HPC User Environment 2

Brought to you by

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Outline

- Recap of User Environment 1 training
- Topics to be covered today
  - Job management on clusters
    - Job priority
    - Backfill
  - Compiling and Analyzing programs
    - Serial program
    - Parallel program
    - Programs using accelerators

Available Computing Resources

- University:HPC@LSU
- State:LONI
- Nation:XSEDE

LSU HPC HIGH PERFORMANCE COMPUTING

Available Clusters

- University:HPC@LSU

  superMike-2, superMIC, philip,

  shelob & pandora

- State:LONI

  QB-2 & Eric

- Nation:XSEDE

  superMIC

HPC Cluster Architectures

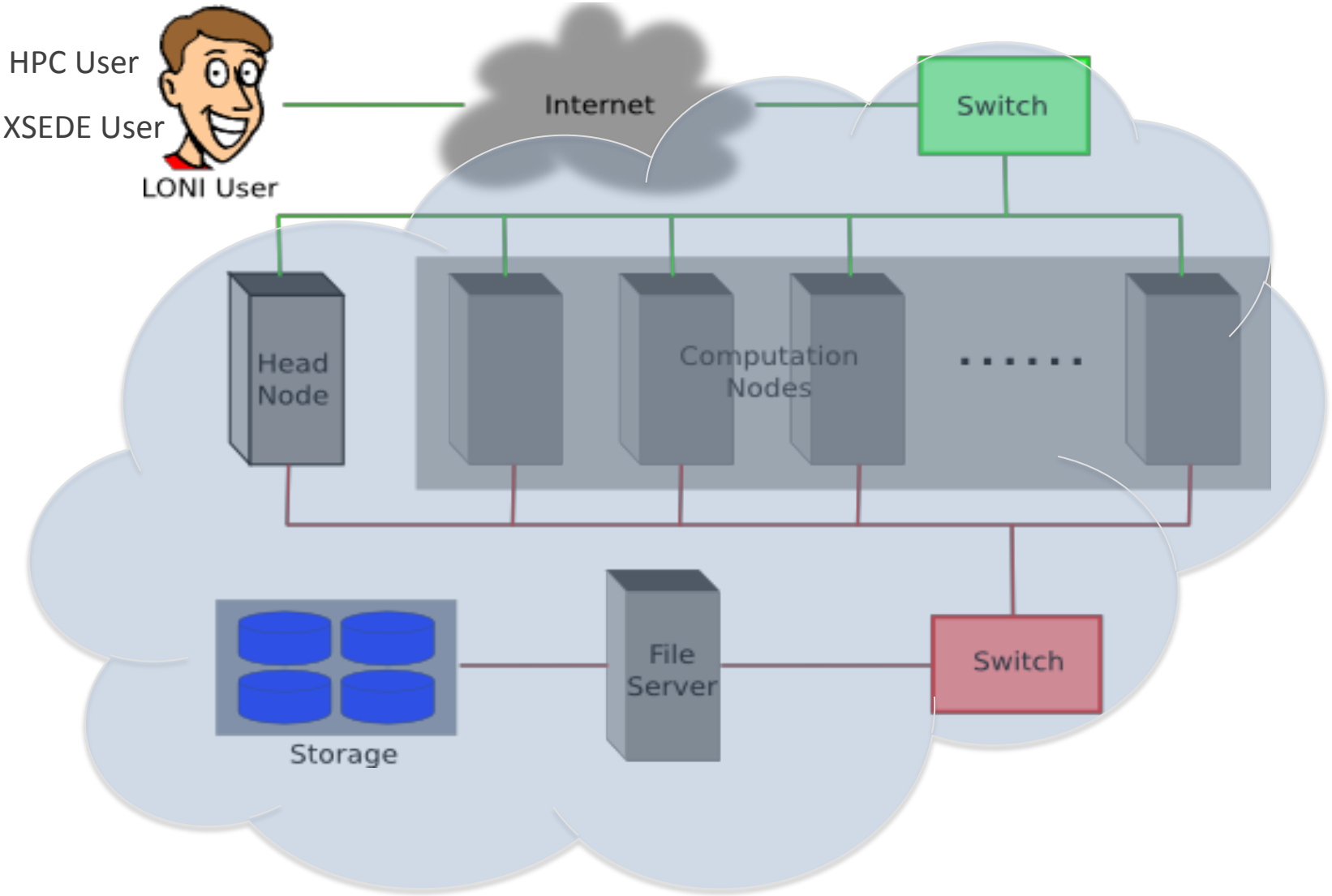
Two major HPC architectures

- Intel x86_64 clusters: SuperMike, SuperMIC, QB-2, Eric, Philip
  - Vendor: Dell
  - Operating System: Linux (RHEL 4/5/6)
  - Processor: Intel
- IBM PowerPC clusters: pandora
  - Vendor: IBM
  - Operating System: AIX
  - Processor: IBM power7

You have learned how to …

- Apply HPC/LONI accounts and allocations
  http://www.hpc.lsu.edu/users/accounts.php
- Reset passwd
  http://www.hpc.lsu.edu/users/password.php
- Login clusters from Linux/Mac/Window machines
  Window: Putty/MobaXterm
- File transfer
- Software management on clusters
  - Module: SuperMIC, QB-2
  - Softenv: SuperMike2, Eric, Philip, Shelob

What is a HPC cluster?



Basic HPC cluster resource terms

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 in the cluster.
Core	An individual CPU on a node. 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 the work.

Cluster Environment

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

Software for managing and scheduling jobs is required.

Resource Manager/ Job Scheduler

- Software to manage resources (CPU time, memory etc.) and management workload
  - Linux clusters: Portable Batch System (PBS)
  - AIX clusters: Loadleveler
- HPC/LONI:
  - Torque: resource manager (open-source version of PBS)
  - Moab: job scheduler
  - Gold: allocation manager
- A batch queuing system determines
