# High Performance Computing at the Oak Ridge Leadership Computing Facility

# Outline

- Our Mission
- Computer Systems: Present, Past, Future
- Challenges Along the Way
- Resources for Users

# Our Mission

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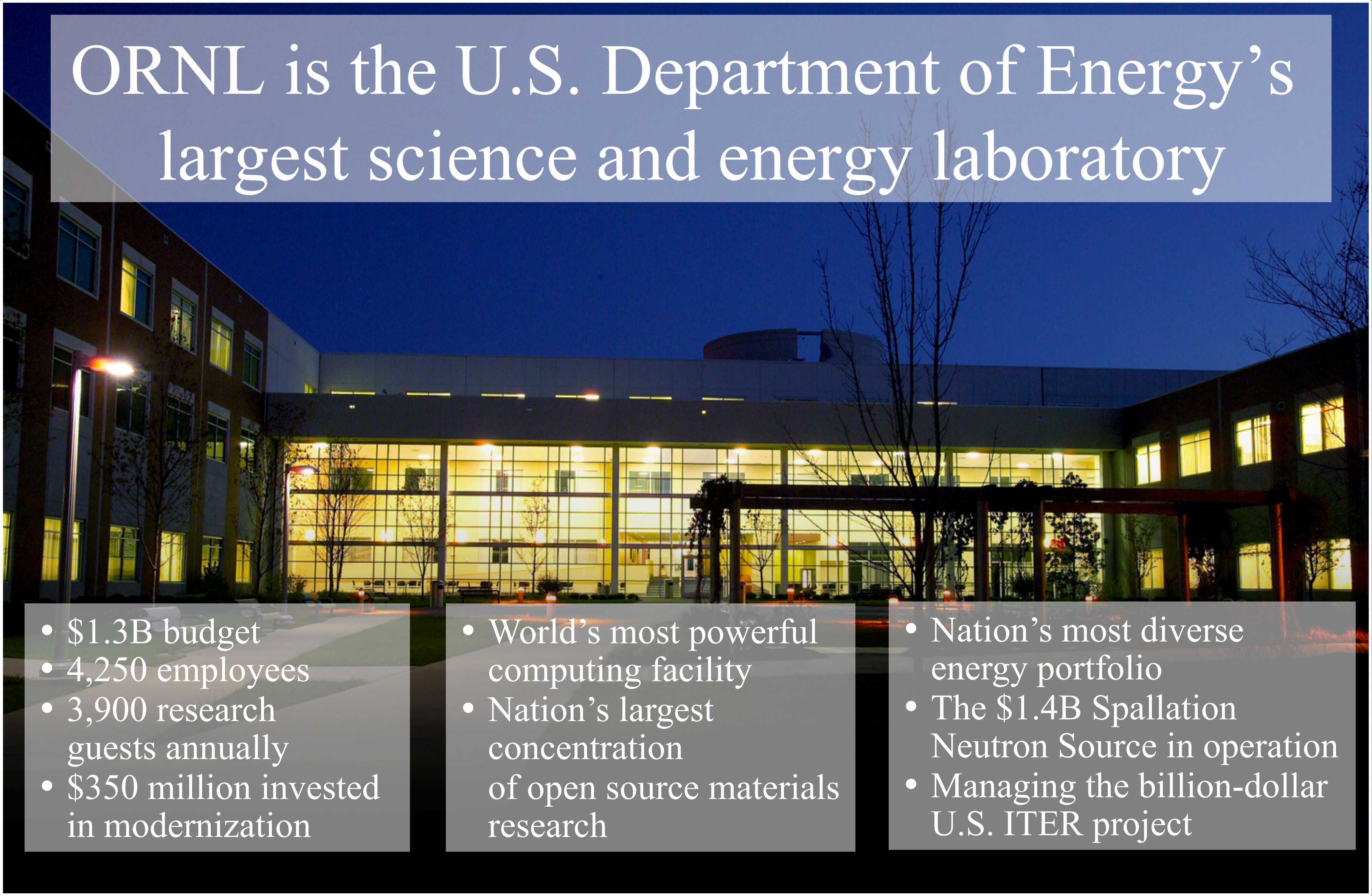
# ORNL is the U.S. Department of Energy's largest science and energy laboratory



- $1.3B budget
- 4,250 employees
- 3,900 research guests annually
- $350 million invested in modernization

- World's most powerful computing facility
- Nation's largest concentration of open source materials research

- Nation's most diverse energy portfolio
- The $1.4B Spallation Neutron Source in operation
- Managing the billion-dollar U.S. ITER project

## Computing Complex @ ORNL

**$70M Operating budget to deploy and operate the computational resources required to tackle global challenges**

- Providing world-leading computational resources and specialized services for the most computationally intensive problems
- Providing stable hardware/software path of increasing scale to maximize productive applications development
- Delivering transforming discoveries in materials, biology, climate, energy technologies, etc.


World's most powerful computer for open science

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# Computer Systems: Present, Past, Future

