Argonne Training Program on Extreme-Scale Computing (ATPESC)

Quick Start on ATPESC Computing Resources

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EXASCALE COMPUTING PROJECT

National Nuclear Security Administration
U.S. DEPARTMENT OF ENERGY | Office of Science
Argonne NATIONAL LABORATORY

AVAILABLE RESOUCE FOR ATPESC

- ALCF Systems
  - KNL (Theta)
  - x86+K80 GPU (Cooley)
  - x86+A100 GPUs (thetaGPU)
- OLCF
  - IBM Power9+NVIDIA V100 GPU (Ascent)
- NERSC
  - x86 + NVIDIA A100 GPU (Perlmutter)
- Cloud resources
  - NVIDIA cloud GPU resources
  - Intel DevCloud
  - AMD Accelerator Cloud (AAC)

The DOE Leadership Computing Facility

- Collaborative, multi-lab, DOE/SC initiative ranked top national priority in *Facilities for the Future of Science: A Twenty-Year Outlook.*
- Mission: Provide the computational and data science resources required to solve the most important scientific & engineering problems in the world.
- Highly competitive user allocation program (INCITE, ALCC).
- Projects receive 100x more hours than at other generally available centers.
- LCF centers partner with users to enable science & engineering breakthroughs (Liaisons, Catalysts).

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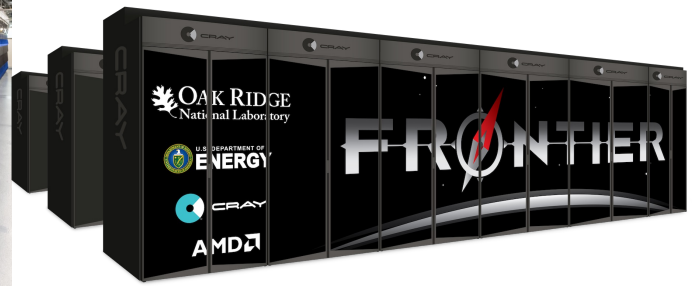
OAK RIDGE National Laboratory



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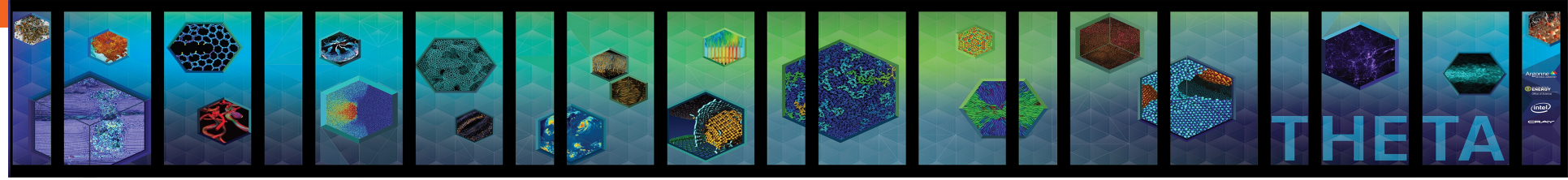
Leadership Computing Facility System

	Argonne LCF			Oak Ridge LCF	
System	Cray XC40	HPE	HPE	IBM	HPE
Name	Theta	Polaris	Aurora in 2022	Summit	Frontier in 2022
Compute nodes	4,392	560	-	4608	-
Node architecture	Intel Knights Landing, 64 cores	AMD Milan + 4x NVIDIA A100 GPU	Intel Xeon + Intel GPU	2 x IBM POWER9 22 cores 6 x NVIDIA V100 GPUs	AMD CPU + AMD GPU
Processing Units	281,088 Cores	17,920 AMD Milan Cores + 2240 GPUs	-	202,752 POWER9 Cores + 27648 GPUs	-
Memory per node, (gigabytes)	192 DDR4 + 16 MCDRAM	512 DDR4 + 160 HBM2 + 1600 SSD	-	512 DDR4 + 96 HBM2 + 1600 NVM	-
Peak performance, (petaflops)	11.69	44	Exascale	200	Exascale

ALCF Systems

- ***Theta - Cray* XC40**
  - 4,392 nodes / 281,088 cores
- ***ThetaGPU – NVIDIA DGX A100***
  - 24 DGX A100 nodes, each with
    - *Two AMD Rome 64-core processors*
    - *Eight NVIDIA A100 GPUs with 40 GB HBM per GPU*
    - *1 TB DDR4 memory*
- ***Cooley (visualization & data analysis)* – Cray CS**
  - 126 nodes, each with
    - Two Intel Xeon E5-2620 Haswell 2.4 GHz 6-core processors
    - NVIDIA Tesla K80 graphics processing unit with 24 GB memory
    - 384 GB DDR4 memory

