ALCF System Architectures - Software and Job Submission

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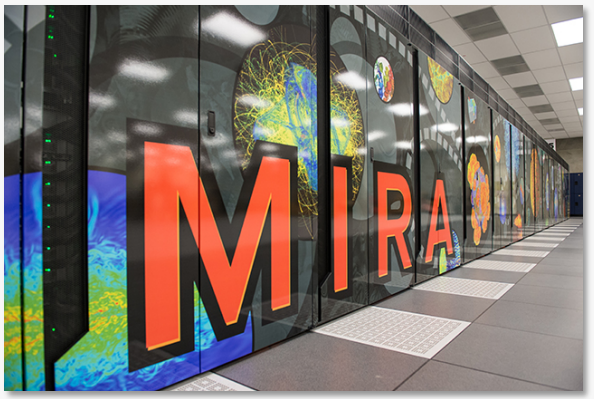
Outline

https://www.alcf.anl.gov/user-guides

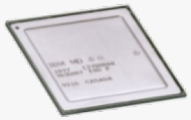
- Mira (Blue Gene Q)
  - System Overview
  - Software & SoftEnv
  - Building your code
  - Queuing and running jobs with qsub & runjob
- Theta (KNL)
  - System Overview
  - Software & Environment Modules
  - Building your code
  - Queuing and running jobs with qsub & aprun
- Tips for troubleshooting



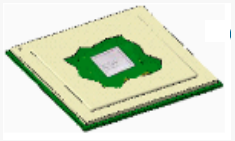
Mira - System Overview

https://www.alcf.anl.gov/mira

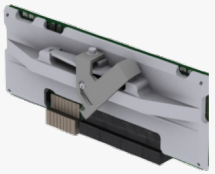
Chip
16+2 cores



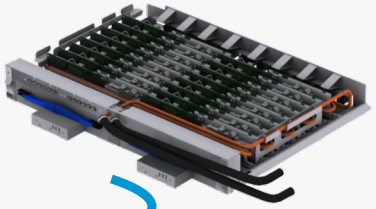
Module
Single chip



Compute card
One single chip module
16 GB DDR3 Memory
Heat Spreader for H_2O Cooling



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

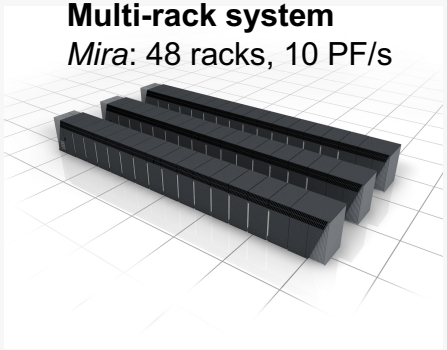


Midplane
16 node boards

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

81 inches tall

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

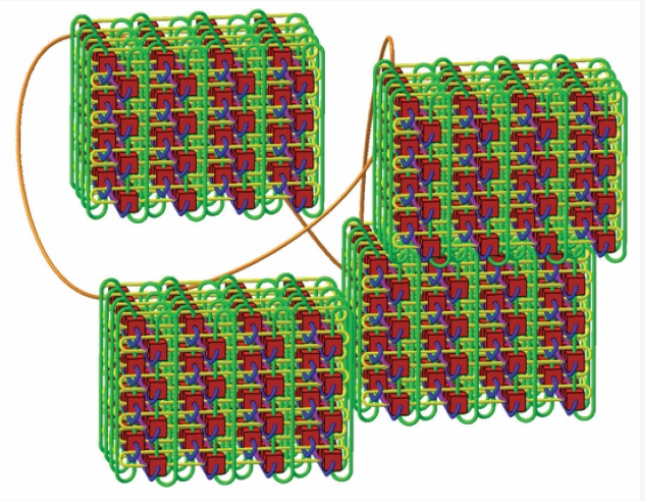


Mira - System Overview

https://www.alcf.anl.gov/user-guides/torus-network-bgq-system

- 5D torus network
  - High nearest neighbor bandwidth while increasing bisection bandwidth and reducing hops vs 3D torus
  - Machine can be partitioned into independent sub-networks
  - Hardware assists for collective and barrier functions over COMM_WORLD and rectangular sub communicators
  - Single network used for P2P, collectives, and barriers.

