Theta
Software and Job Submission

Christopher Knight
Catalyst Team

Argonne NATIONAL LABORATORY

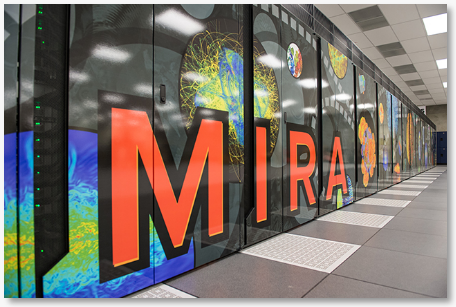
Outline

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

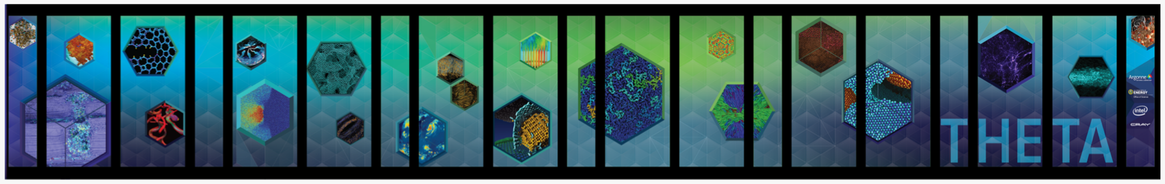
- Theta (KNL)
  - System Overview
  - Software & Environment Modules
  - Building your code
  - Queuing and running jobs with qsub & aprun

- Cooley (x86)
  - System Overview
  - Compiling and queuing jobs

- Tips for troubleshooting



Theta

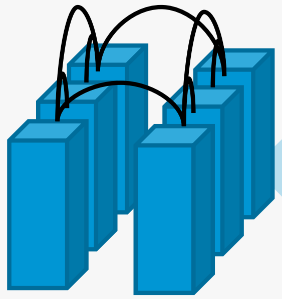


https://www.alcf.anl.gov/theta

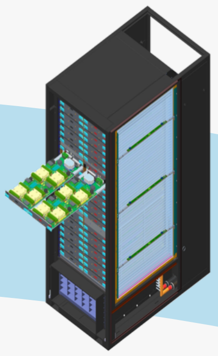
- Serves as a bridge between Mira and Aurora; simulation, data & learning system
- Cray XC40 system running the Cray software stack
- 11.69 PF peak performance
- 4392 nodes with 2nd Generation Intel® Xeon Phi™ processor
  - codenamed Knights Landing (KNL), 7230 SKU 64 cores, 1.3 GHz
  - 4 hardware threads/core
- 192 GB DDR4 & 16 GB MCDRAM memory on each node
- 128 GB SSD on each node
- Cray Aries high-speed interconnect in dragonfly topology
- Project filesystem is 10 PB Lustre with 210 GB/s throughput

Theta - System Overview

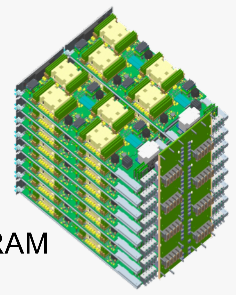
https://www.alcf.anl.gov/theta



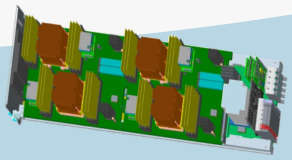
System: 24 Cabinets
4392 Nodes, 1152 Switches
Dual-plane, 12 groups, Dragonfly 12.1 TB/s Bi-Sec
11.7 PF Peak
70 TB MCDRAM, 843 TB DRAM



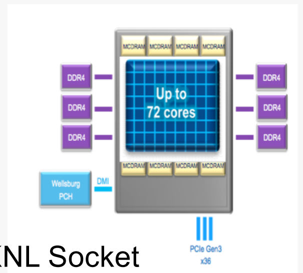
Cabinet: 3 Chassis, 75kW liquid/air cooled
510.72 TF 3TB MCDRAM, 36TB DRAM