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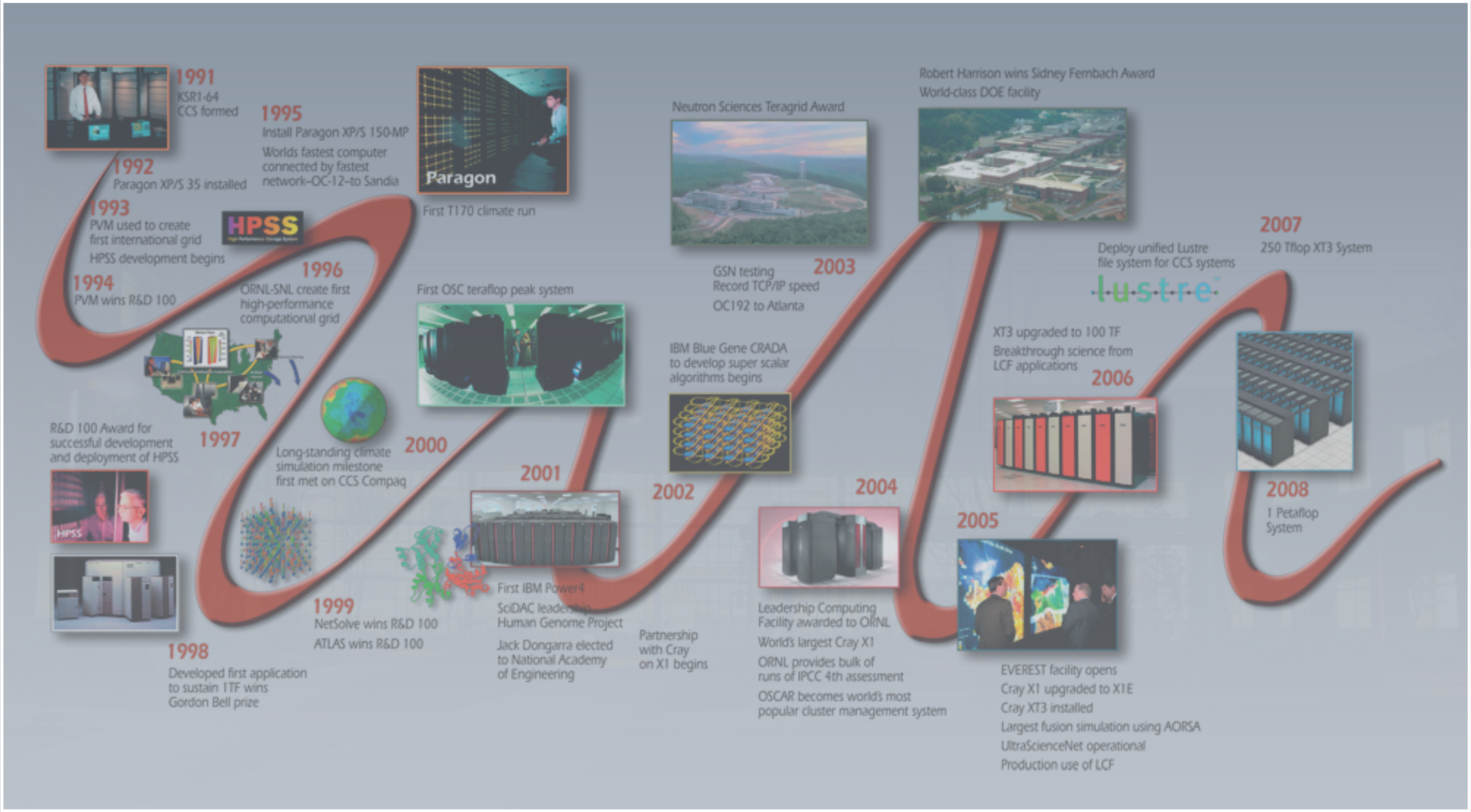
# OLCF systems, 1991–2008

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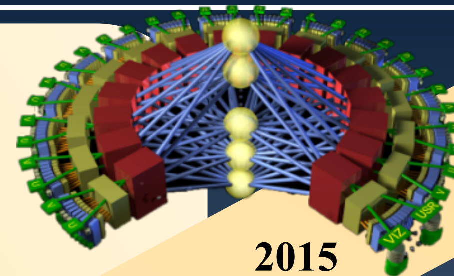
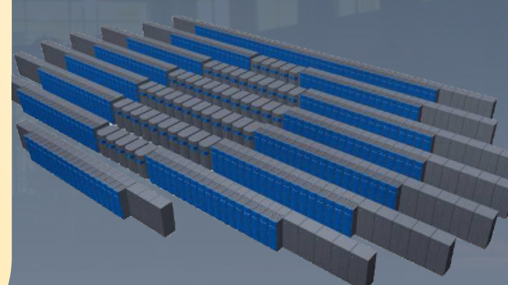
OLCF
Oak Ridge Leadership Computing Facility

# Million-fold increase in computing and data capabilities





2004 — Cray X1 3 TF

2005 — Cray XT3 Single-core 26 TF

2006 — Cray XT3 Dual-core 54 TF

2007 — Cray XT4 119 TF

2008 — Cray XT4 Quad-core 166 TF 18TB, 0.3 PB

2008 — Cray XT4 Quad-core 263 TF 62 TB, 1 PB

2009 — Cray XT5 8/12-core, dual-socket SMP ~1 PF 100TB, 3.3 PB

2009 — Jaguar 8-core, dual-socket SMP 1.64PF 362 TB, 10 PB

2009 — Jaguar 8/12-core, dual-socket SMP 2.60PF 362 TB, 10 PB

2015 — Future system 100–250 PF

2018 — Future system 1000 PF (1 EF)

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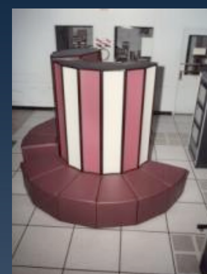
# A Growth-Factor of a Billion in Performance in a Single Career



