Welcome! We will begin soon.

- Please set your microphone to ‘mute’ unless you are asking a question.
- Please leave your camera ON so our speakers can better interact with you.
- This BlueJeans videoconference is meant to be interactive. If you have a question for the presenter, please unmute your mic and speak or post to chat. You may also hold your question for the end of the topic.
- Sessions may be recorded for future playback online.
- BlueJeans software support: please email tdonnelly@anl.gov or call 1-630-899-9044
- CRYPTOCard token or ALCF resource support: please email support@alcf.anl.gov
- We will use Cetus or Vesta for the hands-on. Please make sure you can log in:
  - > ssh username@cetus.alcf.anl.gov or > ssh username@vesta.alcf.anl.gov
Welcome to
Getting Started at the ALCF
Agenda

- **Part I**
  - Blue Gene/Q hardware overview
  - Building your code
  - Considerations before you run
  - Hands-on session

- **Part II**
  - Queuing and running
  - After your job is submitted
  - Potential problems
  - Hands-on session
Part I
Section:

Blue Gene/Q hardware overview
**ALCF resources**

- **Mira** (Production) – IBM Blue Gene/Q
  - 49,152 nodes / 786,432 cores
  - 768 TB of memory
  - Peak flop rate: 10 PF
  - Linpack flop rate: 8.1 PF

- **Cetus** (Test & Devel.) – IBM Blue Gene/Q
  - 4,096 nodes / 65,536 cores
  - 64 TB of memory
  - 838 TF peak flop rate

- **Vesta** (Test & Devel.) – IBM Blue Gene/Q
  - 2,048 nodes / 32,768 cores
  - 32 TB of memory
  - 419 TF peak flop rate

- **Cooley** (Visualization) – Cray + NVIDIA
  - 126 nodes / 1512 x86 cores (Haswell)
  - 126 NVIDIA Tesla K80 GPUs
  - 47 TB x86 memory / 3 TB GPU memory
  - 293 TF peak flop rate

- **Storage**
  - Scratch: 27 PB usable capacity, 330 GB/s bw (GPFS) aggregate over 2 file systems
  - Home: 1.1 PB usable capacity, 45 GB/s bw (GPFS)
ALCF Resources

**Mira**
- 48 racks/768K cores
- 768 TB RAM
- 10 PF

**Cetus (Dev)**
- 4 rack/64K cores
- 64 TB RAM
- 838 TF

**Cooley (Viz)**
- 126 nodes/1512 cores
- 126 NVIDIA GPUs
- 47 x86 TB / 3 TB GPU RAM
- 293 TF

**Networks – 100Gb**
- (via ESnet, internet2, UltraScienceNet, )

**Vesta (Dev)**
- 2 racks/32K cores
- 32TB RAM
- 419 TF

**Mira-fs1**
- (6) DDN 12Ke couplets
- 7 PB (usable), 90 GB/s

**Mira-fs0**
- (16) DDN 12Ke couplets
- 20 PB (usable), 240 GB/s

**Mira-home**
- (3) DDN 12Ke couplets
- 1.1 PB (usable), 45 GB/s

**HPSS**
- (2) Spectralogic T-950
- 10,000 slot libraries
- (48) LTO6 Tape Drives

**DTN**
- (1) DDN 12Ke – 600 TB (raw), 15 GB/s
Blue Gene Features

- **Low speed, low power**
  - Embedded PowerPC core with custom SIMD floating point extensions
  - Low frequency: 1.6 GHz on Blue Gene/Q

- **Massive parallelism**
  - Many cores: 786,432 on Mira

- **Fast communication network(s)**
  - 5D Torus network on Blue Gene/Q

- **Balance**
  - Processor, network, and memory speeds are well balanced

- **Minimal system overhead**
  - Simple lightweight OS (CNK) minimizes noise

- **Standard programming models**
  - Fortran, C, C++ & Python languages supported
  - Provides MPI, OpenMP, and Pthreads parallel programming models

- **System-on-a-Chip (SoC) & Custom designed ASIC (Application Specific Integrated Circuit)**
  - All node components on one chip, except for memory
  - Reduces system complexity and power, improves price / performance

- **High reliability**
  - Sophisticated RAS (Reliability, Availability, and Serviceability)

- **Dense packaging**
  - 1024 nodes per rack
Blue Gene/Q

**Chip**
- 16+2 cores

**Module**
- Single chip

**Compute card**
- One single chip module
- 16 GB DDR3 Memory
- Heat Spreader for H₂O Cooling

**Node board**
- 32 compute cards, optical Modules, link chips; 5D Torus

**Rack**
- 1 or 2 midplanes
- 0, 1, 2, or 4 I/O drawers

**Midplane**
- 16 node boards

**Multi-rack system**
- *Mira*: 48 racks, 10 PF/s

81 inches tall
Blue Gene/Q system components

- **Front-end nodes** – dedicated for user’s to login, compile programs, submit jobs, query job status, debug applications. **RedHat Linux OS.**

- **Service nodes** – perform partitioning, monitoring, synchronization and other system management services. Users do not run on service nodes directly.

- **I/O nodes** – provide a number of Linux/Unix typical services, such as files, sockets, process launching, signals, debugging; run Linux.