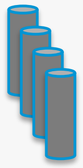
Chassis: 16 Blades, 16 Cards
64 Nodes, 16 Switches
170.24 TF 1TB MCDRAM, 12TB DRAM



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



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

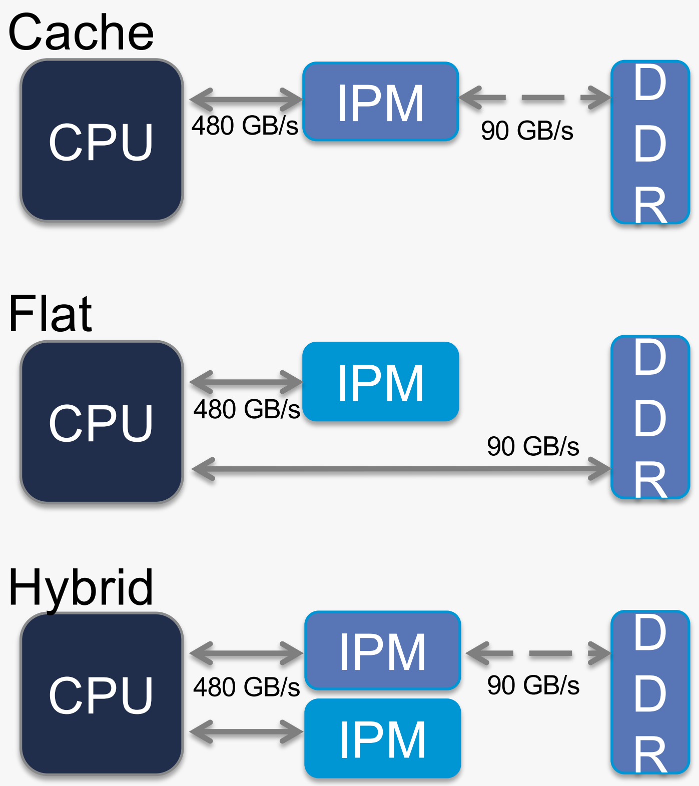


Sonexion Storage
4 Cabinets
Lustre file system
10 PB usable
210 GB/s

Theta - Memory Modes

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

Programming Languages
- Fortran
- C
- C++
- Python

Programming models
- Distributed Memory (Cray MPT)
  - MPI
  - SHMEM
  - GA
- Shared Memory
  - OpenMP 3.1
  - OpenACC 2.0
- PGAS
  - UPC
  - CAF
  - CoArray C++

Compilers
- Cray Compiling Environment (CCE)
- GNU
- 3rd party compilers (Intel)
- Environment setup
- Modules

Tools
- Debuggers
  - DDT
  - lgdb
- Debugging Tools
  - ATP
  - STAT
- Performance Analysis
  - Cray Apprentice
- Porting Tools
  - Reveal
  - CCDB

Optimized Scientific Libraries
- Dense
  - BLAS
  - LAPACK
  - ScaLAPACK
  - Iterative Refinement Toolkit
- Sparse
  - Cray PETSc (with CASK)
  - Cray Trilinos (with CASK)
- FFT
  - FFTW

I/O Libraries
- NetCDF
- HDF5

Cray developed
Licensed ISV SW
3rd party packaging
Cray added value to 3rd party

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, vtk, visit, ffmpeg
- Machine/Deep Learning & workflow
  - Intel Optimized Tensorflow, Keras, Neon, MXNet, Caffe2, Theano, CNTK, PyTorch, Sci-kit Learn, Graph Analytics (Cray Graph Engine), Horovod
  - Optimized with performance libraries Intel MKL, MKL-DNN, LibXSMM, etc…
  - Workflow/Data analysis: Singularity containers, Jupyter Hub, MongoDB, Apache Spark, R, Balsam
  - Python: Intel, Cray, Anaconda

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
  - Can disable automatic linking with libsci: module unload cray-libsci