- Nodes have 10 links with 2 GB/s raw bandwidth each
  - Bi-directional: send & receive gives 4 GB/s
  - 90% bandwidth available to user
  - Additional 11th link for I/O



Mira - Software & Libraries

https://www.alcf.anl.gov/user-guides/software-and-libraries

- IBM system and provided libraries: /bgsys/drivers/ppcfloor
  - glibc
  - mpi
  - PAMI (Parallel Active Messaging Interface)

- Site-supported libraries: /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 number, BLACS

- Additional tuned libraries: /soft/libraries/alcf
  - BLAS, FFTW, LAPACK, PARMETIS, PARPACK, SCALAPACK, SZIP, ZLIB

Mira - Software & Libraries

https://www.alcf.anl.gov/user-guides/software-and-libraries

- Applications: /soft/applications
  - LAMMPS, NAMD, QMCPACK, CP2K, etc…
- Build Tools: /soft/buildtools
  - autotools, cmake, doxygen, etc…
- Compilers: /soft/compilers
  - IBM XL, BGCLANG, GNU
- Debuggers: /soft/debuggers
  - DDT
- Performance Tools: /soft/perftools
  - TAU, HPCToolkit, PAPI, Autoperf, Scalasca, HPCTW, etc…

Mira - SoftEnv

https://www.mcs.anl.gov/hs/software/systems/soften/soften-intro.html

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

- Settings
  - Maintained in the file ~/.soft
  - Add/remove keywords from ~/.soft to change environment
  - Make sure @default is at the very end
  - Use .bash_profile for user-specific environment modifications

- Commands
  - List all keywords defined on the system: softenv
  - Reload initial environment from ~/.soft file: resoft
  - Temporarily modify environment: soft add|remove <keyword>

Mira - Compiler Wrappers

https://www.alcf.anl.gov/user-guides/compiling-and-linking-bgq

- IBM XL cross-compilers
  - SoftEnv key: +mpiwrapper-xl
  - mpixlc_r, mpixlcxx_r, mpixlf77_r, mpixlf90_r, mpixlf95_r, etc…
  - List complete command executed by mpi wrapper: –show

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

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

Mira - SoftEnv Example

https://www.alcf.anl.gov/user-guides/bgq-compiling-and-linking-faqs

- A minimal ~/.soft file needed to build code for compute nodes

```
> cat ~/.soft
  +mpiwrapper-xl
  @default

> resoft
> mpixlc_r -qversion
  IBM XL C/C++ for Blue Gene, V12.1
  Version: 12.01.0000.0015
```

- Remember, after editing ~/.soft file, run resoft command to refresh environment.

Mira - IBM XL Optimization Tips

https://www.alcf.anl.gov/user-guides/bgq-compiling-and-linking-faqs

- Optimization level
  - Best for debugging: –O0
  - Good for correctness check, baseline performance: –O2
  - Loop transformations & additional optimizations: –O3
    - Can alter program semantics unless used with –qstrict

- Tips
  - Performance can decrease at higher levels: –O4 or –O5
  - Use –qlistopt to generate a listing of all flags used in compilation
  - Use –qreport to generate a listing showing how code was optimized
  - Compiler option –g must be used to resolve code line numbers

Mira - Threading

https://www.alcf.anl.gov/user-guides/threading-bgq

- OpenMP
  - IBM XL compilers: –qsmp=omp:noauto
  - GNU: –fopenmp
  - BGCLANG: –fopenmp

- Pthreads
  - NPTL Pthreads implementation in glibc requires no modification

- Tips
  - Auto thread parallelization with –qsmp=auto not always effective
  - Number of threads controlled with runjob command
  - Each core needs at least 2 (possibly 4) threads for peak efficiency

Mira - Preparing to Submit Job

https://www.alcf.anl.gov/user-guides/allocation-accounting-sbank

- Check that you are a member of a project: projects

- Check available disk space
  - $HOME directory: myquota
  - Project directories: myprojectquotas
  - Project directories should be used for production work

- Check that your project has core-hours available
  - Use sbank command to query allocation details
  - Allocation available to project: sbank l a –p <project_name>
  - Charges against project by user: sbank l u –p <project_name> –u <user>
  - Charges on BG/Q are based on partition size, not number of nodes

Mira - Cobalt

https://www.alcf.anl.gov/user-guides/cobalt-job-control

- Resource management software on all ALCF systems
  - Similar to PBS

- Job management commands
  - Submit a job: qsub
  - Query job status: qstat
  - Delete a job: qdel
  - Alter job parameters: qalter
  - Move job to different queue: qmove
  - Place queued job (non-running) on hold: qhold
  - Release hold on job: qrls

- Examples in /soft/cobalt/examples

Mira - qsub

https://www.alcf.anl.gov/user-guides/cobalt-job-control

- Standard options
  - Project to charge: –A <project_name>
  - Queue: –q <queue>
  - Maximum walltime: –t <time_in_minutes>
  - Number of nodes: –n <number_of_nodes>
  - Number of processes: --proccount <number_of_processors>
  - Running mode: --mode <cX | script>
  - Environment variables: --env <VAR1=1:VAR2=1>
  - Prefix for output files: –O <file_prefix>
  - E-mail notifications: –M <email_address>
  - Dependencies: --dependencies <jobid1>:<jobid2>
  - Interactive job: –I or --interactive

