Using a Computing Cluster

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Buzz-Words

- Compute Cluster
- Supercomputers
- Cluster
- High Performance Computing
- High Throughput Computing
- Cyber-Infrastructure
- Advanced Computing Hardware

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Agenda

- **What is a compute cluster?**
- How do you use a compute cluster
  - Navigating, Developing and testing
  - Accessing installed software
  - Submitting jobs to Scheduler

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Example: XSEDE

- Formerly TeraGrid
- Funded by the National Science Foundation

"XSEDE is a single virtual system that scientists can use to interactively share computing resources, data and expertise. People around the world use these resources and services — things like supercomputers, collections of data and new tools — to improve our planet."

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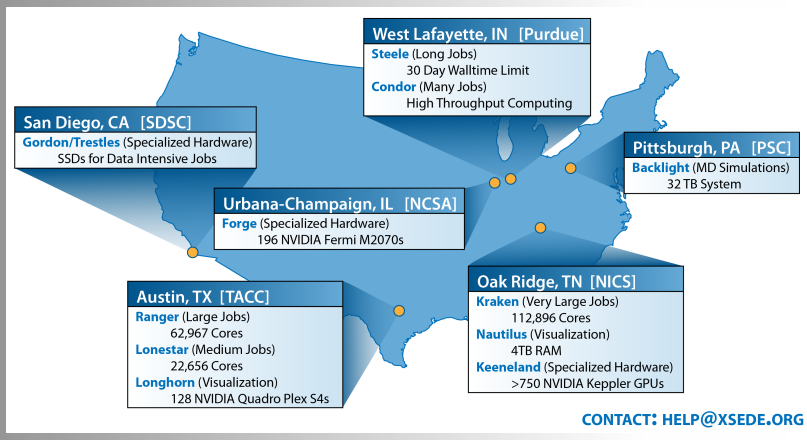
XSEDE Computing Resources



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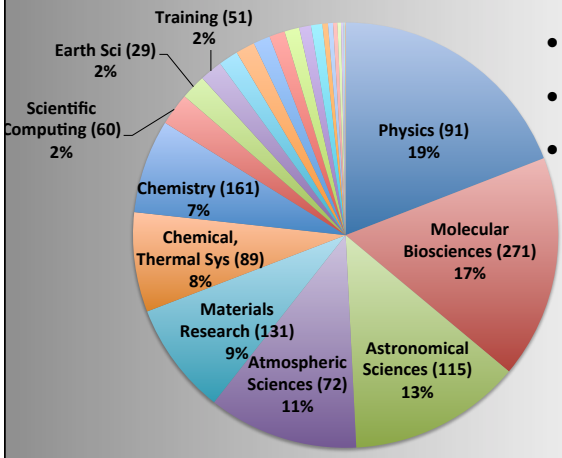
Who Uses XSEDE?

- >2 billion cpu-hours allocated
- 1400 allocations
- 350 institutions
- 32 research domains



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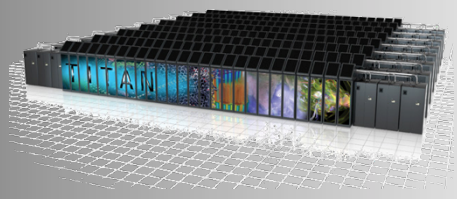
Advanced Computing Hardware

XSEDE
Extreme Science and Engineering Discovery Environment

NASA

Open Science Grid

BLUE WATERS
SUSTAINED PETASCALE COMPUTING



amazon web services™

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Local Resources

- Lab computers
- Department Resources
- College systems
- Institution systems
  - High Performance Computing Center
- Look for a system near you…

