Getting Started on ThetaGPU

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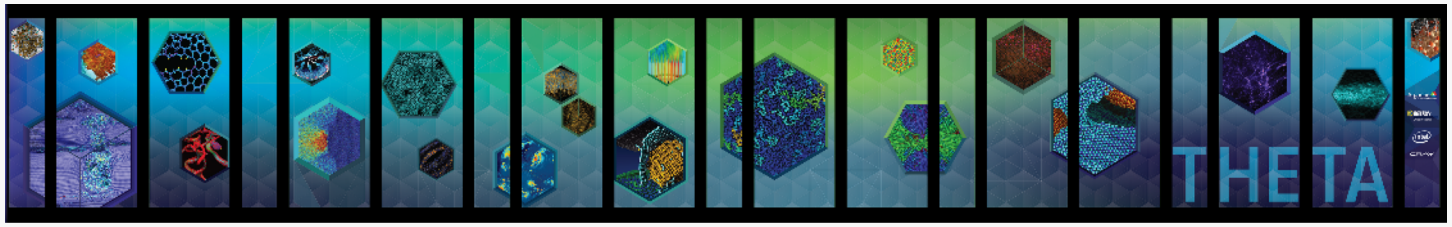
Outline

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

- ThetaGPU (DGX A100)
  - System Overview
  - Software & Environment Modules
  - Building your code
  - Queuing and running jobs with qsub

ThetaGPU



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

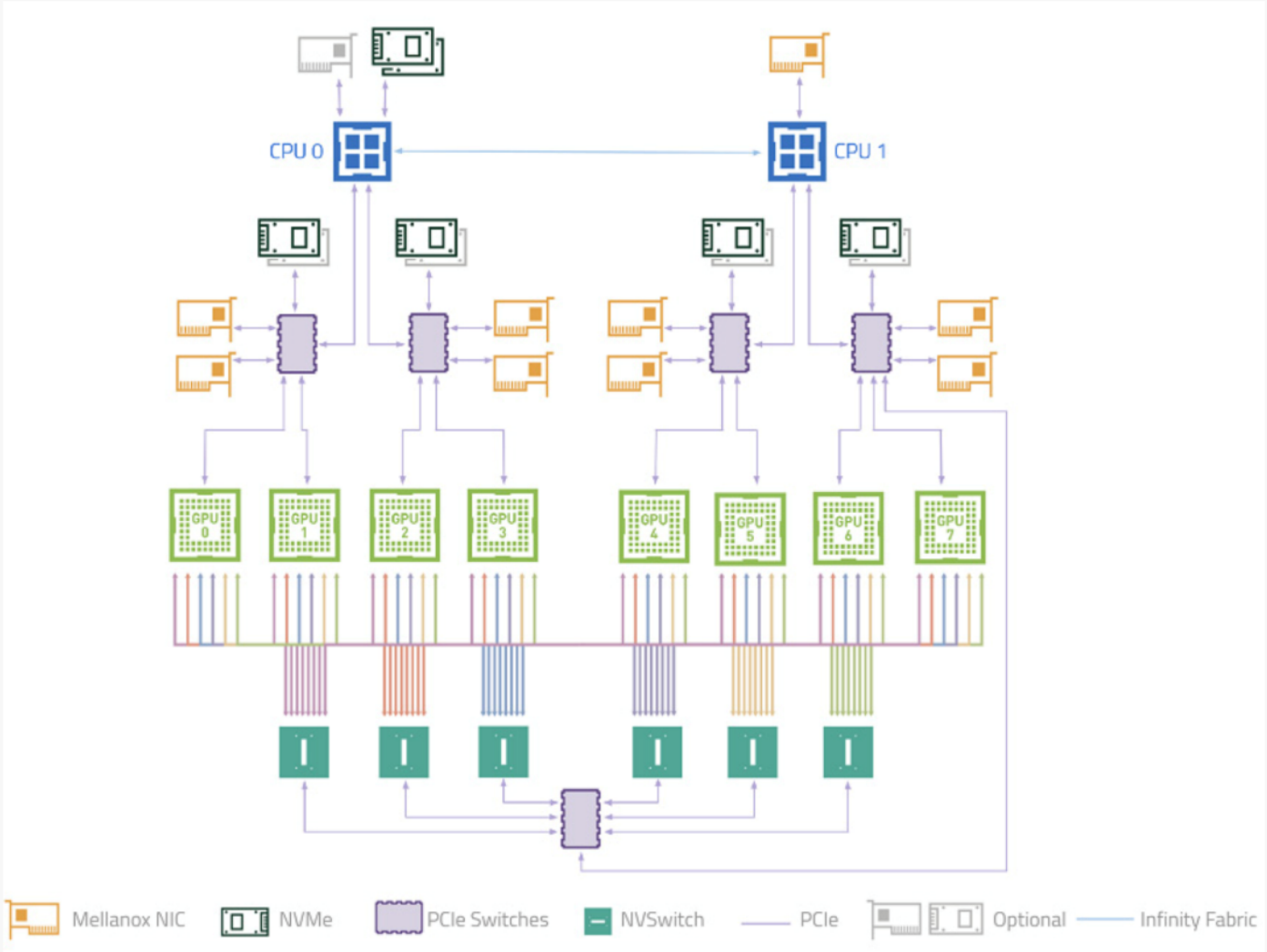
- Theta expansion to support coronavirus research that is now open for general use