Theta



Theta serves as a bridge to the exascale system coming to Argonne

- Serves as a bridge between Mira and Aurora, transition and data analytics system
- Cray XC40 system. Runs Cray software stack
- 11.69 PF peak performance
- 4392 nodes with 2nd Generation Intel® Xeon Phi™ processor
  - Knights Landing (KNL), 7230 SKU 64 cores 1.3GHz
  - 4 hardware threads/core
- 192GB DDR4 memory 16GB MCDRAM on each node
- 128GB SSD on each node
- Cray Aries high speed interconnect in dragonfly topology
- Initial file system: 10PB Lustre file system, 200 GB/s throughput

Theta - Filesystems

- Lustre
  - Home directories (/home) are in /lus/swift/home
    - Default quota 50GiB
    - Your home directory is backed up
  - Project directory locations (/grand) in /lus/grand/projects
    - Theta, ThetaGPU, Cooley: **/grand/projects/ATPESC2022**
      - **CREATE A SUBDIRECTORY /grand/projects/ATPESC2022/usr/your_username**
    - Access controlled by unix group of your project
    - Default quota 1TiB
    - Project directories are NOT backed up
  - With large I/O on Lustre, be sure to consider **stripe width**

Theta – Modules (Theta, ThetaGPU ONLY)

- 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*
  - *help*
  - *list ← what is currently loaded*
  - *avail*
  - *load*
  - *unload*
  - *switch|swap*
  - *use ← add a directory to MODULEPATH*
  - *display|show*

Theta - Compilers

- For all compilers (Intel, Cray, Gnu, etc):
  - **Use:** cc, CC, ftn
  - **Do not use** mpicc, MPICC, mpic++, mpif77, mpif90
    - *they do not generate code for the compute nodes*
- Selecting the compiler you want using **"module swap"** or **"module unload"** followed by **"module load"**
  - Intel
    - PrgEnv-intel *This is the default*
  - Cray
    - module swap PrgEnv-intel PrgEnv-cray
    - **NOTE:** links libsci by default
  - Gnu
    - module swap PrgEnv-intel PrgEnv-gnu
  - Clang/LLVM
    - module swap PrgEnv-intel PrgEnv-llvm

Theta - Job script

```
#!/bin/bash
#COBALT -t 10
#COBALT –n 2
#COBALT -A  ATPESC2022

# Various env settings are provided by Cobalt
echo $COBALT_JOBID  $COBALT_PARTNAME  $COBALT_JOBSIZE

aprun -n 16 -N 8 -d 1 -j 1 -cc depth ./a.out
status=$?

# could do another aprun here...

exit $status
```

Theta - aprun overview

- Start a parallel execution (equivalent of *mpirun*, *mpiexec* on other systems)
  - *Must be invoked from within a batch job that allocates nodes to you!*
- Options
  - -n *total_number_of_ranks*
  - -N *ranks_per_node*
  - -d *depth* [number of cpus (hyperthreads) per rank]
  - -cc **depth** [Note: **depth** is a keyword]
  - -j *hyperthreads* [cpus (hyperthreads) per compute unit (core)]
- Env settings you may need
  - -e OMP_NUM_THREADS=*nthreads*
  - -e KMP_AFFINITY=...
- See also **man aprun**

Submitting a Cobalt job

- qsub –A <project> -q <queue> -t <time> -n <nodes> ./jobscript.sh

  E.g.

  qsub –A Myprojname –q default –t 10 –n 32 ./jobscript.sh

- If you specify your options in the script via #COBALT, then just:
  - qsub jobscript.sh
- Make sure jobscript.sh is executable
- Without "-q", submits to the queue named "**default**"
  - For ATPESC reservations, specify e.g. "–q **ATPESC2022**" (see ***showres*** output)
  - For small tests outside of reservations, use e.g. "-q debug-cache-quad"
- ***Theta "default" (production) queue has 128 node minimum job size***
  - The ATPESC reservation does not have this restriction
- **man qsub** for more options

