HPC User Environment 2

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September 14, 2016

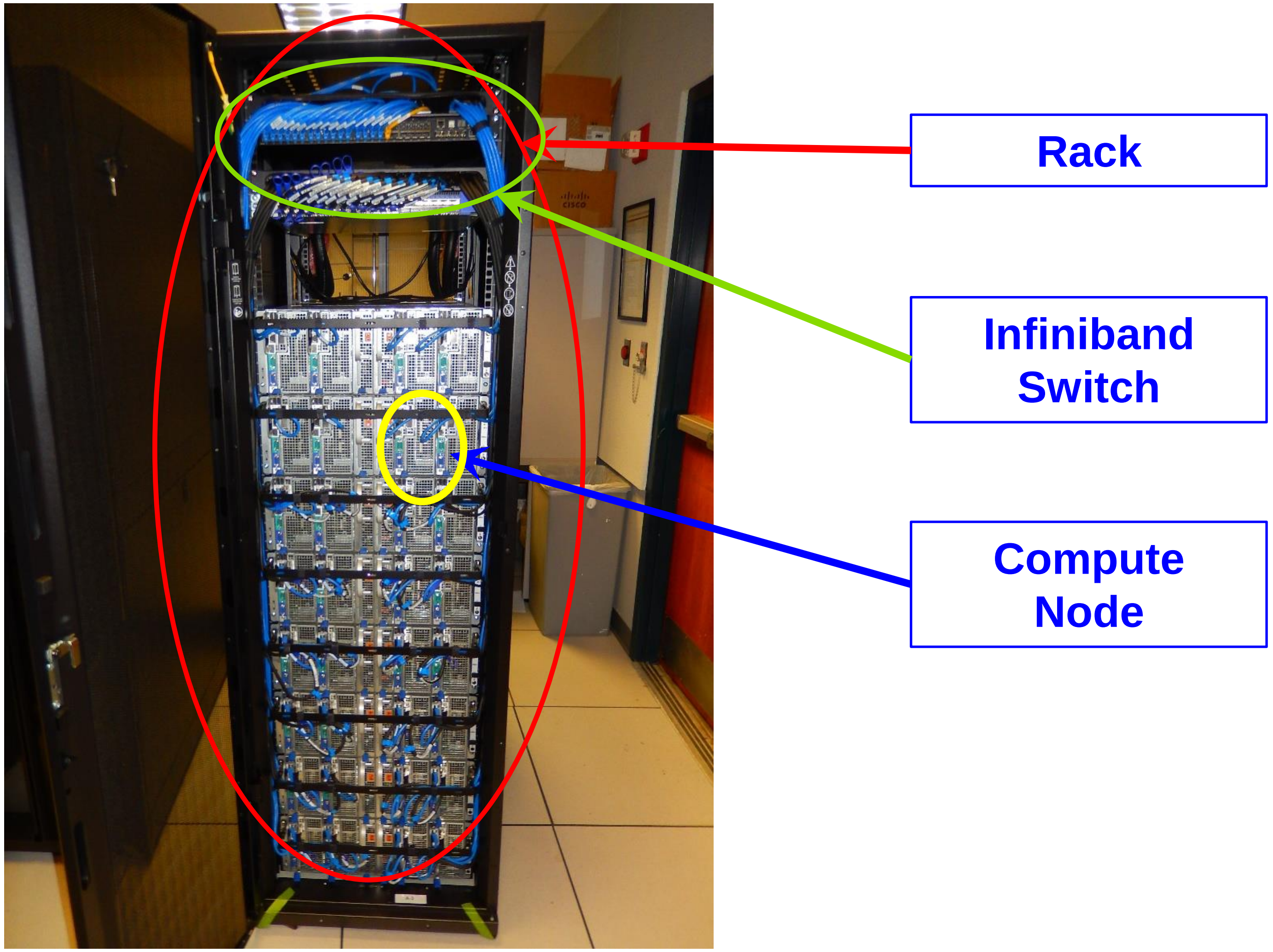
Outline

- **Review HPC User Environment 1 topics**
  - Available HPC resources
  - Accounts and Allocations
  - Cluster architecture
  - Connect to clusters
  - Software management using softenv and module
- **Things to be covered in this training**
  - Job management
    - More on job queues
    - Submit and monitor your jobs
    - Job scheduling basics
      - Job priority
      - Backfill
  - Compiling and analyze codes on cluster
    - Serial program
    - Parallel program