- **Compute nodes** – run user applications, use simple **compute node kernel (CNK)** operating system, ships I/O-related system calls to I/O nodes.
# Partition dimensions on Blue Gene/Q systems

## Mira

<table>
<thead>
<tr>
<th>Nodes</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>512</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>1024</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>2048</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>4096</td>
<td>4/8</td>
<td>4</td>
<td>8/4</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>8192</td>
<td>4</td>
<td>4</td>
<td>16</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>12288</td>
<td>8</td>
<td>4</td>
<td>12</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>16384</td>
<td>4/8</td>
<td>8/4</td>
<td>16</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>24576</td>
<td>4</td>
<td>12</td>
<td>16</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>32768</td>
<td>8</td>
<td>8</td>
<td>16</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>49152</td>
<td>8</td>
<td>12</td>
<td>16</td>
<td>16</td>
<td>2</td>
</tr>
</tbody>
</table>

## Cetus

<table>
<thead>
<tr>
<th>Nodes</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>128</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>256</td>
<td>4</td>
<td>2</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>512</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>1024</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>2048</td>
<td>4/8</td>
<td>4/4</td>
<td>8/4</td>
<td>8/8</td>
<td>2</td>
</tr>
<tr>
<td>4096(*)</td>
<td>8</td>
<td>4</td>
<td>8</td>
<td>8</td>
<td>2</td>
</tr>
</tbody>
</table>

## Vesta

<table>
<thead>
<tr>
<th>Nodes</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>64</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>2</td>
<td>2</td>
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<tr>
<td>128</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>256</td>
<td>4</td>
<td>2</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>512</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>1024</td>
<td>4</td>
<td>4</td>
<td>4/8</td>
<td>8/4</td>
<td>2</td>
</tr>
<tr>
<td>2048(*)</td>
<td>4</td>
<td>4</td>
<td>8</td>
<td>8</td>
<td>2</td>
</tr>
</tbody>
</table>

**Command:** `partlist`


(*) Partition not active.
Mira multiple rack partitions ("blocks")

The number of large block sizes possible is:

<table>
<thead>
<tr>
<th># of nodes</th>
<th># of blocks</th>
</tr>
</thead>
<tbody>
<tr>
<td>49152</td>
<td>1</td>
</tr>
<tr>
<td>32768</td>
<td>3</td>
</tr>
<tr>
<td>24576</td>
<td>2</td>
</tr>
<tr>
<td>16384</td>
<td>9</td>
</tr>
<tr>
<td>12288</td>
<td>12</td>
</tr>
<tr>
<td>8192</td>
<td>6</td>
</tr>
<tr>
<td>4096</td>
<td>12</td>
</tr>
<tr>
<td>2048</td>
<td>24</td>
</tr>
<tr>
<td>1024</td>
<td>64</td>
</tr>
<tr>
<td>512</td>
<td>96</td>
</tr>
</tbody>
</table>


partlist will show you if a large free block is busy due to a wiring dependency
### Minimum partition sizes on Blue Gene/Q systems

<table>
<thead>
<tr>
<th>System</th>
<th>Racks</th>
<th>Minimum Partition Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mira</td>
<td>48</td>
<td>512 nodes</td>
</tr>
<tr>
<td>Cetus</td>
<td>4</td>
<td>128 nodes</td>
</tr>
<tr>
<td>Vesta</td>
<td>2</td>
<td>32 nodes</td>
</tr>
</tbody>
</table>
Questions?
Section:

Building your code
SoftEnv

- A tool for managing a user’s environment
  - Sets your PATH to access desired front-end tools
  - Your compiler version can be changed here

- Settings:
  - Maintained in the file ~/.soft (Mira/Cetus & Vesta) or ~/.soft.cooley (Cooley)
  - Add/remove keywords from ~/.soft or ~/.soft.cooley to change environment
  - Make sure @default is at the very end

- Commands:
  - softenv
    - A list of all keywords defined on the systems
  - resoft
    - Reloads initial environment from ~/.soft or ~/.soft.cooley file
  - soft add|remove keyword
    - Temporarily modify environment by adding/removing keywords

Using compiler wrappers

- **IBM XL cross-compilers:**
  - SoftEnv key: +mpiwrapper-xl
  - Non-thread-safe: mpixlc, mpixlcxx, mpixlf77, mpixlf90, mpixlf95, mpixlf2003, etc.
  - Thread-safe (add _r suffix): mpixlc_r, mpixlcxx_r, mpixlf77_r, etc.
  - “-show” option: shows complete command used to invoke compiler. E.g.: `> mpixlc -show`

- **GNU cross-compilers:**
  - SoftEnv key: +mpiwrapper-gcc
  - mpicc, mpicxx, mpif77, mpif90

- **CLANG cross-compilers:**
  - SoftEnv key: +mpiwrapper-bgclang
  - mpiclang, mpiclang++, mpiclang++11

http://www.alcf.anl.gov/user-guides/software-and-libraries
# IBM XL Optimization Settings Options

<table>
<thead>
<tr>
<th>Level</th>
<th>Implies</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>-O0</td>
<td>-qstrict -qfloat=nofltint:norsqrt:rngchk -qstrict_induction</td>
<td>Preserves program semantics, minimal optimization. <strong>Best for debugging</strong></td>
</tr>
<tr>
<td>-O2 (or -O)</td>
<td>-qstrict -qfloat=nofltint:norsqrt:rngchk -qnostrict_induction -qmaxmem=8192</td>
<td>Preserves program semantics, eliminates redundant code, basic loop optimization. <strong>Good for correctness check, baseline performance</strong></td>
</tr>
<tr>
<td>-O3</td>
<td>-qnostrict -qfloat=fltint:rsqrt:norngchk -qnostrict_induction -qmaxmem=-1 -qhot=level=0</td>
<td>High order loop analysis and transformations, better loop scheduling, inlining, in-depth memory access analysis. <strong>Can alter program semantics unless used with -qstrict</strong></td>
</tr>
<tr>
<td>-O4</td>
<td><strong>All -O3 options plus</strong> -qhot=level=1 -qhot=vector -qipa=level=1</td>
<td>Additional loop analysis, basic interprocedural optimization.</td>
</tr>
<tr>
<td>-O5</td>
<td><strong>All -O4 options plus</strong> -qipa=level=2</td>
<td>Advanced interprocedural analysis (IPA).</td>
</tr>
</tbody>
</table>
IBM XL Optimization Tips