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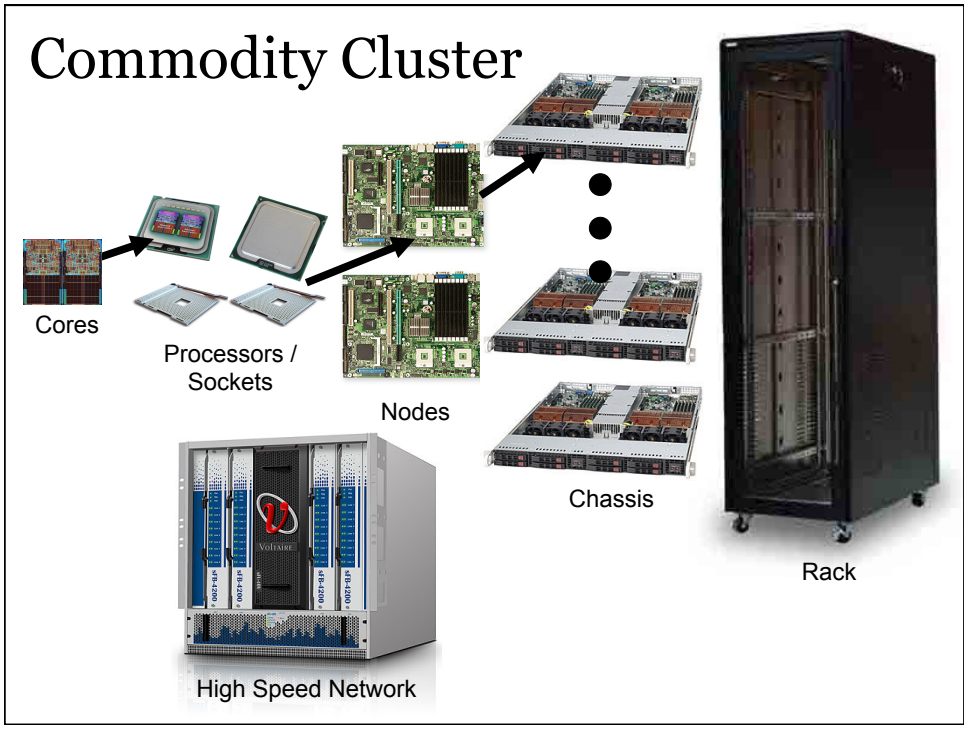
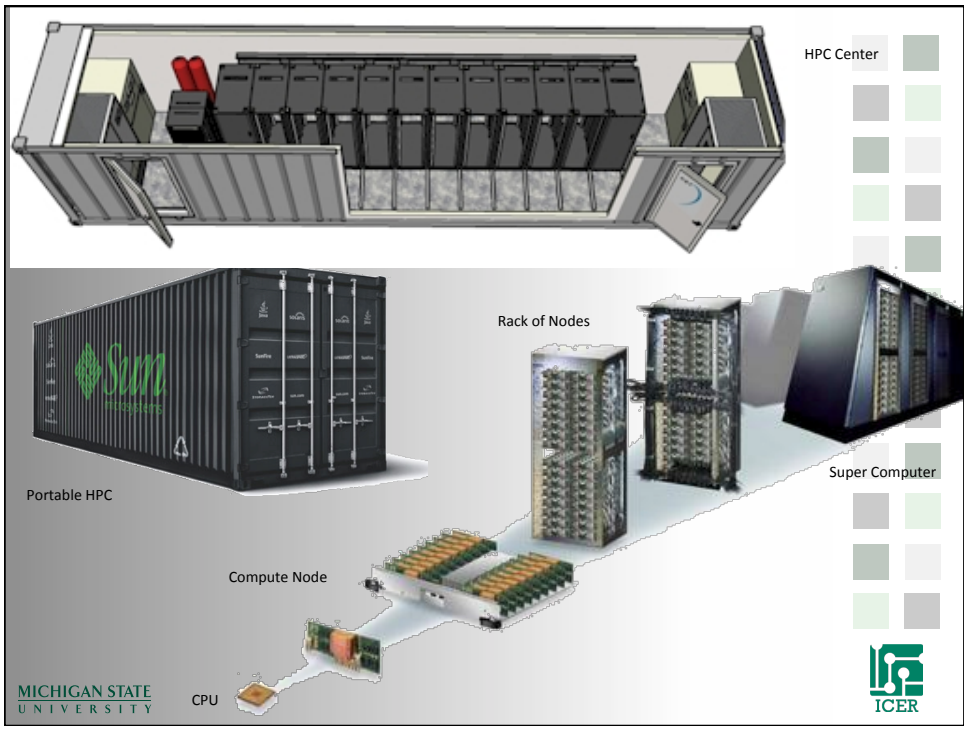

Commodity Cluster
Cores
Processors / Sockets
Nodes
Chassis
Rack
High Speed Network


HPC Center
Rack of Nodes
Super Computer
Portable HPC
Compute Node
CPU
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Large Shared Memory Systems (Fat Nodes)

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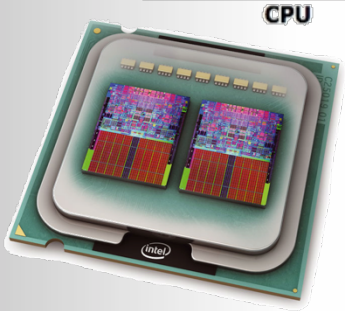
Shared Memory Communication

- Cores on a processor share the same memory
- Many Processors in a box
- OpenMP
- Fat nodes
  - 96 cores
  - 6TB of memory

CPU



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Accelerators

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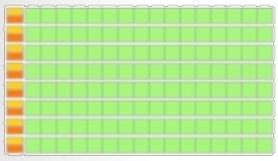
GPGPUs

- Cards used to render graphics on a computer
- Hundreds of cores
- Not very smart cores
- But, if you can make your research look like graphics rendering you may be able to run really fast!