Managing your job

- qstat – show what's in the queue
  - qstat –u <username> # Jobs only for user
  - qstat <jobid> # Status of this particular job
  - qstat –fl <jobid> # Detailed info on job
- qdel <jobid>
- showres – show reservations currently set in the system
- **man qstat** for more options

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

Interactive job

- Useful for short tests or debugging
- Submit the job with –I (letter I for Interactive)
  - Default queue and default project
    - qsub –I –n 32 –t 30
  - Specify queue and project:
    - qsub –I –n 1 –t 30 –q ATPESC2022 –A ATPESC2022
- Wait for job's shell prompt
  - *This is a new shell* with env settings e.g. COBALT_JOBID
  - Exit this shell to end your job
- From job's shell prompt, run just like in a script job, e.g. on Theta
  - aprun –n 512 –N 16 –d 1 –j 1 –cc depth ./a.out
- After job expires, apruns will fail. *Check* **qstat $COBALT_JOBID**

Core files and debugging

- Abnormal Termination Processing (ATP)
  - Set environment **ATP_ENABLED=1** in your job script before aprun
  - On program failure, generates a merged stack backtrace tree in file **atpMergedBT.dot**
  - View the output file with the program **stat-view** (module load stat)

- Notes on linking your program
  - make sure you load the "atp" module before linking
    - to check, *module list*

- Other debugging tools
  - You can generate STAT snapshots asynchronously
  - Full-featured debugging with DDT
  - More info at
    - https://www.alcf.anl.gov/sites/default/files/2020-05/Loy-comp_perf_workshop-debugging-2020-v1.2.pdf

Machine status web page

Running Jobs

Queued Jobs

Reservations

http://status.alcf.anl.gov/theta/activity (a.k.a. The Gronkulator)

ALCF ThetaGPU (x86+GPU)

- ThetaGPU is an extension of Theta and is comprised of 24 NVIDIA DGX A100 nodes for training artificial intelligence (AI) datasets, while also enabling GPU-specific and -enhanced high-performance computing (HPC) applications for modeling and simulation.

- Machine Specs
  - Architecture: AMD Rome CPU
  - Peak Performance: 3.8 petaflops
  - Processors per node: Two 64-core
  - GPU per node: 8 NVIDIA A100
  - Nodes: 24
  - Cores: 3,072
  - Number of GPUs: 192
  - Memory: 24 TB
  - GPU memory: 7.68 TB
  - Interconnect: 20 Mellanox QM9700 HDR200 40-port switches wired in a fat-tree topology

ThetaGPU - Environment

- ThetaGPU Login nodes
  - **`$ ssh thetagpusn1`** (or **`$ ssh thetagpusn2`**) from the Theta login nodes
- Use module commands on thetaGPU login nodes
- Module examples
  - openmpi for mpi
  - nvhpc for NVIDIA OpenMP compilers
- Update your .bashrc and .bash_profile as follows:

```
$ cat ~/.bashrc
# .bashrc
# Source global definitions
if [ -f /etc/bashrc ]
then
    . /etc/bashrc
elif [ -f /etc/bash.bashrc ]
then
    . /etc/bash.bashrc
fi
```

```
$ cat ~/.bash_profile
# .bash_profile
# Get the aliases and functions
if [ -f ~/.bashrc ]; then
        . ~/.bashrc
fi
# proxy settings
export HTTP_PROXY=http://theta-proxy.tmi.alcf.anl.gov:3128
export HTTPS_PROXY=http://theta-proxy.tmi.alcf.anl.gov:3128
export http_proxy=http://theta-proxy.tmi.alcf.anl.gov:3128
export https_proxy=http://theta-proxy.tmi.alcf.anl.gov:3128
```

- ALL bash jobscripts must also begin with **`#!/bin/bash -l`**(that's a lower-case L)

ThetaGPU Job Script

- More like a typical Linux cluster
- Job script
  - Example test.sh:

```
#!/bin/bash -l
NODES=`cat $COBALT_NODEFILE | wc -l`
PROCS=$((NODES * 16))
mpirun -n $PROCS myprog.exe
```

  - Submit on 1 node/gpu for 30 minutes

```
qsub -n 1 -t 30 -q training-gpu -A ATPESC2022 ./test.sh     # For 1 node with 8 GPUs
qsub -n 1 -t 30 -q single-gpu -A ATPESC2022 ./test.sh       # For 1 GPU
```

  - Submit on 1 node/gpu for 30 minutes for an interactive job

```
qsub -I -n 1 -t 30 -q training-gpu -A ATPESC2022            # For 1 node with 8 GPUs
qsub -I -n 1 -t 30 -q single-gpu -A ATPESC2022              # For 1 GPU
```

  - Refer to online user guide for more info
    - https://www.alcf.anl.gov/support-center/theta-gpu-nodes

ALCF Cooley (x86+GPU)

- Cooley, the ALCF's visualization cluster, enables users to analyze and visualize large-scale datasets, helping them to gain deeper insights into simulations and data generated on the facility's supercomputers.