  - order of queuing jobs to be executed
  - which node(s) to be assigned for jobs

Job management basics

- Find appropriate queue: **qstat –q**
- Submit jobs
- Monitor jobs
- Understand the queuing system and requirements

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 < =8
QB2	workq	3 days	20	44	128	Unpreemptable
	checkpt		20		256	Preemptable
	single	7 days	<=20		1	Single-node jobs
	bigmem	3 days	12,24,36,48	4	1	Big-memory jobs

Typically, workq and checkpt queues are for parallel jobs, while single queue is for serial jobs. The ppn of workq and checkpt has to be equal to the number of cores per node. Single queue can be also used for parallel jobs with the number of threads that is less than the number of cores per node.

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	<=4		1	Single node jobs
Philip	workq	3 days	8	5	4	Unpreemptable
	checkpt		8		4	Preemptable
	bigmem		8		2	Big memory jobs
	single	14 days	4	50	1	Single processor
SuperMIC	workq	3 days	20	34	128	Unpreemptable
	checkpt		20		360	Preemptable

Job management basics

- Find appropriate queue: **qstat –q**
- Submit jobs
- Monitor jobs
- Understand the queuing system and requirements

Two Job Types

- Interactive job
  - Purpose: testing, debugging, compiling
  - Set up an interactive environment on compute nodes for users
    - Advantage: can run programs interactively
    - Disadvantage: must be present when the job starts
    - Try not to run interactive jobs with large core count
- Batch job
  - Purpose: production run
  - Executed without user intervention using a job script
    - Advantage: the system takes care of everything
    - Disadvantage: user control is surrendered

Do not run jobs on the head node!!!

Submitting Jobs (interactive job)

```
qsub -I -V \
    -l walltime=<hh:mm:ss> \
    -l nodes=<num_nodes>:ppn=<num_cores> \
    -A <Allocation> \
    -q <queue name>
    -X <enable X11 forwarding>
```

DO NOT directly ssh to compute nodes,

unless the nodes assigned to you by the job scheduler.

