SuperMike-III User Environment

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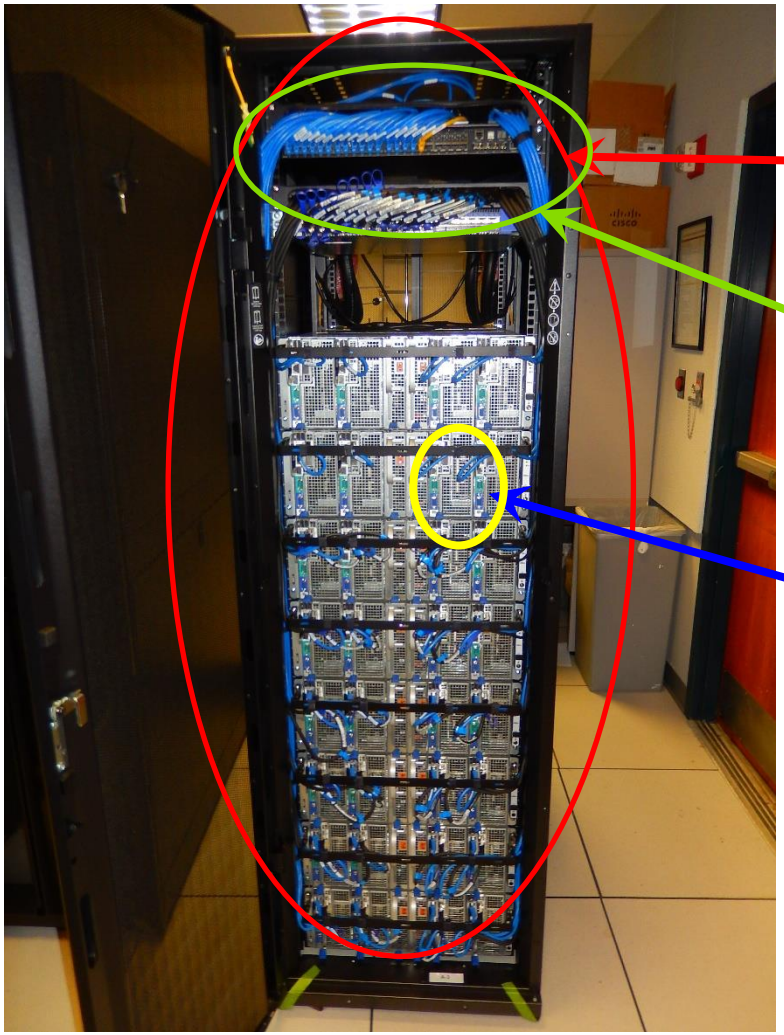
Outline

- **Things to be covered in this section**
  - SuperMike-III job queues
  - Job submission on SuperMike-III
    - Interactive and batch jobs using SLURM
    - Serial and parallel jobs
    - Monitor your jobs

