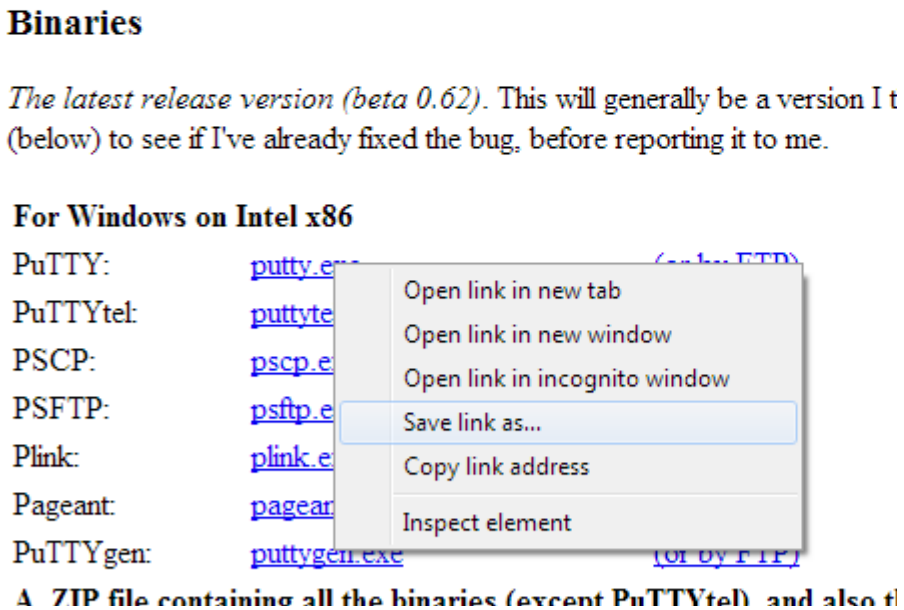
Introduction to ARC Systems

Advanced Research Computing

Sep 8, 2016

Before We Start

- Sign in
- Request account if neces:
- Windows Users:
  - Download PuTTY
    - Google PuTTY
    - First result
    - Save putty.exe to Desktop
  - ALTERNATIVE:
    - ETX newriver.arc.vt.edu



Today's goals

- Introduce ARC
- Give overview of HPC today
- Give overview of VT-HPC resources
- Familiarize audience with interacting with VT-ARC systems

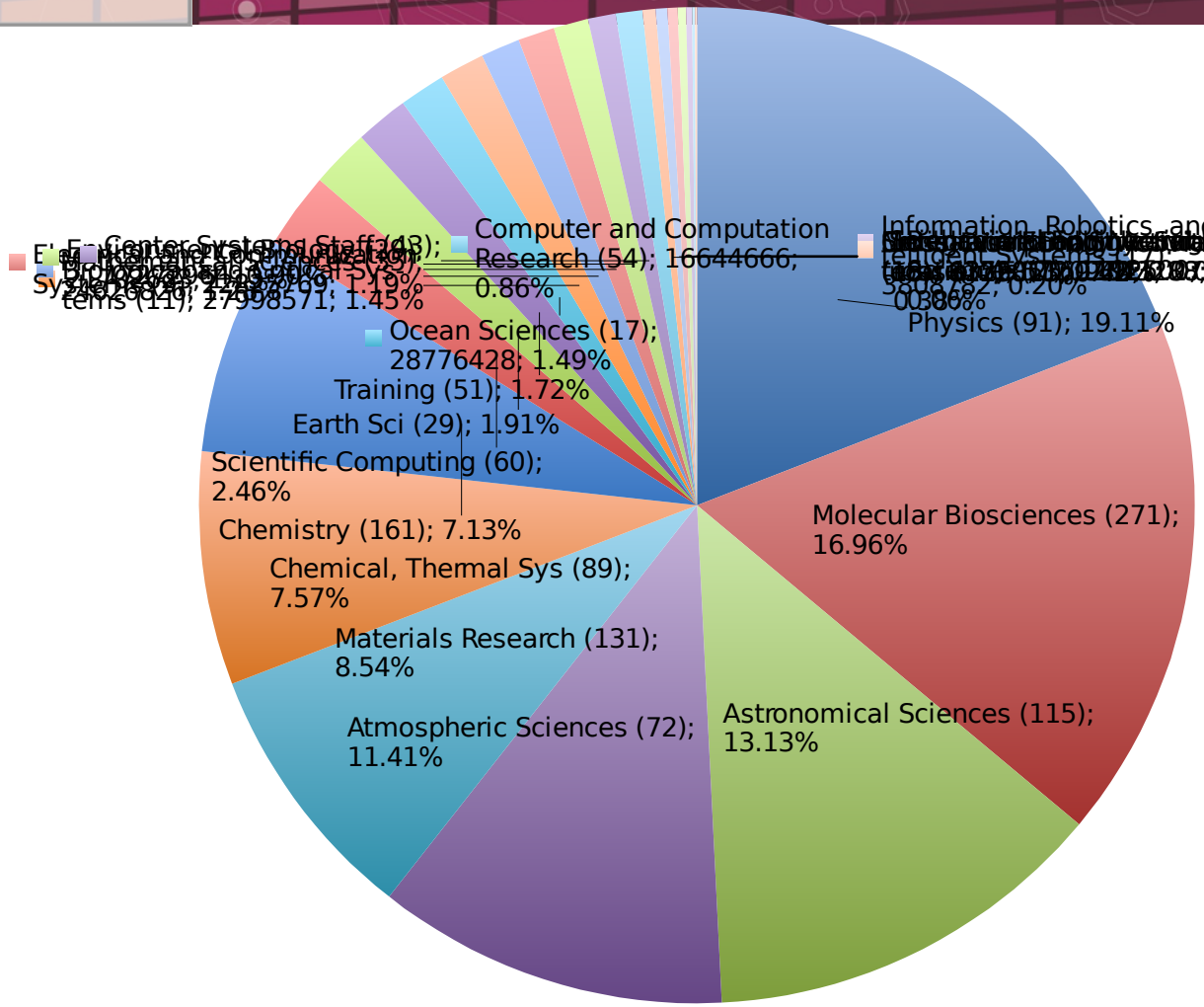
Should I Pursue HPC?