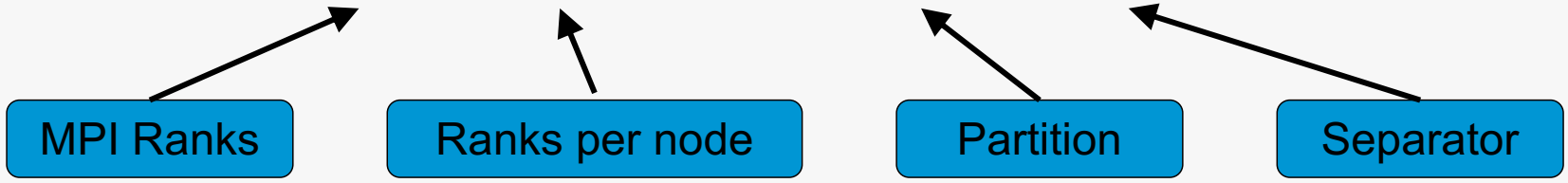
Mira - Submitting Script Jobs

https://www.alcf.anl.gov/user-guides/cobalt-job-control

- Executable is invoked within script (bash, csh, …)

- Example #1 specifies job attributes on command-line

```
> cat myscript.sh
  #!bin/sh
  echo “Starting Cobalt job script”
  runjob --np 131072 –p 16 --block $COBALT_PARTNAME : <app> <app_args>
```




```
> qsub –A <project_name> –t 10 –n 8192 –O <prefix_name> --mode script myscript.sh
  123456
```

Mira - Submitting Script Jobs

https://www.alcf.anl.gov/user-guides/cobalt-job-control

- Executable is invoked within script (bash, csh, …)

- Example #2 specifies job attributes within script

```
> cat myscript.sh
  #!bin/sh
  #COBALT –A <project_name> –t 10 –n 8192 –O <prefix_name>
  echo “Starting Cobalt job script”
  runjob --np 131072 –p 16 --block $COBALT_PARTNAME --verbose=INFO
         --env OMP_NUM_THREADS=4 : <app> <app_args>


> qsub myscript.sh
  123456
```

Mira - Cobalt Files For Submitted Job

https://www.alcf.anl.gov/user-guides/cobalt-job-control

- Cobalt will create three files per job
  - Prefix defaults to jobid if not set with qsub's –O option

- Cobalt log file: <prefix_name>.cobaltlog
  - Create when job is submitted, additional info written while job runs
  - Contains submission information from qsub, runjob, and environment

- Job stderr file: <prefix_name>.error
  - Created at start of job
  - Contains job startup information and any output sent to standard error

- Job stdout file: <prefix_name>.output
  - Created at start of job
  - Contains content sent to standard output

Mira - Now That Your Job Is Queued

https://www.alcf.anl.gov/user-guides/cobalt-job-control

- Check status of submitted jobs

```
> qstat
JobID      User      WallTime   Nodes    State         Location
================================================================
123456     user1     00:30:00     512    dep_fail      None
123457     user2     01:00:00    1024    running       CET-40400-73771-1024
123458     user3     00:30:00    2048    queued        None
123459     user1     01:00:00     512    running       CET-40040-73371-512
123460     user4     00:30:00    2048    user_hold     None
```