1949 Edsac

1954 ORACLE

1959 IBM 7094

1976 Cray 1

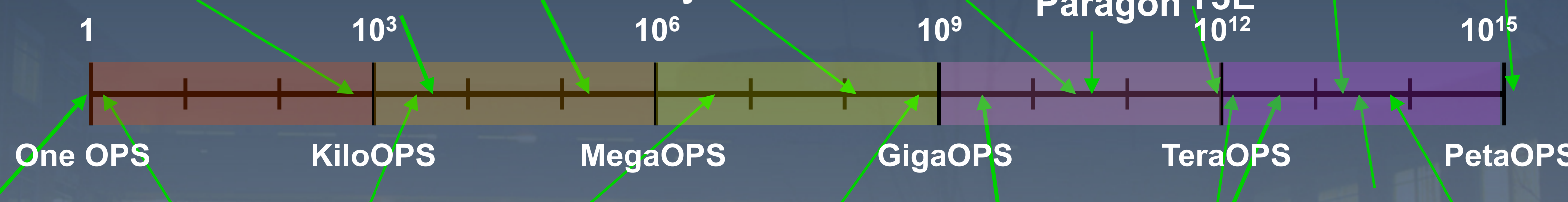
1991 Intel Delta

1995 Intel Paragon

1996 Cray T3E

2003 Cray X1

2008 Cray XT5




1823 Babbage Difference Engine

1943 Harvard Mark 1

1951 Univac 1

1964 CDC 6600

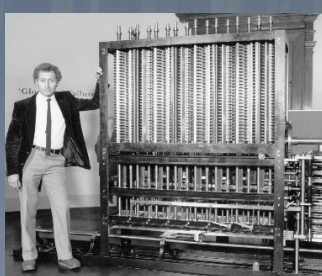
1982 Cray XMP

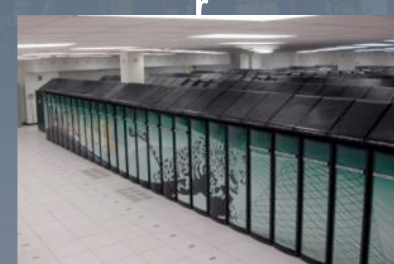
1988 Cray YMP

1997 ASCI Red

2001 Earth Simulato r

2005 Cray XT3





# OLCF resources

**October 2009 summary**

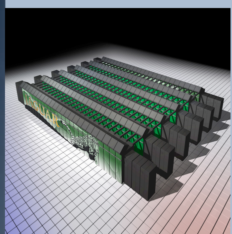
**6 Systems**

**Supercomputers**

**>265,000 cores**
**>360 TB Memory**

**>2,6 PFLOPS**

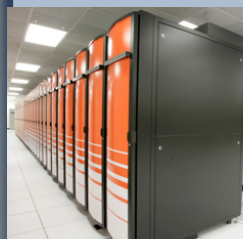
**CRAY XT5 JAGUAR**



(224,256)
2.6GHz
292 TB Memory

10,000 TB

**CRAY XT4 JAGUAR**



(31,328)
2.1GHz
61 TB Memory

750 TB

**IBM BLUE/GENE P**

(8192)
850 MHz
4 TB Memory

60 TB

**LINUX CLUSTER SMOKY**


(1280)
2.4 GHz
2.5 TB

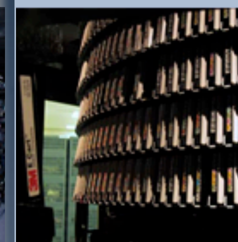
4.5 TB

**LINUX CLUSTER LENS**

(128)
2.2 GHz
128 GB

9 TB

**IBM HPSS**

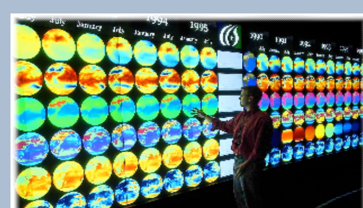


Many storage devices supported

Max. 30 PB

**Scientific visualization lab EVEREST**

27-projector PowerWall
35 million pixels



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# OLCF resources: Jaguar Supercomputer

Jaguar: World's Most Powerful Computer Designed for Science from the Ground Up


| | jaguar XT4 | jaguarpf XT5 |
|---|---|---|
| Peak Performance | 263.16 TFLOPS | 2.33 PFLOPS |
| System Memory | 61 TB | 292 TB |
| Disk Space | 750 TB | 10,000 TB |
| Disk Bandwidth | 44 GB/s | 240 GB/s |
| Interconnect Bandwidth | 157 TB/s | 374 TB/s |

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## OLCF resources: Visualization Facilities

- The visualization capabilities of OLCF include:
  - visualization/data analysis cluster called Lens
  - large PowerWall display called EVEREST
- Scientists can make use of the EVEREST facility by contacting any member of the visualization team and booking a time.

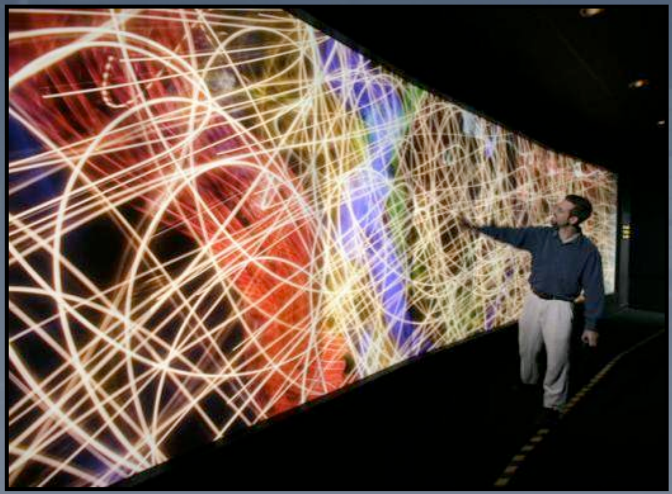
# OLCF resources: Lens

- Resource for data visualization
- 32 node Linux cluster dedicated to data analysis and high-end visualization
- Each node:
  - Four quad-core 2.3 GHz AMD Opteron processors
  - 64 GB memory
  - 2 NVIDIA 8800 GTX GPUs.

# OLCF resources: Visualization PowerWall (EVEREST)

EVEREST - Exploratory Visualization Environment for REsearch in Science and Technology

- 27-projector PowerWall
- Viewing at a 30 feet by 8 feet
- 11,520 by 3,072 pixels, or a total of 35 million pixels
- The wall is integrated with the rest of the computing center, creating a high-bandwidth data path between large-scale high-performance computing and large-scale data visualization.



- EVEREST is controlled by a 14 node cluster with GPUs for remote visualization.
- Each node contains four dual-core AMD Opteron processors.
- These 14 nodes have nVidia QuadroFX 3000G graphics cards connected to the projectors, providing a very-high-throughput visualization capability.

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# OLCF resources: High Performance Storage System (HPSS)

- HPSS is an archival Back-up system which consists of
  - two types of storage technology:
    - disk – "on-line" for frequently/recently accessed files
    - tape – "off-line" for very large or infrequently accessed files
  - Linux servers
  - High Performance Storage System software
- Tape storage is provided by robotic tape libraries.


- HPSS has three SL8500 tape libraries. Each can hold up to 10,000 cartridges.
- The StorageTek SL8500 libraries house a total of
  - twenty-four T10000A tape drives (500 gigabyte cartridges, uncompressed)
  - thirty-six T10000B tape drives (1 terabyte cartridges, uncompressed).
- Each drive has a bandwidth of 120 MB/s
- As of October, 2009, HPSS has 7.2 PB stored in over 16.1 million files.