- Machine Specs
  - Architecture: Intel Haswell
  - Peak Performance: 293 teraflops
  - Processors per node: Two 6-core, 2.4-GHz Intel E5-2620
  - GPU per node: 1 NVIDIA Tesla K80
  - Nodes: 126
  - Cores: 1,512
  - Memory: 47 TB
  - GPU memory: 3 TB
  - Interconnect: FDR InfiniBand network
  - Racks: 6

Cooley - Softenv (Cooley)

- Similar to **modules** package
- Keys are read at login time to set environment variables like PATH.
  - Cooley: ~/.soft.cooley
- To get started:

```
# This key selects Intel compilers to be used by mpi wrappers
+openmpi-2.1.5-intel
+intel-composer-xe
@default
# the end – do not put any keys after the @default
```

- After edits to .soft, type "resoft" or log out and back in again

Cooley Job Script

- More like a typical Linux cluster
- Job script
  - Example test.sh:

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

  - Submit on 5 nodes for 10 minutes

```
qsub -n 5 -t 10 –q training -A ATPESC2022 ./test.sh
```

  - Refer to online user guide for more info

ALCF References

- Sample files (Theta, ThetaGPU, Cooley)
  - /grand/projects/ATPESC2022/EXAMPLES/track-0-getting-started/GettingStarted

- Online docs
  - https://www.alcf.anl.gov/support-center
  - Getting Started Presentations (*slides and videos*)
    - Theta and Cooley
    - https://www.alcf.anl.gov/workshops/2019-getting-started-videos
  - Debugging:
    - https://www.alcf.anl.gov/sites/default/files/2020-05/Loy-comp_perf_workshop-debugging-2020-v1.2.pdf

Cryptocard tips

- The displayed value is a hex string. Type your PIN followed by all letters as CAPITALS.
- If you fail to authenticate the first time, you may have typed it incorrectly
  - Try again with the **same crypto string** (do NOT press button again)
- If you fail again, try a different ALCF host with a fresh crypto #
  - A successful login resets your count of failed logins
- Too many failed logins → your account locked
  - Symptom: You get password prompt but login denied even if it is correct
- Too many failed logins from a given IP → the IP will be blocked
  - Symptom: connection attempt by ssh or web browser will just time out

ATPESC Resources

Theta, ThetaGPU and Cooley

- **Project name: ATPESC2022**
- **Note:** use your ALCF Username. The password will be your old/newly established PIN + token code displayed on the token.
- **Support:** ALCF staff available to help you **via slack**!! and support@alcf.anl.gov
- **Reservations:** Please check the details of the reservations directly on each machine (**command**: showres)
- **Queue**
  - **Theta: ATPESC2022, ThetaGPU: training-gpu, or single-gpu, Cooley: training (check *showres*) or default for running without reservation**

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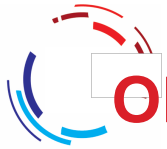
ATPESC Resources



OLCF –Ascent

- *Ascent User Guide https://docs.olcf.ornl.gov/systems/ascent_user_guide.html*
- *Tools to learn how to use the `jsrun` job launcher*
  - *Hello_jsrun – A "Hello, World!"-type program to help understand resource layouts on Summit/Ascent nodes.*
  - *Jsrun Quick Start Guide – A very brief overview to help get you started*
  - *Job-step-viewer – A graphical tool to learn the basics of jsrun*
- *OLCF Tutorials at https://github.com/olcf-tutorials*

- See documents in your Argonne Folder for additional information
- *For other questions, email: help@olcf.ornl.gov*

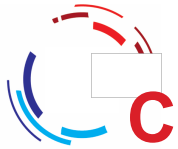
ATPESC Resources

NERSC – Perlmutter (HPE Cray XE)