Submitting Jobs (Batch)

```
#!/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 only queue accepts serial jobs
#PBS -A <loni_allocation>      # Allocation name
#PBS -m bea                    # Send mail when job begin/end/abort
#PBS -M <email address>        # Send mail to this address
<shell commands>
/path/to/executable <options>
<shell commands>
```

Batch Job submission: `qsub job_script`

Job management basics

- Find appropriate queue: **qstat –q**
- Submit jobs
- Monitor jobs
- Understand the queuing system and requirements

Queue Querying – Linux Clusters

"**showq**": information about active, eligible, blocked, recently completed jobs

```
$ 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
...
```

Job Monitoring - Linux Clusters

- Check details on a job

```
qstat -n -u $USER    : detials of node assignment
qstat -f jobid       : details on your job
```

- Delete a job

```
qdel jobid           : delete job
```

- Check approximate start time

```
showstart jobid
```

- Check details of a job

```
checkjob jobid
```

- Check health of a job

```
qshow -j jobid
```

PBS Environmental Variables

```
$ echo $PBS_XXX
```

$PBS_ENVIRONMENT	$PBS_MOMPORT	$PBS_NUM_PPN	$PBS_O_MAIL
$PBS_QUEUE	$PBS_WALLTIME	$PBS_GPUFILE	$PBS_TASKNUM
$PBS_SERVER	$PBS_NODEFILE	$PBS_O_HOME	$PBS_O_PATH
$PBS_JOBCOOKIE	$PBS_NODENUM	$PBS_O_HOST	$PBS_O_QUEUE
$PBS_JOBID	$PBS_JOBNAME	$PBS_O_LOGNAME	$PBS_O_WORKDIR
$PBS_VERSION	$PBS_NP	$PBS_O_LANG	$PBS_O_SHELL
$PBS_VNODENUM	$PBS_NUM_NODES		

“top” command

- Pay attention to load and the memory consumption of your jobs!
- “ssh" to assigned compute nodes
- "top” to obtain a real-time view of the running jobs.

```
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
```

Pay attention to single queue usage

- Single queue – jobs only execute on a part of a single node i.e. `nodes=1:ppn=1/2/4/8`
- Memory concern --- jobs in the single queue should not use:
  - more than 2GB (= 32G / 16) memory per core on Eric, Philip, Pandora and SuperMike II
  - more than 3.2GB (= 64G / 20) memory per core on QB2 and Super MIC
  - Scale up # cores (ppn) if more memory is required
- Typical warnings:
  - 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 points…

- Service unit (SU) = (# cores) * (actual wall-time)
  - also apply to clusters with accelerators (GPU/Phi)
- Eric will be retired in the near future, migrating codes to QB-2 should be taken into consiseration for LONI users
- Bigmem queue on QB-2 is for jobs need > 64 GB memory, not for jobs using more number of cores
- Accelerator usage is highly encouraged.
  Applications requesting such allocations get approved first

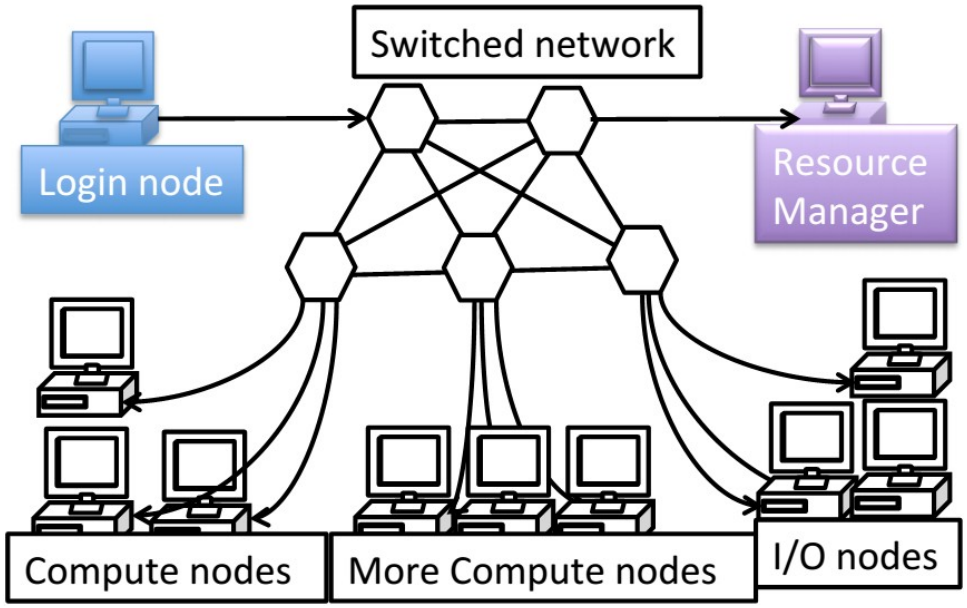
Outline

- Recap of User Environment 1

- Topics to be covered today
  - Job management on clusters
    - Job priority
    - Backfill
  - Compiling and Analyzing programs
    - Serial programs
    - Parallel programs
    - Programs using accelerators