Tips:
- **qlistopt** generates a listing with all flags used in compilation
- **qreport** produces a listing, shows how code was optimized
- Performance can decrease at higher levels of optimization, especially at -O4 or -O5
- May specify different optimization levels for different routines/files
- The compiler option ‘-g’ must be used to resolve the code line numbers in the debugger
Threading

- **OpenMP** is supported
  - IBM XL compilers: `-qsmp=omp:noauto`
  - GNU: `-fopenmp`
  - BGCLANG: `-fopenmp`

- **Pthreads** is supported
  - NPTL Pthreads implementation in glibc requires no modifications

- Compiler **auto thread parallelization** is available
  - Use `-qsmp=auto`
  - Not always effective

- The runjob mode will determine maximum total number of threads (including the master thread)
  - `runjob --ranks-per-node` (or for non-script jobs, `qsub --mode`)
  - Maximum 4 threads per core
  - Each core needs at least 2 (possibly more) threads for peak efficiency
OpenMP

- Shared-memory parallelism is supported within a single node

- Hybrid programming model
  - MPI at outer level, across compute nodes
  - OpenMP at inner level, within a compute node

- For XL compilers, thread-safe compiler version should be used (mpixlc_r etc.) with any threaded application (either OMP or Pthreads)

- OpenMP standard directives are supported (version 3.1):
  - parallel, for, parallel for, sections, parallel sections, critical, single
  - #pragma omp <rest of pragma> for C/C++
  - !$OMP <rest of directive> for Fortran

- Compiler functions
  - omp_get_num_procs, omp_get_num_threads
  - omp_get_thread_num, omp_set_num_threads

- Number of OpenMP threads
  - set using environment variable OMP_NUM_THREADS
  - must be exported to the compute nodes using runjob --envs (or for non-script jobs, qsub --env)
Software & libraries on Blue Gene/Q systems

- ALCF supports two sets of libraries:
  - IBM system and provided libraries: `/bgsys/drivers/ppcfloor`
    - glibc
    - mpi
    - PAMI (Parallel Active Messaging Interface)

- Site supported libraries and programs: `/soft/libraries`
  - ESSL, PETSc, HDF5, netCDF, Parallel netCDF, Boost
    - ESSL is IBM’s optimized Engineering and Scientific Subroutine library for BG/Q: BLAS, LAPACK, FFT, sort/search, interpolation, quadrature, random numbers, BLACS
  - Additional tuned libraries in `/soft/libraries/alcf` subdirectory
    - BLAS, CBLAS, FFTW2, FFTW3, LAPACK, METIS, PARMETIS, PARPACK, SCALAPACK, SILO, SZIP, ZLIB

For a complete list visit:

http://www.alcf.anl.gov/user-guides/software-and-libraries
Tools: performance, profiling, debugging

Non-system libraries and tools are under the /soft directory:

- /soft/applications - applications
  - LAMMPS, NAMD, QMCPACK, etc.

- /soft/buildtools - build tools
  - autotools, cmake, doxygen, etc.

- /soft/compilers - IBM Compiler versions

- /soft/debuggers - debuggers
  - DDT, Totalview

- /soft/libraries - libraries
  - ESSL, PETSc, HDF5, NetCDF, etc.

- /soft/perftools - performance tools
  - TAU, HPCToolkit, PAPI, OpenSpeedshop, Scalasca, HPCTW, etc.
Questions?
Section:
Considerations before you run
Accounts, projects, allocations, etc.

- **ALCF Account**
  - Login username
    - /home/username
  - Access to at least one machine
  - CRYPTOCard token for authentication
    - PIN
    - Must call ALCF Help Desk to activate your token

- **Project**
  - Corresponds to allocation of core-hours on at least one machine
  - User can be member of one or more projects
    - /projects/ProjectName

- **Logging in**
  - ssh -Y username@mira.alcf.anl.gov
    - Click button on CRYPTOCard
    - Password: PIN + CRYPTOCard display

Manage your account at:
http://accounts.alcf.anl.gov
(password needed)

http://www.alcf.anl.gov/user-guides/accounts-access
Allocation Management

- Every user must be assigned to at least one project:
  - Use ‘projects’ command to query.

- Projects are given allocations:
  - Allocations have an amount, start, and end date, and are tracked separately; Charges will cross allocations automatically. The allocation with the earliest end date will be charged first, until it runs out, then the next, and so on.

- NEW: Use ‘sbank’ command to query allocation, balance:
  - sbank allocation –p <projectname>  # show balance of the project
  - sbank-list-users -p <projectname> –u <user> # charges against this project by this user
  - sbank-list-allocations -S geYYYY-MM-DD # allocations with start greater or equal to date
  - Other useful options:
    - -r <resource> : show results for a specific computer resource, default is current login
    - -E lt<DATE> : show info before this date
    - -S ge<DATE1> -E lt<DATE2> : show info for DATE1 =< date < DATE2
    - -h : list of commands with numerous examples

Note: sbank is updated once an hour.