Theta - 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 Theta are based on number of nodes
    - Jobs smaller than 128 nodes are allocated 128 nodes

Theta - Cobalt

https://www.alcf.anl.gov/user-guides/cobalt-job-control-xc40

- Resource management software on all ALCF systems
  - Syntax is similar to a PBS-style script

- 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

Theta - qsub

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

- Standard options
  - Project to charge: –A <project_name>
  - Queue: –q <queue>
  - Maximum walltime: –t <time_in_minutes>
  - Number of nodes: –n <number_of_nodes>
  - Prefix for output files: –O <file_prefix>
  - E-mail notifications: –M <email_address>
  - Dependencies: --dependencies <jobid1>:<jobid2>
  - Interactive job: –I or --interactive

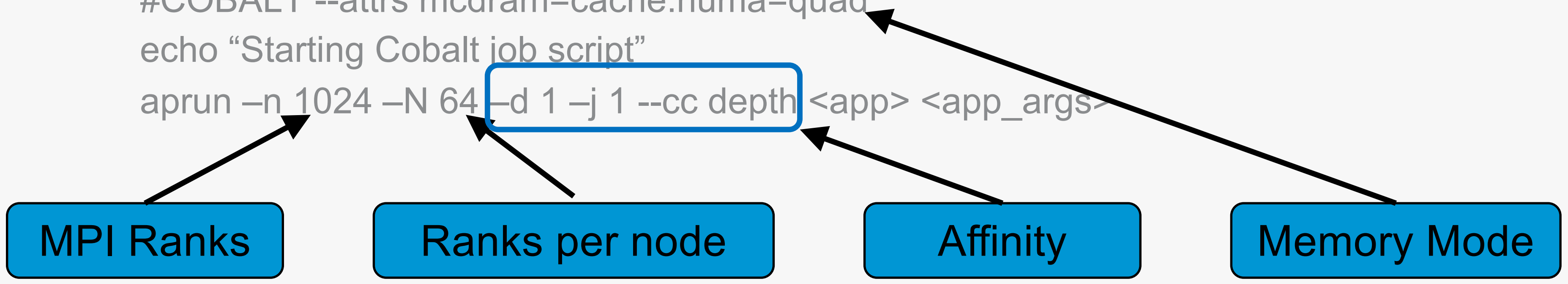
Theta - Submitting Script Jobs

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>

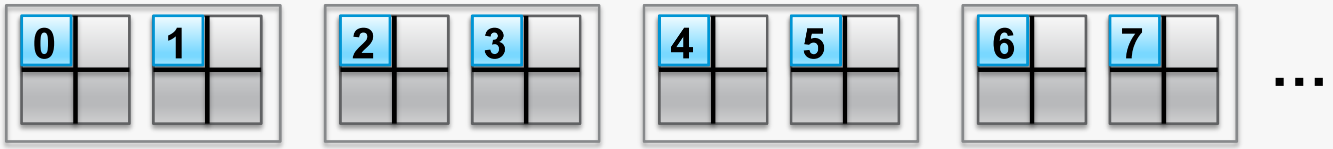
- Environment settings you may need
  - -e OMP_NUM_THREADS=<num_threads>
  - --cc none -e KMP_AFFINITY=<affinity>