- NVIDIA DGX A100 partition
  - 24 nodes each with
    - 8 NVIDIA A100 Tensor Core GPUs & 320 GB HBM memory
    - 2 AMD Rome 64-core CPUs & 1 TB DDR4
    - 15 TB SSD (4 x 3.84 TB), 25 Gb/s bandwidth
    - 8 HDR 200 NICs (compute network)
    - 2 HDR 200 NICs (storage network)

- Dedicated Compute Fabric
  - 20 Mellanox QM9700 HDR200 40-port switches in fat-tree topology

- Project filesystem is Theta's 10 PB Lustre with 210 GB/s throughput

ThetaGPU – Node Overview



https://docs.nvidia.com/dgx/pdf/dgxa100-user-guide.pdf
https://www.nvidia.com/content/dam/en-zz/Solutions/Data-Center/dgx-a100/dgxa100-system-architecture-white-paper.pdf

ThetaGPU - Logging in and Environment

https://www.alcf.anl.gov/support-center/theta/theta-thetagpu-overview#theta-gpu

- Use Theta login nodes

  $ ssh user@theta.alcf.anl.gov

- Load ThetaGPU scheduler

  $ module load cobalt/cobalt-gpu

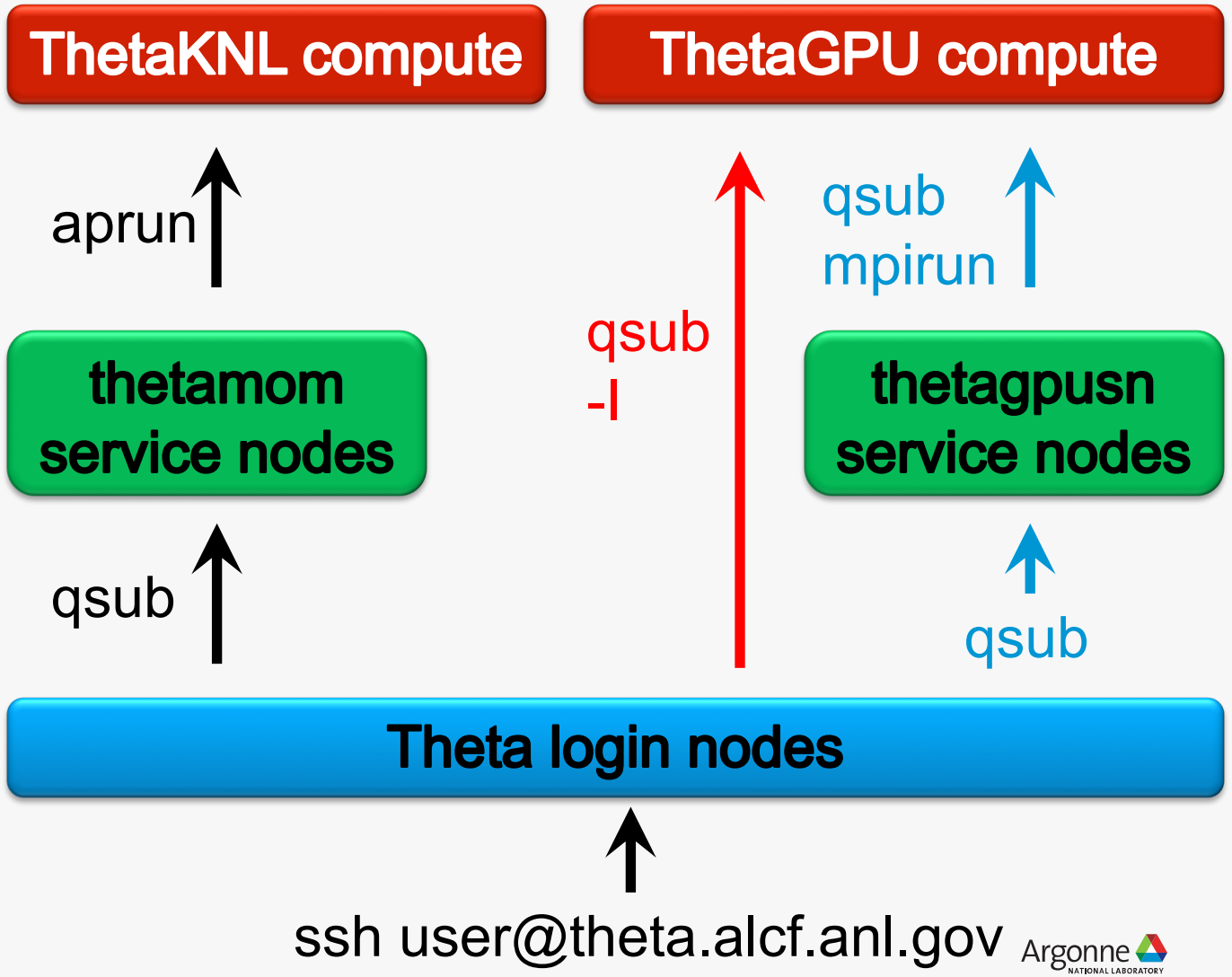
- Use ThetaGPU compute nodes for building and development