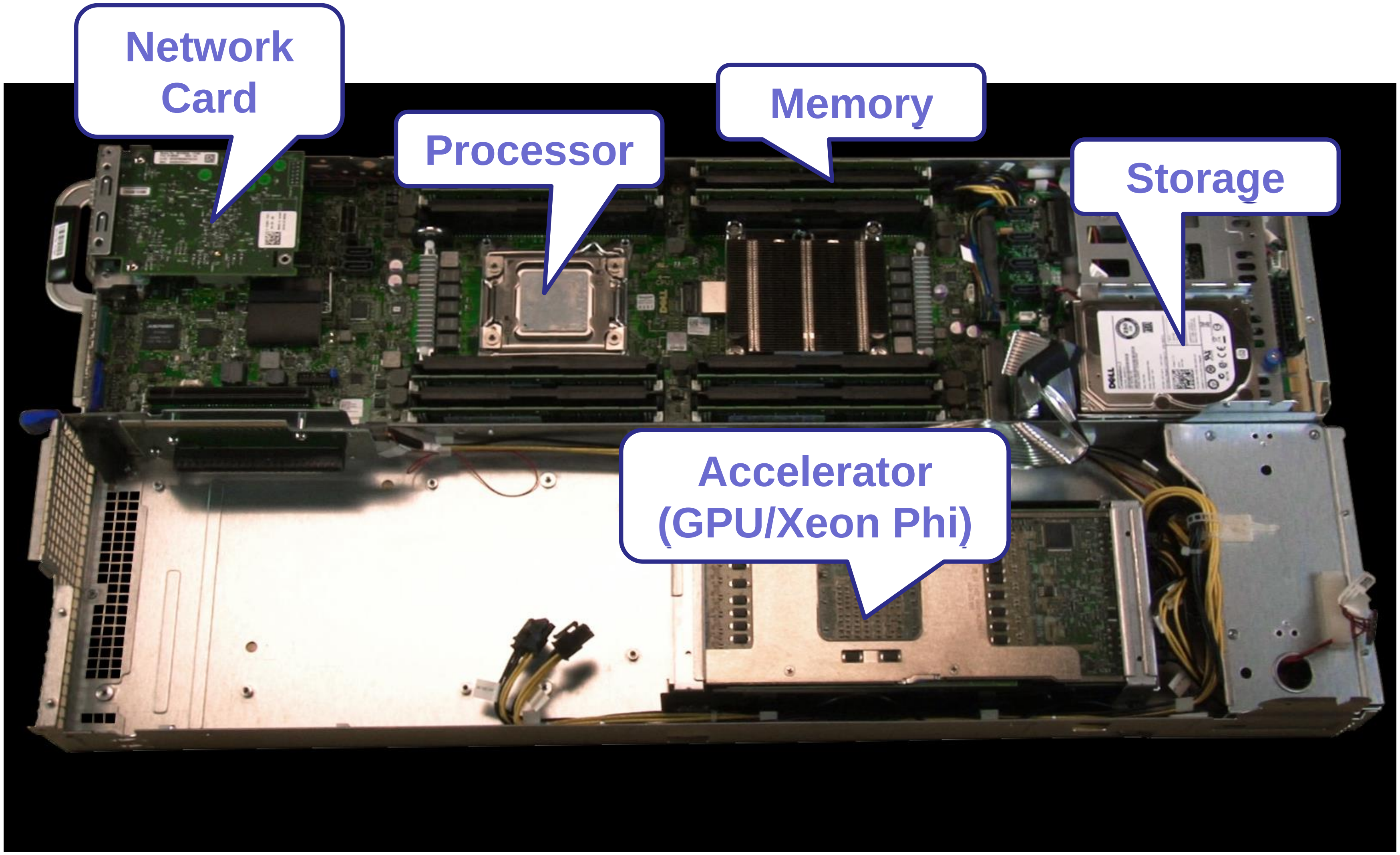
HPC User Environment 2

Brief Review of Session 1

Inside A Cluster Rack

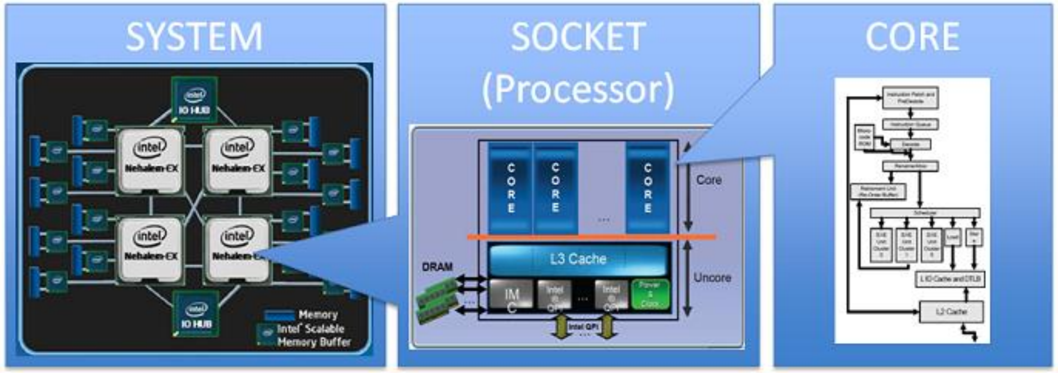


Inside A Compute Node



Cluster Nomenclature

Term	Definition
Cluster	The top-level organizational unit of an HPC cluster, comprising a set of nodes, a queue, and jobs.
Node	A single, named host machine in the cluster.
Core	The basic computation unit of the CPU. For example, a quad-core processor is considered 4 cores.
Job	A user's request to use a certain amount of resources for a certain amount of time on cluster for his work.



HPC Cluster Architectures

- **Major architecture**
  - Intel x86_64 clusters
    - Vendor: Dell
    - Operating System: Linux (RHEL 4/5/6)
    - Processor: Intel

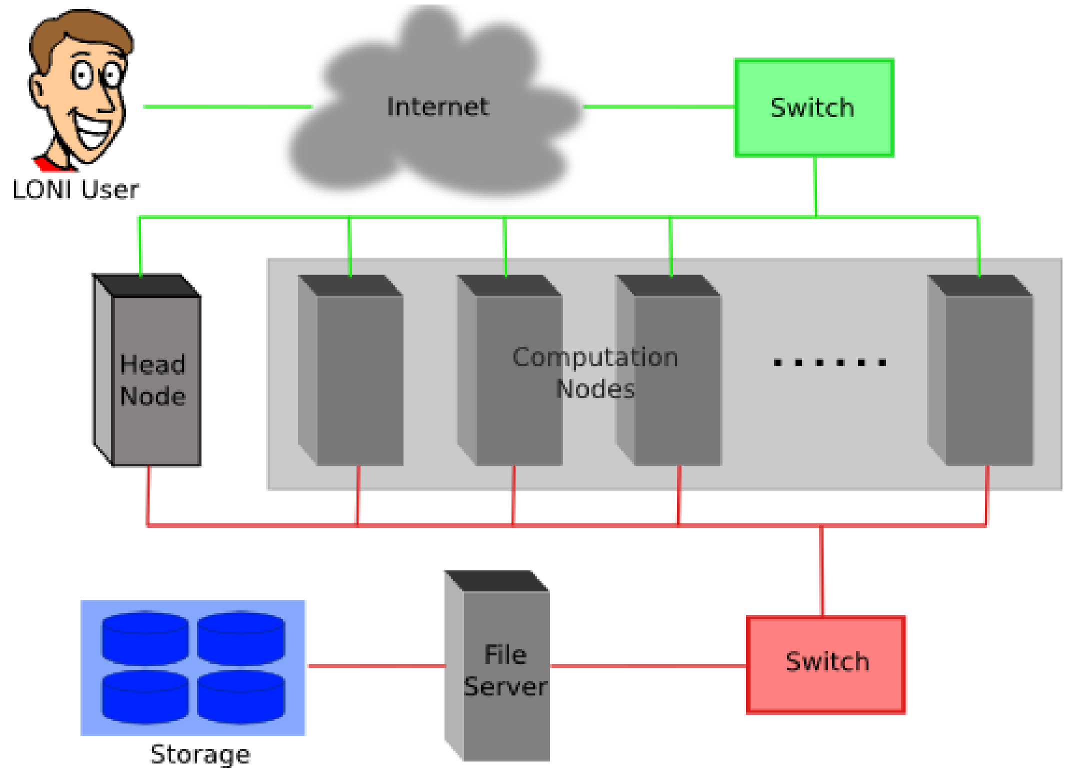
Accessing cluster using ssh (Secure Shell)

- **On Unix and Mac**
  - use ssh on a terminal to connect
- **Windows box (ssh client):**
  - Putty, Cygwin (http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html)
  - MobaXterm (http://mobaxterm.mobatek.net/)
- `ssh username@mike.hpc.lsu.edu`
- **Host name**
  - LONI: <cluster_name>.loni.org
    - <cluster_name> can be:
      - `eric.loni.org`
      - `qb.loni.org`
  - LSU HPC: <cluster_name>.hpc.lsu.edu
    - <cluster_name> can be:
      - `mike.hpc.lsu.edu`
      - `smic.hpc.lsu.edu`
      - `philip.hpc.lsu.edu`

More on 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

- **Find appropriate queue**
- **Understand the queuing system and your requirements and proceed to submit jobs**
- **Monitor jobs during execution**

Job Queues

- **Nodes are organized into queues. Nodes can be shared.**
- **Each job queue differs in**
  - Number of available nodes
  - Max run time
  - Max running jobs per user
  - Nodes may have special characteristics: GPU/Xeon Phi’s, Large memory, etc.
- **Jobs need to specify resource requirements**
  - Nodes, time, queue
- **Its 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 – LONI clusters

Machine	Queue	Max Runtime	ppn	Max running jobs	Max nodes per job	Use
Eric	workq	3 days	8	16	24	Unpreemptable
	checkpt		8		48	Preemptable
	single		1	32	1	ppn=1/2/4/8
QB2	workq	3 days	20	44	128	Unpreemptable
	checkpt		20		256	Preemptable
	single	7 days	1,2,4,8		1	Single node jobs

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Queue Characteristics – LSU Linux clusters

Machine	Queue	Max Runtime	ppn	Max running jobs	Max nodes per job	Use
SuperMike II	workq	3 days	16	34	128	Unpreemptable
	checkpt		16		128	Preemptable
	bigmem	2 days	16		1	Big memory
	gpu	3 days	16		16	Job using GPU
	single	3 days	1,2,4,8		1	Single node jobs
Philip	workq	3 days	8	5	4	Unpreemptable
	checkpt		8		4	Preemptable
	bigmem		8		2	Big memory
	single	14 days	4	50	1	Single processor
SuperMIC	workq	3 days	20	34	128	Unpreemptable
	checkpt		20		360	Preemptable