- See also man aprun

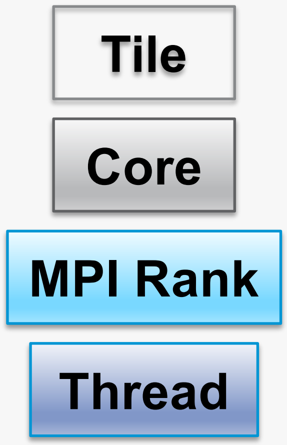
Theta - aprun Overview

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>



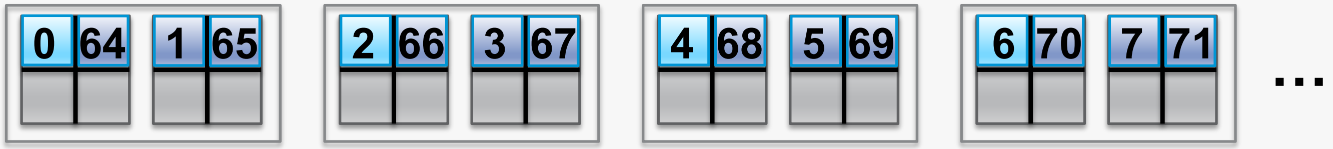
```
nname= nid02937  rnk= 0  tid= 0  ht= {0}
nname= nid02937  rnk= 1  tid= 0  ht= {1}
nname= nid02937  rnk= 2  tid= 0  ht= {2}
nname= nid02937  rnk= 3  tid= 0  ht= {3}
nname= nid02937  rnk= 4  tid= 0  ht= {4}
nname= nid02937  rnk= 5  tid= 0  ht= {5}
```



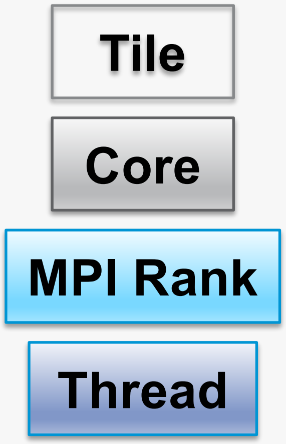
Theta - aprun Overview

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 - Now That Your Job Is Queued

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

- Check status of submitted jobs with qstat
- Format of output can be customized with --header

```
> qstat --header JobID:User:WallTime:Nodes:State:Queue
  JobID     User     WallTime   Nodes    State       Queue
  ===================================================================
  123456    user1    24:00:00    4000    running     default
  123457    user2    03:00:00    2048    queued      default
  123458    user3    03:00:00     128    running     default
  123459    user1    00:30:00       1    running     debug-cache-quad
  123460    user4    00:30:00      64    queued      training
```