- Necessity: Are local resources insufficient to meet your needs?
  - Very large jobs
  - Very many jobs
  - Large data
- Convenience: Do you have collaborators?
  - Share projects between different entities
  - Convenient mechanisms for data sharing

Research in HPC is Broad

- Earthquake Science and Civil Engineering
- Molecular Dynamics
- Nanotechnology
- Plant Science
- Storm modeling
- Epidemiology
- Particle Physics
- Economic analysis of phone network patterns
- Brain science
- Analysis of large cosmological simulations
- DNA sequencing
- Computational Molecular Sciences
- Neutron Science
- International Collaboration in Cosmology and Plasma Physics

Who Uses HPC?



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

Popular Software Packages

- Molecular Dynamics: Gromacs, LAMMPS, NAMD, Amber
- CFD: OpenFOAM, Ansys, Star-CCM+
- Finite Elements: Deal II, Abaqus
- Chemistry: VASP, Gaussian, PSI4, QCHEM
- Climate: CESM
- Bioinformatics: Mothur, QIIME, MPIBLAST
- Numerical Computing/Statistics: R, Matlab, Julia
- Visualization: ParaView, VisIt, Ensight

Learning Curve

- Linux: Command-line interface
- Scheduler: Shares resources among multiple users
- Parallel Computing:
  - Need to parallelize code to take advantage of supercomputer's resources
  - Third party programs or libraries make this easier

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- Unit within the Office of the Vice President of Information Technology
- Provide centralized resources for:
  - Research computing
  - Visualization
- Staff to assist users
- Website: http://www.arc.vt.edu

ARC Goals

- Advance the use of computing and visualization in VT research
- Centralize resource acquisition, maintenance, and support for research community
- Provide support to facilitate usage of resources and minimize barriers to entry
- Enable and participate in research collaborations between departments

Personnel

- Associate VP for Research Computing: Terry Herdman
- Director, HPC: Terry Herdman
- Director, Visualization: Nicholas Polys
- Computational Scientists
  - Justin Krometis
  - James McClure
  - Brian Marshall
  - Srijith Rajamohan
  - Bob Settlage

Personnel (Continued)

- System Administrators (UAS)
  - Tim Rhodes
  - Chris Snapp
  - Brandon Sawyers
  - Josh Akers
- Business Manager: Alana Romanella
- User Support GRAs: Umar Kalim, Sangeetha Srinivasa

Personnel (Continued)

- System & Software Engineers
  - Nathan Liles

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Computational Resources

- NewRiver
  - –Cluster targeting data-Intensive problems
- DragonsTooth
  - –jobs that don't require low latency interconnect i.e. pleasingly parallel
  - –long running, e.g. 30 day wall time
- Blue Ridge
  - –Large scale cluster equipped with Intel Xeon Phi Co-Processors
- Cascades – large general compute with GPU nodes
- Machine Learning cluster coming soon (Tinker??)
- Cloud based access coming soon

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Compute Resources

System	Usage	Nodes	Node Description	Special Features
HokieOne	Shared, Large Memory	82	6 cores, 32GB (Intel Westmere)	2.6TB shared-memory
HokieSpeed	GPGPU	201	12 cores, 24 GB (2× Intel Westmere)	402 Tesla C2050 GPU
BlueRidge	Large-scale CPU, MIC	408	16 cores, 64 GB (2× Intel Sandy Bridge)	260 Intel Xeon Phi 4 K40 GPU 18 128GB nodes
NewRiver	Large-scale, Data Intensive	134	24 cores, 128 GB (2× Intel Haswell)	8 K80 GPGPU 16 “big data” nodes 24 512GB nodes 2 3TB nodes
DragonsTooth	Pleasingly parallel, long jobs	48	24 cores, 256 GB (2× Intel Haswell)	2TB SSD local storage 30 day walltime

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Computational Resources

Name	NewRiver	DragonsTooth	BlueRidge	HokieSpeed	HokieOne
Key Features, Uses	Scalable CPU, Data Intensive	Pleasingly parallel, long running jobs	Scalable CPU or MIC	GPU	Shared Memory
Available	August 2015	August 2016	March 2013	Sept 2012	Apr 2012
Theoretical Peak (TFlops/s)	152.6	.806	398.7	238.2	5.4
Nodes	134	48	408	201	N/A
Cores	3,288	576	6,528	2,412	492
Cores/Node	24	24	16	12	N/A*
Accelerators/Co processors	8 Nvidia K80 GPU	N/A	260 Intel Xeon Phi 8 Nvidia K40 GPU	408 Nvidia C2050 GPU	N/A
Memory Size	34.4 TB	12.3 TB	27.3 TB	5.0 TB	2.62 TB
Memory/Core	5.3 GB*	10.6 GB	4 GB*	2 GB	5.3 GB
Memory/Node	128 GB*	256 GB	64 GB*	24 GB	N/A*

NewRiver

- 134 Nodes
- 3,288 Cores
- 34.4 TB Memory
- EDR InfiniBand (IB) Interconnect
- Data-intensive, large-memory, visualization, and GPGPU special-purpose hardware
  - –8 K80 GPGPU
  - –16 “big data” nodes
  - –24 512GB nodes
  - –2 3TB nodes