Queue Characteristics

- **“qstat -q” will give you more info on the queues**

```
 [fchen14@mike2 ~]$ qstat -q

server: mike3

Queue            Memory CPU Time Walltime Node  Run Que Lm  State
---------------- ------ -------- -------- ----  --- --- --  -----
workq              --      --    72:00:00   128  31   6 --   E R
mwfa               --      --    72:00:00     8   3   0 --   E R
bigmem             --      --    48:00:00     1   0   0 --   E R
lasigma            --      --    72:00:00    28  28   7 --   E R
bigmemtb           --      --    48:00:00     1   0   0 --   E R
priority           --      --    168:00:0   128   0   0 --   E R
single             --      --    72:00:00     1  62   0 --   E R
gpu                --      --    24:00:00    16   1   0 --   E R
preempt            --      --    72:00:00   --    0   0 --   E R
checkpt            --      --    72:00:00   128  31 137 --   E R
admin              --      --    24:00:00   --    0   0 --   E R
scalemp            --      --    24:00:00     1   0   0 --   E R
                                               ----- -----
                                                 156   150
```

- **For a more detailed description use mdiag**

Queue Querying – Linux Clusters

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

```
$ showq
active jobs------------------------
JOBID              USERNAME      STATE PROCS   REMAINING            STARTTIME
236875              ebeigi3    Running    16     1:44:29  Mon Sep 15 20:00:22
236934                 mwu3    Running    16    00:03:27  Mon Sep 15 19:04:20
...
eligible jobs----------------------
JOBID              USERNAME      STATE PROCS     WCLIMIT            QUEUETIME
236795              dmarce1       Idle  1456    00:15:00  Mon Sep 15 16:38:45
236753               rsmith       Idle  2000     4:00:00  Mon Sep 15 14:44:52
236862              dlamas1       Idle   576     2:00:00  Mon Sep 15 17:28:57
...
121 eligible jobs
blocked jobs-----------------------
JOBID              USERNAME      STATE PROCS     WCLIMIT            QUEUETIME
232741              myagho1       Idle  2000  1:00:00:00  Mon Sep  8 07:22:12
235545              tanping       Idle     1  2:21:10:00  Fri Sep 12 16:50:49
235546              tanping       Idle     1  2:21:10:00  Fri Sep 12 16:50:50
...
```

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Submit and Monitor Your Jobs

Two Job Types

- **Interactive job**
  - Set up an interactive environment on compute nodes for users
    - Advantage: can run programs interactively
    - Disadvantage: must be present when the job starts
  - Purpose: testing and debugging, compiling
    - **Do not run on the head node!!!**
    - Try not to run interactive jobs with large core count, which is a waste of resources)
- **Batch job**
  - Executed without user intervention using a job script
    - Advantage: the system takes care of everything
    - Disadvantage: can only execute one sequence of commands which cannot changed after submission
  - Purpose: production run

Submitting Jobs on Linux Clusters

- **Interactive job example:**

```
qsub –I -X -V \
     -l walltime=<hh:mm:ss>,nodes=<num_nodes>:ppn=<num_cores> \
     -A <Allocation> \
     -q <queue name>
```

DO NOT `directly` `ssh` to compute nodes,
unless the nodes are assigned to you by the job scheduler.

  – Add `-X` to enable X11 forwarding

- **Batch Job example:**

```
qsub job_script
```

PBS Job Script – Serial Job

```
#!/bin/bash
#PBS -l nodes=1:ppn=1        # Number of nodes and processor
#PBS -l walltime=24:00:00    # Maximum wall time
#PBS -N myjob                # Job name
#PBS -o <file name>          # File name for standard output
#PBS -e <file name>          # File name for standard error
#PBS -q single               # The queue for serial jobs
#PBS -A <loni_allocation>    # Allocation name
#PBS -m e                    # Send mail when job ends
#PBS -M <email address>      # Send mail to this address

<shell commands>
<path_to_executable> <options>
<shell commands>
```

Tells the job scheduler how much resource you need.

How will you use the resources?

PBS Job Script – Parallel Job

```
#!/bin/bash
#PBS -l nodes=2:ppn=16             #Number of nodes and processors per node
#PBS -l walltime=24:00:00          #Maximum wall time
#PBS -N myjob                      #Job name
#PBS -o <file name>                #File name for standard output
#PBS -e <file name>                #File name for standard error
#PBS -q checkpt                    #Queue name
#PBS -A <allocation_if_needed>     #Allocation name
#PBS -m e                          #Send mail when job ends
#PBS -M <email address>            #Send mail to this address

<shell commands>
mpirun -machinefile $PBS_NODEFILE -np 32 <path_to_executable> <options>
<shell commands>
```

Tells the scheduler how much resource you need.

How will you use the resources?

Job Monitoring - Linux Clusters

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

```
$ qstat -n -u $USER  : For quick look at nodes assigned to you
$ qstat -f jobid     : For details on your job
$ qdel jobid         : To delete job
```

- **Check approximate start time using `showstart`**

```
$ showstart jobid
```

- **Check details of your job using `checkjob`**

```
$ checkjob jobid
```

- **Check health 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 - 19:39:56 up 89 days,  4:13,  1 user,  load average: 0.63, 0.18, 0.06
Tasks: 489 total,   2 running, 487 sleeping,   0 stopped,   0 zombie
Cpu(s):  6.3%us,  0.0%sy,  0.0%ni, 93.7%id,  0.0%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:  65909356k total,  3389616k used, 62519740k free,   151460k buffers
Swap: 207618040k total,     5608k used, 207612432k free,   947716k cached

   PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
 39595 fchen14   20   0  266m 257m  592 R 99.9  0.4   0:06.94 a.out
 39589 fchen14   20   0 17376 1612  980 R  0.3  0.0   0:00.05 top
 38479 fchen14   20   0  108m 2156 1348 S  0.0  0.0   0:00.03 bash
 39253 fchen14   20   0  103m 1340 1076 S  0.0  0.0   0:00.00 236297.mike3.SC
 39254 fchen14   20   0  103m 1324 1060 S  0.0  0.0   0:00.00 bm_laplace.sh
 39264 fchen14   20   0 99836 1908  992 S  0.0  0.0   0:00.00 sshd
 39265 fchen14   20   0  108m 3056 1496 S  0.0  0.0   0:00.03 bash
```

PBS Environmental Variables