- Charges are based on the partition size, NOT the number of nodes or cores used!

http://www.alcf.anl.gov/user-guides/allocation-accounting-sbank
HPC storage file systems at ALCF

<table>
<thead>
<tr>
<th>Name</th>
<th>Accessible from</th>
<th>Type</th>
<th>Path</th>
<th>Backed Up to HPSS</th>
<th>*Daily Snapshots</th>
<th>Uses</th>
</tr>
</thead>
<tbody>
<tr>
<td>vesta-home</td>
<td>Vesta</td>
<td>GPFS</td>
<td>/home or /gpfs/vesta-home</td>
<td>No</td>
<td>Yes</td>
<td>General use</td>
</tr>
<tr>
<td>projects</td>
<td>Vesta</td>
<td>GPFS</td>
<td>/projects</td>
<td>No</td>
<td>No</td>
<td>Intensive job output, large files</td>
</tr>
<tr>
<td>mira-home</td>
<td>Mira Cetus Cooley</td>
<td>GPFS</td>
<td>/home or /gpfs/mira-home</td>
<td>Yes</td>
<td>Yes</td>
<td>General use</td>
</tr>
<tr>
<td>projects</td>
<td>Mira Cetus Cooley</td>
<td>GPFS</td>
<td>/projects</td>
<td>No</td>
<td>No</td>
<td>Intensive job output, large files</td>
</tr>
</tbody>
</table>

* Daily snapshots are stored for 1 week on-disk in /gpfs/{vesta,mira}-home/.snapshots/. These snapshots do NOT persist in the event of disk failure.

http://www.alcf.anl.gov/user-guides/bgq-file-systems
Disk quota management

- Disk storage
  - /home directories:
    - Default of **100 GB** for Mira and **50 GB** for Vesta
    - Check your quota with the ‘myquota’ command
  - /projects directories:
    - Default of **1000 GB** for Mira and **500 GB** for Vesta
    - Check the quota in your projects with the ‘myprojectquotas’ command

Backups and tape archiving

- **Backups**
  - On-disk snapshots of `/home` directories are done nightly
    - If you delete files accidentally, check:
      - `/gpfs/mira-home/.snapshots` on Mira
      - `/gpfs/vesta-home/.snapshots` on Vesta
  - **Only Mira/Cetus/Cooley home directories** are backed up to tape
    - The Vesta home directories are **not** backed up to tape (just daily snapshots)
    - Project directories are **not** backed up (`/projects`)

- **Manual data archiving to tape (HPSS)**
  - HSI is an interactive client
  - GridFTP access to HPSS is available
Data transfer to/from ALCF

The Blue Gene/Q connects to other research institutions using a total of 60 Gbits/s of public network connectivity

• Data management webinar:
  https://www.youtube.com/watch?feature=player_embedded&v=pEkgf2KnaU4

Data Transfer Utilities

- **GridFTP** (for large transfers)
  - Other site must accept our Certificate Authority (CA)
  - CRYPTOCard access available
- **sftp** and **scp** (for “small” transfers)
  - For local transfers of small files, not recommended for large data transfers due to poor performance and excess resource utilization on the login nodes.

Data Transfer Service

- **Globus** (for large transfers)
  - Globus addresses the challenges faced by researchers in moving, sharing, and archiving large volumes of data among distributed sites.
  - ALCF Blue Gene/Q endpoints: alcf#dtn_mira, alcf#dtn_vesta, alcf#dtn_hpss
  - Ask your laboratory or university system administrator if your institution has an endpoint.
  - Globus Connect Personal to share and transfer files to/from a local machine.

http://www.alcf.anl.gov/user-guides/data-transfer
Questions?
Section:

Hands-on session
Hands-on session (Part I)

- Log into Cetus or Vesta:
  > ssh username@cetus.alcf.anl.gov  or  > ssh username@vesta.alcf.anl.gov

http://www.alcf.anl.gov/user-guides/connect-log

- Project:
  - Check that you are a member of the project used for this hands-on session:
    > projects
    … ALCF_Getting_STARTED …
  - Check the allocation of core-hours available for this project:
    > sbank-list-allocations -p ALCF_Getting_STARTED
  - Check the disk space in your $HOME and the projects that you are part of:
    > myquota
    > myprojectquotas
Hands-on session (Part I)

- The reservation for today’s event is: training
  - Check the name of the queue created for the hands-on session:
    > showres

- Select MPI wrapper scripts:
  - The default user environment does not provide a set of MPI compiler wrappers. A wrapper may be selected by using the appropriate SoftEnv key.
  - For the following examples, ensure that you have the `+mpiwrapper-xl` key uncommented and that it is located before the `@default` line.

> cat ~/.soft
  +mpiwrapper-xl
  @default
> resoft
> mpixlc -qversion

Note: after editing your `~/.soft` file, run command ‘resoft’ to refresh your environment.

[http://www.alcf.anl.gov/user-guides/overview-how-compile-and-link](http://www.alcf.anl.gov/user-guides/overview-how-compile-and-link)
Part II
Section:

Queuing and running
Mira job scheduling

- Restrictions in queues
  - **prod-long**: restricted to the row 0
  - **prod-short, prod-capability**: can run in the full machine

http://www.alcf.anl.gov/user-guides/machine-partitions

<table>
<thead>
<tr>
<th>User Queued</th>
<th>Underlying Queue</th>
<th>Nodes</th>
<th>Wall-clock Time (hours)</th>
<th>Max. Running per User</th>
<th>Max. Queued per User</th>
</tr>
</thead>
<tbody>
<tr>
<td>prod</td>
<td>prod-short</td>
<td>512 - 4096</td>
<td>0 - ≤6</td>
<td>5</td>
<td>20</td>
</tr>
<tr>
<td>prod</td>
<td>prod-long</td>
<td>512 - 4096</td>
<td>&gt;6 - 12</td>
<td>5</td>
<td>20</td>
</tr>
<tr>
<td>prod</td>
<td>prod-capability</td>
<td>4097 - 49152</td>
<td>0 - 24</td>
<td>5</td>
<td>20</td>
</tr>
<tr>
<td>prod</td>
<td>backfill (*)</td>
<td>512 - 49152</td>
<td>0 - 6</td>
<td>5</td>
<td>20</td>
</tr>
<tr>
<td>prod-1024-torus</td>
<td>prod-1024-torus</td>
<td>1024</td>
<td>0 - 12</td>
<td>5</td>
<td>16</td>
</tr>
<tr>
<td>prod-32768-torus</td>
<td>prod-32768-torus</td>
<td>32768</td>
<td>0 - 24</td>
<td>1</td>
<td>20</td>
</tr>
</tbody>
</table>

(*) This queue is automatically selected based on the scheduling policy.