SuperMike-III HPC User Environment

Overview of SuperMike-III

Inside A Cluster Rack

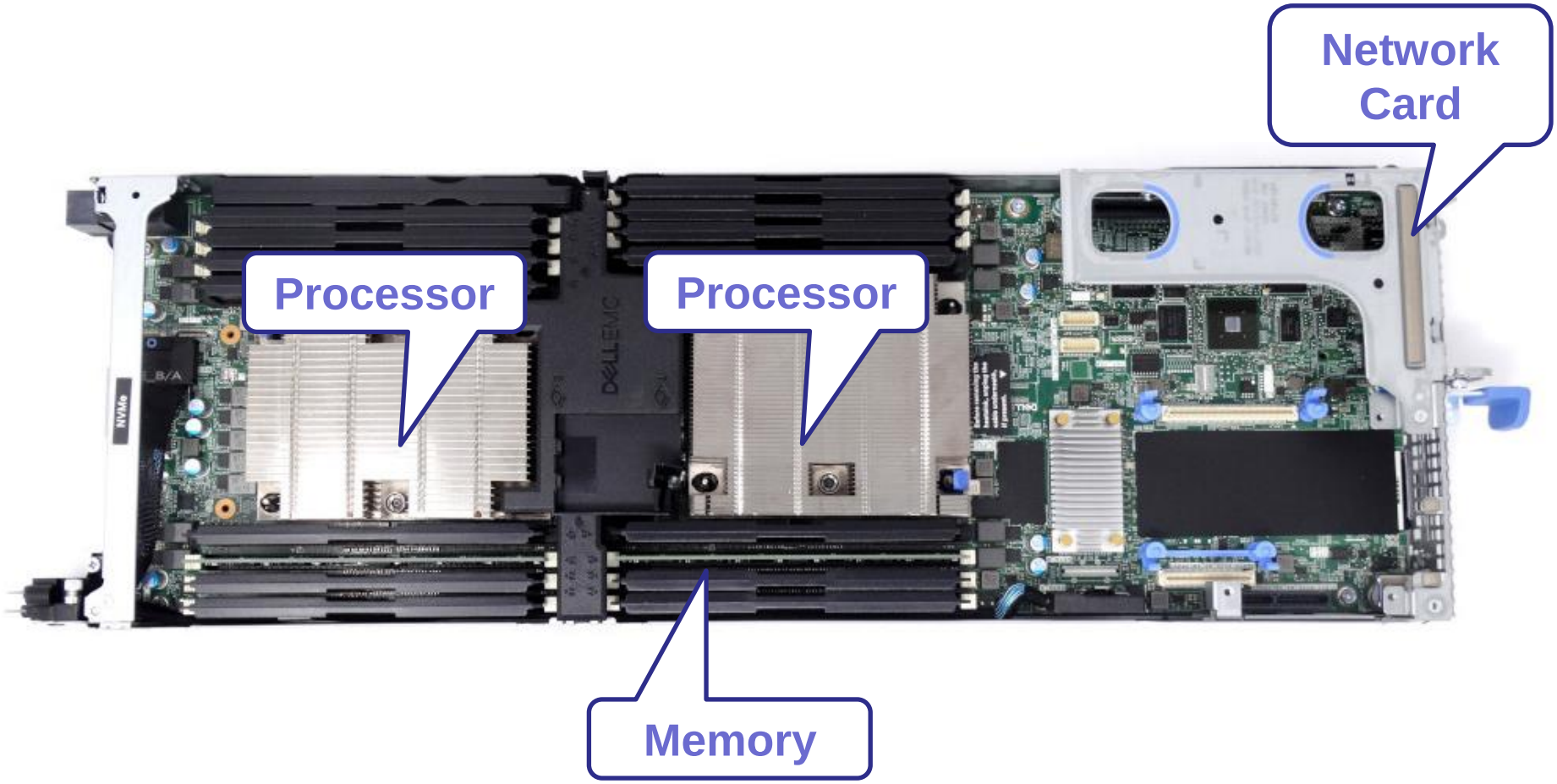


Rack

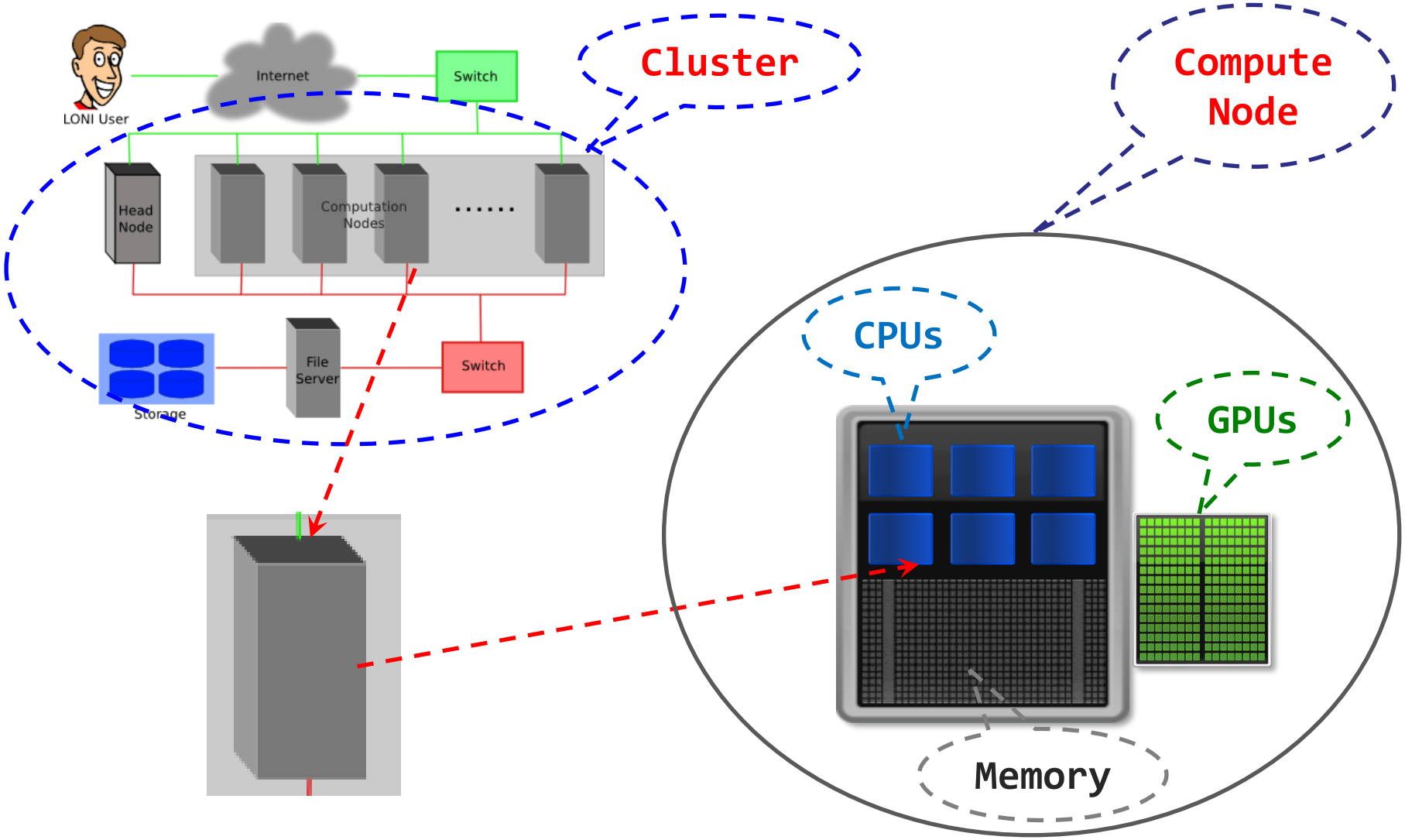
Infiniband Switch

Compute Node

Inside A SuperMike-III Compute Node



Conceptual Relationship



Summary of SuperMike-III

- **SuperMike-III is a 1.3 PetaFlop peak performance cluster with the latest CPUs from Intel and GPUs from NVIDIA, comprised of 183 compute nodes connected by 200 Gbps Infiniband fabric:**
  - 171 regular nodes: two 32-core Intel Ice Lake CPUs, 256 GB RAM
  - 8 GPU nodes: two 32-core Intel Ice Lake CPUs, 256 GB RAM, four NVIDIA Tesla A100 GPUs
  - 4 bigmem nodes: two 32-core Intel Ice Lake CPUs, 2 TB RAM