```
[fchen14@mike315 ~]$ echo $PBS_
$PBS_ENVIRONMENT  $PBS_MOMPORT      $PBS_NUM_PPN      $PBS_O_MAIL
$PBS_QUEUE        $PBS_WALLTIME     $PBS_GPUFILE      $PBS_NODEFILE
$PBS_O_HOME       $PBS_O_PATH       $PBS_SERVER       $PBS_JOBCOOKIE
$PBS_NODENUM      $PBS_O_HOST       $PBS_O_QUEUE      $PBS_TASKNUM
$PBS_JOBID        $PBS_NP           $PBS_O_LANG       $PBS_O_SHELL
$PBS_VERSION      $PBS_JOBNAME      $PBS_NUM_NODES    $PBS_O_LOGNAME
$PBS_O_WORKDIR    $PBS_VNODENUM
```

Pay attention to single queue usage

- **Single queue - Used for jobs that will only execute on a single node, i.e. `nodes=1:ppn=1/2/4/8`.**
- **Jobs in the single queue should not use:**
  - More than 2GB memory per core for Eric, Philip and SuperMike2 (32G/16).
  - More than 3.2GB memory per core for QB2 (64G/20).
- **If applications require more memory, scale the number of cores (ppn) to the amount of memory required: i.e. max memory available for jobs in single queue is 8GB for ppn=4 on SuperMikeII.**
- **Typical type of warning:**
  - E124 - Exceeded memory allocation. This Job XXXX appears to be using more memory (GB) than allocated (9 > 3).
  - E123 - Exceeded ppn/core allocation. This Job XXXX appears to be using more cores than allocated (6 > 1). Please allocate the number of cores that the job will use, (ppn=6). This Job has 1 core(s) allocated (ppn=1).

More things to be noticed

- Eric is old and will be retired in the near future LONI users are encouraged to migrate their codes to QB-2 as soon as possible.
- The purpose of bigmem queue on QB-2 is for jobs costing big (larger than 64 GB) memory not for jobs using more number of cores.
- GPU is available to workq or checkpt queues on QB2.
- Xeon Phi is available to workq or checkpt queues on SuperMIC.
- There is no single queue on SuperMIC.
- Users are encouraged to use accelerators (GPU/Xeon Phi) whenever possible. Application for allocation involving with usage of accelerators will be easier to be approved.

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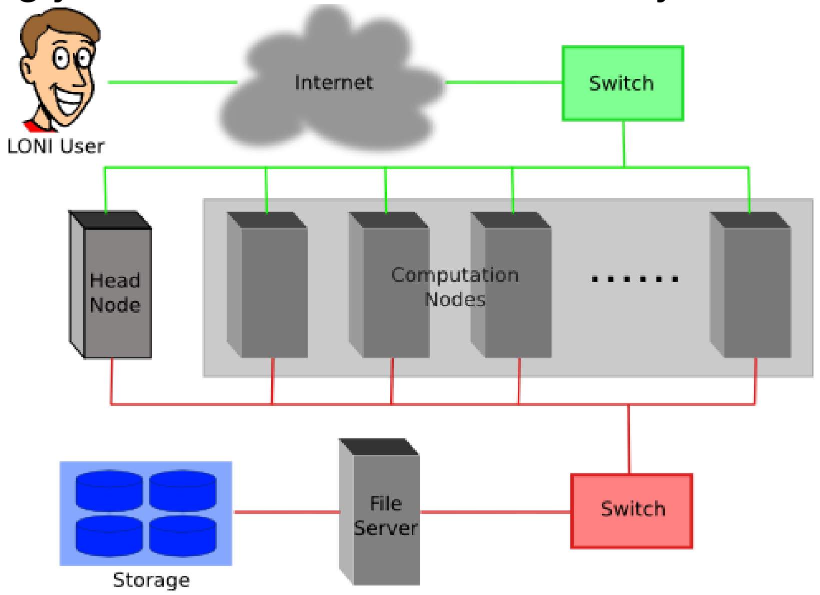
Job Scheduling Basics

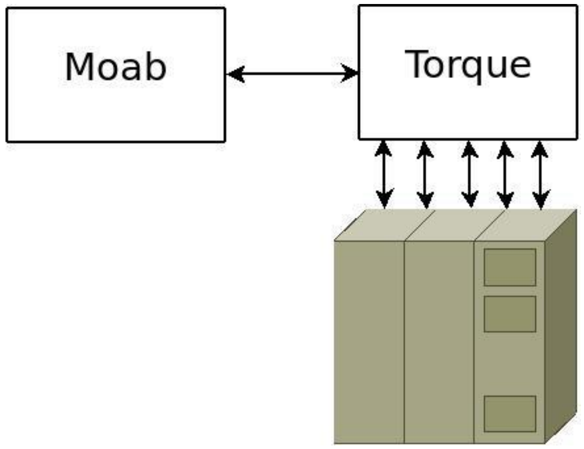
Back to Cluster Architecture

- **As a user, you interact with the scheduler and/or resource manager whenever you submit a job, or query on the status of your jobs or the whole cluster, or seek to manage your jobs.**
- **Resource managers give access to compute resource**
  - Takes in a resource request (job) on login node
  - Finds appropriate resource and assigns you a priority number
  - Positions your job in a queue based on the priority assigned.
  - Starts running jobs until it cannot run more jobs with what is available.



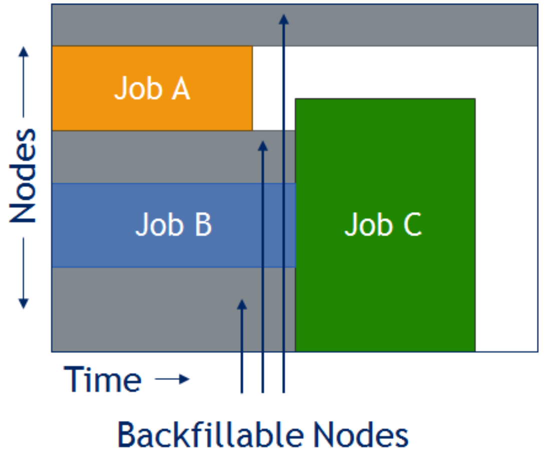
Job Scheduler

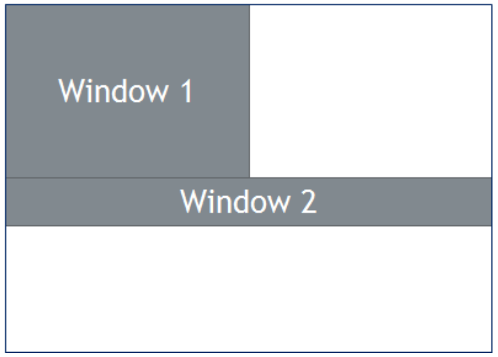
- **HPC & LONI Linux clusters use TORQUE, an open source version of the Portable Batch System (PBS) together with the MOAB Scheduler, to manage user jobs.**
- **Resource Manager - Torque**
  - Manages a queue of jobs for a cluster of resources
  - Launches job to a simple FIFO job queue
- **Workload Manager - Moab**
  - A scheduler that integrates with one or more Resource Managers to schedule jobs across domains of resources (servers, storage, applications)
  - Prioritizes jobs
  - Provides status of running and queued jobs, etc.
- **The batch queuing system determines**
  - The order jobs are executed
  - On which node(s) jobs are executed



Job management philosophy

- **Working Philosophy**
  - Prioritize workload into a queue for jobs
  - ***Backfill*** idle nodes to maximize utilization
    - Will be detailed later...





Job Priorities

- **Jobs with a higher job priority are scheduled ahead of jobs with a lower priority.**
- **Job priorities have contributions from the following:**
  - credential priority
  - fairshare priority
  - resource priority
  - service priority
- Priority determination for each queued job, use
  - `mdiag -p`:

```
$ mdiag -p
diagnosing job priority information (partition: ALL)
Job            PRIORITY*    Cred( User:Class)    FS( User:  WCA)  Serv(QTime:XFctr)   Res( Proc)
       Weights --------      100(   10:   10)   100(   10:   50)     2(    2:   20)    30(   10)