- **I/O to compute node ratio 1:128**
Cetus job scheduling

<table>
<thead>
<tr>
<th>User Queue</th>
<th>Partition Sizes in Nodes</th>
<th>Wall-clock Time (hours)</th>
<th>Max. Running per User</th>
<th>Max. Queued Node-Hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>default</td>
<td>128, 256, 512, 1024, 2048</td>
<td>0 - 1</td>
<td>5</td>
<td>1024</td>
</tr>
<tr>
<td>low</td>
<td>128, 256, 512, 1024, 2048</td>
<td>0 - 1</td>
<td>3</td>
<td>2048</td>
</tr>
</tbody>
</table>

Cetus scheduling is designed to support application testing and debugging, not production work.

- I/O to compute node ratio 1:128

Vesta job scheduling

<table>
<thead>
<tr>
<th>User Queue</th>
<th>Partition Sizes in Nodes</th>
<th>Wall-clock Time (hours)</th>
<th>Max. Running per User</th>
<th>Max. Queued Node-hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>default</td>
<td>32, 64, 128, 256, 512, 1024</td>
<td>0 - 2</td>
<td>5</td>
<td>1024</td>
</tr>
<tr>
<td>singles</td>
<td>32, 64, 128, 256, 512, 1024</td>
<td>0 - 2</td>
<td>1</td>
<td>1024</td>
</tr>
<tr>
<td>low</td>
<td>32, 64, 128, 256, 512, 1024</td>
<td>0 - 2</td>
<td>None</td>
<td>2048</td>
</tr>
</tbody>
</table>

- I/O to compute node ratio 1:32

http://www.alcf.anl.gov/user-guides/job-scheduling-policy-bgq-systems
Mira job boot times

- Each time a job is submitted using a standard `qsub` command, all nodes in a partition are rebooted.
- Boot times depend on the size of the partition:

<table>
<thead>
<tr>
<th>Nodes in partition</th>
<th>Boot time (minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \leq 2048 )</td>
<td>1</td>
</tr>
<tr>
<td>4096</td>
<td>1.5</td>
</tr>
<tr>
<td>8192</td>
<td>3</td>
</tr>
<tr>
<td>16384</td>
<td>4</td>
</tr>
<tr>
<td>32768</td>
<td>6</td>
</tr>
<tr>
<td>49152</td>
<td>7</td>
</tr>
</tbody>
</table>

The scheduler will attempt to boot the block up to three times if the boot procedure fails, so it may take as much as three times as long under rare circumstances.
Cobalt resource manager and job scheduler

- Cobalt is the resource management software on all ALCF systems
  - Similar to PBS but not the same

- Job management commands:
  - `qsub`: submit a job
  - `qstat`: query a job status
  - `qdel`: delete a job
  - `qalter`: alter batched job parameters
  - `qmove`: move job to different queue
  - `qhold`: place queued (non-running) job on hold
  - `qrls`: release hold on job
  - `qavail`: list current backfill slots available for a particular partition size

- For reservations:
  - `showres`: show current and future reservations
  - `userres`: release reservation for other users
qsub Options

Syntax:

```
qsub [-d] [-v] -A <project name> -q <queue> --cwd <working directory>
   --env envvar1=value1:envvar2=value2 --kernel <kernel profile>
   -K <kernel options> -O <outputprefix> -t time <in minutes>
   -e <error file path> -o <output file path> -i <input file path>
   -n <number of nodes> -h --proccount <processor count>
   --mode <mode> -M <email> --dependencies <jobid1>:<jobid2> <command> <args>
```

- Standard options:

  -A project  project to charge
  -q queue  queue
  -t <time_in_minutes>  required runtime
  -n <number_of_nodes>  number of nodes
  --proccount <number_of_cores>  number of CPUs
  --mode <cX | script>  running mode
  --env VAR1=1:VAR2=1  environment variables
  <command> <args>  command with arguments
  -O project <output_file_prefix>  prefix for output files (default jobid)
  -M <email_address>  e-mail notification of job start, end
  --dependencies <jobid1>:<jobid2>  set dependencies for job being submitted
  -l or --interactive  run an interactive command

Further options and details may be found in the man pages (> man qsub) or at:

http://trac.mcs.anl.gov/projects/cobalt/wiki/CommandReference
Cobalt job control: basic method

- **Basic**: submit a BG/Q executable
  
  `qsub -n nodes --proccount P --mode cN … path/executable`

  - $N$ is number of processes (MPI ranks) per node

- Node has 16 cores
  - `--mode c1` — 1 rank/node
  - `--mode c2` — 2 rank/node
  - ...
  - `--mode c16` — 1 rank/core
  - `--mode c32` — 2 rank/core
  - `--mode c64` — 4 rank/core

- Threads
  - `qsub --mode c1 --env OMP_NUM_THREADS=64`
  - `qsub --mode c2 --env OMP_NUM_THREADS=32`
  - ...
  - `qsub --mode c16 --env OMP_NUM_THREADS=4`
  - ...
**Cobalt job control: script method**

- **Script:** submit a script (bash, csh, ....)
  ```
  qsub --mode script ... path/script
  ```

- **Example:**
  ```
  > qsub -A myproject -t 10 -n 8192 --mode script myscript.sh
  ```

  ```bash
  #!/bin/sh
  echo "Starting Cobalt job script"
  runjob --np 131072 -p 16 --block $COBALT_PARTNAME : <executable> <args...>
  ```