Back to Cluster Architecture

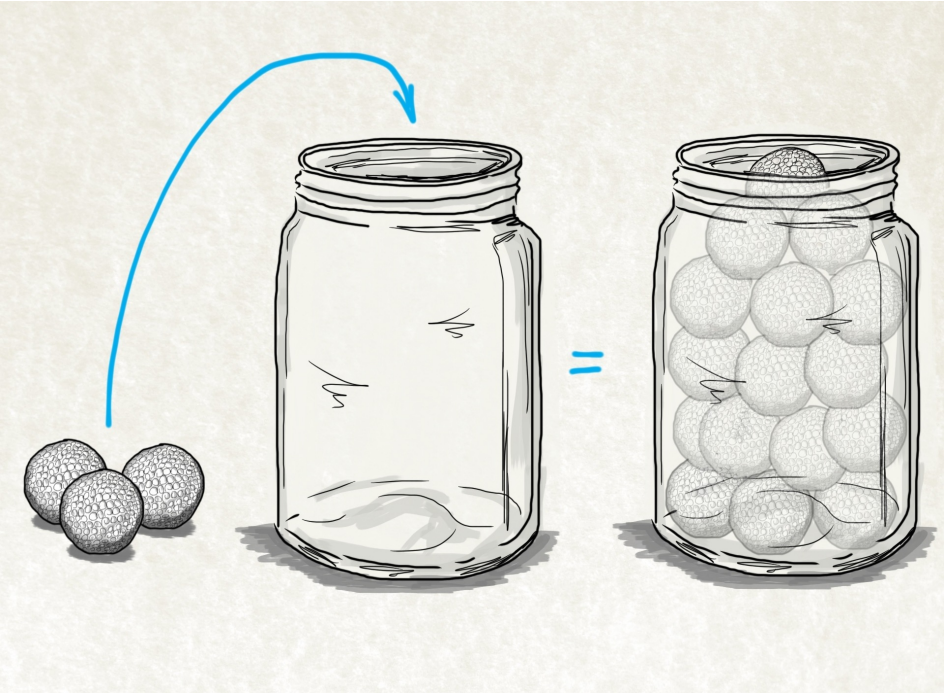
- Resource/scheduling managers
  - Take resource request (job) from the login node
  - Check available resources and assign a priority number to the job
  - Queue the job
  - Start the job if available resources match the request



Resource manager philosophy

Maximize the usage of a cluster

- Prioritize workload (jobs) into a queue
- *Backfill* idle nodes to maximize utilization



Job Priority

- Not “First Come First Served”
- Jobs with higher priorities scheduled first
- Factors determine job priority:
  - credential priority
  - fairshare priority
  - resource priority
  - service priority
- Priority determination for queued/waiting jobs
  - `mdiag -p`