Mira - Now That Your Job Is Queued

https://www.alcf.anl.gov/user-guides/cobalt-job-control

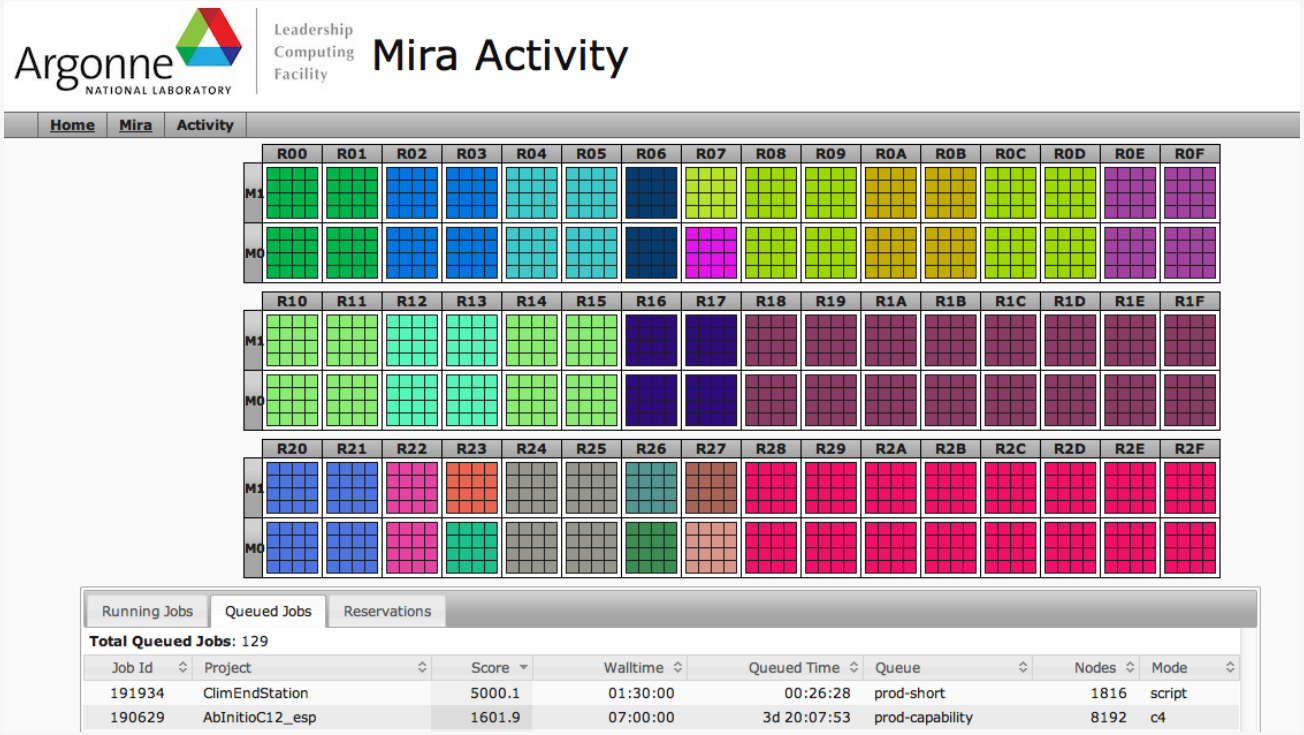
- Additional qstat queries
  - Show more job details: qstat –f <jobid>
  - Show all job details: qstat –fl <jobid>
  - Show all jobs from user: qstat –u <user>
  - Show information about queues: qstat –Q

- Delete job from queue: qdel <jobid>

- Alter properties of queued job
  - Change walltime: qalter –t <new_time> <jobid>
  - Change number of nodes: qalter –n <new_number_of_nodes> <jobid>
  - Change queue: qmove <new_queue> <jobid>

Mira - Checking Status of Job

https://status.alcf.anl.gov/mira/activity



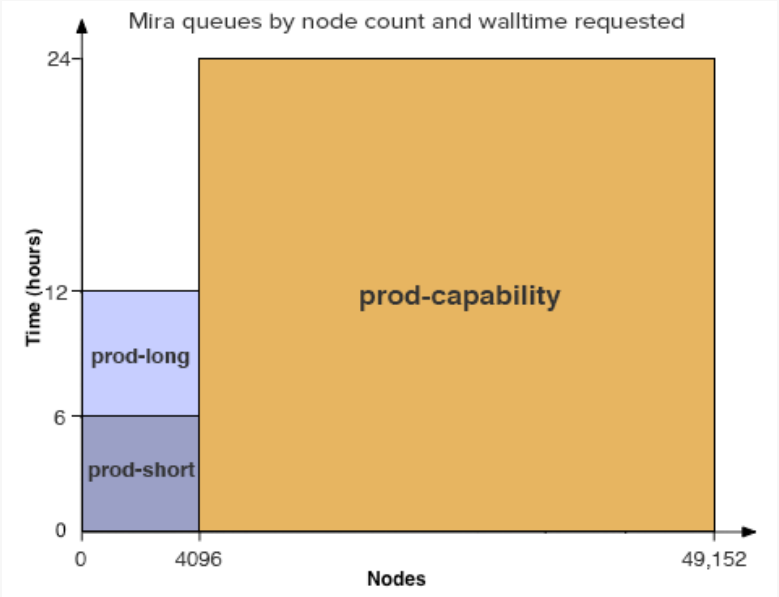
Mira - Optimizing For Queue Throughput

https://www.alcf.anl.gov/user-guides/job-scheduling-policy-bgq-systems

- Small (≤ 4096 nodes), long (6-12 hours) jobs redirected to prod-long queue, which is restricted to row 0

- Consider instead
  - Small (≤ 4096 nodes), short (≤ 6 hours) jobs redirected to prod-short queue, which run anywhere
  - Large (> 4096 nodes) jobs redirected to prod-capability queue, which run anywhere

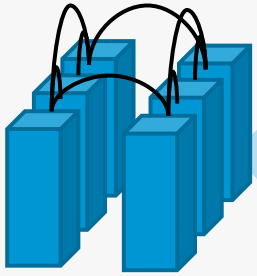
- For long sequences of jobs, chain them together with dependencies
  - Dependent jobs inherit score boost from previous successful job in chain.