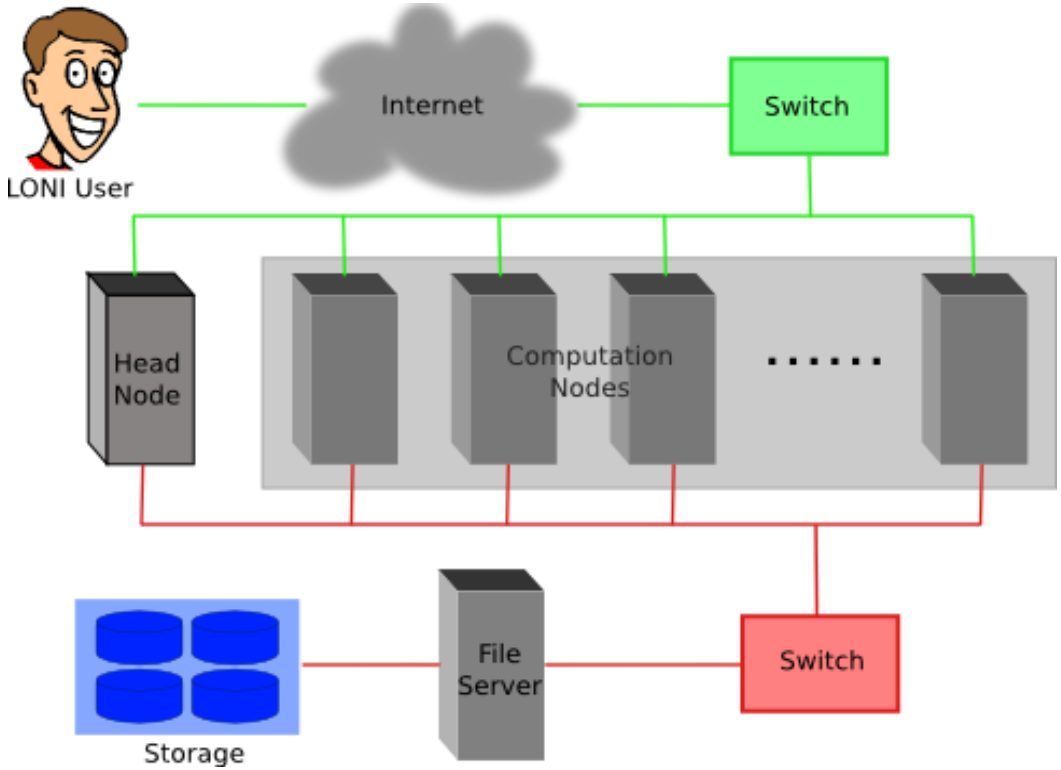
- **log in SuperMike-III with your current LSU HPC credentials using**
  - `ssh <username>@mike.hpc.lsu.edu`
- **Before you submit jobs on SuperMike-III, please make sure that you review the user guide here:**
  - http://www.hpc.lsu.edu/docs/guides.php?system=SuperMike3
- **The biggest difference SuperMIC users would notice on SuperMike-III is that, instead of Torque/Moab (PBS), *SLURM* is employed as the workload and resource manager.**

SuperMike-III HPC User Environment

SuperMike-III Job Queues

Cluster Environment

- **Multiple compute nodes**
- **Multiple users**
- **Each user may have multiple jobs running simultaneously**
- **Multiple users may share the same node**



Job submission basics

1. **Find appropriate queue**

2. **Understand the queuing system and your requirements and proceed to submit jobs**

3. **Monitor jobs during execution**

Job Queues (Partitions)

- **Nodes are organized into queues. Nodes can be shared.**
- **Each job queue (partition) differs in**
  - Number of available nodes
  - Max run time
  - Max running jobs per user
  - Nodes may have special characteristics: GPU, Large memory, etc.
- **Jobs need to specify resource requirements**
  - Nodes, time, queue
- **It's called a queue for a reason, but jobs don't run on a "First Come First Served" policy,**
  - This will be detailed in later slides

Queue Characteristics – LSU clusters

Machine	Queue	Max Runtime (h)	ppn	Max nodes per job
SuperMIC	workq	72	20	128
	checkpt		20	256
	single	168	1,2,4,6,8	1
	bigmem	72	48	1

Machine	Partition	Max Runtime (h)	cores per node	Max nodes per job
SuperMike-III	workq	72	64	84
	checkpt	72	64	84
	single	168	64	1
	gpu	72	64	4
	bigmem	72	64	1

- By default, you job will be submitted to “single” queue (partition).

Queue Characteristics

- **"sinfo" will give you more info on the queues**

```
[fchen14@mike2 slurmdoc]$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
admin        up   infinite      4    mix mike[001-003,192]
admin        up   infinite    197   idle mike[004-190,193-202]
admin        up   infinite      1   down mike191
single*      up 3-00:00:00      4    mix mike[001-003,192]
single*      up 3-00:00:00    187   idle mike[004-190]
single*      up 3-00:00:00      1   down mike191
checkpt      up 3-00:00:00      4    mix mike[001-003,192]
checkpt      up 3-00:00:00    187   idle mike[004-190]
checkpt      up 3-00:00:00      1   down mike191
workq        up 3-00:00:00      4    mix mike[001-003,192]
workq        up 3-00:00:00    187   idle mike[004-190]
workq        up 3-00:00:00      1   down mike191
gpu          up 3-00:00:00      8   idle mike[193-200]
bigmem       up 3-00:00:00      2   idle mike[201-202]
```

Queue Querying – Linux Clusters

- **Displays information about active, eligible, blocked, and/or recently completed jobs: `showq` command**

```
[fchen14@mike1 ~]$ showq
ACTIVE JOBS--------------------
JOBID     JOBNAME    USERNAME      STATE   CORE   REMAINING  STARTTIME
================================================================================
4896      cellranger lyan1         Running 64      21:42:43  Tue Jul 26 14:55:23
4924      bash       fchen14       Running 64      11:05:50  Tue Jul 26 16:18:30
4946      xhpcg_skx  lyan1         Running 2048    11:33:16  Tue Jul 26 16:45:56
4956      supernova. lyan1         Running 64      23:42:50  Tue Jul 26 16:55:30
4964      test       yexu          Running 64       3:52:34  Tue Jul 26 17:05:14
4968      gmx_mpi    lyan1         Running 128     11:59:19  Tue Jul 26 17:11:59
4969      bash       lyan1         Running 64      11:59:41  Tue Jul 26 17:12:21

       7 active jobs

Total Jobs: 7     Active Jobs: 7     Idle Jobs: 0     Blocked Jobs: 0
```

SuperMike-III HPC User Environment

Job Submission Through SLURM

PBS to SLURM

- **Why SLURM?**
  - SLURM has a more open model
  - SLURM also feels more modern in its design and implementation
  - SLURM scales well, job starts faster, etc.