- 1536 GPU-accelerated nodes, each with
  - 64 AMD Milan cores with 4 NVIDIA A100 GPUs
  - 256 GB DDR4 memory
  - 160 GB HBM2 memory on 4 GPUs
- 3072 AMD Milan (64-core) nodes, each with
  - 128 physical cores
  - 512 GB memory
- Reference

  https://docs.nersc.gov/systems/perlmutter/

ATPESC Resources



Cloud resources for Tools track

- NVIDIA Cloud GPU resources
  - Attendees interested in the NVIDIA tools hands-on session will need an NVIDIA developer account. They can sign up here ahead of time: https://developer.nvidia.com/
  - On the day of the tools track, we will screenshare this landing page URL and the accompanying access code: https://courses.nvidia.com/dli-event/
- Intel DevCloud (TBD)
- AMD Accelerator Cloud (TBD)

Questions?

- *Use this presentation as a reference during ATPESC!*
- Supplemental info will be posted as well

Hands-on exercise

- On Theta
- On ThetaGPU
- On Cooley

Hands-on exercise: Theta

- $ ssh -Y {your_username} @theta.alcf.anl.gov # Login to Theta

- $ module list # See loaded modules

```
jkwack@thetalogin5:~> module li
Currently Loaded Modulefiles:
  1) modules/3.2.11.4                                 9) dmapp/7.1.1-7.0.2.1_2.104__g38cf134.ari          17) perftools-base/20.06.0
  2) intel/19.1.0.166                                10) gni-headers/5.0.12.0-7.0.2.1_2.38__g3b1768f.ari  18) PrgEnv-intel/6.0.7
  3) craype-network-aries                            11) xpmem/2.2.20-7.0.2.1_2.75__g87eb960.ari          19) craype-mic-knl
  4) craype/2.6.5                                    12) job/2.2.4-7.0.2.1_2.91__g36b56f4.ari             20) cray-mpich/7.7.14
  5) cray-libsci/20.06.1                             13) dvs/2.12_2.2.177-7.0.2.1_13.10__g0b75e43d        21) nompirun/nompirun
  6) udreg/2.3.2-7.0.2.1_2.59__g8175d3d.ari          14) alps/6.6.59-7.0.2.1_3.90__g872a8d62.ari          22) adaptive-routing-a3
  7) ugni/6.0.14.0-7.0.2.1_3.83__ge78e5b0.ari        15) rca/2.2.20-7.0.2.1_2.98__g8e3fb5b.ari            23) darshan/3.3.0
  8) pmi/5.0.16                                      16) atp/3.6.4                                        24) xalt
```

- $ module avail # See available modules

- $ showres # Check reservation
- $ qstat -u {your_username} # To see your jobs
- $ qstat -fu {your_username} # To see your jobs with more verbose information

Hands-on exercise: Theta

- $ cd /grand/projects/ATPESC2022 # Go to the project folder
- $ cd usr # Go to user space under project
- $ mkdir {your_username} # Create your space
- $ cd {your_username}

- $ cp -rf /grand/projects/ATPESC2022/EXAMPLES/track-0-getting-started/GettingStarted .
- $ cd GettingStarted/theta/
- $ more hellompi.c # See the example source
- $ more Makefile # An example of how to compile a code
- $ more submit.sh # An example of job script

Hands-on exercise: Theta

- $ export CRAYPE_LINK_TYPE=dynamic # For dynamic linking
- $ module swap PrgEnv-intel PrgEnv-cray; module swap PrgEnv-cray PrgEnv-intel # To avoid a bug

- $ cc -o hellompi hellompi.c # Build the example
- $ make clean; make # Another way to build the example