NewRiver Nodes

Description	#	Hosts	CPU	Cores	Memory	Local Disk	Other Features
General	100	nr027-nr126	2 x E5-2680 v3 (Haswell)	24	128 GB, 2133 MHz	1.8 TB	
GPU	8	nr019-nr026	2 x E5-2680 v3 (Haswell)	24	512 GB	3.6 TB (2 x 1.8 TB)	NVIDIA K80 GPU
I/O	16	nr003-nr018	2 x E5-2680 v3 (Haswell)	24	512 GB	43.2 TB (24 x 1.8 TB)	2x 200 GB SSD
Large Memory	2	nr001-nr002	4 x E7-4890 v2 (Ivy Bridge)	60	3 TB	10.8 TB (6 x 1.8 TB)	
Interactive	8	newriver1-newriver8	2 x E5-2680 v3 (Haswell)	24	256 GB		NVIDIA K1200 GPU

Storage Resources

Name	Intent	File System	Environment Variable	Per User Maximum	Data Lifespan	Available On
Home	Long-term storage of files	GPFS (NewRiver) NFS (Other)	$HOME	500 GB (NewRiver) 100 GB (Other)	Unlimited	Login and Compute Nodes
Group	Shared Data Storage for Research Groups	GPFS (NewRiver)	$GROUP	10 TB Free per faculty researcher	Unlimited	Login and Compute Nodes
Work	Fast I/O, Temporary storage	GPFS (NewRiver) Lustre (BlueRidge) GPFS (Other)	$WORK	20 TB (NewRiver) 14 TB (Other) 3 million files	120 days	Login and Compute Nodes

Storage Resources (continued)

Name	Intent	File System	Environment Variable	Per User Maximum	Data Lifespan	Available On
Archive	Long-term storage for infrequently-accessed files	CXFS	$ARCHIVE	-	Unlimited	Login Nodes
Local Scratch	Local disk (hard drives)		$TMPDIR	Size of node hard drive	Length of Job	Compute Nodes
Memory (tmpfs)	Very fast I/O	Memory (RAM)	$TMPFS	Size of node memory	Length of Job	Compute Nodes

Visualization Resources

- VisCube: 3D immersion environment with three 10′ by 10′ walls and a floor of 1920×1920 stereo projection screens
- DeepSix: Six tiled monitors with combined resolution of 7680×3200
- ROVR Stereo Wall
- AISB Stereo Wall

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Getting Started with ARC

- Review ARC's system specifications and choose the right system(s) for you
  - Specialty software
- Apply for an account online the Advanced Research Computing website
- When your account is ready, you will receive confirmation from ARC's system administrators

Resources

- ARC Website: http://www.arc.vt.edu
- ARC Compute Resources & Documentation: http://www.arc.vt.edu/hpc
- New Users Guide: http://www.arc.vt.edu/newusers
- Frequently Asked Questions: http://www.arc.vt.edu/faq
- Linux Introduction: http://www.arc.vt.edu/unix

Thank you

Questions?

Log In

- Log in via SSH
  - Mac/Linux have built-in client
  - Windows need to download client (e.g. PuTTY)

System	Login Address (xxx.arc.vt.edu)
NewRiver	newriver1 to newriver8
Dragonstooth	dragonstooth1
BlueRidge	blueridge1 or blueridge2
HokieSpeed	hokiespeed1 or hokiespeed2
HokieOne	hokieone

Browser-based Access

- Browse to http://newriver.arc.vt.edu
- Xterm: Opens an SSH session with X11 forwarding (but faster)
- Other profiles: VisIt, ParaView, Matlab, Allinea
- Create your own!

ALLOCATION SYSTEM

Allocations

- "System unit" (roughly, core-hour) account that tracks system usage
- Applies only to NewRiver and BlueRidge

http://www.arc.vt.edu/allocations

Allocation System: Goals

- Track projects that use ARC systems and document how resources are being used
- Ensure that computational resources are allocated appropriately based on needs
  - Research: Provide computational resources for your research lab
  - Instructional: System access for courses or other training events

Allocation Eligibility

To qualify for an allocation, you must meet at least one of the following:

- Be a Ph.D. level researcher (post-docs qualify)
- Be an employee of Virginia Tech and the PI for research computing
- Be an employee of Virginia Tech and the co-PI for a research project led by non-VT PI

Allocation Application Process

- Create a research project in ARC database
- Add grants and publications associated with project
- Create an allocation request using the web-based interface
- Allocation review may take several days
- Users may be added to run jobs against your allocation once it has

Allocation Tiers

- Research allocations fall into three tiers:
- Less than 200,000 system units (SUs)
  - –200 word abstract
- 200,000 to 1 million SUs
  - –1-2 page justification
- More than 1 million SUs
  - –3-5 page justification

Allocation Management

- Web-based:
  - User Dashboard -> Projects -> Allocations
  - Systems units allocated/remaining
  - Add/remove users
- Command line:
  - Allocation name and membership: `glsaccount`
  - Allocation size and amount remaining:
    `gbalance -h -a <name>`
  - Usage (by job): `gstatement -h -a <name>`

USER ENVIRONMENT

Consistent Environment

- Operating system (CentOS)
- Storage locations
- Scheduler
- Hierarchical module tree for system tools and applications

Modules

- Modules are used to set the PATH and other environment variables
- Modules provide the environment for building and running applications
  - Multiple compiler vendors (Intel vs GCC) and versions
  - Multiple software stacks: MPI implementations and versions
  - Multiple applications and their versions
- An application is built with a certain compiler and a certain software stack (MPI, CUDA)
  - Modules for software stack, compiler, applications
- User loads the modules associated with an application, compiler, or software stack
  - modules can be loaded in job scripts