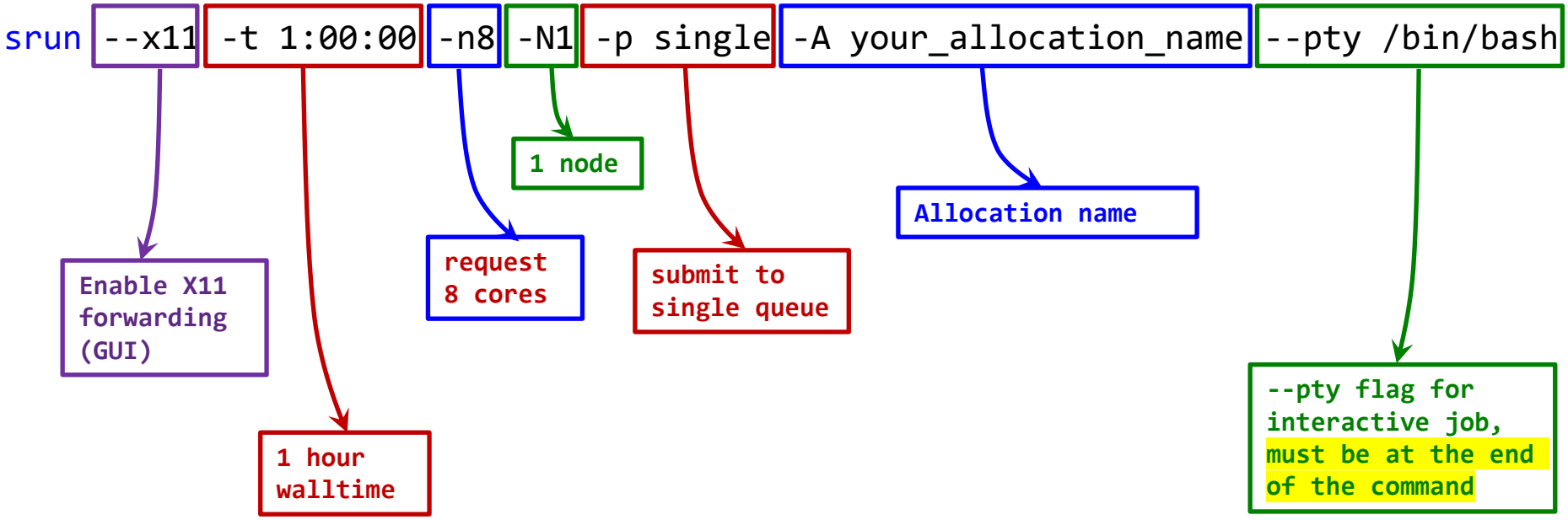
- **What will we cover in this session?**
  - Basic SLURM job submission
    - Interactive job
    - Batch job

Two Job Types

- **Interactive job**
  - User can interact with the terminal on the compute node.
  - Interactive jobs can be used for ***testing and troubleshooting*** code.
  - Requesting an interactive job will allocate resources and log you into a shell on a compute node.
- **Batch job**
  - Executed without user intervention using a job script
  - Batch jobs are used for production runs.
  - Requesting an interactive job will allocate resources and execute the job commands in a non-interactive shell

SLURM Interactive Job Command

- **To start an interactive job, use the `srun` command like the example below:**



Check Available Allocations

```
[fchen14.fchen14-t460] ➤ ssh fchen14@mike.hpc.lsu.edu
##############################################################################
Send questions and comments to the email ticket system at sys-help@loni.org.
##############################################################################
SuperMike-3 at LSU (Open in friendly user mode)
17-May-2022
SuperMike-3 is a 1.3 PetaFlop peak performance cluster with 11,712 CPU cores,
...Message Of The Day...
[fchen14@mike1 ~]$ showquota
User filesystem quotas for fchen14 (uid 32584):
     Filesystem         MB used       quota       files      fquota
     /homem                 433       10000       21532           0
     /work /project      302299           0     2325239     4000000
Storage allocation      MB used       quota       files  expiration
     sa_fchen14               -           -           -  2000-01-01
CPU Allocation SUs:        remaining   allocated  expiration
    hpc_hpcadmin8:         393715.16  2000000.00  2022-07-01
    hpc_train_2022:         49301.54
```

Start an SLURM Interactive Job

```
[fchen14@mike1 ~]$ srun --x11 -t 1:00:00 -n8 -N1 -p single -A hpc_train_2022 --pty /bin/bash
srun: Job is in held state, pending scheduler release
srun: job 4799 queued and waiting for resources
Interactive job 4799 running:
srun: job 4799 has been allocated resources
[fchen14@mike156 ~]$ hostname
mike156
[fchen14@mike156 ~]$ some_job_commands # your own job commands
```