- $ aprun -n 4 ./hellompi # It won't work since you are on a login node

  XALT Error: unable to find aprun

Hands-on exercise: Theta

- $ qsub -I -n 1 -t 30 -A ATPESC2022 -q ATPESC2022 # Start an interactive job mode

```
Connecting to thetamom3 for interactive qsub...
Currently Loaded Modulefiles:
  1) modules/3.2.11.4                                 11) nodehealth/5.6.27-7.0.2.1_4.72__g20e015c.ari       21) perftools-base/20.06.0
  2) alps/6.6.59-7.0.2.1_3.90__g872a8d62.ari          12) system-config/3.6.3072-7.0.2.1_8.6__gca557bd7.ari  22) PrgEnv-intel/6.0.7
  3) nodestat/2.3.89-7.0.2.1_2.76__g8645157.ari       13) Base-opts/2.4.142-7.0.2.1_2.75__g8f27585.ari       23) craype-mic-knl
  4) sdb/3.3.812-7.0.2.1_2.97__gd6c4e58.ari           14) intel/19.1.0.166                                   24) cray-mpich/7.7.14
  5) udreg/2.3.2-7.0.2.1_2.59__g8175d3d.ari           15) craype-network-aries                               25) nompirun/nompirun
  6) ugni/6.0.14.0-7.0.2.1_3.83__ge78e5b0.ari         16) craype/2.6.5                                       26) adaptive-routing-a3
  7) gni-headers/5.0.12.0-7.0.2.1_2.38__g3b1768f.ari  17) cray-libsci/20.06.1                                 27) darshan/3.3.0
  8) dmapp/7.1.1-7.0.2.1_2.104__g38cf134.ari          18) pmi/5.0.16                                         28) xalt
  9) xpmem/2.2.20-7.0.2.1_2.75__g87eb960.ari          19) atp/3.6.4
 10) llm/21.4.631-7.0.2.1_3.3__g4fcec58.ari           20) rca/2.2.20-7.0.2.1_2.98__g8e3fb5b.ari
```

- $ cd /grand/projects/ATPESC2022/usr
- $ cd {your_username}/GettingStarted/theta/
- $ aprun -n 4 ./hellompi

```
jkwack@thetamom3:/grand/projects/ATPESC2022/usr/jkwack/GettingStarted/theta> aprun -n 4 ./hellompi
0: Hello!
1: Hello!
2: Hello!
3: Hello!
Application 27120510 resources: utime ~0s, stime ~2s, Rss ~10244, inblocks ~2590, outblocks ~8
```

Hands-on exercise: ThetaGPU

- $ ssh thetagpusn1 # Login to ThetaGPU from Theta, (or, $ ssh thetagpusn2)

- $ module list # See loaded modules
- $ module avail # See available modules

- $ showres # Check reservation (only for thetaGPU, not on theta)
- $ qstat -u {your_username} # To see your jobs (only jobs on thetaGPU, not on theta)
- $ qstat -fu {your_username} # To see your jobs with more verbose information

Hands-on exercise: ThetaGPU

- $ vi ~/.bashrc
- $ cat ~/.bashrc

```
# .bashrc
# Source global definitions
if [ -f /etc/bashrc ]
then
    . /etc/bashrc
elif [ -f /etc/bash.bashrc ]
then
    . /etc/bash.bashrc
fi
```

- $ vi ~/.bash_profile
- $ cat ~/.bash_profile

```
# .bash_profile
# Get the aliases and functions
if [ -f ~/.bashrc ]; then
        . ~/.bashrc
fi
# proxy settings
export HTTP_PROXY=http://theta-proxy.tmi.alcf.anl.gov:3128
export HTTPS_PROXY=http://theta-proxy.tmi.alcf.anl.gov:3128
export http_proxy=http://theta-proxy.tmi.alcf.anl.gov:3128
export https_proxy=http://theta-proxy.tmi.alcf.anl.gov:3128
```

Hands-on exercise: ThetaGPU

- $ source ~/.bashrc
- $ cd /grand/projects/ATPESC2022 # Go to the project folder
- $ cd usr/{your_username} # Go to your space under project
- $ cd GettingStarted/thetaGPU/
- $ more hellompi.c # See the example source
- $ more Makefile # An example of how to compile a code
- $ more submit.sh # An example of job script

Hands-on exercise: ThetaGPU

- $ mpicc -o hellompi hellompi.c # Build the example
- $ make clean; make # Another way to build the example

- $ nvidia-smi # NVIDIA A100 GPUs are visible since you are on a login node

```
jkwack@thetagpusn1:/grand/projects/ATPESC2022/usr/jkwack/GettingStarted/thetaGPU$ nvidia-smi

Command 'nvidia-smi' not found, but can be installed with:

apt install nvidia-340       (You will have to enable component called 'restricted')
apt install nvidia-utils-390 (You will have to enable component called 'restricted')

Ask your administrator to install one of them.
```