  $ qsub -I -n 1 -t 60 -q full-node -A …

- Can also login to ThetaGPU service nodes, if needed

  $ ssh thetagpusn1

  $ qsub -I -n 1 -t 60 -q full-node -A …



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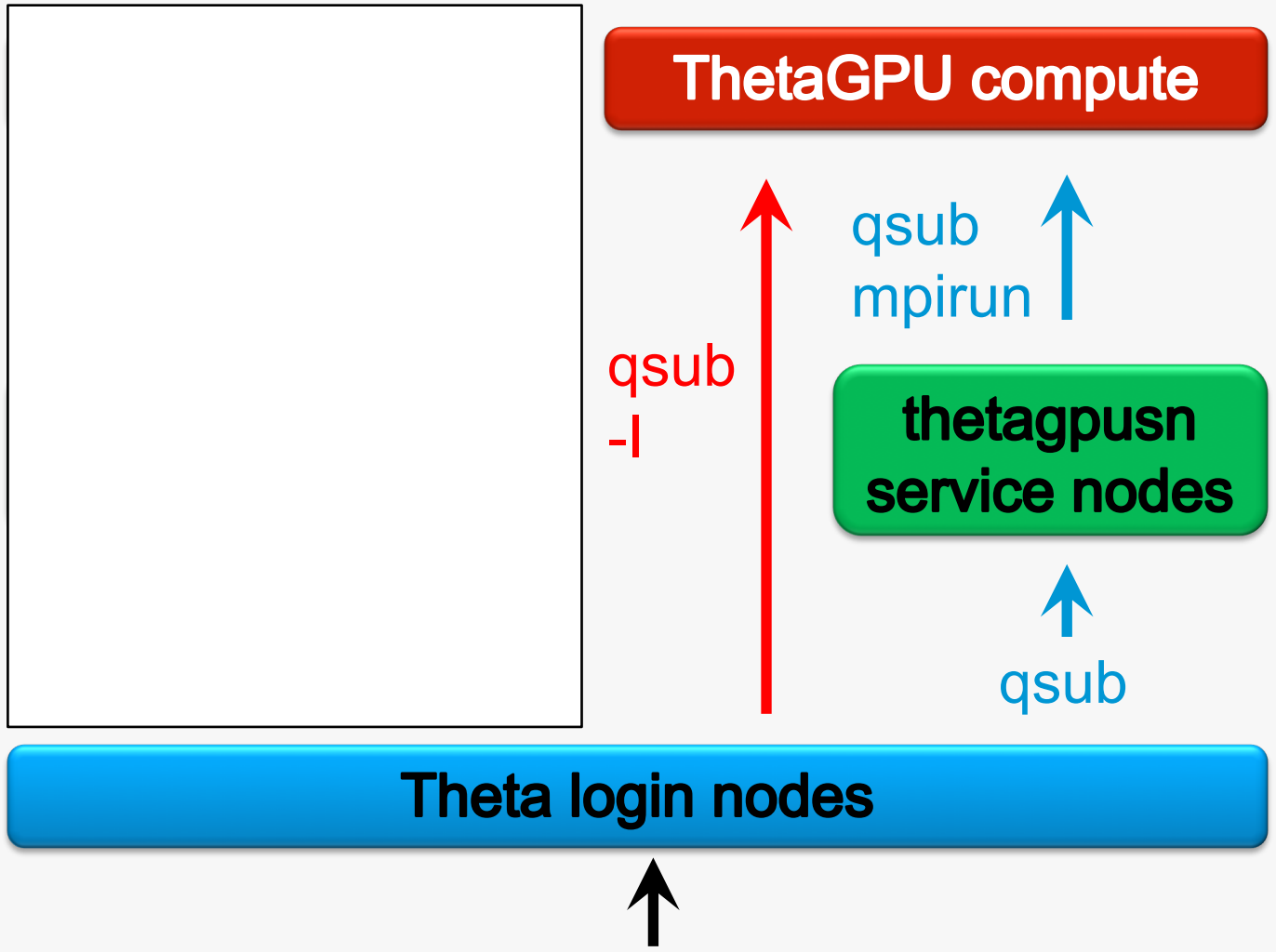