236172           246376     40.6(100.0:   0.0)   8.6( 19.6:  0.3)   4.0(1480.: 99.7)  46.8(2048.)
235440           242365     41.3(100.0:   0.0)   4.6(   8.2:  0.6)   6.6(3959.:  6.5)  47.5(512.0)
235441           242365     41.3(100.0:   0.0)   4.6(   8.2:  0.6)   6.6(3959.:  6.5)  47.5(512.0)
235442           242361     41.3(100.0:   0.0)   4.6(   8.2:  0.6)   6.6(3958.:  6.5)  47.5(512.0)
236396           241821     41.4(100.0:   0.0)   8.8( 19.6:  0.3)   2.2(664.0: 67.4)  47.6(1456.)
```

Priority components

- **Credential priority** = credweight * (userweight * job.user.priority)
  = 100 * (10 * 100) = 100000

  It is a constant for all users.
- **Fairshare priority** = fsweight * min (fscap,(fsuserweight*DeltaUserFSUsage))
  = 100 * (10 * DeltaUserFSUsage)

  If you have not submitted jobs in the past 7 days, DeltaUserFSUsage = 20000
- **Service priority** = serviceweight * (queuetimeweight * QUEUETIME + xfactorweight * XFACTOR)
  = 2 * (2 * QUEUETIME + 20 * XFACTOR),

  where XFACTOR = 1 + QUEUETIME / WALLTIMELIMIT.
- **Resource priority** = resweight * min (rescap, (procweight * TotalProcessorsRequested)
  = 30 * min (3840, (10 * TotalProcessorsRequested)

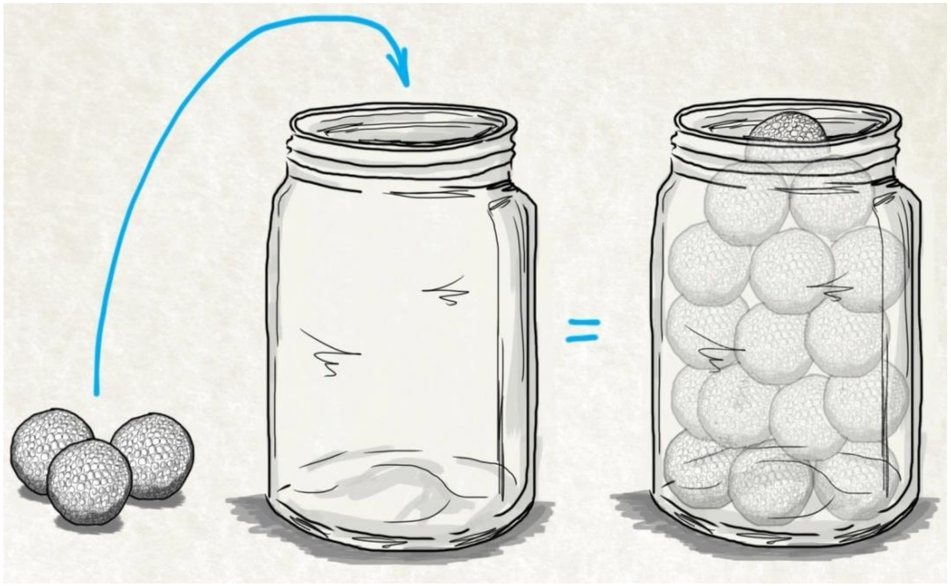
- **See http://www.hpc.lsu.edu/docs/pbs.php , click "Job priority".**

How to get higher priority?

- **Do not submit too many jobs within one week.**
- **Submit your job early to accumulate the queue time.**
- **More on resource priority:**
  - Request more compute nodes.
  - Request a smaller walltime limit.
  - see next few slides...

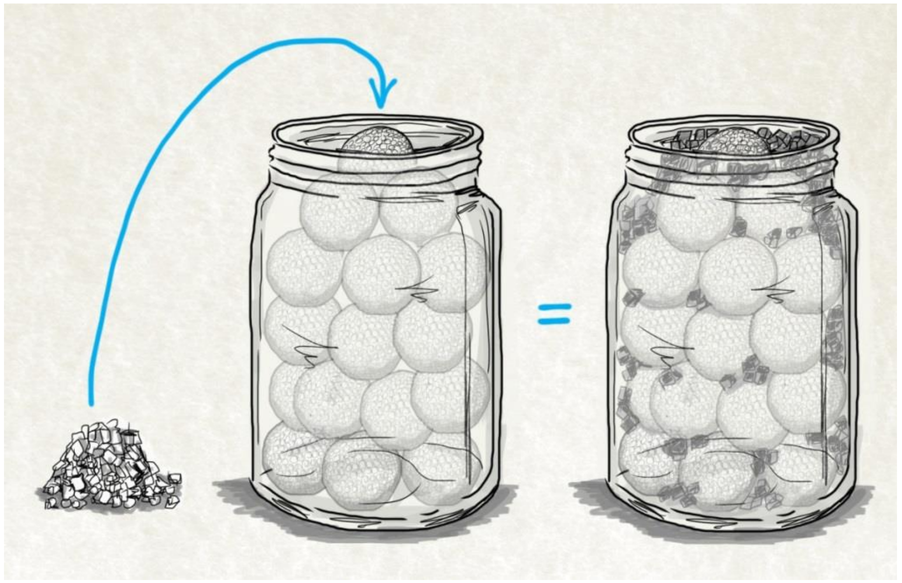
How to maximize the usage of a cluster?

- Fill in high-priority (large) jobs
- Backfill low-priority (small) jobs



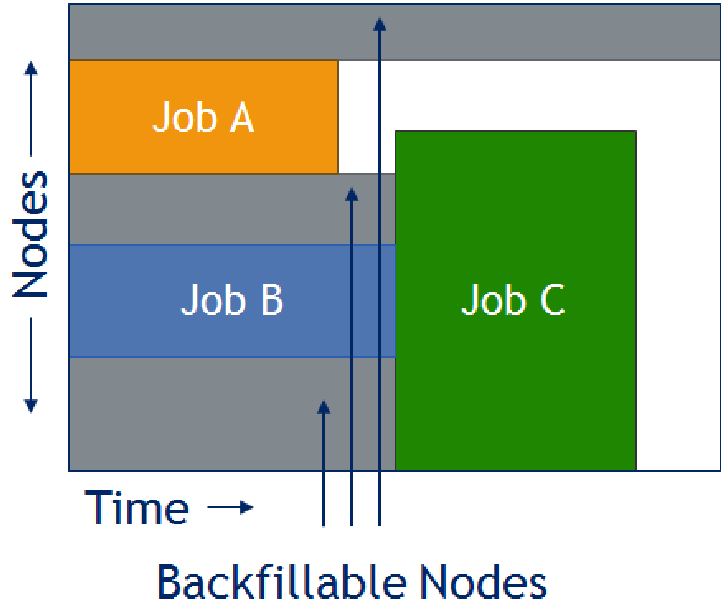
1

2

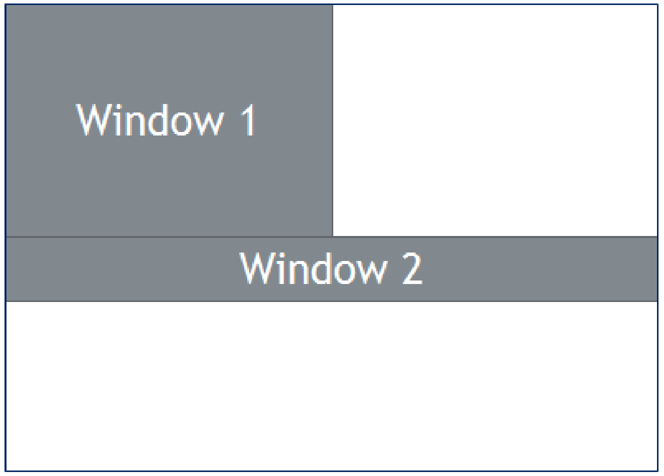


An Overview of Backfilling (1)

- **Backfill is a scheduling optimization that allows a scheduler to make better use of available resources by running jobs out of order.**
- **Enabling backfill allows the scheduler to start other, lower-priority jobs so long as they do not delay the highest priority job.**



- **If the FIRSTFIT algorithm is applied, the following steps are taken:**
  - The list of feasible backfill jobs is filtered, selecting only those that will actually fit in the current backfill window.
  - The first job is started.
  - While backfill jobs and idle resources remain, repeat step 1.



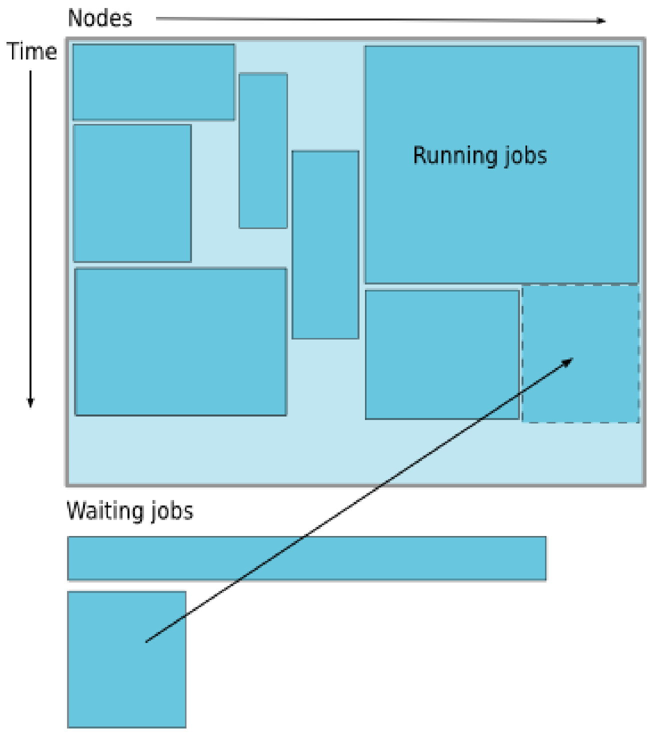
An Overview of Backfilling (2)

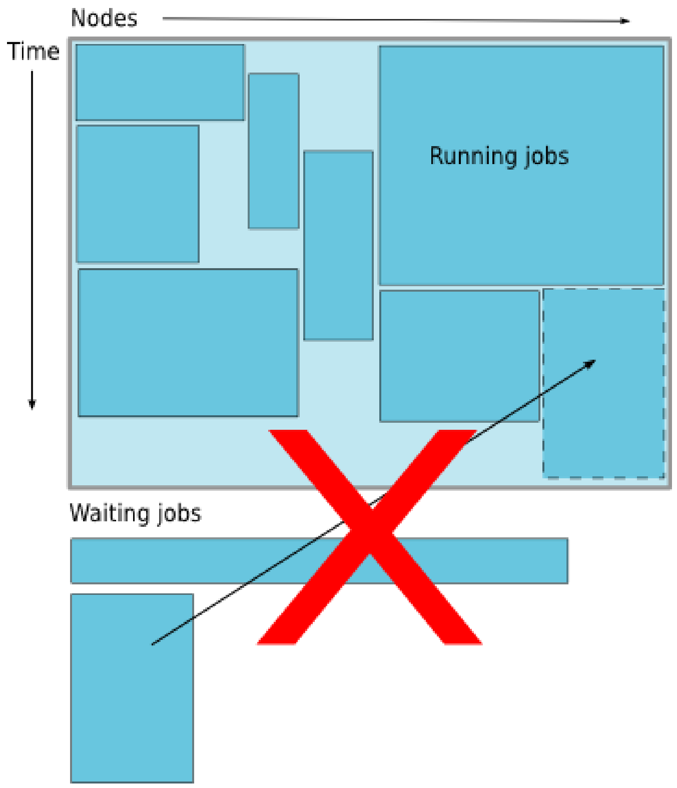
- **Although by default the start time of the highest priority job is protected by a reservation, there is nothing to prevent the third priority job from starting early and possibly delaying the start of the second priority job.**
- **Command to show current backfill windows:**
  - `showbf`
    - Shows what resources are available for immediate use.
    - This command can be used by any user to find out how many processors are available for immediate use on the system. It is anticipated that users will use this information to submit jobs that meet these criteria and thus obtain quick job turnaround times.
  - Example:

```
[fchen14@eric2 ~]$ showbf -c workq
Partition      Tasks  Nodes      Duration   StartOffset       StartDate
---------      -----  -----  ------------  ------------  --------------
ALL               40      5      18:50:35      00:00:00  11:16:49_09/04
ALL                8      1      INFINITY      00:00:00  11:16:49_09/04
```

How Much Time Should I Ask for?

- **It should be**
  - Long enough for your job to complete
  - As short as possible to increase the chance of backfilling





Frequently Asked Questions

- **I submitted job A before job B. Why job B started earlier than job A?**
- **There are free nodes available, why my job is still waiting and not running?**
- **Why my job is not get accelerated when running on cluster?**
  - Is your job utilizing the parallel resource on the cluster?
  - Does you job have lots of I/O tasks?
  - See next section...

HPC User Environment 2

Compile and Analyze Codes on Cluster

Compilers

- **Serial compilers**

Language	Linux cluster		
	Intel	PGI	GNU
Fortran	ifort	pgf77, pgf90	gfortran
C	icc	pgcc	gcc
C++	icpc	pgCC	g++

- **Parallel compilers**

Language	Linux clusters
Fortran	mpif77, mpif90
C	mpicc
C++	mpiCC

Example compiling serial code

- **icc hello_cpu_elapsed.c**
- **gfortran test_hello2.f90**

- **List symbols for executables:**

```
nm - list symbols from object files
```

- **Example:**

```
[fchen14@mike2 hello]$ nm ./a.out | grep intel
000000000060eb60 B __intel_cpu_indicator

[fchen14@mike2 hello]$ nm ./a.out | grep gfortran
                 U _gfortran_set_args@@GFORTRAN_1.0
```

CPU time vs Elapsed time

- **CPU time (or process time):**
  - The amount of time for which a central processing unit (CPU) was used for processing instructions of a computer program or operating system, as opposed to, for example, waiting for input/output (I/O) operations or entering low-power (idle) mode.
- **Elapsed real time (or simply real time, or wall clock time)**
  - The time taken from the start of a computer program until the end as measured by an ordinary clock. Elapsed real time includes I/O time and all other types of waits incurred by the program.
- **If a program uses parallel processing, total CPU time for that program would be more than its elapsed real time.**
  - (Total CPU time)/(Number of CPUs) would be same as elapsed real time if work load is evenly distributed on each CPU and no wait is involved for I/O or other resources.

Compiling and Analyzing C serial program

```c
#include <stdio.h>
#include <time.h>
int main(char *argc, char **argv) {
    double s=0.0;
    // fundamental arithmetic type representing clock tick counts.
    clock_t start, end;
    int i;
    start = clock();
    for (i=0;i<1000000000;i++)
        s+=i*2.0; // doing some floating point operations
    end = clock();
    double time_elapsed_in_seconds = (end - start)/(double)CLOCKS_PER_SEC;
    printf("cputime_in_sec: %e\n", time_elapsed_in_seconds);
    start = clock();
    system ("sleep 5"); // just sleep, does this accumulate CPU time?
    end = clock();
    time_elapsed_in_seconds = (end - start)/(double)CLOCKS_PER_SEC;
    printf(“cputime_in_sec: %e\n", time_elapsed_in_seconds);
    return 0;
}
```

Watch the actual cpu time using “time”

```
[fchen14@mike429 serial]$ gcc hello_cpu_elapsed.c
[fchen14@mike429 serial]$ time ./a.out
cputime_in_sec: 2.740000e+00
cputime_in_sec: 0.000000e+00