Hands-on exercise: ThetaGPU

- $ qsub -I -n 1 -t 30 -A ATPESC2022 -q single-gpu # Start an interactive job mode

```
jkwack@thetagpusn1:/grand/projects/ATPESC2022/usr/jkwack/GettingStarted/thetaGPU$ qsub -I -n 1 -t 30 -A ATPESC2022 -q single-gpu
Job routed to queue "single-gpu".
WARNING: Filesystem attribute not set for this job submission.
This job will be set to request all filesystems.  In the event
of a filesystem outage, this job may be put on hold unnecessarily.
Setting attrs to:  {'filesystems': 'home,grand,eagle,theta-fs0'}
Wait for job 10096966 to start...
Opening interactive session to thetagpu06-gpu0
Welcome to Ubuntu 20.04.4 LTS (GNU/Linux 5.4.0-121-generic x86_64)

 * Documentation:  https://help.ubuntu.com
 * Management:     https://landscape.canonical.com
 * Support:        https://ubuntu.com/advantage

  System information as of Sun 31 Jul 2022 02:09:05 AM CDT

  System load:  1.66             Users logged in:             0
  Usage of /:   1.5% of 1.72TB   IPv4 address for docker0:     172.17.0.1
  Memory usage: 2%               IPv4 address for enp226s0:   10.230.2.194
  Swap usage:   0%               IPv4 address for infinibond0: 172.23.2.194
  Processes:    3262             IPv4 address for infinibond0: 172.22.2.194

Last login: Sun Jul 31 01:22:28 2022 from thetagpusn1.mcp

Currently Loaded Modules:
  1) openmpi/openmpi-4.0.5   2) Core/StdEnv
```

Hands-on exercise: ThetaGPU

- $ cd /grand/projects/ATPESC2022/usr/{your_username}/GettingStarted/thetaGPU/
- $ mpirun -n 4 ./hellompi

```
jkwack@thetagpu06:/grand/projects/ATPESC2022/usr/jkwack/GettingStarted/thetaGPU$ mpirun -n 4 ./hellompi
0: Hello!
1: Hello!
2: Hello!
3: Hello!
```

- $ nvidia-smi

```
jkwack@thetagpu06:/grand/projects/ATPESC2022/usr/jkwack/GettingStarted/thetaGPU$ nvidia-smi
Sun Jul 31 02:10:48 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 470.129.06   Driver Version: 470.129.06   CUDA Version: 11.4     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-SXM...  On   | 00000000:07:00.0 Off |                    0 |
| N/A   21C    P0    52W / 400W |      0MiB / 40536MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

Hands-on exercise: Cooley

- $ ssh -Y {your_username} @cooley.alcf.anl.gov # Login to Cooley

- $ softenv # Check available environment
- $ vi .soft.cooley # Update your environment
- $ cat .soft.cooley

  +openmpi-2.1.5-intel

  +intel-composer-xe

  @default
- $ resoft # Apply the updated environment
- $ which mpicc

  /soft/libraries/mpi/openmpi-2.1.5/intel/bin/mpicc

Hands-on exercise: Cooley

- $ showres # Check reservation
- $ qstat -u {your_username} # To see your jobs
- $ qstat -fu {your_username} # To see your jobs with more verbose information

- $ qsub -I -n 1 -t 30 -A ATPESC2022 -q training # Start an interactive job mode

- $ cd /grand/projects/ATPESC2022/usr/{your_username} # Go to the project folder
- $ cd GettingStarted/cooley/ # Go to the example folder

Hands-on exercise: Cooley

- $ mpicc -o hellompi hellompi.c # Build the example
- $ make clean; make # Another way to build the example

- $ mpirun -n 4 ./hellompi