# OLCF resources: Center-Wide File System (SPIDER)

"Spider" provides a shared, parallel file system for all LCF systems and based on Lustre file system

- Over 10 PB of RAID-6 Capacity
  - 13,440 1Gb SATA Drives (33 tons of discs)
  - 192 OSSs and 1344 OSTs (7 OSTs/OSS)
  - 3 Terabytes of memory
- Demonstrated bandwidth of over 200 GB/s
  - 30,000 files created per second
- Demonstrated stability on a number of LCF Systems
  - Over 26,000 lustre clients at OLCF mounting the file system and performing I/O
- Available from all systems via our high performance scalable I/O network
  - 4 InfiniBand core switches
  - Over 3,000 InfiniBand ports
  - Over 3 miles of cables


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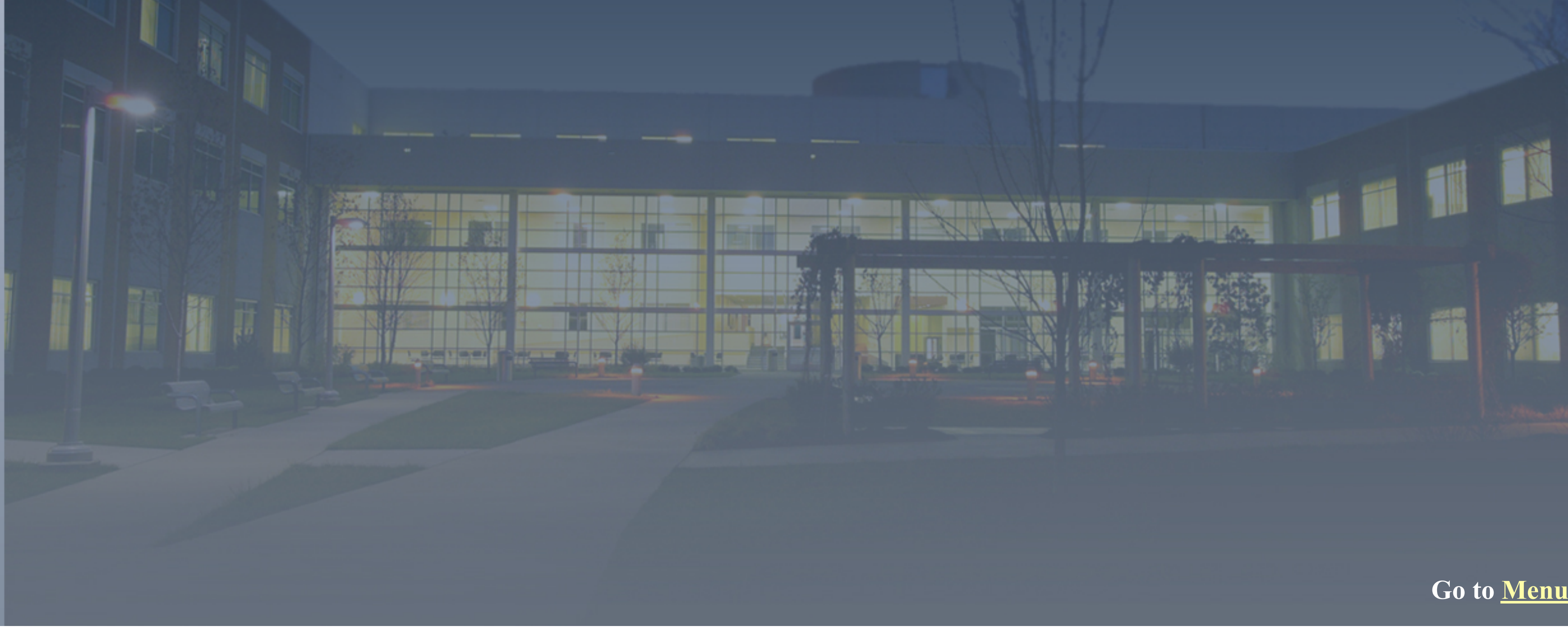
# A Quick Start Guide to OLCF JAGUAR System



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# Outline

# Jaguar System Overview: General Outline

Jaguar is a Cray XT system consisting of XT4 and XT5 partitions.

| Jaguar | XT4 | XT5 |
|---|---|---|
| **CPU Type** | 2.1 GHz Quad-core AMD Opteron (Budapest) | 2.6 GHz Hex-core AMD Opteron (Istanbul) |
| **Interconnect** | Cray SeaStar2 Router | Cray SeaStar2+ Router |
| **Switching Capacity (Router's Peak Bandwidth)** | 45.6GB/s 6 switch ports per Cray SeaStar chip, 7.6 GB/s each | 57.6GB/s 6 switch ports per Cray SeaStar2+ chip, 9.6 GB/s each |
| **Memory type** | DDR2-800 (some nodes use DDR2-667 memory) | DDR2-800 |
| **Memory Bandwidth** | 10.6 to 12.8 GB/sec per AMD Opteron | 21.2 GB/sec to 25.6 GB/sec per compute node |
| **Floor Space** | 1400 feet$^2$ | 4400 feet$^2$ |
| **Cooling Technology** | Air | Liquid |

# Jaguar System Overview: Summary of Resources

Jaguar is a Cray XT system consisting of XT4 and XT5 partitions

| Jaguar | XT4 | XT5 | Total |
|---|---|---|---|
| **Nodes per blade** | 4 | | |
| **CPUs per node**[1] | 1 | 2 | |
| **Cores per node** | 4 | 12 | |
| **Compute nodes**[2] | 7,832 | 18,688 | |
| **AMD Opteron cores** | 31,328 | 224,256 | 255,584 |
| **Memory per CPU** | 8 GB/CPU | | |
| **System Memory** | ~61.2 TB | ~292 TB | ~353.2 TB |
| **Disk Bandwidth** | ~44 GB/s | ~240 GB/s | ~284 GB/s |
| **Disk Space** | ~750 TB | ~10,000 TB | ~10,750 TB |
| **Interconnect Bandwidth** | ~157 TB/s | ~374 TB/s | ~532 TB/s |
| **Floor Space** | 1400 feet$^2$ | 4400 feet$^2$ | 5800 feet$^2$ |
| **Ideal Performance per core**[3] **(4 FLOPs/cycle times $2.1*10^9$ cycles/sec)** | 8.4 GFLOPS | 10.4 GFLOPS | |
| **Overall Ideal Performance** | ~263.16 TFLOPS | ~2.33 PFLOPS | ~2.60 PFLOPS |

[1] In the context of Jaguar CPU is also called a socket.
[2] Note that in addition to compute nodes Jaguar also has input/output (I/O) and login service nodes.
[3] FLOPs = **FL**oating point **OP**erations; FLOPS = **FL**oating point **O**perations **P**er **S**econd

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# Jaguar System Overview: System Software

- Operating system is Cray Linux Environment (CLE) 2.1:
  - Compute Nodes – Compute Node Linux (CNL)
  - Login/Service nodes – SUSE Linux
- Compilers
  - C/C++, Fortran
- MPI implementation
  - Cray MPI based on MPICH
- High Performance Storage System (HPSS) software

# Logging into Jaguar: Connection Requirements

- The only supported remote client on OLCF systems is a secure shell (SSH) client.
- The only supported authentication method is one-time passwords (OTP).