real    0m7.782s
user    0m2.750s
sys     0m0.005s
```

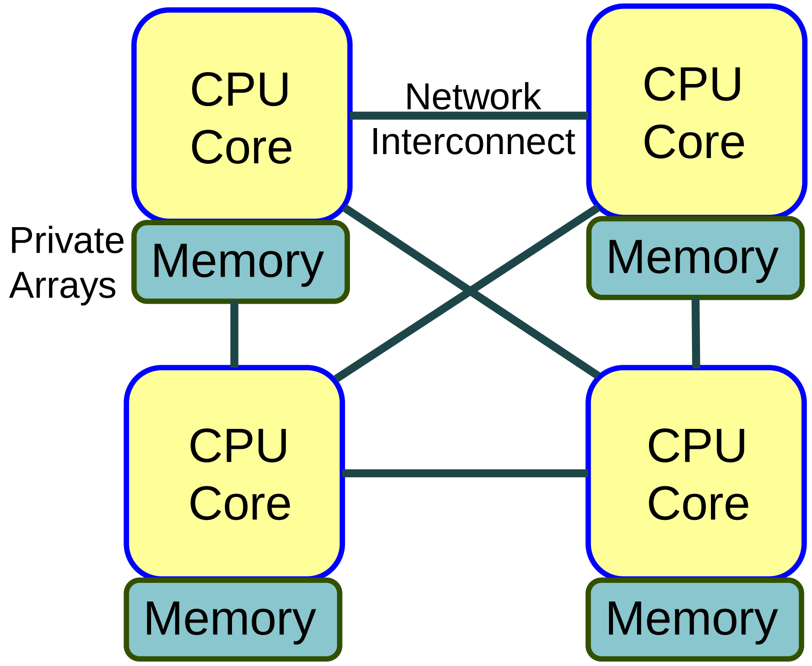
Some additional info about "time"

- **Use the Linux command `time` to evaluate the actual time usage**
  - time a simple command or give resource usage
- **Real refers to actual elapsed time (wall clock time)**
  - Time from start to finish of the call. This is all elapsed time including time used by other processes and time the process spends blocked (for example if it is waiting for I/O to complete).
- **User and Sys refer to CPU time used only by the process.**
  - User is the amount of CPU time spent in user-mode code (***outside the kernel***) within the process.
  - Sys is the amount of CPU time spent ***in the kernel*** within the process.
- **Purpose of this example:**
  - real < user: The process is CPU bound and takes advantage of parallel execution on multiple cores/CPUs.
  - real ≈ user: The process is CPU bound and takes no advantage of parallel execution.
  - real > user: The process is I/O bound. Execution on multiple cores would be of little to no advantage.

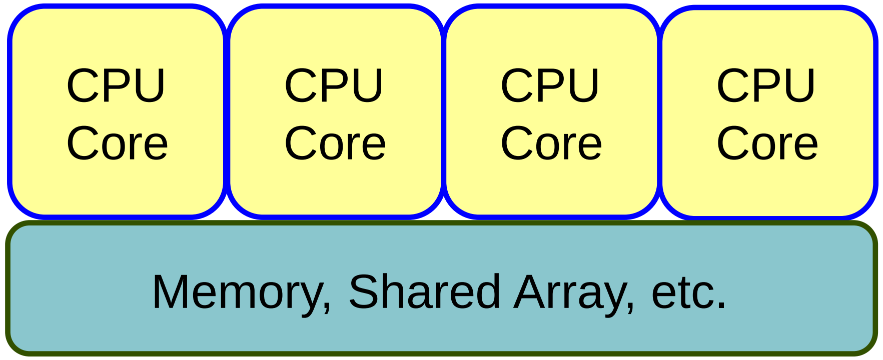
Two parallel schemes

- ➢ **Shared Memory system**
  - – A single multicore compute node
  - – Open Multi-processing (OpenMP)
- ➢ **Distributed Memory system**
  - – Mutliple compute nodes
  - – Message Passing Interface (MPI)

MPI: Distributed Memory System



OpenMP: Shared Memory System



Typically less memory overhead/duplication. Communication often implicit, through cache coherency and runtime.

Example compiling threaded OpenMP code

- **Compiling OpenMP code often requires the** `openmp` **compiler flags, it varies with different compiler**
- **Environment Variable** `OMP_NUM_THREADS` **sets the number of threads**
- **Examples:**

```
[fchen14@mike2 src]$ gcc -fopenmp hello_openmp.c
[fchen14@mike2 src]$ ifort -openmp hello_openmp.f90
```

Compiler	Compiler Options	Default behavior for # of threads (OMP_NUM_THREADS not set)
GNU (gcc, g++, gfortran)	-fopenmp	as many threads as available cores
Intel (icc ifort)	-openmp	as many threads as available cores
Portland Group (pgcc,pgCC,pgf77,pgf90)	-mp	one thread

Sample OpenMP C code

```c
#include <omp.h>
#include <stdio.h>
#include <stdlib.h>
int main (int argc, char *argv[]) {
    int nthreads, tid;
    /* Fork a team of threads with their own copies of variables */
#pragma omp parallel private(nthreads, tid)
    {
        /* Obtain thread number */
        tid = omp_get_thread_num();
        printf("Hello World from thread = %d\n", tid);
        /* Only master thread does this */
        if (tid == 0) {
            nthreads = omp_get_num_threads();
            printf("Number of threads = %d\n", nthreads);
        }
    } /* All threads join master thread and disband */
}
```

Sample OpenMP Fortran code

```
program hello

integer nthreads,tid,omp_get_num_threads,omp_get_thread_num
! fork a team of threads giving them their own copies of variables
!$omp parallel private(nthreads, tid)
! obtain thread number
tid = omp_get_thread_num()
print *, 'hello world from thread = ', tid
! only master thread does this
if (tid .eq. 0) then
    nthreads = omp_get_num_threads()
    print *, 'number of threads = ', nthreads
end if
! all threads join master thread and disband
!$omp end parallel
end
```

Analyzing a parallel (OpenMP) program

- **What will be the CPU time and elapsed time for the following code segment:**

  See (on SuperMike II):
  `/home/fchen14/userenv/src/openmp/hello_openmp_cpu_elapse.c`

```
// fundamental arithmetic type representing clock tick counts.
clock_t start, end;
struct timeval r_start, r_end;
int i;
gettimeofday(&r_start, NULL);
start = clock();
#pragma omp parallel for // spawn the openmp threads
for (i=0;i<N;i++) a = i*2.0; // doing some floating point operations
end = clock();
gettimeofday(&r_end, NULL);
double cputime_elapsed_in_seconds = (end -
start)/(double)CLOCKS_PER_SEC;
double realtime_elapsed_in_seconds = ((r_end.tv_sec * 1000000 +
r_end.tv_usec) - (r_start.tv_sec * 1000000 +
r_start.tv_usec))/1000000.0;
```

Available MPI libraries on LONI & HPC

	Name	**MPI Library**				**Default serial compiler**
Cluster Resource		Mvapich	Mvapich2	OpenMPI	MPICH	
LONI	Eric	0.98, 1.1	1.4, 1.6, 1.8.1	1.3.4	X	Intel 11.1
	QB2	X	2.0	1.8.1	3.0.3	Intel 14.0.2
LSU	SuperMikeII	X	1.9, 2.0.1	1.6.2 1.6.3 1.6.5	3.0.2	Intel 13.0.0
	Philip	X	X	1.4.3, 1.6.1	1.2.7, 1.3.2, 1.4.1	Intel 11.1
	SuperMIC	X	2.0	1.8.1	3.0.3 3.1.1	Intel 14.0.2

MPI Compilers (1)

Language	Linux clusters	AIX clusters
Fortran	mpif77, mpif90	mpxlf, mpxlf90
C	mpicc	mpcc
C++	mpiCC	mpCC

```
mpif90 hello.f90

mpicc hello.c

mpicxx hello.cpp
```

MPI Compilers (2)

- **These MPI compilers are actually wrappers**
  - They still use the compilers we've seen on the previous slide
    - Intel, PGI or GNU
  - They take care of everything we need to build MPI codes
    - Head files, libraries etc.
  - What they actually do can be reveal by the `-show` option
- **It's extremely important that you compile and run your code with the same version of MPI!**
  - Use the default version if possible

Compiling a MPI C program

- **Compiling Hello world in C version:**
  - mpicc hello_mpi.c

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char** argv) {
    int name_len, world_size, world_rank;
    char processor_name[MPI_MAX_PROCESSOR_NAME];
    //Initialize the MPI environment
    MPI_Init(NULL, NULL);
    // Get the number and rank of processes
    MPI_Comm_size(MPI_COMM_WORLD, &world_size);
    MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);
    // Get the name of the processor
    MPI_Get_processor_name(processor_name, &name_len);
    // Print off a hello world message
    printf("Iam from processor %s, rank %d out of %d processors\n",
            processor_name, world_rank, world_size);
    // Finalize the MPI environment.
    MPI_Finalize();
}
```