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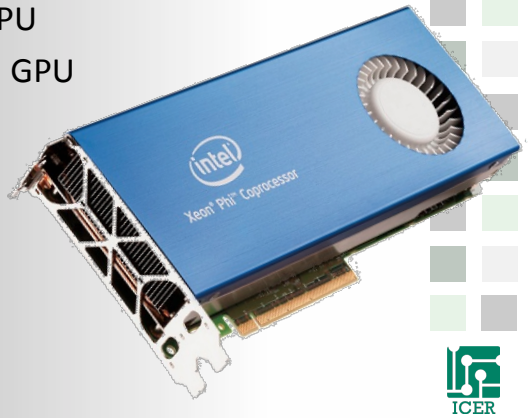
Intel Xeon Phi

- Cross between CPU and GPU
- About 60 Pentium I cores
  - Less cores than GPU
  - Easier to use than GPU
    - OpenMP
    - MPI



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High Throughput HTCondor Cluster

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MSU HTCondor Cluster

- Runs like a screen saver and Scavenges CPU cycles:
  - Little/No communication between nodes
  - Pleasantly parallel
  - Great for lots-o-small jobs

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Example: HPCC@MSU

FREE*

- Large Memory Nodes (up to 6TB!)
- GPU Accelerated cluster (K20, M1060)
- PHI Accelerated cluster (5110p)
- Over 600 nodes, 10000 computing cores
- Access to high throughput condor cluster
- 363TB high speed parallel scratch file space
- 50GB replicated file spaces (up to 1TB for free)
- Over 1800 preinstalled user level software packages
- Specialized VMs

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Which solution is better?

- Depends on what you are doing and your needs:
  - Resources
    - Software
    - Memory
    - File I/O
    - CPU scaling
    - Specialty Hardware
  - Flexibility
  - Price
  - Speed
    - Queue time
    - Run time

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Exercise: Connect to HPCC

- Step 1: ssh to gateway.hpcc.msu.edu

- Step 2: ssh into a dev node (developer node)

```
> ssh dev-intel10
```

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Key Difference 1

- Gateway vs.
  Head node /Development node vs.
  compute node

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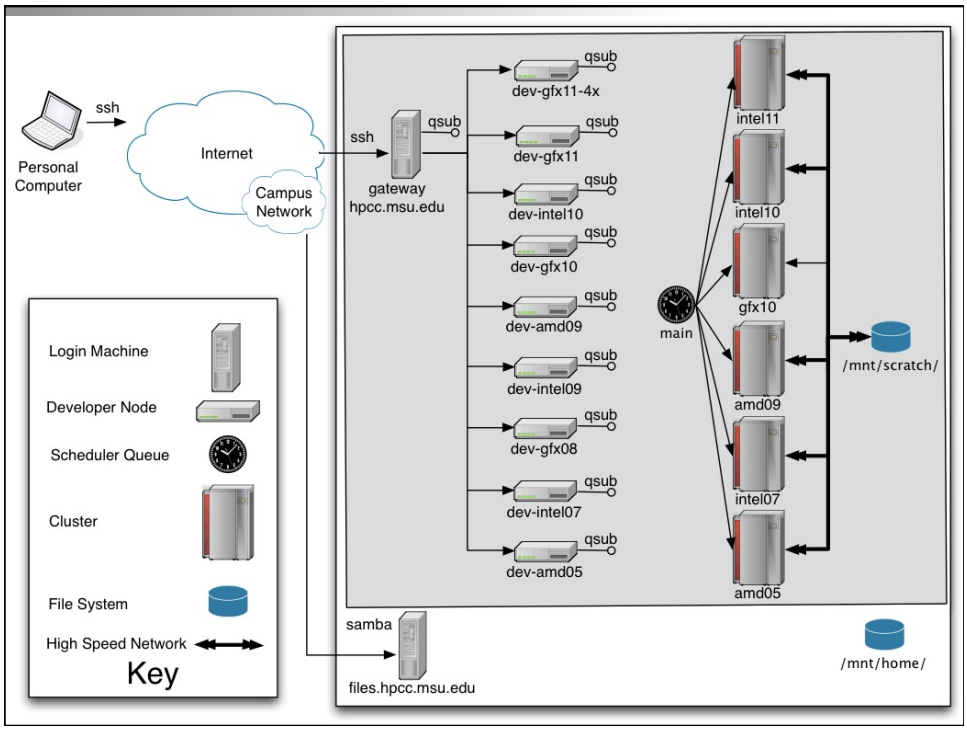