SLURM Environmental Variables

```
[fchen14@mike2 slurmdoc]$ srun --x11 -t 1:00:00 -n8 -N1 -p single -A
LSU_LSUadmin1 --pty /bin/bash
[fchen14@mike156 slurmdoc]$ echo $SLURM_
$SLURM_CLUSTER_NAME          $SLURM_JOB_NAME
$SLURM_NPROCS                $SLURM_STEP_NODELIST
$SLURM_CPU_BIND              $SLURM_JOB_NODELIST
$SLURM_NTASKS                $SLURM_STEP_NUM_NODES
$SLURM_CPU_BIND_LIST         $SLURM_JOB_NUM_NODES
$SLURM_PRIO_PROCESS          $SLURM_STEP_NUM_TASKS
$SLURM_CPU_BIND_TYPE         $SLURM_JOB_PARTITION
$SLURM_PROCID                $SLURM_STEP_TASKS_PER_NODE
...
$SLURM_JOB_GID               $SLURM_NNODES
$SLURM_STEPID                $SLURM_TOPOLOGY_ADDR_PATTERN
$SLURM_JOBID                 $SLURM_NODEID
$SLURM_STEP_ID               $SLURM_UMASK
$SLURM_JOB_ID                $SLURM_NODELIST
$SLURM_STEP_LAUNCHER_PORT    $SLURM_WORKING_CLUSTER
```

Notes about srun inside interactive job

- **If you need to start another MPI job using `srun` inside an interactive job, you need to add "`--overlap`" after the srun command to avoid command hang:**

```
[fchen14@mike1 ~]$ srun -N1 -n8 -p single --pty bash # interactive job
srun: Job is in held state, pending scheduler release
srun: job 5224 queued and waiting for resources
Interactive job 5224 waiting:
srun: job 5224 has been allocated resources
[fchen14@mike001 ~]$ srun -n 4 hostname # this command will hang
[fchen14@mike001 ~]$ srun --overlap -n 4 hostname # this command will work
mike001
mike001
mike001
mike001
```

- **For batch job, you don't need to add** `--overlap`

SLURM Batch Job Script

- **To create a batch SLURM script, use your favorite editor (e.g. vi or emacs, nano) to create a text file with both SLURM instructions and commands how to run your job.**
- **All SLURM directives (special instructions) are prefaced by the #SBATCH.**

```
#!/bin/bash
#SBATCH -N 1         # request one node
#SBATCH -t 2:00:00   # request two hours
#SBATCH -p single    # in single partition (queue)
#SBATCH -A your_allocation_name
#SBATCH -o %x-%j.out-%N # optional, name of the stdout, using the job number (%j) and the
hostname of the node (%N)
#SBATCH -e %x-%j.err-%N # optional, name of the stderr, using job and hostname values
# below are job commands

date
cd /work/$USER/myjob
./mydemo
# Mark the time it finishes.
date
# exit the job
exit 0
```

Tells the job scheduler how much resource you need.

How will you use the resources?

Common SLURM Switches

- **`#SBATCH -A allocation_name`:**
  - short for --account, charge jobs to your allocation named allocation_name.
- **`#SBATCH -N <number_of_nodes>:`**
  - short for --nodes, number of nodes on which to run.
- **`#SBATCH -n <number_of_cores/processes>:`**
  - short for --ntasks, number of tasks (CPU cores) to run job on. The memory limit for jobs is 4 GB of MEM per CPU core requested.
- **`#SBATCH -c <cores_per_process>:`**
  - short for --ncpus-per-task, number of threads per process.
- **`#SBATCH -p partition:`**
  - short for --partition, submit job to the partition queue. Allowed values for partition: single, checkpt, workq, gpu, bigmem. Depending on cluster (use `sinfo` command)
- **`#SBATCH -t hh:mm:ss:`**
  - short for --time, request walltime.
- **`#SBATCH -o filename.out:`**
  - short for --output, write standard output.
- **`#SBATCH -e filename.err:`**
  - short for --error, write standard error.
  - Note that by default, SLURM will merge standard error and standard output.

Submit SLURM Batch Job

- **To submit the above job to the scheduler, save the above script as a text file, e.g., singlenode.sh, then use the `sbatch` command to submit, the output will be something like the below:**

```
[fchen14@mike2 slurmdoc]$ sbatch singlenode.slm
Submitted batch job 37355 estimates 9 SUs from allocation LSU_train_2020.
Estimated remaining SUs: 37352
See running job information with: scontrol show job 37355
```

- **To check the status of your job, use the `squeue` command:**

```
[fchen14@mike2 slurmdoc]$ squeue -u $USER
JOBID PARTITION     QOS      NAME     USER  ACCOUNT       STATE  PRIORITY       TIME
SUBMIT_TIM TIME_LIMI  NODES   CPUS MIN_MEMORY NODELIST(REASON)
             37480   checkpt normal batch.sl  fchen14 LSU_tra    RUNNING
1       0:06 2020-09-18   1:00:00      2     96 3958M mike[161-162]
```

Common SLURM Commands (1)

- **`squeue` is used to show the partition (queue) status. Useful options:**
  - `-u <username>:` limit output to jobs by username --state=pending: limit output to pending (i.e. queued) jobs --state=running: limit output to running jobs
  - Below is an example to query all jobs submitted by current user (fchen14)

```
[fchen14@mike2 slurmdoc]$ squeue -u fchen14
JOBID  PARTITION  NAME       USER    ST  TIME_LIMIT TIME CPUS  NODES  NODELIST(REASON)
37876  workq      hybrid_job fchen14 CF  5:00       0:04 96    2      mike[005-006]
```

Common SLURM Commands (2)

- **`sinfo` is used to view information about SLURM nodes and partitions.**

```
[fchen14@mike156 ~]$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
admin        up   infinite      2  inval mike[147,175]
admin        up   infinite      1   comp mike183
admin        up   infinite      1    mix mike156
admin        up   infinite    178   idle mike[001-146,148-155,157-174,176-181]
admin        up   infinite      1   down mike182
single*      up 7-00:00:00      1  inval mike147
single*      up 7-00:00:00      1    mix mike156
single*      up 7-00:00:00    169   idle mike[001-146,148-155,157-171]
checkpt      up 3-00:00:00      1  inval mike147
checkpt      up 3-00:00:00      1    mix mike156
checkpt      up 3-00:00:00    169   idle mike[001-146,148-155,157-171]
workq        up 3-00:00:00      1  inval mike147
workq        up 3-00:00:00      1    mix mike156
workq        up 3-00:00:00    169   idle mike[001-146,148-155,157-171]
bigmem       up 3-00:00:00      1  inval mike175
bigmem       up 3-00:00:00      3   idle mike[172-174]
gpu          up 3-00:00:00      1   comp mike183
gpu          up 3-00:00:00      6   idle mike[176-181]
gpu          up 3-00:00:00      1   down mike182
```