- **Options may appear within script using #COBALT (similar to #PBS):**
  ```
  > qsub myscript.sh
  ```

  ```bash
  #!/bin/bash
  #COBALT -A myproject -t 10 -n 8192 -O My_Run
  runjob --np 131072 -p 16 --block $COBALT_PARTNAME --verbose=INFO : <executable> <args...>
  ```
Job dependencies

- Following job in sequence depends on completion of current job

```
> qsub -A MyProject -t 12:00:00 -n 8192 --mode c32 myprogram
** Project 'MyProject'; job rerouted to queue 'prod-capability'

234439
```

```
> qsub -A MyProject -t 12:00:00 -n 8192 --mode c32 myprogram \ --dependencies 234439
** Project 'MyProject'; job rerouted to queue 'prod-capability'

234440
```

```
> qstat -u myusername
JobID  User     WallTime  Nodes  State     Location
====================================================
234439  myusername  12:00:00  8192   queued    None
234440  myusername  12:00:00  8192  dep_hold  None
```
Job dependencies (cont’d)

○ Job 234439 fails (ends with error code), Job 234440 goes into dep_fail:

```bash
> qstat -u myusername
```

<table>
<thead>
<tr>
<th>JobID</th>
<th>User</th>
<th>WallTime</th>
<th>Nodes</th>
<th>State</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>234440</td>
<td>myusername</td>
<td>12:00:00</td>
<td>8192</td>
<td>dep_fail</td>
<td>None</td>
</tr>
</tbody>
</table>

○ Release 234440 to allow it to run:

```bash
> qrls --dependencies 234440
> qstat -u myusername
```

<table>
<thead>
<tr>
<th>JobID</th>
<th>User</th>
<th>WallTime</th>
<th>Nodes</th>
<th>State</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>234440</td>
<td>myusername</td>
<td>12:00:00</td>
<td>8192</td>
<td>queued</td>
<td>None</td>
</tr>
</tbody>
</table>
Advanced runs using script mode

- Multiple (consecutive) runs in a single job
- Multiple simultaneous runs in a single job
- Combinations of the above

See:
- [http://www.alcf.anl.gov/user-guides/cobalt-job-control](http://www.alcf.anl.gov/user-guides/cobalt-job-control)
Advanced runs using ensemble and subblock jobs

Example of ensemble jobs

Example of subblock jobs

Minimum partition size on Mira

http://www.alcf.anl.gov/user-guides/cobalt-job-control
MPI mapping

- A mapping defines the assignment of MPI ranks to BG/Q processors

- Default mapping is \textit{ABCDE}T
  - \textbf{(ABCDE)} are 5D torus coordinates, \textit{T} is a CPU number
  - Rightmost letter of the mapping increases first as processes are distributed (\textit{T} then \textit{E})

- Mappings may be specified by user using the \texttt{RUNJOB\_MAPPING} environment variable:
  
  - With a \texttt{mapping string}:
    - \texttt{qsub --env RUNJOB\_MAPPING=TEDACB --mode c32...}
    - String may be any permutation of ABCDET
    - \textit{E} dimension of torus is always of size 2
  
  - With a \texttt{mapping file}:
    - \texttt{qsub --env RUNJOB\_MAPPING=<FileName> --mode c32...}
    - mapfile: each line contains 6 coordinates to place the task, first line for task 0, second line for task 1...
    - allows for use of any desired mapping
    - file must contain one line per process and not contain conflicts (no verification)
    - use high-performance toolkits to determine communication pattern

http://www.alcf.anl.gov/user-guides/machine-partitions
Reservations

- Reservations allow exclusive use of a partition for a specified group of users for a specific period of time
  - a reservation prevents other users’ jobs from running on that partition
  - often used for system maintenance or debugging
  - **R.pm** (preventive maintenance), **R.hw** or **R.sw** (addressing HW or SW issues)
  - reservations are sometimes idle, but still block other users’ jobs from running on a partition
  - should be the exception not the rule

- Requesting
  - See: [http://www.alcf.anl.gov/user-guides/reservations](http://www.alcf.anl.gov/user-guides/reservations)
  - Email reservation requests to support@alcf.anl.gov
  - View reservations with **showres**
  - Release reservations with **userres**

- When working with others in a reservation, these qsub options are useful:
  - **--run_users** <user1>:<user2>:… All users in this list can control this job
  - **--run_project** <projectname> All users in this project can control this job
Questions?
Section:

After your job is submitted
qstat: show status of a batch job(s)

- **qstat**          # list all jobs
  
<table>
<thead>
<tr>
<th>JobID</th>
<th>User</th>
<th>WallTime</th>
<th>Nodes</th>
<th>State</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>301295</td>
<td>smith</td>
<td>00:10:00</td>
<td>16</td>
<td>queued</td>
<td>None</td>
</tr>
</tbody>
</table>

- **About jobs**
  - JobID is needed to kill the job or alter the job parameters
  - Common states: queued, running, user_hold, maxrun_hold, dep_hold, dep_fail

- **qstat -f <jobid>**     # show more job details
- **qstat -fl <jobid>**    # show all job details
- **qstat -u <username>**  # show all jobs from <username>

- **qstat -Q**
  - Instead of jobs, this shows information about the queues
  - Will show all available queues and their limits
  - Includes special queues used to handle reservations
Machine status web page

http://status.alcf.anl.gov/mira/activity (a.k.a. The Gronkulator)
Machine status web page (cont’d)

http://status.alcf.anl.gov/cetus/activity

http://status.alcf.anl.gov/vesta/activity
Machine status web page (cont’d)

http://status.alcf.anl.gov/cooley/activity
Cobalt files for a job

- Cobalt will create 3 files per job, the basename `<prefix>` defaults to the jobid, but can be set with “qsub -O myprefix”
  - jobid can be inserted into your string e.g. "-O myprefix_${jobid}"