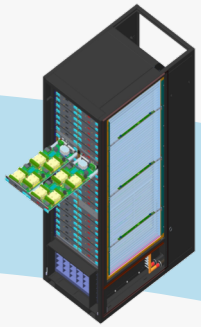



ANY QUESTIONS?

Theta - System Overview

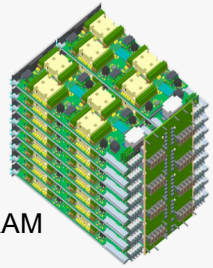
https://www.alcf.anl.gov/theta



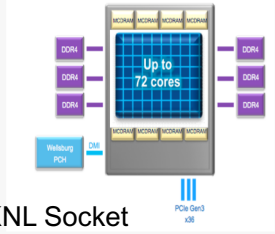


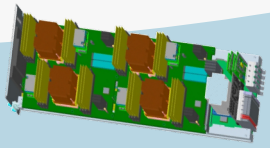
Cabinet: 3 Chassis, 75kW liquid/air cooled
510.72 TF 3TB MCDRAM, 36TB DRAM

System: 24 Cabinets
4392 Nodes, 1152 Switches
Dual-plane, 12 groups, Dragonfly 12.1 TB/s Bi-Sec
11.7 PF Peak
70 TB MCDRAM, 843 TB DRAM

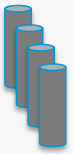


Chassis: 16 Blades, 16 Cards
64 Nodes, 16 Switches
170.24 TF 1TB MCDRAM, 12TB DRAM





Compute Blade:
4 Nodes/Blade + Aries switch
10.64 TF 64GB MCDRAM
768GB DRAM



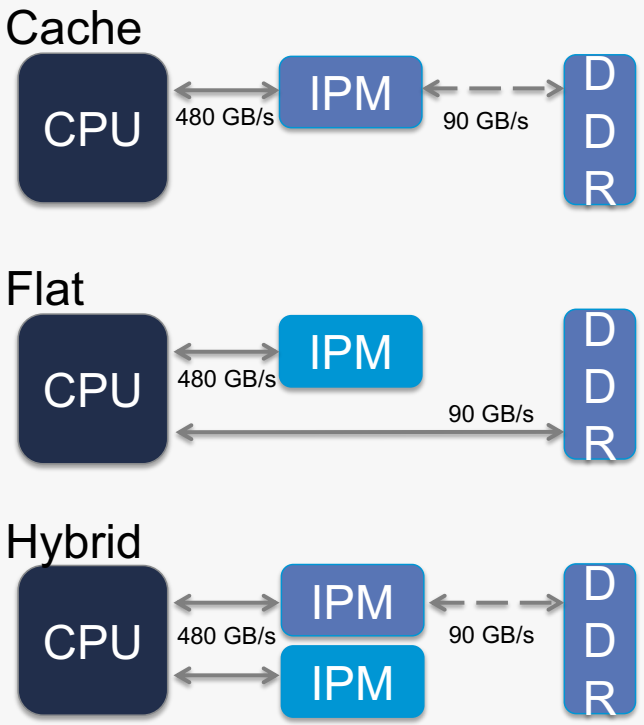
Sonexion Storage
4 Cabinets
Lustre file system
10 PB usable
210 GB/s