Common SLURM Commands (3)

- **scancel is used to signal or cancel jobs. Typical usage with squeue.**

```
[fchen14@mike1 ~]$ squeue -u fchen14
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
               341   checkpt     bash  fchen14  R       0:13      1 mike001
               340   checkpt     bash  fchen14  R    1:50:57      1 mike002
# cancel (delete) job with JOBID 340
[fchen14@mike1 ~]$ scancel 340
# job status might display a temporary "CG" ("CompletinG") status immediately after
scancel
[fchen14@mike1 ~]$ squeue -u fchen14
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
               340   checkpt     bash  fchen14 CG    1:51:08      1 mike002
               341   checkpt     bash  fchen14  R       0:41      1 mike001
[fchen14@mike1 ~]$ squeue -u fchen14
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
               341   checkpt     bash  fchen14  R       1:08      1 mike001
```

Common SLURM Commands (4)

- **`scontrol` is used to view or modify SLURM configuration and state. Typical usage for the user is to check job status:**

```
[fchen14@mike1 ~]$ squeue -u fchen14 # show all jobs
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
               341   checkpt     bash  fchen14  R    1:29:20      1 mike001
[fchen14@mike1 ~]$ scontrol show job 341
JobId=341 JobName=bash
   UserId=fchen14(32584) GroupId=Admins(10000) MCS_label=N/A
   Priority=1 Nice=0 Account=hpc_hpcadmin6 QOS=normal
   JobState=RUNNING Reason=None Dependency=(null)
   ... some details omitted...
   MinCPUsNode=1 MinMemoryNode=22332M MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   OverSubscribe=NO Contiguous=0 Licenses=(null) Network=(null)
   Command=/bin/bash
   WorkDir=/home/fchen14/test
   Power=
```

Serial and Parallel (Multi-Threaded and MPI) Job Templates

- **Serial Jobs**

- **Parallel Jobs**
  - SMP (Shared Memory Parallelism)
    - OpenMP
    - Python's Multiprocessing
    - Pthread
    - R's mcapply
  - MPI
  - Hybrid

Serial Job Script Template

```
#!/bin/bash
#SBATCH --job-name=serial_job_test    # Job name
#SBATCH --ntasks=1                    # Using a single core
#SBATCH --time=00:10:00      # Time limit hh:mm:ss
#SBATCH --output=%x_%j.log   # Standard output and error log,
                             # %x: job name
                             # %j: job-id

module load python

echo "Running job on a single CPU core"

date
/home/user/single_core_job.py
date
```

Shared Memory Parallelism (SMP) Jobs

- **Shared-Memory Parallelism (SMP) is when workload is shared among different CPU cores using multiple threads or processes running within a single compute node and these cores have access to common (shared) memory.**
  - SMP jobs cannot make use of multiple nodes and all the cores must be physically located the same node.
  - When running SMP jobs, you must make the SMP application aware of how many cores to use.
  - How that is done depends on the specific type of application. Typical examples:
    - OpenMP (Open Multi-Processing)
      - First set `--ntasks=1`, and then set OMP_NUM_THREADS to a value less than or equal to the number of cpus-per-task
    - Pthreads
    - Python's multiprocessing module
    - R's mcapply

SMP Job Script (OpenMP Based)

```
#!/bin/bash
#SBATCH --job-name=smp_job           # Job name
#SBATCH --nodes=1                    # Run all processes on a single node
#SBATCH --ntasks=1                   # Run a single task
#SBATCH --cpus-per-task=8            # Number of CPU cores per task
#SBATCH --time=00:10:00              # Time limit hh:mm:ss
#SBATCH --output=%x_%j.log           # Standard output and error log

date
# use this line if your job uses OpenMP
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

/home/user/smp_job.out
date
```

MPI (Message Passing Interface) Job

- **According to SLURM documentation (https://slurm.schedmd.com/mpi_guide.html), "there are three fundamentally different modes of operation used by various MPI implementation with SLURM:**

  - *“SLURM directly launches the tasks and performs initialization of communications through the PMI2 or PMIx APIs. (Supported by most modern MPI implementations.)*
  - *Use mpirun launches tasks using SLURM's infrastructure (not using PMIx).*
  - *SLURM creates a resource allocation for the job and then mpirun launches tasks using some mechanism other than SLURM." (We do not recommend HPC/LSU users use this method to launch their MPI jobs.)”*

MPI Job - (PMIx Versions)

- **If you compiled your MPI application using our default intel-mpi libraries, it is recommended to start the application directly using the `srun` command.**

```
#!/bin/bash
#SBATCH --job-name=mpi_job_test      # Job name
#SBATCH --partition=workq            # For jobs using more than 1 node, submit to workq
#SBATCH --nodes=2                    # Number of nodes to be allocated
#SBATCH --ntasks=128                 # Number of MPI tasks (i.e. processes/cores)
#SBATCH --time=00:05:00              # Wall time limit (hh:mm:ss)
#SBATCH --output=%x_%j.log     # Standard output and error

echo ""
echo "SLURM Nodes Allocated          = $SLURM_JOB_NODELIST"
echo "Number of Nodes Allocated      = $SLURM_JOB_NUM_NODES"
echo "Number of Tasks Allocated      = $SLURM_NTASKS"

module load intel-mpi/2021.5.1
srun -n $SLURM_NTASKS ./a.out
```

MPI Job - (Non-PMIx Versions)