- **Cobalt log file: `<prefix>`.cobaltlog**
  - created by Cobalt when job is submitted, additional info written during the job
  - contains submission information from qsub command, runjob, and environment variables

- **Job stderr file: `<prefix>`.error**
  - created at the start of a job
  - contains job startup information and any content sent to standard error while the user program is running

- **Job stdout file: `<prefix>`.output**
  - contains any content sent to standard output by user program
qdel: kill a job

- `qdel <jobid1> <jobid2>`
  - delete the job from a queue
  - terminate a running job
qalter, qmove: alter parameters of a job

- Allows user to alter the parameters of queued jobs without resubmitting
  - Most parameters may only be changed before the run starts

- Usage: `qalter [options] <jobid1> <jobid2> …`

- Example:
  > `qalter -t 60 123 124 125`
  (changes wall time of jobs 123, 124 and 125 to 60 minutes)

- Type ‘`qalter -help`’ to see full list of options

- qalter cannot change the queue; use `qmove` instead:
  > `qmove <destination_queue> <jobid>`
qhold, qrls: holding and releasing

- **qhold** - Hold a submitted job (will not run until released)
  qhold <jobid1> <jobid2>

- To submit directly into the hold state, use `qsub -h`

- **qrls** - Release a held job (in the `user_hold` state)
  qrls <jobid1> <jobid2>

- Jobs in the `dep_hold` state released by removing the dependency
  qrls --dependencies <jobid>
  or qalter --dependencies none <jobid>

- Jobs in the `admin_hold` state may only be released by a system administrator
Reasons why a job may not be running yet

- There is a reservation which interferes with your job
  - `showres` shows all reservations currently in place
- There are no available partitions for the requested queue
  - `partlist` shows all partitions marked as functional
  - `partlist` shows the assignment of each partition to a queue

<table>
<thead>
<tr>
<th>Name</th>
<th>Queue</th>
<th>State</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIR-04800-37B71-1-1024</td>
<td>prod-short:backfill</td>
<td>busy</td>
</tr>
<tr>
<td>MIR-04880-37BF1-1-1024</td>
<td>prod-short:backfill</td>
<td>blocked (MIR-048C0-37BF1-512)</td>
</tr>
<tr>
<td>MIR-04C00-37F71-1-1024</td>
<td>prod-short:backfill</td>
<td>blocked (MIR-04C00-37F31-512)</td>
</tr>
<tr>
<td>MIR-04C80-37FF1-1-1024</td>
<td>prod-short:backfill</td>
<td>idle</td>
</tr>
</tbody>
</table>

- Job was submitted to a queue that is restricted from running at this time
Optimizing for queue throughput

- Small (≤ 4K), long (6h < time < 12h) jobs submitted to prod will be redirected to prod-long, which is restricted to row 0.

- Consider instead:
  - Small (≤ 4K), short (≤ 6h) jobs in prod queue will be redirected to prod-short, which can run anywhere.
  - Large (> 4K) jobs in prod queue will be redirected to prod-capability, which can run anywhere.

- Shotgun approach:
  - If your code is amenable, submit a mix of job sizes and lengths.

- Check for drain windows:
  - `partlist | grep idle`
  - `full partlist output`:

<table>
<thead>
<tr>
<th>Name</th>
<th>Queue</th>
<th>State</th>
<th>Backfill</th>
<th>Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MIR-04800-37B71-1-1024</td>
<td>prod-short:backfill</td>
<td>busy</td>
<td>-</td>
<td>4x4x4x8x2</td>
</tr>
<tr>
<td>MIR-04880-37BF1-1-1024</td>
<td>prod-short:backfill</td>
<td>blocked (MIR-048C0-37BF1-512)</td>
<td>-</td>
<td>4x4x4x8x2</td>
</tr>
<tr>
<td>MIR-04C00-37F71-1-1024</td>
<td>prod-short:backfill</td>
<td>blocked (MIR-04C00-37F31-512)</td>
<td>-</td>
<td>4x4x4x8x2</td>
</tr>
<tr>
<td>MIR-04C80-37FF1-1-1024</td>
<td>prod-short:backfill</td>
<td>idle</td>
<td>0:49</td>
<td>4x4x4x8x2</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

In this case, a job submitted for 1024 nodes can run immediately if its time is < 49 minutes (might need to be a few minutes shorter to allow for scheduling delay)
Questions?
Section:

Potential problems
When things go wrong... logging in

- Check to make sure it’s not a scheduled system maintenance day:
  - Login nodes on Blue Gene/Q and data analytics systems are often closed off during system maintenance to allow for activities that would impact users.
  - Look for reminders in the weekly maintenance announcement to users and in the pre-login banner message.
  - An all-clear email will be sent out to users at the close of maintenance.