Theta - 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

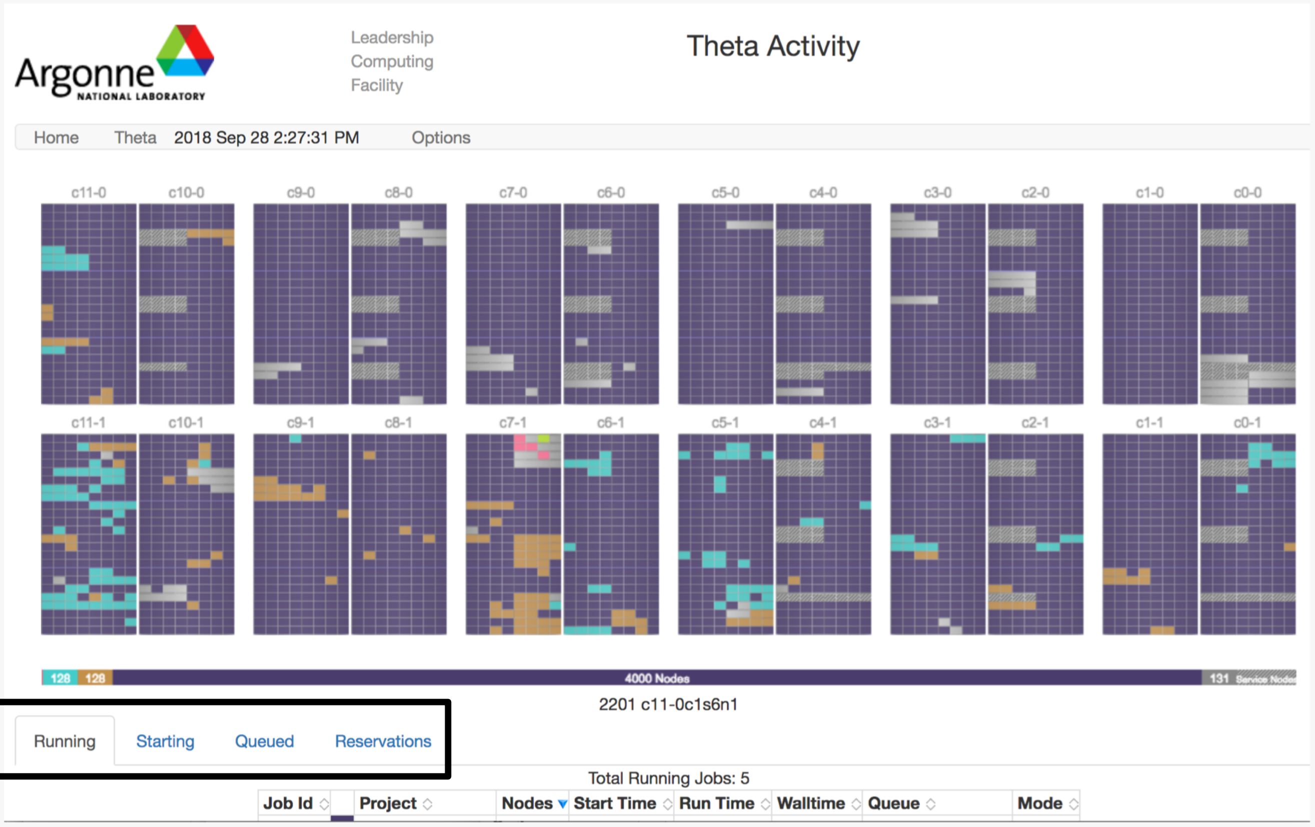
- Delete job from queue: qdel <jobid>

- 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>

Theta - Checking Status of Job

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

Running
Starting
Queued
Reservations



Total Running Jobs: 5

Job Id	Project	Nodes	Start Time	Run Time	Walltime	Queue	Mode

Theta - 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

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: 128 nodes, maximum walltime 3 hours
  - capability jobs: >= 802 nodes, maximum walltime 24 hours
  - Check website for current policies

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

Theta - Queues

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

- Jobs smaller than 128 nodes in default queue will be allocated 128 nodes

- Consider ensembles instead
  - Bundling multiple smaller jobs into single submission (e.g. multiple apruns)
  - Use a workflow system such as Balsam: https://www.alcf.anl.gov/balsam

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

ANY QUESTIONS?

Cooley

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

- Cooley serves as an analysis and visualization resource for projects
- x86+GPU system with 126 compute nodes
- 293 TF peak performance
- Each compute node has
  - two 2.4 GHz Intel Haswell processors (6 cores per CPU, 12 cores total)
  - one NVIDIA Tesla K80 (with two GPUs)
  - 384 GB CPU RAM, 12 GB RAM per GPU
  - 345 GB local scratch space
- FDR Infiniband interconnect
- Mira's GPFS and Theta's Lustre project filesystems mounted

Cooley - Softenv

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

- Cooley uses softenv instead of modules
- Keys are read at login time to set environment variables
  - Mira, Cetus, Vesta: ~/.soft
  - Cooley: ~/.soft.cooley
- To get started:

```
# Select latest version of mvapich2 with GNU compilers
+mvapich2
@default
# the end - do not put any keys after @default
```

- After edits to .soft.cooley, type resoft or log out and back in again
- Type softenv to see list of all available keys

Cooley - Compilers

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

- Choose compiler via softenv keys
- Non-MPI compilers
  - GNU: +gcc-8.2.0 (gcc, g++, gfortran)
  - Intel: +intel-composer-xe (icc, ifort)
  - Clang: @clang (clang)
- MPI Compiler wrappers
  - mvapich (mpicc, mpicxx, mpifort
    - GNU: +mvapich2
    - Intel: +mvapich2-intel
    - Clang: @mvapich2-clang (no mpifort)
  - mpich (mpicc, mpicxx, mpif77, mpif90)
    - GNU: +mpich2-1.4.1p1
    - Intel: +mpich2-1.4.1p1-intel