- **You can still run the MPI job using mpirun with intel-mpi.**

```
#!/bin/bash
#SBATCH --job-name=mpi_job_test      # Job name
#SBATCH --partition=workq            # For jobs using more than 1 node, submit to workq
#SBATCH --nodes=2                    # Number of nodes to be allocated
#SBATCH --ntasks=128                 # Number of MPI tasks (i.e. processes/cores)
#SBATCH --time=00:05:00              # Wall time limit (hh:mm:ss)
#SBATCH --output=mpi_test_%j.log     # Standard output and error

echo ""
echo "SLURM Nodes Allocated          = $SLURM_JOB_NODELIST"
echo "Number of Nodes Allocated      = $SLURM_JOB_NUM_NODES"
echo "Number of Tasks Allocated      = $SLURM_NTASKS"

module load intel-mpi/2021.5.1
mpirun -n $SLURM_NTASKS ./a.out
```

Hybrid (MPI + SMP) Job

- **Hybrid jobs are MPI applications where each MPI process is multi-threaded and can use multiple cores across multiple nodes. If the MPI implementation is compiled with PMIx enabled, use the `srun` command to start the hybrid job, otherwise, use the `mpirun` command to start it.**

```
#!/bin/bash
#SBATCH --partition=workq            # Need to submit workq for multiple node jobs
#SBATCH --nodes=2                    # Maximum number of nodes to be allocated
#SBATCH --ntasks=4                   # Number of MPI tasks (i.e. processes)
#SBATCH --cpus-per-task=32           # Number of cores per MPI task
#SBATCH --time=00:05:00              # Wall time limit (hh:mm:ss)
#SBATCH --output=hybrid_test_%j.log  # Standard output and error file

echo "Number of Nodes Allocated      = $SLURM_JOB_NUM_NODES"
echo "Number of Tasks Allocated      = $SLURM_NTASKS"
echo "Number of Cores/Task Allocated = $SLURM_CPUS_PER_TASK"

module load intel-mpi/2021.5.1
# PMIx version
srun -n $SLURM_NTASKS -c $SLURM_CPUS_PER_TASK ./a_pmix.out
# Non-PMIx version
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
mpirun -n $SLURM_NTASKS ./a_hydra.out
```

Inspect Job Results

- **Check job standard output/standard error by inspecting the redirected files:**

```
[fchen14@mike2 slurm]$ cat lmp_hybrid_5287.log
Date              = Thu Jul 28 07:51:11 CDT 2022
Hostname          = mike003
Working Directory = /home/fchen14/lsusm3workshop/slurm
Number of Nodes Allocated      = 2
Slurm Nodes Allocated          = mike[003-004]
Number of Tasks Allocated      = 4
Number of Cores/Task Allocated = 32
Autoloading intel/2021.5.0
Autoloading intel-mpi/2021.5.1
Loading lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1
  Loading requirement: intel/2021.5.0 intel-mpi/2021.5.1
LAMMPS (23 Jun 2022)
OMP_NUM_THREADS environment is not set. Defaulting to 1 thread.
(src/comm.cpp:98)
  using 1 OpenMP thread(s) per MPI task
using multi-threaded neighbor list subroutines
set 32 OpenMP thread(s) per MPI task
...
```

SuperMike-III HPC User Environment

Job Monitoring

Job Monitoring on SuperMike-III

- **Check details on your job using `qstat`**

```
$ squeue -u $USER  : For quick look at nodes assigned to you
$ scontrol show job <jobid>     : For details on your job
$ scancel jobid          : To delete job
```

- **Check memory usage of your job using `qshow`**

```
$ qshow jobid
```

- **Please pay close attention to the load and the memory consumed by your job!**

Using the “top” command

- **The top program provides a dynamic real-time view of a running system.**

```
top - 23:30:16 up 51 days, 16:18,  4 users,  load average: 0.16, 0.05, 0.06
Tasks: 692 total,   2 running, 690 sleeping,   0 stopped,   0 zombie
%Cpu(s):  1.1 us,  1.0 sy,  0.0 ni, 97.9 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
KiB Mem : 19647060+total, 18699553+free,  8677504 used,   797560 buff/cache
KiB Swap: 13421772+total, 13405440+free,   163328 used. 18702988+avail Mem

   PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
208754 fchen14   20   0 7731040   5.5g  20108 R 100.0  2.9   0:16.50 lmp
208999 fchen14   20   0  172868   2948   1624 R   0.7  0.0   0:00.07 top
     1 root      20   0  191624   2832   1544 S   0.0  0.0  21:18.21 systemd
     2 root      20   0       0      0      0 S   0.0  0.0   0:04.81 kthreadd
     4 root       0 -20       0      0      0 S   0.0  0.0   0:00.00 kworker/0:0H
     6 root      20   0       0      0      0 S   0.0  0.0   1:06.85 ksoftirqd/0
```