Node: KNL Socket
192 GB DDR4 (6 channels) **2.66 TF** 16GB MCDRAM
128 GB SSD

Theta - System Overview

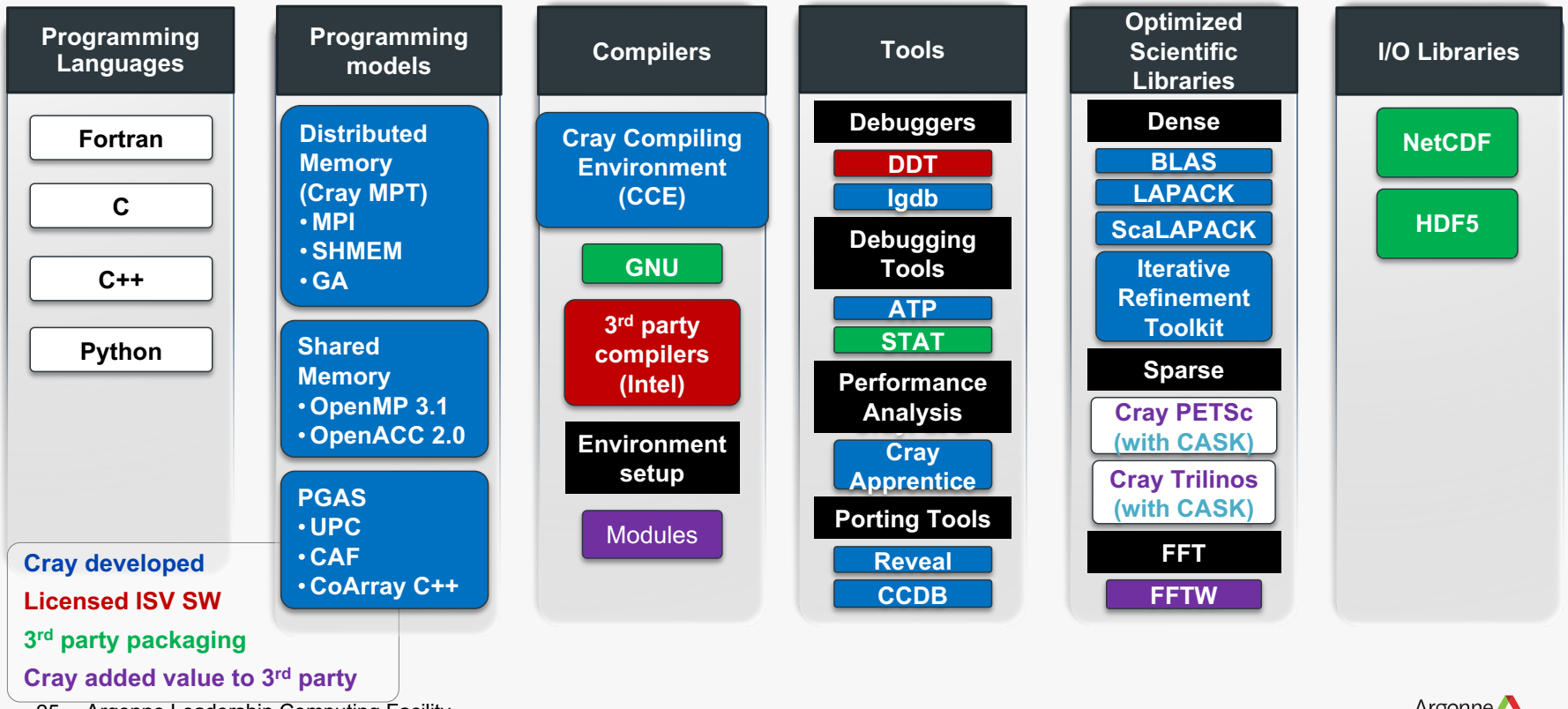
https://www.alcf.anl.gov/user-guides/xc40-memory-modes

- Two memory types
  - In Package Memory (IPM)
    - 16 GB MCDRAM @ ~480 GB/s
  - Off Package Memory (DDR)
    - 192 GB @ ~90GB/s
- Single address space; multiple NUMA domains
- Memory configurations
  - Cached: DDR fully cached by IPM
  - Flat: User managed
  - Hybrid: ¼, ½, IPM used as cache
- Managing memory
  - jemalloc & memkind libraries
  - Pragmas for static memory allocations



Theta - Cray Programming Environment

https://www.alcf.anl.gov/user-guides/software-and-libraries



Theta - Non-system Software & Libraries

https://www.alcf.anl.gov/user-guides/software-and-libraries

- Compilers: /soft/compilers
  - llvm and intel beta releases
- Debuggers: /soft/debuggers
  - DDT
- Libraries: /soft/libraries
  - argobots, bolt, breakpad
- Performance tools: /soft/perftools
  - Darshan, HPCToolkit, memlog, TAU
- Visualization: /soft/visualization
  - Paraview, R

Theta - Modules

https://modules.sourceforge.net

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

- Module commands
  - List available module commands: module help
  - List currently loaded modules: module list
  - List all available modules: module avail
  - Add module to environment: module load <mod>
  - Remove module from environment: module unload <mod>
  - Swap loaded module with new one: module switch <mod_old> <mod_new>
  - List information about module: module show <mod>

Theta - Compiler Wrappers

https://www.alcf.anl.gov/user-guides/compiling-and-linking-xc40

- For all compilers (Intel, Cray, GNU, Clang)
  - Use cc, CC, ftn
  - Do not use mpicc, mpiCC, mpic++, mpif77, mpif90, etc… as they do not generate code for compute nodes

- Select compiler you want: module swap <PrgEnv-old> <PrgEnv-new>
  - Intel (default): PrgEnv-intel
  - Cray: module swap PrgEnv-intel PrgEnv-cray
  - GNU: module swap PrgEnv-intel PrgEnv-gnu
  - Clang: module swap PrgEnv-intel PrgEnv-llvm

