq --nodelist=qbd[046-047] -N2 –n128 -t 1-00:00:00

squeue --me

Auxiliary information

Running LAMMPS jobs using 1 GPU

```
#!/bin/bash
#SBATCH --partition=gpu
#SBATCH --gres=gpu:1
#SBATCH --nodes=1
#SBATCH --ntasks=16
#SBATCH --cpus-per-task=1
#SBATCH --time=D-HH:MM:SS
#SBATCH --account=allocation-name
#SBATCH --job-name=test
#SBATCH --output=lammps.%j.out
#SBATCH --error=lammps.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END

module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

echo $SLURM_JOBID
echo $SLURM_NTASKS
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun -N1 -n16 lmp_mpi -sf gpu -pk gpu 1 neigh yes newton off -in lj.in > lj.out
```

Running LAMMPS jobs using 2 GPUs

```
#!/bin/bash
#SBATCH -p gpu
#SBATCH –-gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32
#SBATCH -c 1
#SBATCH -t D-HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o lammps.%j.out
#SBATCH -e lammps.%j.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=BEGIN,END

module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

echo $SLURM_JOBID
echo $SLURM_NTASKS
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun -N1 –n32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Auxiliary information

SLURM_JOB_ID	- This ID can be used to track the job status and retrieve logs
SLURM_JOB_NAME	- The name of the job as specified by the user in command or script.
SLURM_NTASKS	- **The total number of tasks (processes) allocated for the job.**
SLURM_CPUS_PER_TASK	- **The number of CPUs allocated per task.**
SLURM_NODES	- **A list of nodes allocated for the job.**
SLURM_NODELIST	- A comma-separated list of nodes that are allocated for the job.
SLURM_SUBMIT_DIR	- **The directory from which the job was submitted.**
SLURM_ARRAY_JOB_ID	- The job ID of the array job if the job is part of a job array.
SLURM_ARRAY_TASK_ID	- The ID of the specific task in an array job.
SLURM_JOB_NODELIST	- List of nodes allocated for the job, specifically formatted for easier parsing.
SLURM_JOB_DEPENDENCY.	- Indicating which jobs must complete before this job can start.
SLURM_MEM_PER_CPU	- The amount of memory allocated per CPU core for the job.

Standard error and output

command > output.log 2>&1

In Unix-like operating systems, processes have three standard file descriptors:

1. Standard Input (stdin): File descriptor 0 (used for input).
2. Standard Output (stdout): **File descriptor 1** (used for normal output).
3. Standard Error (stderr): **File descriptor 2** (used for error messages).