Module commands

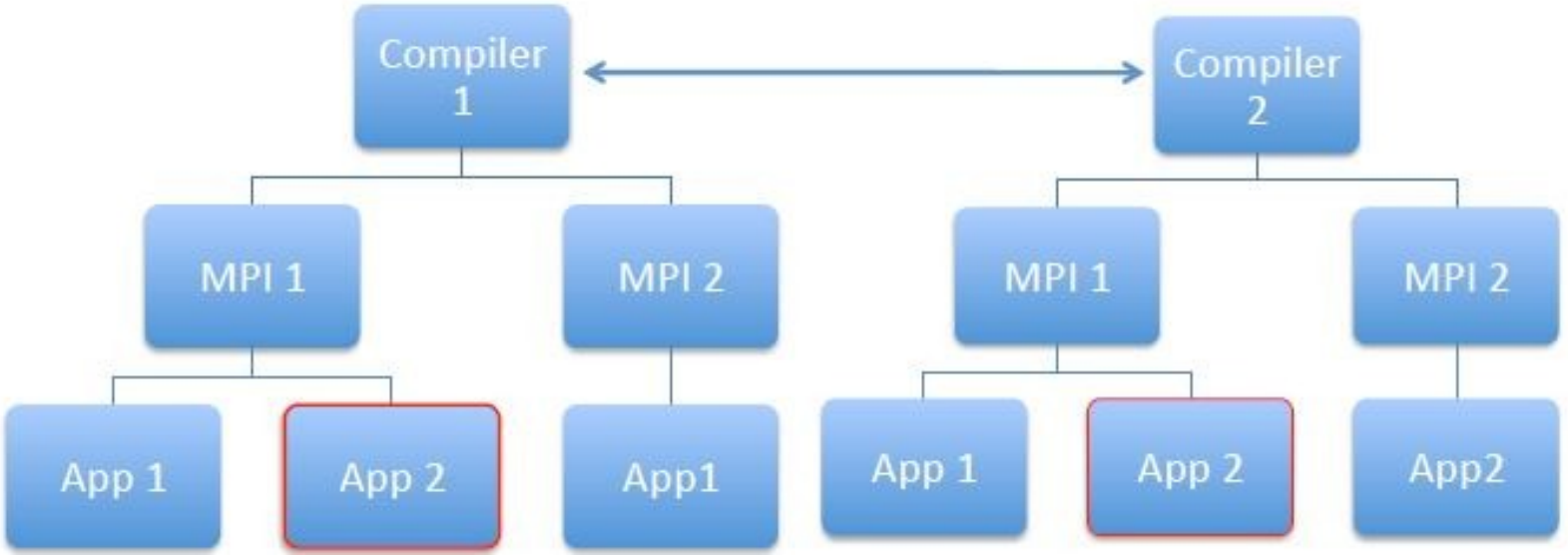
Command	Result
`module`	List options
`module list`	List loaded modules
`module avail`	List available modules
`module load <module>`	Add a module
`module unload <module>`	Remove a module
`module swap <mod1> <mod2>`	Swap two modules
`module help <module>`	Module environment
`module show <module>`	Module description
`module spider <module>`	Search modules
`module reset`	Reset to default
`module purge`	Unload all modules

Modules

- Available modules depend on:
  - The compiler (eg. Intel, gcc) and
  - The MPI stack selected

- Defaults:
  - BlueRidge: Intel + mvapich2
  - HokieOne: Intel + MPT
  - HokieSpeed: Intel + OpenMPI
  - NewRiver, DragonsTooth: none