- UNIX-based operating systems generally have an SSH client built in.
- Windows users may obtain free clients online, such as PuTTY.

Any SSH client:

- must support the SSH-2 protocol (supported by all modern SSH clients).
- must allow keyboard-interactive authentication to access OLCF systems. For UNIX-based SSH clients, the following line should be in either the default ssh_config file or your $HOME/.ssh/config file:

```
PreferredAuthentications keyboard-interactive,password
```

The line may also contain other authentication methods, so long as keyboard-interactive is included.

# Logging into Jaguar: Connection Procedure

To connect to Jaguar from a UNIX-based system type the following in your terminal:

```
ssh userid@jaguar.ccs.ornl.gov
```

← Cray XT4

```
ssh userid@jaguarpf.ccs.ornl.gov
```

← Cray XT5

Enter PASSCODE: $\underbrace{\text{PIN}}_{\text{4-6 digits}} + \underbrace{\text{6 digits}}_{\text{Changes every 30 seconds}}$ from RSA® SecurID

OLCF RSA Key Fingerprints:

```
jaguar   0d:c9:db:37:55:da:41:26:55:4a:80:bb:71:55:dd:01
jaguarpf 80:58:21:03:96:47:1a:15:2c:25:d3:ca:e6:04:e8:a7
```

# Login Nodes

- When you login to Jaguar you will be placed on a "login node"
- Login nodes are used for basic tasks such as file editing, code compilation, data backup, and job submission
- These nodes provide a full SUSE Linux environment, complete with compilers, tools, and libraries
- The login nodes should not be used to run production jobs. Production work should be performed on the systems compute resources.
- Serial jobs (post-processing, *etc*) may be run on the compute nodes as long as they are statically linked (will be discussed later)

# Compute (Batch) Nodes

- All MPI/OpenMP user applications execute on batch or compute nodes
- Batch nodes provide **limited** Linux environment – Compute Node Linux (CNL)
- Compute nodes can see only the Lustre scratch directories
- Access to compute resources is managed by the PBS/TORQUE – batch system manager
- Job scheduling is handled by Moab, which interacts with PBS/TORQUE and the XT system software.

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# File Systems: Basics

- The Network File Service (NFS) server contains user's home directories, project directories, and software directories.
- Compute nodes can only see the Lustre work space
  - The NFS-mounted home, project, and software directories are not accessible to the compute nodes.
- Shared Lustre area (SPIDER) is now available on compute nodes and is the only scratch area for the XT5.
- Executables must be executed from within the Lustre work space:
  - `/tmp/work/$USER` (XT4 and XT5)
  - `/lustre/scr144/$USER` (XT4 only)
- Batch jobs can be submitted from the home or work space. If submitted from a user's home area, a batch script should cd into the Lustre work space directory (`cd $PBS_O_WORKDIR`) prior to running the executable through aprun.
- All input must reside in the Lustre work space
- All output must also be sent to the Lustre work space

# File Systems: User's Directories

*Each user is provided the following space resources:*

- Home directory - NFS Filesystem
  `/ccs/home/$USER`
- Work directory/Scratch space - Lustre Filesystem
  `/tmp/work/$USER`
- Project directory - NFS Filesystem
  `/ccs/proj/projectid`
- HPSS storage

## Software Environment: Modules

- Software is loaded, unloaded or swapped using modules.

- Use of modules allows software, libraries, paths, etc. to be cleanly entered into and removed from your programming environment.

- Conflicts are detected and module loads that would cause conflicts are not allowed.

# Software Environment: `module` command

## Loading Commands

- **`module [load||unload] my_module`**
  - Loads/Unloads module *`my_module`*
  - e.g., `module load subversion`
- **`module swap module#1 module#2`**
  - Replaces *`module#1`* with *`module#2`*
  - e.g., `module swap PrgEnv-pgi PrgEnv-gnu`

## Informational Commands

- **`module help my_module`**
  - Lists available commands and usage
- **`module show my_module`**
  - Displays the actions upon loading `my_module`
- **`module list`**
  - Lists all loaded modules
- **`module avail [name]`**
  - Lists all modules [beginning with *`name`*]
  - e.g., `module avail gcc`

# Compiling: System Compilers

The following compilers should be used to build codes on Jaguar.

| Language | Compiler |
| --- | --- |
| C | `cc` |
| C++ | `CC` |
| Fortran 77, 90 and 95 | `ftn` |

Note that `cc`, `CC` and `ftn` are actually the Cray XT Series wrappers for invoking the PGI, GNU, Intel, Cray, or Pathscale compilers (discussed later…)

# Compiling: Default Compilers

- Default compiler is PGI. The list of all packages is obtained by
  - `module avail PrgEnv`

- To use the Cray wrappers with other compilers the programming environment modules need to be swapped, i.e.
  - `module swap PrgEnv-pgi PrgEnv-gnu`
  - `module swap PrgEnv-pgi PrgEnv-cray`

- To just use the GNU/Cray compilers directly load the GNU/Cray module you want:
  - `module load PrgEnv-gnu/2.1.50HD`
  - `module load PrgEnv-cray/1.0.1`

- It is possible to use the GNU compiler versions directly without loading the Cray Programming Environments, but note that the Cray wrappers will probably not work as expected if you do that.