Running Jobs on the HPC

- Submission scripts are used to run jobs on the cluster
- The developer (dev) nodes are used to compile, test and debug programs

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Advantages of running Interactively

- You do not need to write a submission script
- You do not need to wait in the queue
- You can provide input to and get feedback from your programs as they are running

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Disadvantages of running Interactively

- All the resources on developer nodes are shared between all users.
- Any single process is limited to 2 hours of cpu time. If a process runs longer than 2 hours it will be killed.
- Programs that overutilize the resources on a developer node (preventing other to use the system) can be killed without warning.

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Developer Nodes

Name	Cores	Memory	Accelerators	Notes
dev-intel07	8	8GB	-	
dev-gfx08	4	8GB	3 x M1060	Nvidia Graphics Node
dev-intel10	8	24GB	-	
dev-intel14	20	64GB	-	
dev-intel14-phi	20	128GB	2 x Phi	Xeon Phi Node
dev-intel14-k20	20	128GB	2 x K20	Nvidia Graphics Node

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Available Software

- Center Supported Development Software
  - Intel compilers, openmp, openmpi, mvapich, totalview, mkl, pathscale, gnu, ...
- Center Supported Research Software
  - MATLAB, R, fluent, abaqus, HEEDS, amber, blast, ls-dyna, starp...
- Customer Software
  - gromacs, cmake, cuda, imagemagick, java, openmm, siesta…
  - For a more up to date list, see the documentation wiki:
    - http://wiki.hpcc.msu.edu/

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Key Difference 2

- Environment management Systems
  - a.k.a. modules, gnu modules, lua modules, etc

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Module System

- To maximize the different types of software and system configurations that are available to the users, HPCC uses a Module system
- Key Commands
  - **module avail** – show available modules
  - **module list** – list currently loaded modules
  - **module load** modulename – load a module
  - **module unload** modulename – unload a module
  - **module spider keyword** – Search modules for a keyword

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Exercise – Module

- List loaded modules

  `>module list`
- Show available modules:

  `>module avail`
- Try an example (Shouldn't work):

  `>powertools`

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Exercise: getexample

- Load a newly available module:

  `>module load powertools`
- Show powertools (should work now):

  `>powertools`
- Run the "getexample" powertool

  `>getexample`
- Download the helloMPI example

  `>getexample mothur_example`

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Navigating the example

- Change to the helloworld directory:

```
> cd ./mothur_example
> ls -la
> less README
```

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Key Difference 3

- Scheduling system.
- Ex:
  - SLERM
  - PBS Torque / Moab
  - Condor
- Requires a submission script

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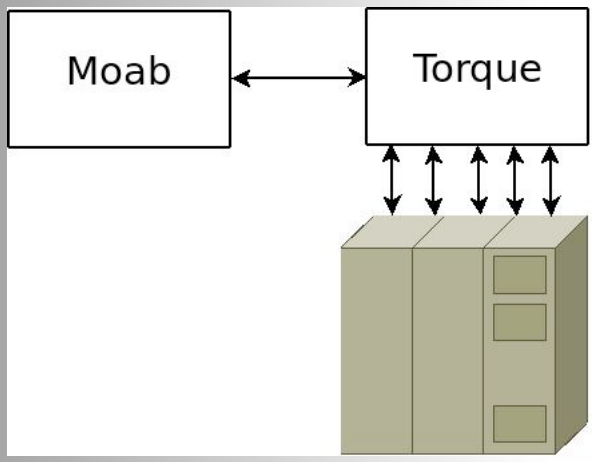
Resource Manager and scheduler



Not First In First Out!!