Job Priorities

```
$ 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: a constant
  credweight * (userweight * job.user.priority) =100*(10*100) = 100000

- Fairshare priority: usage in the last 7 days
  fsweight * min (fscap, (fsuserweight * DeltaUserFSUsage)) = 100 * (10 * 20),
  where max(DeltaUserFSUsage) = 20

- Service priority: queuing time / wall-time
  serviceweight * (queuetimeweight * QUEUETIME +xfactorweight * XFACTOR)
  = 2 * (2 * QUEUETIME + 20 * XFACTOR), where XFACTOR
  = 1 + QUEUETIME /WALLTIMELIMIT

- Resource priority: # processors requested
  resweight * min (rescap, (procweight * TotalProcessorsRequested)
  = 30 * min (3840, (10 * TotalProcessorsRequested))

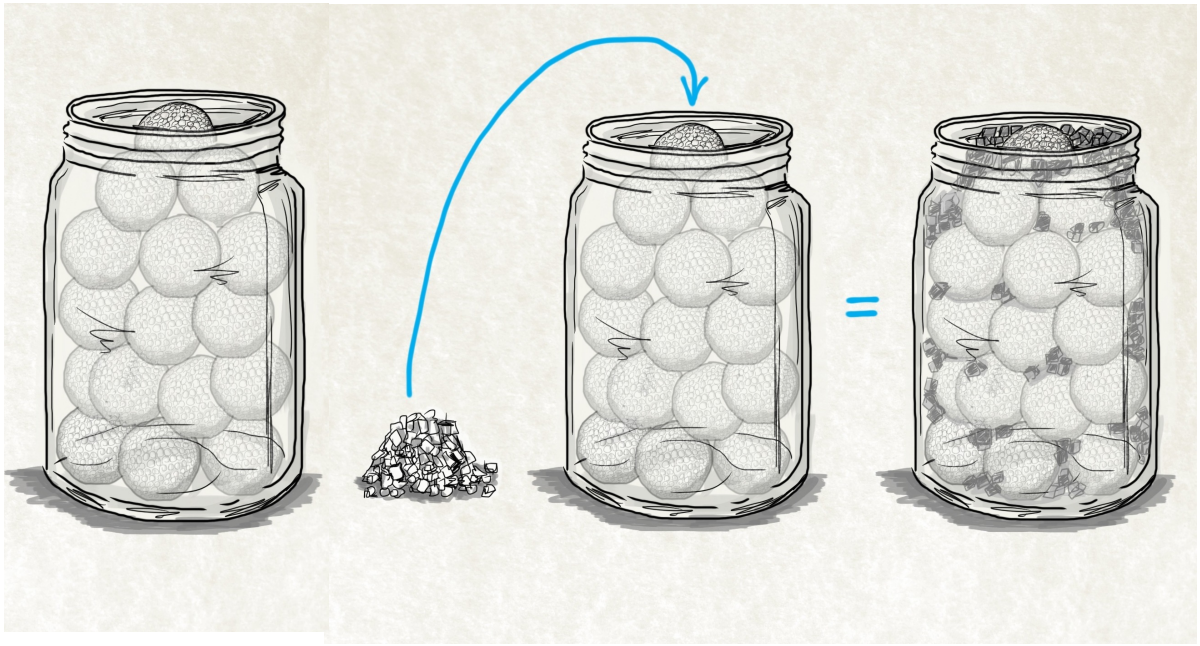
http://www.hpc.lsu.edu/docs/pbs.php

How to get higher priority?

- Request more compute nodes
- Request a smaller walltime
- Do not submit too many jobs within one week
- Submit your job early to accumulate the queue time

How to maximize the usage of a cluster?

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



Backfilling

- FIRSTFIT
  - Filter the list of feasible backfill jobs and select those fit in the current backfill window
  - Start the first fitting job

- Scheduling optimization allows a job schedule to
  - Running jobs out of order to better utilize available resources
  - So long as NOT delay the highest priority job in the queue.

Backfilling

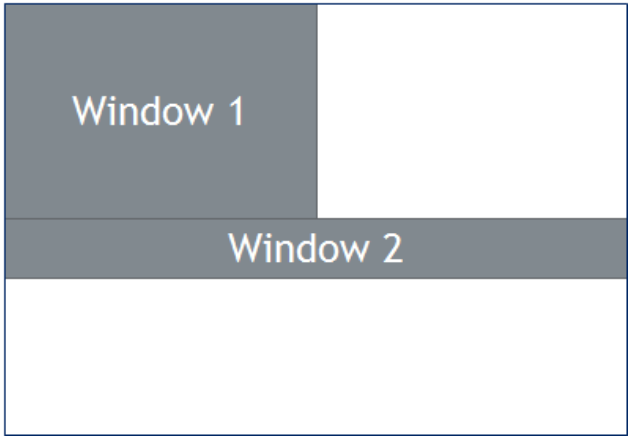
"showbf"

- Display available resources for immediate usage.
- Use this information to customize job submission script in order to obtain a quick job turnaround

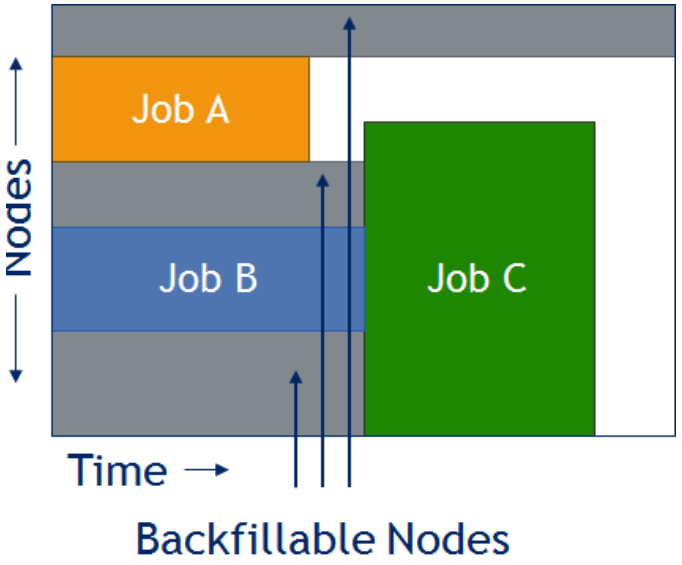
```
$showbf -c workq