Check memory Usage for Multi-Node Job

- Check health of your job using `qshow`

  `$ qshow <jobid>`

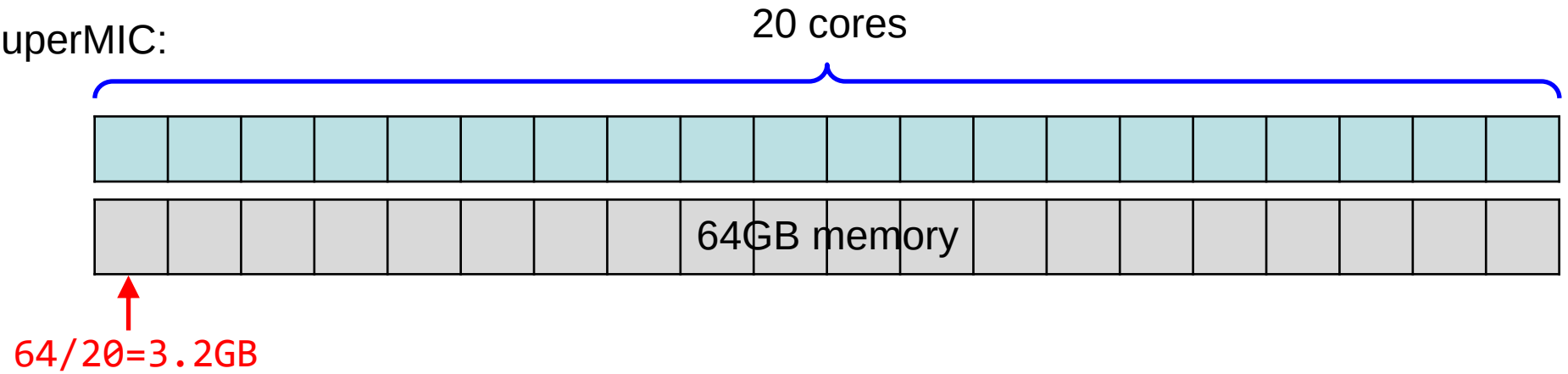
```
[fchen14@mike2 slurmdoc]$ sbatch ex_lmp_hybrid.sh
Submitted batch job 37888 estimates 8 SUs from allocation LSU_LSUadmin1.
Estimated remaining SUs: 521696
JOBID      NAME               PARTITION  TIME_LIMIT  ST  CPUS  NODES  REASON
37888      hybrid_job_test    workq      5:00        PD  96    2      None
[fchen14@mike2 slurmdoc]$ qshow 37888
PBS job: 37888, nodes: 2
Hostname  Days Load CPU U# (User:Process:VirtualMemory:Memory:Hours)
mike005       0 Autoloading 211  6 fchen14:lmp:5847M:3.2G fchen14:lmp:5846M:3.3G
fchen14:slurm_scr+:113M:2M fchen14:srun:388M:5M fchen14:srun:50M:1M
mike006       0 Autoloading 216  3 fchen14:lmp:5870M:5.1G fchen14:lmp:4447M:3.3G
PBS_job=37888 user=fchen14 allocation=LSU_LSUadmin1 queue=workq total_load=0.00
cpu_hours=0.00 wall_hours=0.00 unused_nodes=0 total_nodes=2 ppn=48 avg_load=0.00
avg_cpu=213% avg_mem=7640mb avg_vmem=11746mb
top_proc=fchen14:lmp:mike006:5870M:5.1G:0.0hr:105%  node_processes=3
```

Pay attention to single queue usage

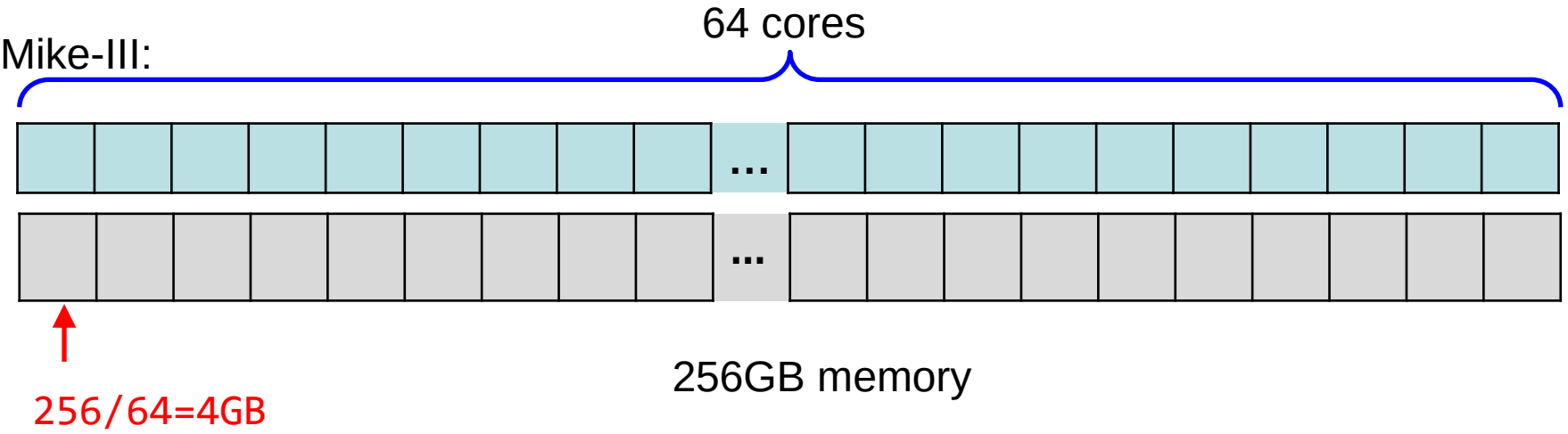
- **Single queue - Used for jobs that will only execute on a single node, i.e. `–N1 -n1-64`.**
- **Jobs in the single queue should not use:**
  - More than 3GB memory per core for QB2 (64G/20).
  - More than 4GB memory per core for SuperMike-III (256G/64).
- **If applications require more memory, scale the number of cores (`--ntasks/-n`) to the amount of memory required: i.e. max memory available for jobs in single queue is 16GB for `--ntasks 4` on SuperMike-III.**

Core and Memory in Single queue

SuperMIC:



SuperMike-III:



Question:

On SuperMIC, if my job needs 17GB memory, what `-ppn` value should I use?

On SuperMike-III, if my job needs 17GB memory, what `--ntasks (-n)` value should I use?

Short Summary

- **How to check queue (partition) information in SLURM?**
- **How to submit SLURM interactive job?**
  - Note the usage of `--overlap`
- **How to submit SLURM batch job?**
  - SMP (OpenMP)
  - MPI
  - Hybrid
- **Monitor your job?**

❖ ***Questions?***

Next Sessions

- **11:15 - 12:00**
  - Performance benchmarks and tuning
- **12:00 - 01:30**
  - Lunch break
- **01:30 - 03:30**
  - Q&A + On-ramp sessions (breakout sessions)