Hierarchical Module Structure



JOB SUBMISSION & MONITORING

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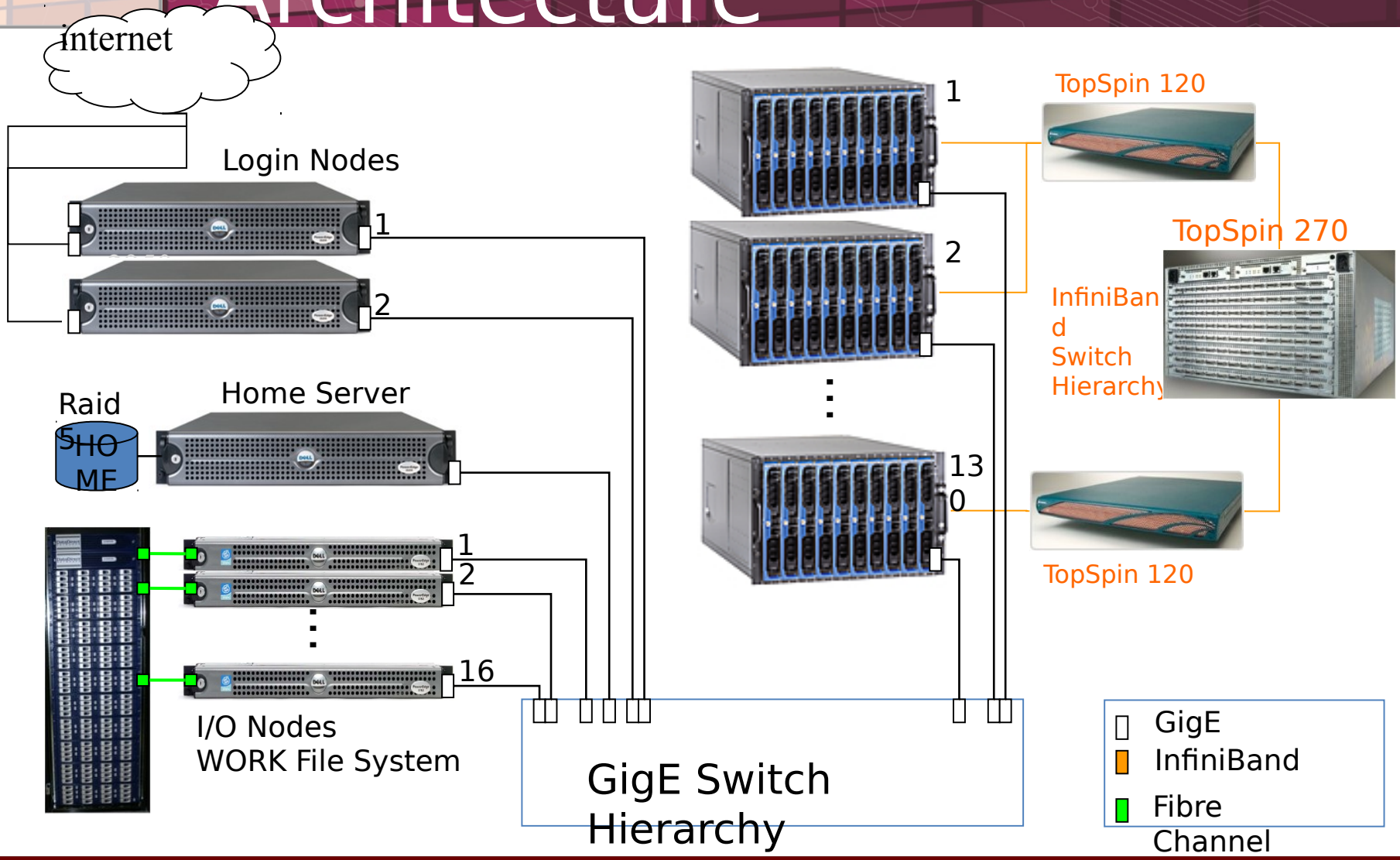
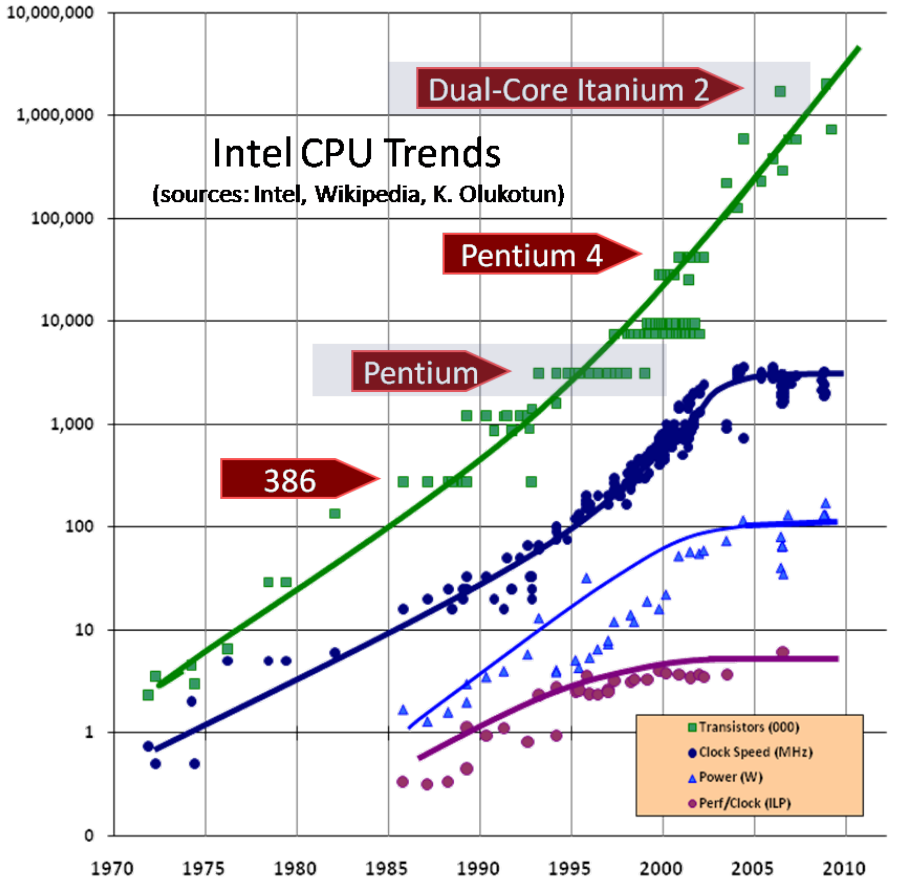
Cluster System Architecture



Parallelism is the New Moore's Law

- Power and energy efficiency impose a key constraint on design of micro-architectures
- Clock speeds have plateaued
- Hardware parallelism is increasing rapidly to make up the difference



Essential Components of HPC

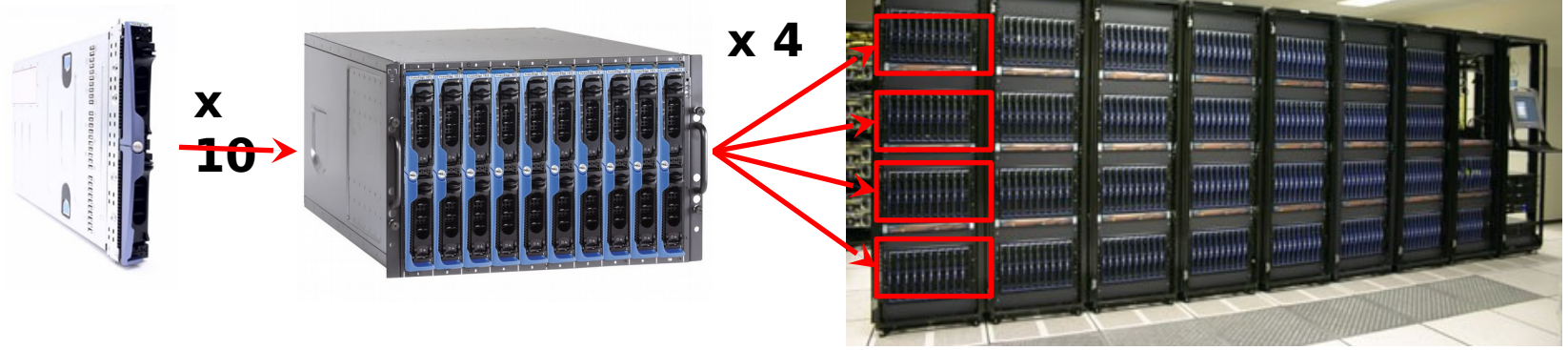
- Supercomputing resources
- Storage
- Visualization
- Data management
- Network infrastructure
- Support