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 and how many nodes?

- Long enough for your job to complete, as short as possible to increase the chance of backfilling



- Enough nodes to complete your job, as less nodes as possible



Frequently Asked Questions

1) I submitted job A before job B. Why did job B start earlier than job A?

2) There are free nodes available, why is my job still waiting?

3) Why my job does not get accelerated when using a cluster?
   1. does your job utilize the parallel resource on the cluster?
   2. does you job have lots of I/O tasks?
   3. see next section...

Outline

- Recap of User Environment 1

- Topics to be covered today
  - More on job management
    - Job priority
    - Backfill
  - Compiling and Analyzing programs
    - Serial programs
    - Parallel programs
    - Programs using accelerators

Compilers

- Serial compilers

Language	Linux cluster			AIX cluster
	Intel	PGI	GNU	XL
Fortran	ifort	pgf77, pgf90	gfortran	xlf, xlf90
C	icc	pgcc	gcc	xlc
C++	icpc	pgCC	g++	xlC

- Parallel compilers

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

Compiling and Analyzing C serial program

```
#include <stdio.h>
#include <math.h>
#include <time.h>
int main(char *argc, char **argv) {
    double s=0.0;
    clock_t start, end;
    int i;
    start = clock();
    for (i=0;i<1000000000;i++)
        s = i / 2.0 * 4.9; // do some floating point operations
    end = clock();
    double time_computing_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_sleeping_in_seconds = (end - start)/(double)CLOCKS_PER_SEC;
    printf("\ncputime_in_sec: %e\n", time_elapsed_in_seconds);
    return 0;
}
```

Watch the actual cpu time

```
$ gcc hello.c
$ time ./a.out
time_computing_in_sec: 4.540000e+00
time_sleeping_in_sec: 0.000000e+00

Real    0m9.547s
user    0m4.543s
sys     0m0.002s

$ gfortran hello.f90
```

CPU time vs Elapsed time

- CPU time (or process time):
  - CPU time for processing instructions of a computer program or operating system.
- Elapsed real time (real time /wall clock time)
  - Time taken from the start of a computer program until the end including 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.