Cooley - Job Script

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

- Job script similar to Theta except mpirun instead of aprun
  - Example test.sh

```
#!/bin/sh
NODES=`cat $COBALT_NODEFILE | wc -l`
PROCS=$((NODES * 12))
mpirun -f $COBALT_NODEFILE -n $PROCS myprog.exe
```

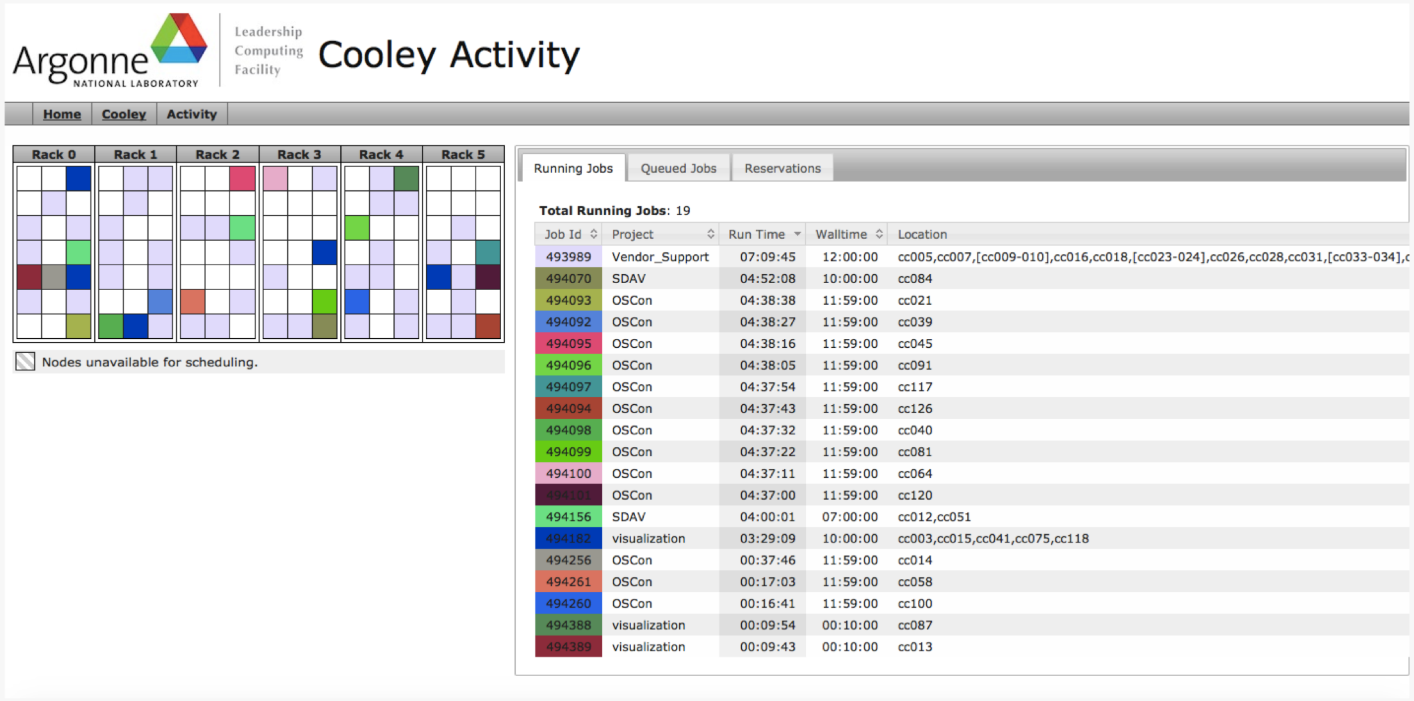
  - Submit executable script on 5 nodes for 10 minutes

```
qsub -q training -n 5 -t 10 -A Comp_Perf_Workshop ./test.sh
```

  - Queues
    - default for large/long jobs, debug for short/small jobs
    - pubnet to get public network visibility
    - nox11 queues to suppress X server for CUDA jobs