Terminology

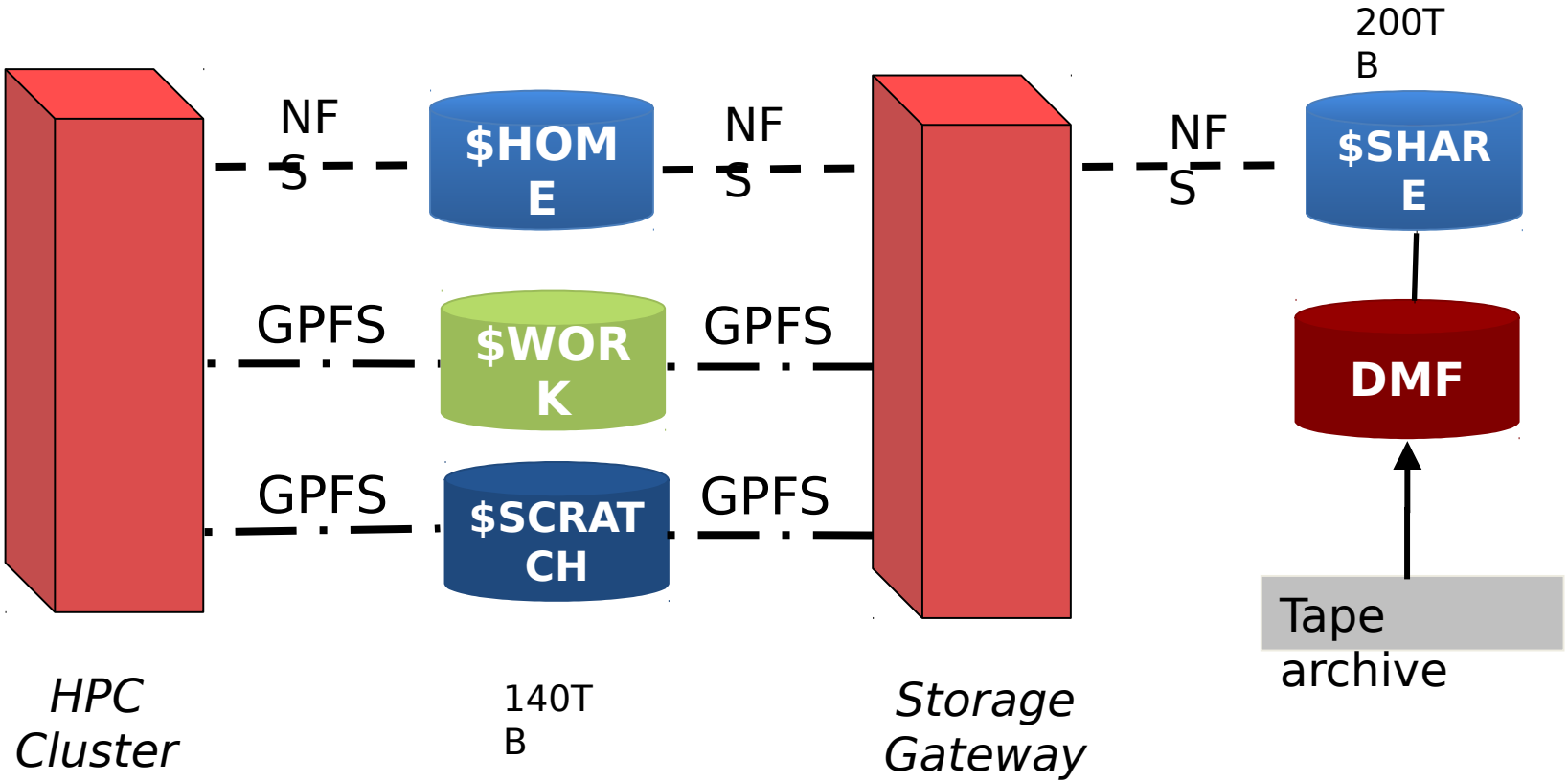
- Core: A computational “unit”
- Socket: A single CPU (“processor”). Includes roughly 4-15 cores.
- Node: A single “computer”. Includes roughly 2-8 sockets.
- Cluster: A single “supercomputer” consisting of many nodes.
- GPU: Graphics processing unit. Attached to some nodes. General purpose GPUs (GPGPUs) can be used to speed up certain kinds of codes.
- Xeon Phi: Intel’s product name for its GPU competitor. Also called “MIC”.

Blade : Rack : System

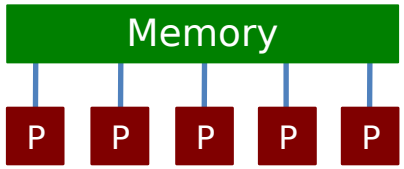
- 1 node : 2 x 8 cores= 16 cores
- 1 chassis : 10 nodes = 160 cores
- 1 rack (frame) : 4 chassis = 640 cores
- system : 10 racks = 6,400 cores



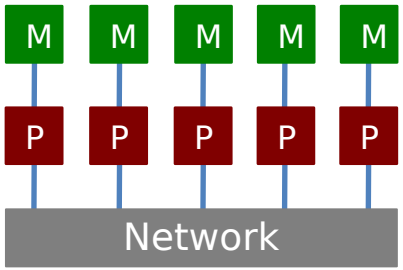
HPC Storage


NFS
$HOME
NFS
NFS
200TB
$SHARE
GPFS
$WORK
GPFS
DMF
GPFS
$SCRATCH
GPFS
Tape archive
HPC Cluster
140TB
Storage Gateway