# Compiling: Useful Compiler Flags (PGI)

## General:

| Flag | Comments |
| --- | --- |
| **`-mp=nonuma`** | Compile multithreaded code using OpenMP directives |

## Debugging:

| Flag | Comments |
| --- | --- |
| **`-g`** | For debugging symbols; put first |
| **`-Ktrap=fp`** | Trap floating point exceptions |
| **`-Mchkptr`** | Checks for unintended dereferencing of null pointers |

## Optimization:

| Flag | Comments |
| --- | --- |
| **`-Minfo`** | Provides info on compiler performed optimizations |
| **`-Mneginfo`** | Instructs the compiler to produce information on why certain optimizations are not performed. |
| **`-fast`** | Equivalent to **`-Mvect=sse -Mscalarsse -Mcache_align -Mflushz`** |
| **`-fastsse`** | Same as **`-fast`** |
| **`-Mcache_align`** | Makes certain that arrays are on cache line boundaries |
| **`-Munroll=c:`*`n`*** | Unrolls loops ***n*** times (e.g., ***n***=4) |
| **`-Mipa=fast,inline`** | Enables interprocedural analysis (IPA) and inlining, benefits for C++ and Fortran |
| **`-Mconcur`** | Automatic parallelization |

# Running Jobs: Introduction

- When you log into Jaguar, you are placed on one of the login nodes.
- Login nodes should be used for basic tasks such as file editing, code compilation, data backup, and job submission.
- The login nodes should not be used to run production jobs. Production work should be performed on the system's compute resources.
- On Jaguar, access to compute resources is managed by the PBS/TORQUE. Job scheduling and queue management is handled by Moab which interacts with PBS/TORQUE and the XT system software.
- Users either submit the job scripts for batch jobs, or submit a request for interactive job.
- The following pages provide information for getting started with the batch facilities of PBS/TORQUE with Moab as well as basic job execution.

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# Running Jobs: Batch Scripts

- Batch scripts can be used to run a set of commands on a systems compute partition.
- The batch script is a shell script containing PBS flags and commands to be interpreted by a shell.
- Batch scripts are submitted to the batch manager, PBS, where they are parsed. Based on the parsed data, PBS places the script in the queue as a job.
- Once the job makes its way through the queue, the script will be executed on the head node of the allocated resources.

# Running Jobs: Example Batch Script

```
1: #!/bin/bash
2: #PBS -A XXXYYY
3: #PBS -N test
4: #PBS -j oe
5: #PBS -l walltime=1:00:00,size=192
6:
7: cd $PBS_O_WORKDIR
8: date
9: aprun -n 192 ./a.out
```

NOTE: Since users cannot share nodes, size requests must be
- Шa multiple of 4 on the XT4 or
- Шa multiple of 12 on the XT5.

This batch script can be broken down into the following sections:

- Shell interpreter
  - Line 1
  - Can be used to specify an interpreting shell.
- PBS commands
  - The PBS options will be read and used by PBS upon submission.
  - Lines 2–5
    - 2: The job will be charged to the XXXYYY project.
    - 3: The job will be named “test.”
    - 4: The jobs standard output and error will be combined.
    - 5: The job will request 192 cores for 1 hour.
  - Please see the PBS Options page for more options.
- Shell commands
  - Once the requested resources have been allocated, the shell commands will be executed on the allocated nodes head node.
  - Lines 6–9
    - 6: This line is left blank, so it will be ignored.
    - 7: This command will change directory into the script's submission directory. We assume here that the job was submitted from a directory in /lustre/scratch/.
    - 8: This command will run the date command.
    - 9: This command will run the executable a.out on 192 cores with a.out.

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# Running Jobs: Submitting Batch Jobs - `qsub`

- To submit the batch script named `test.pbs` do:

```
qsub test.pbs
```

- All job resource management handled by Torque.
- Batch scripts can be submitted for execution using the `qsub` command.
- If successfully submitted, a PBS job ID will be returned. This ID can be used to track the job.

# Running Jobs: Interactive Batch Jobs

- Batch scripts are useful for submitting a group of commands, allowing them to run through the queue, then viewing the results. It is also often useful to run a job interactively. However, users are not allowed to directly run on compute resources from the login module. Instead, users must use a batch-interactive PBS job. This is done by using the `-I` option to `qsub`.
- For interactive batch jobs, PBS options are passed through `qsub` on the command line:

```
qsub -I -A XXXYYY -q debug -V -l size=24,walltime=1:00:00
```

This request will…

| | |
|---|---|
| `-I` | Start an interactive session |
| `-A` | Charge to the "XXXYYY" project |
| `-q debug` | Run in the debug queue |
| `-V` | Import the submitting users environment |
| `-l size=24,walltime=1:00:00` | Request 24 compute cores for one hour |

# Running Jobs: Altering Batch Jobs – `qdel`, `qhold`, `qrls`

- Command: `qdel`
  - Jobs in the queue in any state can be stopped and removed from the queue using the command qdel.
  - For example, to remove a job with a PBS ID of 1234, use the following command: `qdel 1234`

- Command: `qhold`
  - Jobs in the queue in a non-running state may be placed on hold using the qhold command. Jobs placed on hold will not be removed from the queue, but they will not be eligible for execution.
  - For example, to move a currently queued job with a PBS ID of 1234 to a hold state, use the following command: `qhold 1234`

- Command: `qrls`
  - Once on hold the job will not be eligible to run until it is released to return to a queued state. The qrls command can be used to remove a job from the held state.
  - For example, to release job 1234 from a held state, use the following command: `qrls 1234`

# Running Jobs: Monitoring Job Status - `qstat`

PBS and Moab provide multiple tools to view queue, system, and job statuses.
Command: `qstat`
Use `qstat -a` to check the status of submitted jobs:

```
nid00004:
                                                          Req'd  Req'd    Elap
Job ID Username Queue Jobname SessID NDS Tasks Memory Time   S Time
------ -------- ----- ------- ------ --- ----- ------ -----  - -----
29668   user1   batch job2    21909   1  256   --     08:00 R 02:28
29894   user2   batch run128   --     1  128   --     02:30 Q --
29895   user3   batch STDIN   15921   1  1     --     01:00 R 00:10
29896   user2   batch jobL    21988   1  2048  --     01:00 R 00:09
29897   user4   debug STDIN   22367   1  2     --     00:30 R 00:06
29898   user1   batch job1    25188   1  1     --     01:10 C 00:00
```

| | |
|---|---|
| **Job ID** | PBS assigned job ID. |
| **Username** | Submitting user's user ID. |
| **Queue** | Queue into which the job has been submitted. |
| **Jobname** | PBS job name. This is given by the PBS -n option in the PBS batch script. Or, if the -n option is not used, PBS will use the name of the batch script. |
| **SessID** | Associated session ID. |
| **NDS** | PBS node count. Not accurate; will be one. |
| **Tasks** | Number of cores requested by the job's -size option. |
| **Req'd Memory** | Job's requested memory. |
| **Req'd Time** | Job's given wall time. |
| **S** | Job's current status. See the status listings below. |
| **Elap Time** | Job's time spent in a running status. If a job is not currently or has not been in a run state, the field will be blank. |

| **Status Value** | **Meaning** |
|---|---|
| E | Exiting after having run |
| H | Held |
| Q | Queued; eligible to run |
| R | Running |
| S | Suspended |
| T | Being moved to new location |
| W | Waiting for its execution time |
| C | Recently completed (within the last 5 minutes) |

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# Running Jobs: `showq, checkjob`

Command : `showq`

The Moab utility `showq` gives a more detailed description of the queue and displays it in the following states:

**Active** These jobs are currently running.

**Eligible** These jobs are currently queued awaiting resources. A user is allowed five jobs in the eligible state.

**Blocked** These jobs are currently queued but are not eligible to run. Common reasons for jobs in this state are jobs on hold, the owning user currently having five jobs in the eligible state, and running jobs in the longsmall queue.