- Cray wrappers
  - List complete command executed: –craype-verbose
  - Disable automatic linking with libsci: –mkl

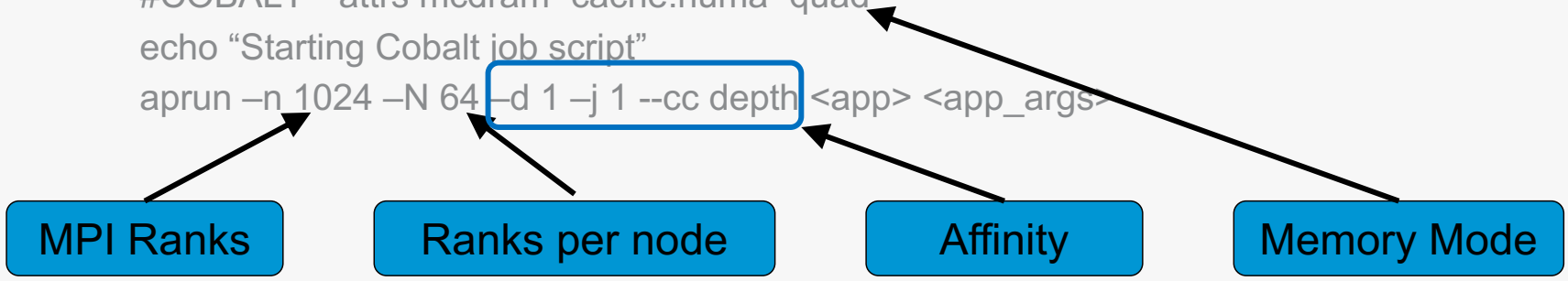
Theta - Submitting Script Jobs

https://www.alcf.anl.gov/user-guides/running-jobs-xc40

- Executable is invoked within script (bash, csh, …)

- aprun is used to launch executables on compute nodes

```
> cat myscript.sh
  #!bin/sh
  #COBALT –A <project_name> –t 10 –n 16 –O <prefix_name> –q default
  #COBALT --attrs mcdram=cache:numa=quad
  echo “Starting Cobalt job script”
  aprun –n 1024 –N 64 –d 1 –j 1 --cc depth <app> <app_args>
```




```
> qsub myscript.sh
  123456
```

Theta - aprun Overview

https://www.alcf.anl.gov/user-guides/running-jobs-xc40

- aprun options
  - Total number of MPI ranks: –n <total_number_ranks>
  - Number of MPI ranks per node: –N <number_ranks_per_node>
  - Number of hyperthreads per MPI rank (depth): –d <num_hardware_threads_per_rank>
  - Number of hyperthreads per core: –j <number_hardware_threads_per_core>
  - MPI rank and thread placement: --cc depth
  - Environment variables: –e <VAR1=1> –e <VAR2=1>
  - Core specialization: –r <number_hardware_threads>

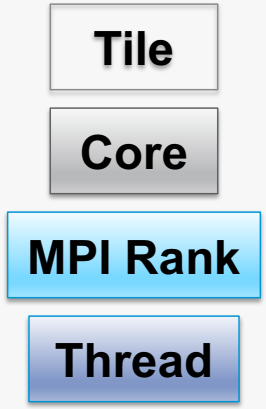
- See also man aprun

Theta - aprun Overview

https://www.alcf.anl.gov/user-guides/running-jobs-xc40

- Theta's KNL nodes have 32 tiles with 2 cores each (4 hardware threads per core)
- Example #1: 2 nodes, 64 ranks/node, 1 thread/rank, 1 rank/core
  - aprun –n 128 –N 64 –d 1 –j 1 --cc depth <app> <app_args>


```
nname= nid02937  rnk= 0  tid= 0  ht= {0}
nname= nid02937  rnk= 1  tid= 0  ht= {1}
nname= nid02937  rnk= 2  tid= 0  ht= {2}
nname= nid02937  rnk= 3  tid= 0  ht= {3}
nname= nid02937  rnk= 4  tid= 0  ht= {4}
nname= nid02937  rnk= 5  tid= 0  ht= {5}
```