Shared vs. Distributed memory

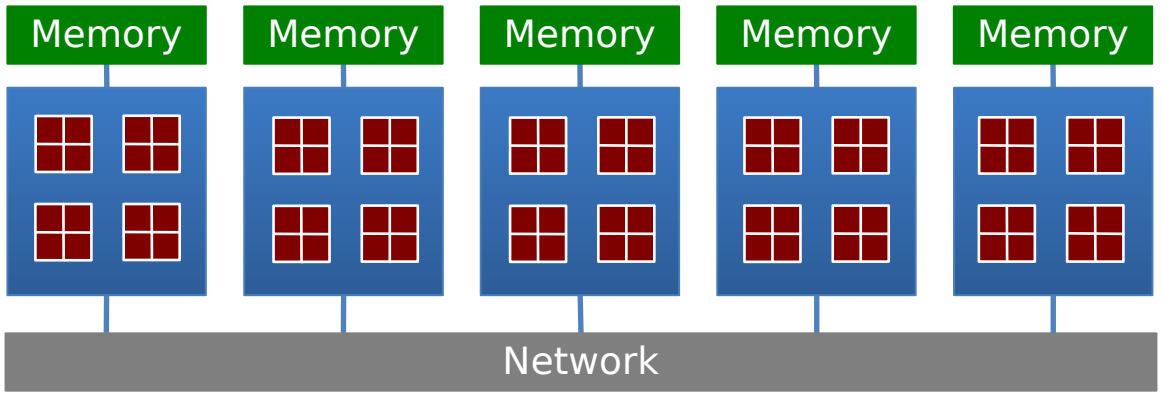


- All processors have access to a pool of shared memory
- Access times vary from CPU to CPU in NUMA systems
- Example: SGI UV, CPUs on same node



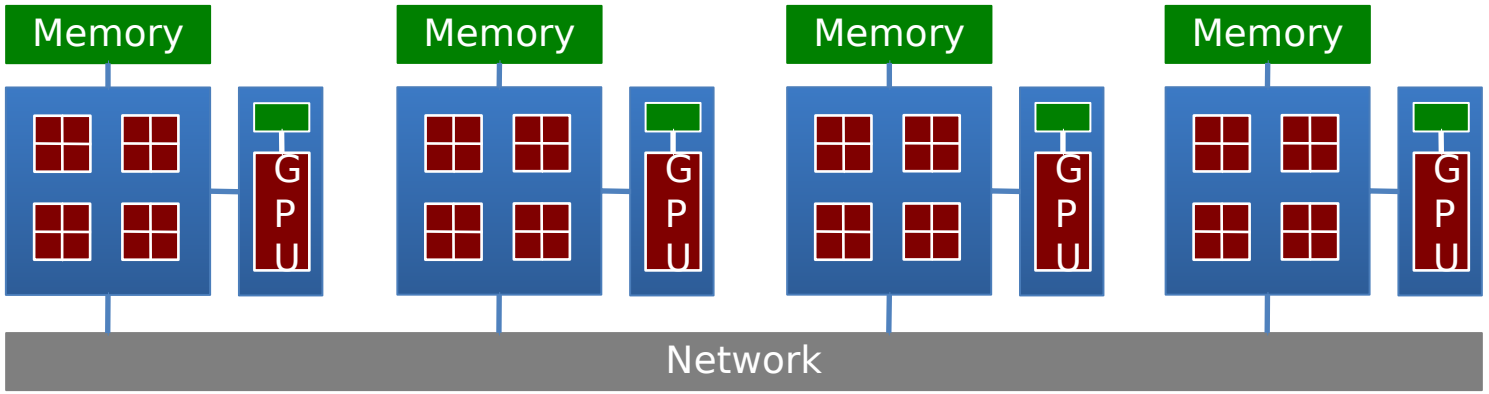
- Memory is local to each processor
- Data exchange by message passing over a network
- Example: Clusters with single-socket blades

Multi-core systems



- Current processors place multiple processor cores on a die
- Communication details are increasingly complex
  - Cache access
  - Main memory access
  - Quick Path / Hyper Transport socket connections
  - Node to node connection via network

Accelerator-based Systems



- Calculations made in both CPUs and GPUs
- No longer limited to single precision calculations
- Load balancing critical for performance
- Requires specific libraries and compilers (CUDA, OpenCL)
- Co-processor from Intel: MIC (Many Integrated Core)

Submitting a Job

- Submission via a shell script
  - Job description: Resources required, run time, allocation
  - Modules & dependencies
  - Execution statements
- Submit job script: `qsub <job_script>`

- Interactive options:
  - Interactive job: `qsub -I …`
  - Interactive job with X11 forwarding: `qsub -I -X …`

Job Monitoring

- Determine job status, and if pending when it will run

Command	Meaning
`checkjob -v JOBID`	Get the status and resources of a job
`showq`	See what jobs are running and cluster utilization
`showstart JOBID`	Get expected job start time
`qdel JOBID`	Delete a job

Job Execution

- Order of job execution depends on a variety of parameters:
  - Submission Time
  - Queue Priority
  - Backfill Opportunities
  - Fairshare Priority
  - Advanced Reservations
  - Number of Actively Scheduled Jobs per User

Examples: ARC Website

- See the Examples section of each system page for sample submission scripts and step-by-step examples:
  - http://www.arc.vt.edu/newriver
  - http://www.arc.vt.edu/dragonstooth
  - http://www.arc.vt.edu/blueridge
  - http://www.arc.vt.edu/hokiespeed
  - http://www.arc.vt.edu/hokieone

A Step-by-Step Example

Getting Started

- Find your training account (hpcXX)
- Log into NewRiver
  - Mac: `ssh hpcXX@cascades1.arc.vt.edu`
  - Windows: Use PuTTY
    - Host Name: `cascades1.arc.vt.edu`

Example: Running MPI Quad

- Or copy from training directory:

```
cp /home/TRAINING/newriver/* ./
```

- Build the code

Compile the Code

- Intel compiler is already loaded

```
module list
```

- Compile command (executable is mpiqd)

```
mpicc -o mpiqd mpi_quad.c
```

- To use GCC instead, swap it out:

```
module swap intel gcc
```

Prepare Submission Script

- Copy sample script:

```
cp /home/TRAINING/ARC_Intro/br.qsub  .
```

- Edit sample script:
  - Walltime
  - Resource request (nodes/ppn)
  - Module commands (add Intel & mvapich2)
  - Command to run your job
- Save it (e.g., mpiqd.qsub)