```
[jkwack@cc043 ~]$ cd /grand/projects/ATPESC2022/usr/jkwack/GettingStarted/cooley/
[jkwack@cc043 cooley]$ make clean; make
/bin/rm -f *.error *.output *.cobaltlog hellompi
which mpicc
/soft/libraries/mpi/openmpi-2.1.5/intel/bin/mpicc
mpicc -g -O0 -o hellompi hellompi.c
[jkwack@cc043 cooley]$ mpirun -n 4 ./hellompi
0: Hello!
1: Hello!
2: Hello!
3: Hello!
```

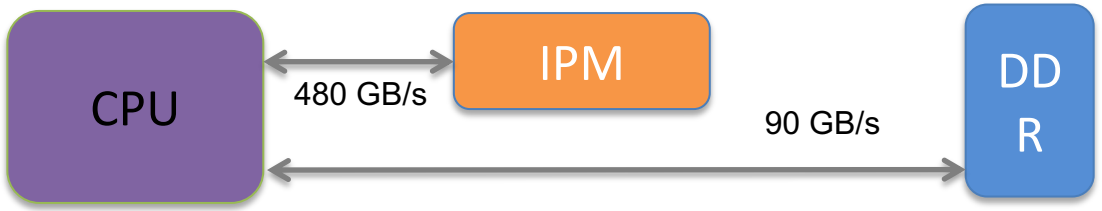
Supplemental Info

Theta Memory Modes - IPM and DDR

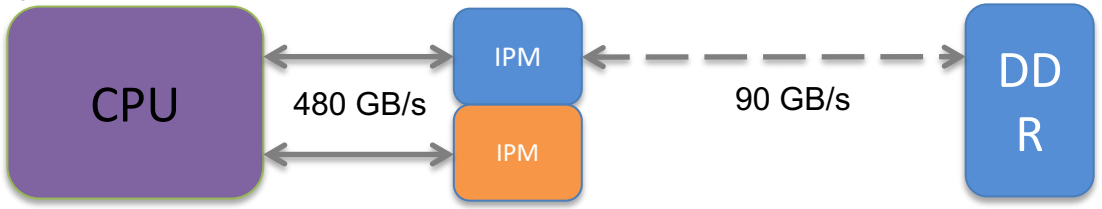
Selected at node boot time

Cache

Flat



Hybrid

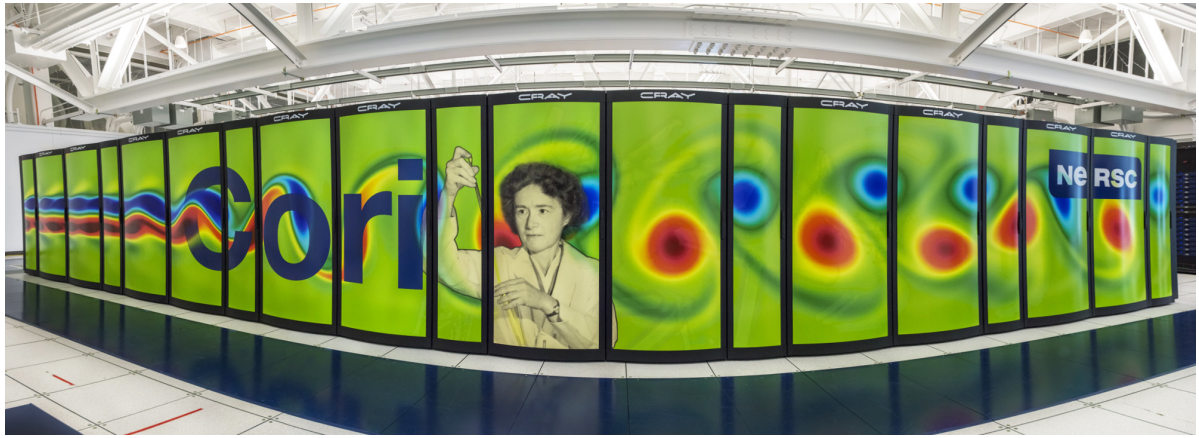


- **Two memory types**
- In Package Memory (IPM)
  - 16 GB MCDRAM
  - ~480 GB/s bandwidth
- Off Package Memory (DDR)
  - Up to 384 GB
  - ~90 GB/s bandwidth
- **One address space**
- Possibly multiple NUMA domains
- **Memory configurations**
- Cached: DDR fully cached by IPM
  - Flat: user managed
- Hybrid: ¼, ½ IPM used as cache
  - **Managing memory:**
- jemalloc & memkind libraries
- Pragmas for static memory allocations

Theta queues and modes

- MCDRAM and NUMA modes can only be set by the system when nodes are rebooted. *Users cannot directly reboot nodes.*
- Submit job with the --attrs flag to get the mode you need. E.g.
  - qsub –n 32 –t 60 –attrs mcdram=cache:numa=quad ./jobscript.sh
- Other mode choices
  - mcdram: cache, flat, split, equal
  - numa: quad, a2a, hemi, snc2, snc4
- Queues
  - Normal jobs use queue named "default"
  - Debugging: debug-cache-quad, debug-flat-quad
    - Note: pre-set for mcdram/numa configuration
  - "qstat –Q" lists all queues

ATPESC Resources



NERSC – Cori (Cray XC40)

- 9688 KNL nodes, each with
  - 68 physical cores
  - 96 GB DDR4 memory
  - 16 GB MCDRAM
- 2388 Haswell (16-core) nodes, each with
  - 32 physical cores
  - 128 GB memory
- Reference

  https://docs.nersc.gov/systems/cori/