Command : `checkjob`

The Moab utility `checkjob` can be used to view details of a job in the queue.

For example, if job 736 is a job currently in the queue in a blocked state, the following can be used to view why the job is in a blocked state:

`checkjob 736` The return may contain a line similar to the following:

```
BlockMsg: job 736 violates idle HARD MAXJOB limit of 2 for
        user (Req: 1 In Use: 2)
```

This line indicates the job is in the blocked state because the owning user has reached the limit of two jobs currently in the eligible state.

# Running Jobs: `showstart, showbf, xtprocadmin`

Command : `showstart`

The Moab utility `showstart` gives an estimate of when the job will start.

```
showstart 100315
job 100315 requires 16384 procs for 00:40:00
Estimated Rsv based start in 15:26:41 on Fri Sep 26
23:41:12
Estimated Rsv based completion in 16:06:41 on Sat Sep 27
00:21:12
```

Since the start time may change dramatically as new jobs with higher priority are submitted, so you need to periodically rerun the command.

Command : `showbf`

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. As such, it is primarily useful for small jobs. This command incorporates down time, reservations, and node state information in determining the available backfill window.

# Running Jobs: Job Execution - `aprun`

- By default, commands will be executed on the job's associated service node.
- The `aprun` command is used to execute a job on one or more compute nodes.
- The XT's layout should be kept in mind when running a job using `aprun`. The XT5 partition currently contains two hex-core processors (a total of 12 cores) per compute node. While the XT4 partition currently contains one quad-core processor (a total of 4 cores) per compute node.
- The `PBS size` option requests compute cores.

# Running Jobs: Basic `aprun` options

| Option | Description |
|---|---|
| `-D` | Debug (shows the layout aprun will use) |
| `-n` | Number of MPI tasks.<br>Note: If you do not specify the number of tasks to aprun, the system will default to 1. |
| `-N` | Number of tasks per Node. (XT5: 1 – 12) and (XT4: 1 – 4)<br>NOTE: Recall that the XT5 has two Opterons per compute node. On the XT5, to place one task per quad-core Opteron, use -S 1 (not -N 1 as on the XT4). On the XT4, because there is only one Opteron per node, the -S 1 and -N1 will result in the same layout. |
| `-m` | Memory required per task. Default:<br>4-core, 8-GB Cray XT4 nodes (8 GB / 4 CPUs = 2 GB)<br>XT4: A maximum of 2GB per core; 2.1GB will allocate two cores for the task |
| `-d` | Number of threads per MPI task.<br>Note: As of CLE 2.1, this option is very important. If you specify OMP_NUM_THREADS but do not give a -d option, aprun will allocate your threads to a single core. You must use OMP_NUM_THREADS to specify the number of threads per MPI task, and you must use -d to tell aprun how to place those threads. |
| `-S` | Number of PEs to allocate per NUMA node. |
| `-ss` | Strict memory containment per NUMA node. |

# Running Jobs: XT5 example

`aprun -n 24 ./a.out` will run a.out across 24 cores. This requires two compute nodes. The MPI task layout would be as follows:

| Compute Node 0 | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Opteron 0 | | | | | | | Opteron 1 | | | | | |
| Core 0 | Core 1 | Core 2 | Core 3 | Core 4 | Core 5 | | Core 0 | Core 1 | Core 2 | Core 3 | Core 4 | Core 5 |
| 0 | 1 | 2 | 3 | 4 | 5 | | 6 | 7 | 8 | 9 | 10 | 11 |

| Compute Node 1 | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Opteron 0 | | | | | | | Opteron 1 | | | | | |
| Core 0 | Core 1 | Core 2 | Core 3 | Core 4 | Core 5 | | Core 0 | Core 1 | Core 2 | Core 3 | Core 4 | Core 5 |
| 12 | 13 | 14 | 15 | 16 | 17 | | 18 | 19 | 20 | 21 | 22 | 23 |

The following will place tasks in a round robin fashion.

```
> setenv MPICH_RANK_REORDER_METHOD 0
> aprun -n 24 a.out
```

```
Rank 0,  Node 0, Opteron 0, Core 0
Rank 1,  Node 1, Opteron 0, Core 0
Rank 2,  Node 0, Opteron 0, Core 1
Rank 3,  Node 1, Opteron 0, Core 1
Rank 4,  Node 0, Opteron 0, Core 2
Rank 5,  Node 1, Opteron 0, Core 2
Rank 6,  Node 0, Opteron 0, Core 3
Rank 7,  Node 1, Opteron 0, Core 3
Rank 8,  Node 0, Opteron 0, Core 4
Rank 9,  Node 1, Opteron 0, Core 4
Rank 10, Node 0, Opteron 0, Core 5
Rank 11, Node 1, Opteron 0, Core 5
Rank 12, Node 0, Opteron 1, Core 0
Rank 13, Node 1, Opteron 1, Core 0
Rank 14, Node 0, Opteron 1, Core 1
Rank 15, Node 1, Opteron 1, Core 1
Rank 16, Node 0, Opteron 1, Core 2
Rank 17, Node 1, Opteron 1, Core 2
Rank 18, Node 0, Opteron 1, Core 3
Rank 19, Node 1, Opteron 1, Core 3
Rank 20, Node 0, Opteron 1, Core 4
Rank 21, Node 1, Opteron 1, Core 4
Rank 22, Node 0, Opteron 1, Core 5
Rank 23, Node 1, Opteron 1, Core 5
```