Submission Script (Typical)

```
#!/bin/bash
#PBS -l walltime=00:10:00
#PBS -l nodes=2:ppn=16
#PBS -q normal_q
#PBS -W group_list=newriver
#PBS -A AllocationName          <--Only for NewRiver/BlueRidge

module load intel mvapich2

cd $PBS_O_WORKDIR
echo "MPI Quadrature!"
mpirun -np $PBS_NP ./mpiqd

exit;
```

Submission Script (Today)

```
#!/bin/bash
#PBS -l walltime=00:10:00
#PBS -l nodes=2:ppn=8
#PBS -q normal_q
#PBS -W group_list=training
#PBS -A training
#PBS -l advres=NLI_ARC_Intro.26

module load intel mvapich2

cd $PBS_O_WORKDIR
echo "MPI Quadrature!"
mpirun -np $PBS_NP ./mpiqd

exit;
```

Submit the job

- Copy the files to $WORK:

```
cp mpiqd $WORK
cp mpiqd.qsub $WORK
```

- Navigate to $WORK

```
cd $WORK
```

- Submit the job:

```
qsub mpiqd.qsub
```

- Scheduler returns job number:

```
25770.master.cluster
```

Wait for job to complete

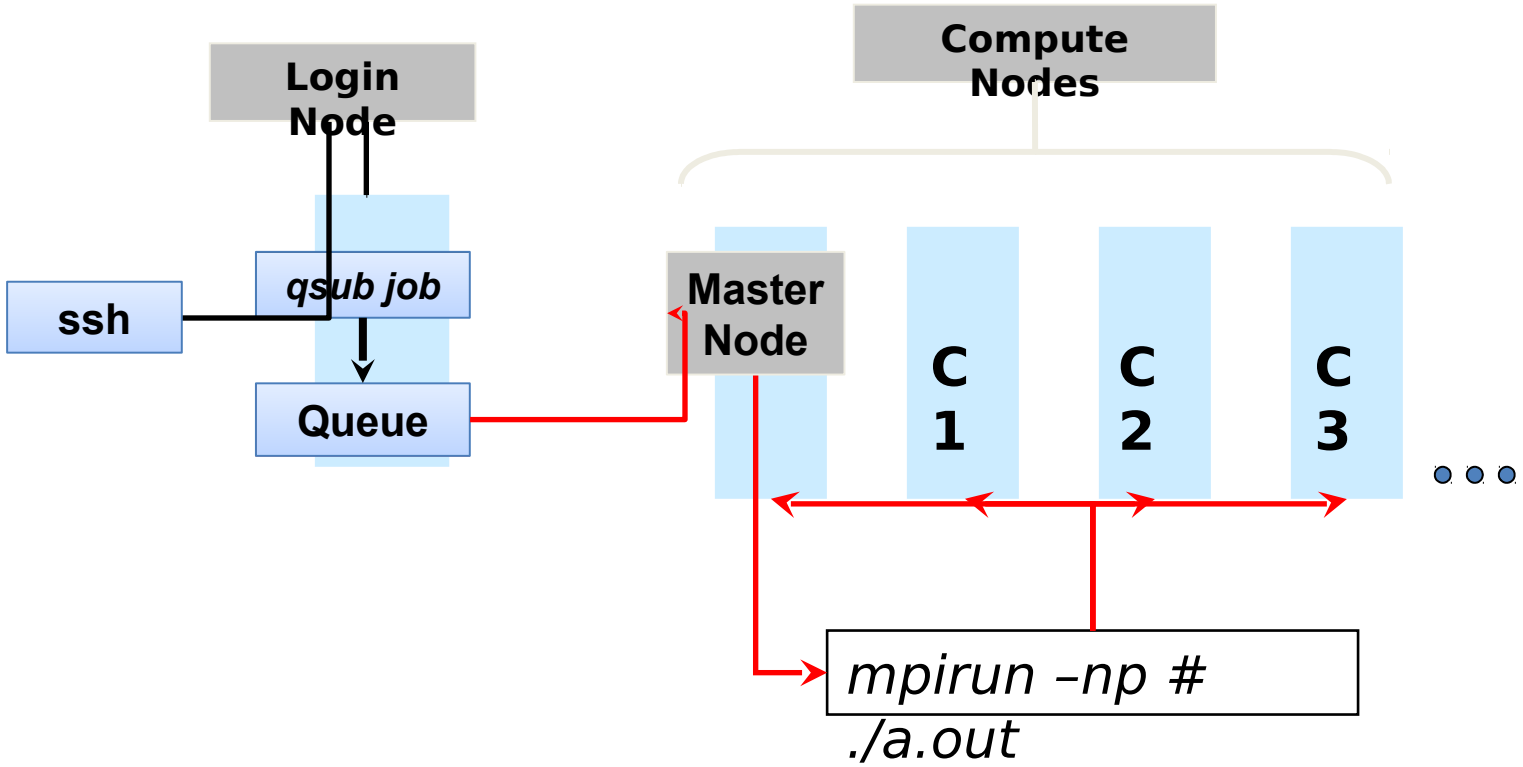
- Check job status:

```
checkjob -v 25770
showq -u hpcXX
```

- When complete:
  - Job output: `mpiqd.qsub.o25770`
  - Errors: `mpiqd.qsub.e25770`
- Copy results back to $HOME:

```
cp mpiqd.qsub.o25770 $HOME
```

What is Job Submission?



Resources

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- Linux Introduction: http://www.arc.vt.edu/unix
- Module Tutorial: http://www.arc.vt.edu/modules
- Scheduler Tutorial: http://www.arc.vt.edu/scheduler