Cooley - Checking Status of Job

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



Total Running Jobs: 19

Job Id	Project	Run Time	Walltime	Location
493989	Vendor_Support	07:09:45	12:00:00	cc005,cc007,[cc009-010],cc016,cc018,[cc023-024],cc026,cc028,cc031,[cc033-034],c
494070	SDAV	04:52:08	10:00:00	cc084
494093	OSCon	04:38:38	11:59:00	cc021
494092	OSCon	04:38:27	11:59:00	cc039
494095	OSCon	04:38:16	11:59:00	cc045
494096	OSCon	04:38:05	11:59:00	cc091
494097	OSCon	04:37:54	11:59:00	cc117
494094	OSCon	04:37:43	11:59:00	cc126
494098	OSCon	04:37:32	11:59:00	cc040
494099	OSCon	04:37:22	11:59:00	cc081
494100	OSCon	04:37:11	11:59:00	cc064
494101	OSCon	04:37:00	11:59:00	cc120
494156	SDAV	04:00:01	07:00:00	cc012,cc051
494182	visualization	03:29:09	10:00:00	cc003,cc015,cc041,cc075,cc118
494256	OSCon	00:37:46	11:59:00	cc014
494261	OSCon	00:17:03	11:59:00	cc058
494260	OSCon	00:16:41	11:59:00	cc100
494388	visualization	00:09:54	00:10:00	cc087
494389	visualization	00:09:43	00:10:00	cc013

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

- Job on Theta is in ”starting” state; nodes being rebooted into memory mode requested.

- 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 status of nodes on Theta & Cooley: nodelist

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/pe/cce/default/cce/x86-64/lib/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!

HANDS-ON SESSION

Hands-on session

- On Theta or Cooley, copy examples from /projects/Comp_Perf_Workshop/examples
  - Can also retrieve examples from GitLab: git clone https://gitlab.com/alcf/training.git

- This week's workshop has its own project and queue names
  - Theta: -A Comp_Perf_Workshop -q training
  - Cooley: -A Comp_Perf_Workshop -q training

- Theta/Cooley: compile & submit
  - make
  - qsub submit.sh

Hands-on session - Theta Compilation Example

- Create directory, copy files, compile and submit

```
> cd /projects/Comp_Perf_Workshop
> mkdir -p $USER
> cp -r examples $USER
> cd $USER/examples/theta/compilation
> make
```

- Submit job and check output

```
> qsub submit.sh
> qstat -u $USER
> cat <JobID>.output
```

- qsub echos a cobalt JobID to the screen. In the absence of a -o argument, three files are created (say JobID was 123456):

  123456.cobaltlog, 123456.error, 123456.output (replaced by hellompi.output with -o)

Hands-on session - Theta Examples

- Example of an OpenMP job submission
  - Change to directory, compile, and submit

```
> cd /projects/Comp_Perf_Workshop/$USER/examples/theta/omp
> make
> qsub submit.sh
```

  - Note, remember that thread affinity is controlled by aprun settings (see slides 14-18 for reference)

- Example of a Python job submission
  - Change to directory, compile, and submit

```
> cd /projects/Comp_Perf_Workshop/$USER/examples/theta/python
> qsub submit.sh
```

  - Note, examine submit.sh script for loading python environment on Theta

Hands-on session - Cooley Examples

- Example of an OpenMP job submission
  - Change to directory, compile, and submit

```
> cd /projects/Comp_Perf_Workshop/$USER/examples/cooley/omp
> make
> qsub submit.sh
```

  - Remember to edit your ~/.soft.cooley file and add compiler & MPI keys. Note, @default should be the last line in your file.

- Example of a Python job submission
  - Edit your ~/.soft.cooley and add “+anaconda” before @default
  - Update your environment to include python paths

```
> resoft
```

  - Change to directory, compile, and submit

```
> cd /projects/Comp_Perf_Workshop/$USER/examples/theta/python
> qsub submit.sh
```