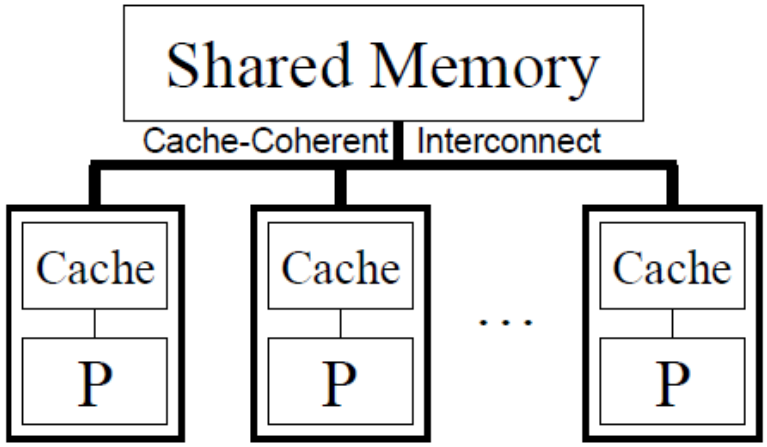
Parallel schemes

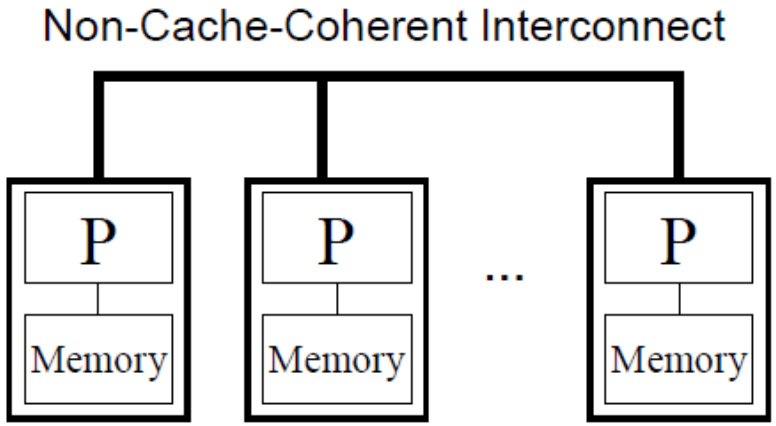
Shared memory

- Single multicore node
- Multi-threading (OpenMP)

Distributed memory

- Mutliple compute nodes
- Message Passing (MPI)





Compiling OpenMP code

- -openmp flag is required to compile OpenMP codes
- export `OMP_NUM_THREADS=` # threads
- Examples:

```
gcc -fopenmp hello_openmp.c
ifort -openmp hello_openmp.f90
```

Compiler	Compiler flag	Default thread # (OMP_NUM_THREADS)
GNU (gcc, g++, gfortran)	-fopenmp	# threads = available cores
Intel (icc, icpc, ifort)	-openmp	# threads = available cores
Portland Group (pgcc,pgCC, pgf77, pgf90)	-mp	one thread

Sample OpenMP - C code

```
#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
```

Available MPI libraries on LONI & HPC

Cluster Name		MPI Library					
		Mvapich	**Mvapich2**	**OpenMPI**	**IMPI**	**MPICH**	**MPICH2**
LONI	Eric	0.98 1.1	1.4 1.6 1.8.1	1.3.4	X	X	1.1
	QB2	X	2.0	1.8.1	4.1.3.048	3.0.3 3.1.1	X
LSU	Super-MikeII	X	1.9 2.0.1 2.1	1.6.2 1.6.3 1.6.5	4.1.3.048	3.0.2	X
	Philip	X	X	1.4.3 1.6.1	X	1.2.7	1.3.2 1.4.1
	SuperMIC	X	2.0	1.8.1	4.1.3.048	3.0.3 3.1.1	X

MPI Compilers (1)

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

- Check current MPI implementation

```
$ which mpicc
/usr/local/packages/openmpi/1.6.2/Intel-13.0.0/bin/mpicc
```

- Compile MPI programs

```
$ mpif90 hello.90
$ mpicc hello.c
```

MPI Compilers (2)

- MPI compilers are wrappers of
  - Intel/ PGI/ GNU compiler
  - Combined with header files/ libraries needed to build MPI codes
  - `mpicc/mpif90 -show` for details
- Please compile and run your code with the same version of MPI!

Compiling MPI programs

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
```

Compiling a MPI C program

```
mpicc hello_mpi.c
```

```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

```
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
```

Compiling MPI programs (2)

Check which libraries are used

```
$ 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)
```

PBS Job Script – run an MPI Job

```
#!/bin/bash

#PBS   -l  nodes=2:ppn=16
#PBS   -l  walltime=02:30:00
#PBS   -N  myjob
#PBS   -o  test.out
#PBS   -e  test.err
#PBS   -q  checkpt
#PBS   -A  hpc_train_2015

export NPROCS=`wc -l $PBS_NODEFILE |gawk '//{print $1}'`
cd $PBS_O_WORKDIR
mpirun -machinefile $PBS_NODEFILE -np $NPROCS ./hello_mpi
```

"mpirun" could be different for different MPI implementations. Use "mpirun --help" to check.