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# Running Jobs: Threads

- The system supports threaded programming within a compute node.
- On the XT5, threads may span both Opterons within a single compute node, but cannot span compute nodes.
- Users have a great deal of flexibility in thread placement. Several examples are shown below.
- Note: Under CNL 2.1, threaded codes must use the

  `aprun -d depth` option

  The -d option specifies the number of threads per task. Without the option all threads will be started on the same core. Under previous CNL versions the option was not required. The number of cores used is calculated by multiplying the value of -d by the value of -n.
- Focus of this discussion will be OpenMP threads

# Running Jobs: Threads – XT5 Example

- Example: Launch 4 MPI tasks, each with 6 threads. Place 1 MPI task per Opteron (this requests 2 compute nodes and requires a size request of 24):

```
export OMP_NUM_THREADS=6
> aprun -n4 -d6 -S1 a.out
Rank 0, Thread 0, Node 0, Opteron 0, Core 0 <-- MASTER
Rank 0, Thread 1, Node 0, Opteron 0, Core 1 <-- slave
Rank 0, Thread 2, Node 0, Opteron 0, Core 2 <-- slave
Rank 0, Thread 3, Node 0, Opteron 0, Core 3 <-- slave
Rank 0, Thread 4, Node 0, Opteron 0, Core 4 <-- slave
Rank 0, Thread 5, Node 0, Opteron 0, Core 5 <-- slave
Rank 1, Thread 0, Node 0, Opteron 1, Core 0 <-- MASTER
Rank 1, Thread 1, Node 0, Opteron 1, Core 1 <-- slave
Rank 1, Thread 2, Node 0, Opteron 1, Core 2 <-- slave
Rank 1, Thread 3, Node 0, Opteron 1, Core 3 <-- slave
Rank 1, Thread 4, Node 0, Opteron 1, Core 4 <-- slave
Rank 1, Thread 5, Node 0, Opteron 1, Core 5 <-- slave
Rank 2, Thread 0, Node 1, Opteron 0, Core 0 <-- MASTER
Rank 2, Thread 1, Node 1, Opteron 0, Core 1 <-- slave
Rank 2, Thread 2, Node 1, Opteron 0, Core 2 <-- slave
Rank 2, Thread 3, Node 1, Opteron 0, Core 3 <-- slave
Rank 2, Thread 4, Node 1, Opteron 0, Core 4 <-- slave
Rank 2, Thread 5, Node 1, Opteron 0, Core 5 <-- slave
Rank 3, Thread 0, Node 1, Opteron 1, Core 0 <-- MASTER
Rank 3, Thread 1, Node 1, Opteron 1, Core 1 <-- slave
Rank 3, Thread 2, Node 1, Opteron 1, Core 2 <-- slave
Rank 3, Thread 3, Node 1, Opteron 1, Core 3 <-- slave
Rank 3, Thread 4, Node 1, Opteron 1, Core 4 <-- slave
Rank 3, Thread 5, Node 1, Opteron 1, Core 5 <-- slave
```

# Third-Party Software

- OLCF has installed many third-party software packages, libraries, etc., and created module files for them
  - Third-party applications (e.g., MATLAB, GAMESS)
  - Latest versions or old versions not supported by vendor (e.g., fftw/3.1.2)
  - Suboptimal versions to do proof-of-concept work (e.g., blas/ref)
  - Debug versions (e.g., petsc/2.3.3-debug)
- OLCF modules available via `module load` command, installed in `/sw/xt/` directory

# Debugging and Profiling

The following tools are availably on Jaguar for debugging and profiling:

| Debugging | Profiling and Analysis |
|---|---|
| DDT, TotalView | Cray PAT, Apprentice2, PAPI, TAU etc. |

Always check the compatibility of the compiler options you want to use.

# Information Resources for Users

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# Resources for Users: Getting Started

- About Jaguar

  http://www.nccs.gov/computing-resources/jaguar/

- Quad Core AMD Opteron Processor Overview

  http://www.nccs.gov/wp-content/uploads/2008/04/amd_craywkshp_apr2008.pdf

- PGI Compilers for XT5

  http://www.nccs.gov/wp-content/uploads/2008/04/compilers.ppt

- OLCF Training & Education – archives of OLCF workshops and seminar series, HPC/ parallel computing references

  http://www.nccs.gov/user-support/training-education/

- 2009 Cray XT5 Quad-core Workshop

  http://www.nccs.gov/user-support/training-education/workshops/2008-cray-xt5-quad-core-workshop/

# Resources for Users: Advanced Topics

- Debugging Applications Using TotalView

  http://www.nccs.gov/user-support/general-support/software/totalview

- Debugging Applications Using DDT

  http://www.nccs.gov/computing-resources/jaguar/software/?software=ddt

- Using Cray Performance Tools - CrayPat

  http://www.nccs.gov/computing-resources/jaguar/debugging-optimization/cray-pat/

- I/O Tips for Cray XT4

  http://www.nccs.gov/computing-resources/jaguar/debugging-optimization/io-tips/

- OLCF Software

  http://www.nccs.gov/computing-resources/jaguar/software/

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- About Jaguar

  http://www.nccs.gov/computing-resources/jaguar/

- Quad Core AMD Opteron Processor Overview

  http://www.nccs.gov/wp-content/uploads/2008/04/amd_craywkshp_apr2008.pdf

- PGI Compilers for XT5

  http://www.nccs.gov/wp-content/uploads/2008/04/compilers.ppt

- OLCF Training & Education – archives of OLCF workshops and seminar series, HPC/ parallel computing references

  http://www.nccs.gov/user-support/training-education/

- 2009 Cray XT5 Quad-core Workshop

  http://www.nccs.gov/user-support/training-education/workshops/2008-cray-xt5-quad-core-workshop/

# Information Resources for Users: Advanced Topics

- Debugging Applications Using TotalView

  http://www.nccs.gov/user-support/general-support/software/totalview

- Using Cray Performance Tools - CrayPat

  http://www.nccs.gov/computing-resources/jaguar/debugging-optimization/cray-pat/

- I/O Tips for Cray XT4

  http://www.nccs.gov/computing-resources/jaguar/debugging-optimization/io-tips/

- OLCF Software

  http://www.nccs.gov/computing-resources/jaguar/software/

- Cray Documentation

  http://docs.cray.com/

## Resources for Users: More Information

- OLCF website

  http://www.nccs.gov/

- How to obtain Access to OLCF Resources

  http://www.nccs.gov/user-support/access/

- Contact us

  help@nccs.gov