- Remember that CRYPTOCard passwords:
  - Require a pin at the start
  - Are all hexadecimal characters (0-9, A-F). Letters are all UPPE...
When things go wrong... running

- Cobalt jobs, by default, produce three files (*.cobaltlog, *.error, *.output)
- Only *.cobaltlog is generated at submit time, the others at runtime
- Boot status (successful or not) written to *.cobaltlog
- After booting, the *.error file will have a non-zero size:
  - Note: If your script job redirects the stderr of cobalt-mpirun, it will not end up in the job’s .error file
- If you think there is an issue, it’s best to save all three files:
  - Send the jobid, machine name and a copy of the files to support@alcf.anl.gov
When things go wrong... running

- **RAS** events appearing in your .error file are not always a sign of trouble:
  - RAS stands for Reliability, Availability, and Serviceability

- Few are signs of a serious issue, most are system noise:
  - Messages have a severity associated with them:
    - INFO
    - WARN
    - ERROR
    - FATAL
  - Only **FATAL** RAS events will terminate your application
  - **ERROR** may degrade performance but will NOT kill your job
  - Still worth watching as they may indicate an application performance issue

- If your run exits abnormally, the system will list the last RAS event encountered in the run. **This RAS event did not necessarily cause the run to die.**
Core files

- Jobs experiencing fatal errors will generally produce a core file for each process

- Examining core files:
  - Core files are in text format, readable with the ‘more’ command
  - `bgq_stack` command provides call stack trace from a core file:
    - Ex: `bgq_stack <program_binary> core.*`
    - Command line interface (CLI)
    - Can only examine one core file at a time
      - [http://www.alcf.anl.gov/user-guides/bgqstack](http://www.alcf.anl.gov/user-guides/bgqstack)
  - `coreprocessor.pl` command provides call stack trace from multiple cores:
    - Ex: `coreprocessor.pl -c=<directory_with_core_files> -b=a.out`
    - CLI and GUI: GUI interface requires X11 forwarding (ssh -X mira.alcf.anl.gov)
    - Provides information from multiple core files
      - [http://www.alcf.anl.gov/user-guides/coreprocessor](http://www.alcf.anl.gov/user-guides/coreprocessor)

- Environment variables control core dump behavior:
  - BG_COREDUMPONEXIT=1 : creates a core dump when the application exits
  - BG_COREDUMPDISABLED=1 : disables creation of any core files
Getting help

Online resources (24/7):
- ALCF web pages:
  - http://www.alcf.anl.gov/user-guides
  - https://accounts.alcf.anl.gov
- Mira/Cetus/Vesta/Cooley status (a.k.a. The Gronkulator):
  - http://status.alcf.anl.gov/{mira,cetus,vesta,cooley}/activity

Contact us:
- E-mail: support@alcf.anl.gov
- ALCF Help Desk: Hours: Monday – Friday, 9 a.m. – 5 p.m. (Central time)
  Phone: 630-252-3111 or 866-508-9181 (toll-free, US only)
- Your Catalyst

News from ALCF:
- ALCF Weekly Updates, ALCF newsletters, email via
  {mira,cetus,vesta,cooley}-notify lists, etc.
Help Us Help You

For better, faster results, provide ALCF these details when you contact us for help (where applicable):

- Machine(s) involved (Mira/Cetus/Vesta/Cooley)
- Job IDs for any jobs involved
- Exact error message received
- Exact command executed
- Filesystem used when the problem was encountered with path to files
- Account username and project name that the problem pertains to
- For connection problems: IP address from which you are connecting
- Application software name/information
Questions?
Section:

Hands-on session
Hands-on session

- Today’s event has its own **project** and **queue** name:
  -A ALCF_Getting_Started -q training

- **Compilation** example, using basic qsub mode:
  - Create directory, copy files, and compile program:
    - mkdir –p ~/training/Hands-on
    - cp -r /soft/cobalt/examples/compilation ~/training/Hands-on
    - cd ~/training/Hands-on/compilation
    - ls
    - cat hello_mpi.cpp
    - cat Makefile
    - make

- Submit job using basic mode and check output:
  - qsub -A ALCF_Getting_Started -q training -t 5 -n 16 --mode c1 -o hello_mpi.output hello_mpi_cpp
  - qstat -u <username>
  - cat hello_mpi.output

- qsub echoes a number to the screen, which is the Cobalt job id. In the absence of a -o argument, three files are created (say JobID was 227076):
  - 227076.cobaltlog, 227076.error, 227076.output (*replaced by hello_mpi.output with -o* )
Hands-on session

- **Example of script job** submission:
  - Copy directory:
    ```bash
    > cp -r /soft/cobalt/examples/script ~/training/Hands-on
    > cd ~/training/Hands-on/script
    ```
  - Open the README file and follow the instructions to submit a script job.
  - Look at the `runHelloMPI.sh` script file. It invokes `runjob` to run the program.
  - Example:
    ```bash
    > mpixlcxx_r -g -o hello_mpi_cpp hello_mpi.cpp
    > qsub -A ALCF_Getting_Started -q training -t 5 -n 16 -o hello_mpi.output --mode script runHelloMPI.sh
    ```

- **Example of interactive job** submission:
  - Copy directory:
    ```bash
    > cp -r /soft/cobalt/examples/interactive ~/training/Hands-on
    > cd ~/training/Hands-on/interactive
    ```
  - Open the README file and follow the instructions to submit an interactive job.
Hands-on session

- Example of a **multi-block** ensemble submission:
  - Copy directory:
    ```
    > cp -r /soft/cobalt/examples/ensemble ~/training/Hands-on
    > cd ~/training/Hands-on/ensemble/1024-2x512
    ```
  - The README file contains instructions to submit a 1-rack job with two 512 blocks.
    **NOTE:** remember to adapt the number of nodes and the block sizes provided in this example to the min./max. partition sizes available in the machine where you want to run the test (see slides 11 for reference).

- Example of **subblock** ensemble submission:
  - Copy directory:
    ```
    > cp -r /soft/cobalt/examples/subblock ~/training/Hands-on
    > cd ~/training/Hands-on/subblock/512-4x128
    ```
  - Open the README file and follow the instructions to submit a job for multiple 128-node runs on a midplane of Mira.

- Example of **python job** submission:
  - Copy directory:
    ```
    > cp -r /soft/cobalt/examples/python ~/training/Hands-on
    > cd ~/training/Hands-on/python
    ```
  - Open the README file and follow the instructions to submit a python job.
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Thank you for attending!