Compiling a MPI Fortran program

- **Compiling Hello world in Fortran:**
  - mpif90 hellp_mpi.f90

```
program hello_mpi
    include 'mpif.h'
    !use mpi
    character 10 name
    ! Initialize the MPI library:
    call MPI_Init(ierr)
    ! Get size and rank
    call MPI_Comm_Size(MPI_COMM_WORLD, numtasks, ierr)
    call MPI_Comm_Rank(MPI_COMM_WORLD, rank, ierr)
    ! print date
    if (nrank == 0) then
        write( , )'System date'
        call system('date')
    endif
    call MPI_Barrier(MPI_COMM_WORLD, ierr)
    ! print rank
    call MPI_Get_Processor_Name(name, len, ierr)
    write( , )"I am ", nrank, "of", numtasks, "on ", name
    ! Tell the MPI library to release all resources it is using:
    call MPI_Finalize(ierr)
end program hello_mpi
```

Notes for compiling a MPI program (1)

➢ **Always verify what compiler/library is being used:**

```
$ mpicc -show
icc -I/usr/local/packages/openmpi/1.6.2/Intel-13.0.0/include -
L/usr/local/packages/openmpi/1.6.2/Intel-13.0.0/lib -lmpi -ldl -lm -
Wl,--export-dynamic -lrt -lnsl -libverbs -libumad -lpthread -lutil

$ mpif90 -show
ifort -I/usr/local/packages/openmpi/1.6.2/Intel-13.0.0/include -
I/usr/local/packages/openmpi/1.6.2/Intel-13.0.0/lib -
L/usr/local/packages/openmpi/1.6.2/Intel-13.0.0/lib -lmpi_f90 -
lmpi_f77 -lmpi -ldl -lm -Wl,--export-dynamic -lrt -lnsl -libverbs -
libumad -lpthread -lutil
```

Notes for compiling a MPI program (2)

- **Always verify what library is being used: Before and after:**

```
$ ldd a.out #ldd - print shared library dependencies
        linux-vdso.so.1 =>  (0x00007fff907ff000)
        libmpi_f90.so.1 => /usr/local/packages/openmpi/1.6.2/Intel-
13.0.0/lib/libmpi_f90.so.1 (0x00002b9ae577e000)
        libmpi_f77.so.1 => /usr/local/packages/openmpi/1.6.2/Intel-
13.0.0/lib/libmpi_f77.so.1 (0x00002b9ae5982000)
        libmpi.so.1 => /usr/local/packages/openmpi/1.6.2/Intel-
13.0.0/lib/libmpi.so.1 (0x00002b9ae5bb9000)
...
        libpthread.so.0 => /lib64/libpthread.so.0 (0x0000003b21800000)
...
        libifport.so.5 =>
/usr/local/compilers/Intel/composer_xe_2013.0.079/compiler/lib/intel64/l
ibifport.so.5 (0x00002b9ae61ee000)
        libifcore.so.5 =>
/usr/local/compilers/Intel/composer_xe_2013.0.079/compiler/lib/intel64/l
ibifcore.so.5 (0x00002b9ae641d000)
```

Running and Analyzing MPI program

- **Make sure you are running your jobs on the correct nodes**
- **Important if you want to run less processes than ppn**
- **Understand the usage of $PBS_NODEFILE**

```
[fchen14@mike2 ~]$ qsub -I -X -l nodes=2:ppn=16 -l walltime=01:00:00 -q gpu
...
[fchen14@mike429 ~]$ echo $PBS_NODEFILE
/var/spool/torque/aux//236660.mike3
[fchen14@mike429 ~]$ cat $PBS_NODEFILE
mike429
...                # 16 repeats of mike429
mike429
mike430
...                # 16 repeats of mike430
mike430
[fchen14@mike429 hybrid]$ cat $PBS_NODEFILE| uniq > hosts
[fchen14@mike429 hybrid]$ cat hosts
mike429
mike430
```

Running and Analyzing MPI program

```
[fchen14@mike315 mpi]$ mpicc hello_mpi.c
[fchen14@mike315 mpi]$ mpirun -np 32 -hostfile $PBSNODEFILE ./a.out
Iam from processor mike315, rank 1 out of 32 processors
Iam from processor mike315, rank 6 out of 32 processors
Iam from processor mike315, rank 9 out of 32 processors
Iam from processor mike315, rank 12 out of 32 processors
Iam from processor mike315, rank 0 out of 32 processors
Iam from processor mike315, rank 2 out of 32 processors
Iam from processor mike315, rank 3 out of 32 processors
Iam from processor mike315, rank 7 out of 32 processors
Iam from processor mike315, rank 10 out of 32 processors
Iam from processor mike315, rank 5 out of 32 processors
Iam from processor mike315, rank 13 out of 32 processors
Iam from processor mike315, rank 4 out of 32 processors
Iam from processor mike315, rank 8 out of 32 processors
Iam from processor mike334, rank 17 out of 32 processors
Iam from processor mike315, rank 11 out of 32 processors
Iam from processor mike315, rank 14 out of 32 processors
Iam from processor mike315, rank 15 out of 32 processors
Iam from processor mike334, rank 18 out of 32 processors
```

Compiling hybrid (MPI+OpenMP) program

- **See** `/home/fchen14/userenv/src/hybrid/hello_hybrid.c` **for complete source**
- **Use command:**
  - `$ mpicc -openmp hello_hybrid.c`

```
#pragma omp parallel default(shared) private(itd, np)
    {
        gtd = omp_get_num_threads(); //get total num of threads in a process
        itd = omp_get_thread_num();  // get thread id
        gid = nrank*gtd + itd;       // global id
        printf("Gid %d from thd %d out of %d from process %d out of %d on %s\n",
                gid, itd, gtd, nrank, numprocs, processor_name);
        if (nrank==0 && itd==0)
        {
            // system("pstree -ap -u $USER");
            system("for f in `cat $PBS_NODEFILE|uniq`; do ssh $f pstree -ap -u
$USER; done;");
            system("sleep 10");
        }
    }
```

Analyzing a hybrid program

```
[fchen14@mike315 hybrid]$ export OMP_NUM_THREADS=4
[fchen14@mike315 hybrid]$ mpirun -np 2 -x OMP_NUM_THREADS ./a.out
Gid 0 from thread 0 out of 4 from process 0 out of 2 on mike315
Gid 2 from thread 2 out of 4 from process 0 out of 2 on mike315
Gid 1 from thread 1 out of 4 from process 0 out of 2 on mike315
Gid 3 from thread 3 out of 4 from process 0 out of 2 on mike315
Gid 4 from thread 0 out of 4 from process 1 out of 2 on mike315
Gid 6 from thread 2 out of 4 from process 1 out of 2 on mike315
Gid 7 from thread 3 out of 4 from process 1 out of 2 on mike315
Gid 5 from thread 1 out of 4 from process 1 out of 2 on mike315
bash,108067
  |-mpirun,110651 -np 2 -x OMP_NUM_THREADS ./a.out
  |   |-a.out,110652
  |   |   |-sh,110666 -c ...
  |   |   |   `-ssh,110670 mike315 pstree -ap -u fchen14
  |   |   |-{a.out},110654
  |   |   |-{a.out},110656
  |   |   |-{a.out},110662
  |   |   |-{a.out},110663
  |   |   |-{a.out},110664
  |   |   `-{a.out},110665
  |
```

Exercise

- **Submit a small job to run “sleep 180”and “print PBS variables”**
  - Create a script to submit a 5 min job and print from within the job script PBS variables $PBS_NODEFILE, $PBS_WORKDIR. Also run “sleep 180” to give you a few minutes to verify status.
  - Once the job is running, find out the Mother Superior node and other slave nodes assigned to your job using qstat.
  - Log into MS node and verify that your job is running and find your temporary output file
  - Modify your script to print hello from each of your assigned nodes
- **Run a shell script using mpirun to print process id of shell**

Future Trainings

- **Next week training: Basic Shell Scripting**
  - Wednesdays 9:00am, September 21, Frey Computing Service Center 307
- **Programming/Parallel Programming workshops**
  - Usually in summer
- **Keep an eye on our webpage: www.hpc.lsu.edu**