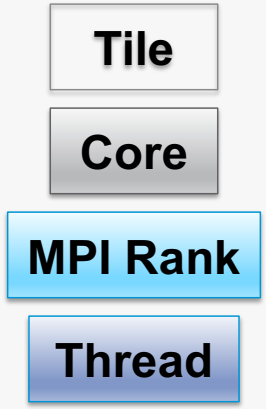


Theta - aprun Overview

https://www.alcf.anl.gov/user-guides/running-jobs-xc40

- Theta's KNL nodes have 32 tiles with 2 cores each (4 hardware threads per core)
- Example #1: 2 nodes, 32 ranks/node, 4 thread/rank, 2 threads/core
  - aprun –n 64 –N 32 –d 4 –j 2 --cc depth -e OMP_NUM_THREADS=4 <app> <app_args>


```
nname= nid02937  rnk= 0  tid= 0  ht= {0}
nname= nid02937  rnk= 0  tid= 1  ht= {1}
nname= nid02937  rnk= 0  tid= 2  ht= {64}
nname= nid02937  rnk= 0  tid= 3  ht= {65}
nname= nid02937  rnk= 1  tid= 0  ht= {2}
nname= nid02937  rnk= 1  tid= 1  ht= {3}
```



Theta - aprun Overview

https://www.alcf.anl.gov/user-guides/running-jobs-xc40

- Affinity
  - Use –d and --cc depth to let ALPS control affinity
  - Use --cc none if you want to use OpenMP (or KMP) env. variables to specify affinity

- Core specialization with –r <number_hardware_threads>
  - Offload OS and MPI to unused hardware threads (e.g. reduce variability)

- Allocating memory in flat mode
  - Default memory allocation in DDR (NUMA 0)
  - Only allocate memory to HBM (NUMA 1): numactl –m 1
  - Prefer memory allocation to HBM: numactl –p 1
  - Example: aprun –n 128 –N 64 –d 1 –j 1 --cc depth numactl –m 1 <app> <app_args>

Theta - Queues

https://www.alcf.anl.gov/user-guides/job-scheduling-policy-xc40-systems

- Jobs are routed to single default queue
  - Nodes allocated to job will be rebooted (if needed) for requested memory mode
  - Best to always specify memory mode (e.g. --attrs mcdram=cache:numa=quad)
  - Pad requested walltime by ~30 minutes to account for possible rebooting
  - Don't delete job if remains in "starting" for several minutes

- Wall-clock limits are function of number of requested nodes
  - minimum allocation: 8 (128) nodes, maximum walltime 2 (3) hours
  - capability jobs: >= 648 (802) nodes, maximum walltime 24 hours
  - Check website for current policies

- Two 16-node debug queues available
  - debug-cache-quad
  - debug-flat-quad


ANY QUESTIONS?

Why Hasn't My Job Started?

- There is a reservation which delays your job from starting
  - List all reservations currently in place: showres
- There are no available nodes for the requested queue
  - Nodes may be down, busy running other jobs, draining next job, or reserved
  - Check queue status: qstat
  - Check machine status: http://status.alcf.anl.gov
  - Check "ALCF Weekly Updates" for training, reservation, and maintenance notices
- List idle resources
  - List status of partitions on Mira: partlist
  - List status of nodes on Theta: nodelist

Mira - Core Files and Debugging

https://www.alcf.anl.gov/user-guides/debugging-profiling

- Examining core files
  - Core files are in text format (e.g. readable with more command)
  - List call stack trace from single core file: bgq_stack <app> core.#
  - List call stack trace from multiple core files: coreprocessor.pl
    - Example: coreprocessor.pl –c=<dir> –b=<exe>
    - Can also connect to running job

- Environment variables
  - Create core dump when application exits: BG_COREDUMPONEXIT=1
  - Disables creation of any core files: BG_COREDUMPDISABLED=1

- Full-featured debugging with DDT

Theta - Core Files and Debugging

https://www.alcf.anl.gov/user-guides/debugging-profiling

- Abnormal Termination Processing (ATP)
  - Set environment variable ATP_ENABLED=1 in job script before aprun
  - Upon failure, generate merged stack backtrace tree in atpMergedBT.dot file
  - View output file with stat-view after loading with module load stat

- Notes on linking your application
  - PrgEnv-cray links everything necessary by default
  - PrgEnv-intel requires –Wl,–T/opt/cray/pc/cce/8.5.2/craylibs/x86-64/2.23.1.cce.ld

- Other debugging tools
  - You can generate STAT snapshots asynchronously
  - Full-featured debugging with DDT

When Things Go Wrong Running…

https://www.alcf.anl.gov/user-support

- Examine core files

- Best to save all three files generated by cobalt
  - <prefix_name>.cobaltlog, <prefix_name>.error, and <prefix_name>.output

- Retain important information
  - Jobid, machine name, copy/location of all files, exact error message

- Contact us
  - Your ALCF contact
  - Email: support@alcf.anl.gov
  - Call the ALCF Help Desk
    - Hours: Monday-Friday, 9am-5pm CT
    - Phone: 630-252-3111 or 866-508-9181 (toll-free, US only)


HAPPY COMPUTING!