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Schedulers vs Resource Managers

- Scheduler
  (Moab)
  - Tracks and assigns
    - Memory
    - CPUs
    - Disk space
    - Software Licenses
    - Power / environment
    - Network
- Resource Manager
  (PBS/Torque)
  - Hold jobs for execution
  - Put the jobs on the nodes
  - Monitor the jobs and nodes

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Common Commands

- **qsub** <Submission script>
  - Submit a job to the queue
- **qdel** <JOB ID>
  - Delete a job from the queue
- **showq** –u <USERNAME>
  - Show the current job queue
- **checkjob** <JOB ID>
  - Check the status of the current job
- **showstart** –e all <JOB ID>
  - Show the estimated start time of the job

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Submission Script

1. List of required resources
2. All command line instructions needed to run the computation

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Typical Submission Script

Shell Comment

Define Shell

```
#!/bin/bash -login
#PBS -l walltime=10:00:00,mem=3Gb,nodes=10:ppn=1
#PBS -j oe

cd ${PBS_O_WORKDIR}

./myprogram -my input arguments

qstat -f ${PBS_JOBID}
```

Resource Requests

Shell Commands

Special Environment Variables

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Example: Submit a job

- Go to the top helloworld directory

```
>cd ~/mothur_example
```

- Create a simple submission script

```
>less run_mothur_quality.qsub
```

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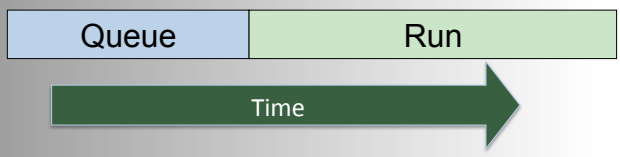
Submitting a job

- qsub –arguments <Submission Script>
  - Returns the job ID. Typically looks like the following:
    - 5945571.cmgr01
- Time to job completion



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Example: Submit a job, cont.

- Submit the file to the queue

```
>qsub run_mothur_quality.qsub
```

- Record jobid number (######) and wait at most 30 seconds
- Check the status of the queue

```
>showq
```

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Example: Monitor a job

- Submit the file to the queue:

```
>qstat -f ######
```

- When will a job start:

```
>showstart -e all ######
```

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Scheduling Priorities

- Jobs that use more resources get higher priority (because these are hard to schedule)
- Smaller jobs are backfilled to fit in the holes created by the bigger jobs
- Eligible jobs acquire more priority as they sit in the queue
- Jobs can be in three basic states:
  - Blocked, eligible or running

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Cluster Resources

Year	Name	Description	ppn	Memory	Nodes	Total Cores
2007	intel07	Quad-core 2.3GHz Intel Xeon E5345	8	8GB	126	1008
2009	amd09	Sun Fire X4600 (Fat Node) AMD Opteron 8384	32	256GB	3	96
2010	gfx10	NVIDIA CUDA Node (no IB)	8	18GB	32	256
2010	intel10	Intel Xeon E5620 (2.40 GHz)	8	24GB	191	1528
2011	intel11	Intel Xeon 2.66 GHz E7-8837	32	512GB	2	64
			32	1TB	1	32
			64	2TB	2	128
2014	intel14	Intel Xeon E5-2670 v2 (2.6 GHz)	20	64GB	128	2560
			20	256GB	24	480
		2 NVIDIA K20 GPUs	20	128GB	40	800
		2 Xeon Phi 5110P	20	128GB	28	560
	Total				577	7512

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System Limitations

- Scheduling
  - 5 eligible jobs at a time
  - 520 running jobs
  - 1000 submitted jobs
- Resources
  - 1 week of walltime
  - 520 cores (nodes * ppn)
  - ppn=64
  - 2TB memory on a single core
  - ~200 GB Hard Drive

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Job completion

- By default the job will automatically generate two files when it completes:
  - Standard Output:
    - Ex: jobname.o5945571
  - Standard Error:
    - Ex: jobname.e5945571
- You can combine these files if you add the join option in your submission script:
  - "#PBS -j oe"
- You can change the output file name
  - #PBS -o /mnt/home/netid/myoutputfile.txt

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Other Job Properties

- resources (-l)
  - Walltime, memory, nodes, processor, network, etc.
- #PBS –l feature=gpgpu,gbe
- #PBS –l nodes=2:ppn=8:gpu=2
- #PBS –l mem=16gb
- Email address (-M)
  - Ex: #PBS –M colbrydi@msu.edu
- Email Options (-m)
  - Ex: #PBS –m abe

Many others, see the wiki:
http://wiki.hpcc.msu.edu/

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Summary Clusters vs. Cloud

- Key differences when using:
  - Different node types (gateway, head/ development, compute)
  - Environment management Systems (modules)
  - Batch Submission Script (Resources needed and commands to execute)

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Discussion
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