Testing a MPI program interactively

- 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

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

Running and Analyzing MPI program

```
[user@mike315 mpi]$ mpicc hello_mpi.c
[user@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

- $ 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

```
[user@mike315 hybrid]$ export OMP_NUM_THREADS=4

[user@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
```

Using Accelerators

- Nvidia GPU: thousands of cores

  Cuda, OpenACC
- Intel Xeon Phi: processor(s)+ coprocessor(s)

  Native, offload to Phi

Pandora – LSU AIX Clusters

- Four 8-core IBM Power7 3.3 GHz processors per node, 4 threads per core (128 cores)
- 8 nodes total
- Advantage: good for multithread jobs, such as applications using OpenMP
- Disadvantage: porting efforts from Linux system

Queue Characteristics – LSU AIX Clusters

"llclass" -- list of queues

Machine	Queue	Max Runtime	Max slots per job	Max nodes per job	Use
Pandora	Interactive	30 minutes	8	1	Unpreemptable
	Workq	3 days	224	7	Preemptable
	Single	3 days	64	2	Small jobs

Jobs management - AIX clusters

- Program compilation

```
xlc test.c –o test
mpcc test_mpi.c –o test_mpi
```

- Job submission

```
llsubmit jobscript : submit job llcancel
```

- Job deletion

```
jobid : delete job
```

Job Monitoring - AIX Clusters

- Command: `showllstatus.py`
  - Show job status and nodes running on
- Command: `llq <options> <job_id>`
  - All jobs are displayed if <`job_id`> is omitted
  - Display detailed information: `llq -l <job_id>`
  - Check the estimated start time: `llq -s <job_id>`
  - Show jobs from a specific user: `llq -u <username>`

```
-bash-3.2$ llq
Id                       Owner      Submitted   ST PRI Class        Running On
------------------------ ---------- ----------- -- --- ------------ -----------
pandora1.19106.0         mainak      9/1  23:41 R  50  workq        pandora008
pandora1.19108.0         ghoshbd     9/2  14:58 R  50  workq        pandora005
pandora1.19109.0         ghoshbd     9/2  15:08 R  50  workq        pandora007
pandora1.19110.0         ghoshbd     9/2  15:33 R  50  workq        pandora002
pandora1.19111.0         ghoshbd     9/2  15:44 R  50  workq        pandora004
pandora1.19112.0         ghoshbd     9/2  15:58 I  50  workq
pandora1.19113.0         ghoshbd     9/2  16:10 I  50  workq
pandora1.19114.0         mainak      9/4  08:16 I  50  workq

8 job step(s) in queue, 3 waiting, 0 pending, 5 running, 0 held, 0 preempted
```

LoadLeveler Job Script - Serial

```
#!/bin/sh
#@ job_type= serial                                    Job type
#@ output = /work/default/username/$(jobid).out Standard output
#@ error = /work/default/username/$(jobid).err  Standard error
#@ notify_user= youremail@domain                      Notification
#@ notification = error                                Notify on error
#@ class = single                                      Queue
#@ wall_clock_limit= 24:00:00                          Wall clock time
#@ requirements = (Arch == “POWER5”)                   Job requirement
#@ environment = COPY_ALL                              Environment
#@ queue

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

LoadLeveler Job Script - Parallel

```
#!/bin/sh
#@ job_type= parallel                                  Job type
#@ output = /work/default/username/$(jobid).out Standard output
#@ error = /work/default/username/$(jobid).err  Standard error
#@ notify_user= youremail@domain                       Notification
#@ notification = error                                Notify on error
#@ class = checkpt                                     Queue
#@ wall_clock_limit= 24:00:00                          Wall clock time
#@ node_usage= shared node usage
#@ node = 2                                            # of nodes
#@ total_tasks= 16                                     # of processors
#@ requirements = (Arch == “POWER7”)                   # Job requirement
#@ environment = COPY_ALL    Environment
#@ queue

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

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_O_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, Sep 23, 2015, Frey 307

- Check out other trainings at HPC webpage:
  www.hpc.lsu.edu