ThetaGPU - Software & Libraries

We recommend Nvidia or LLVM compilers, GNU compilers do not currently offload

https://www.alcf.anl.gov/support-center/theta-gpu-nodes

- List available modules on ThetaGPU compute node

thetagpu##$ module avail

```
------------------------------------------------------------------------ /usr/local/lmod/lmod/modulefiles -------------------------------------------------------------------------
   Core/lmod    Core/settarg

------------------------------------------------------------ /lus/theta-fs0/software/environment/thetagpu/lmod/modulefiles -------------------------------------------------------------
   Core/StdEnv                 (L,D)    conda/tensorflow/2020-12-23        llvm/release-12.0.0       (D)    nvhpc-nompi/21.3
   aocl/blis-3.0                        conda/tensorflow/2021-01-08        nccl/nccl-v2.8.4-1_CUDA11        nvhpc/20.9                        (D)
   cmake/3.19.5                         conda/tensorflow/2021-03-02 (D)    nvhpc-byo-compiler/20.9   (D)    nvhpc/21.2
   conda/pytorch/2020-11-25             hdf5/1.8.13                        nvhpc-byo-compiler/21.2          nvhpc/21.3
   conda/pytorch/2021-03-02    (D)      hdf5/1.12.0                 (D)    nvhpc-byo-compiler/21.3          openmpi/openmpi-4.0.5             (L)
   conda/tensorflow/2020-11-11          llvm/main-20210112                 nvhpc-nompi/20.9          (D)    openmpi/openmpi-4.1.0_ucx-1.10.0
   conda/tensorflow/2020-12-17          llvm/main-20210426                 nvhpc-nompi/21.2                 openmpi/openmpi-4.1.0             (D)

------------------------------------------------------ /lus/theta-fs0/software/spack/share/spack/modules/linux-ubuntu18.04-x86_64 -------------------------------------------------------
   autoconf-2.69-gcc-7.5.0-wmttzuv                gdbm-1.18.1-gcc-10.2.0-ia4egqb       mpfr-4.0.2-gcc-7.5.0-mpv2v7v         readline-8.0-gcc-10.2.0-ephdh34
   autoconf-archive-2019.01.06-gcc-7.5.0-bdyarrk  gdbm-1.18.1-gcc-7.5.0-4av4gyw        ncurses-6.2-gcc-10.2.0-qjpgcs6       readline-8.0-gcc-7.5.0-t54jzdy
   automake-1.16.3-gcc-7.5.0-stmktof              gmp-6.1.2-gcc-7.5.0-3ol3tld          ncurses-6.2-gcc-7.5.0-crhlefo        zlib-1.2.11-gcc-10.2.0-glt2u7u
   berkeley-db-18.1.40-gcc-10.2.0-fle5h4p         libiconv-1.16-gcc-7.5.0-jearpk4      openssl-1.1.1j-gcc-10.2.0-3g4hmwz    zlib-1.2.11-gcc-7.5.0-smoyzzo
   berkeley-db-18.1.40-gcc-7.5.0-vd7vwr5          libsigsegv-2.12-gcc-7.5.0-lbrx7ln    perl-5.32.1-gcc-10.2.0-grji3ix       zstd-1.4.5-gcc-7.5.0-rnf7xyj
   cmake-3.19.5-gcc-10.2.0-felctqr                libtool-2.4.6-gcc-7.5.0-jdxbjft      perl-5.32.1-gcc-7.5.0-op6xocu
   diffutils-3.7-gcc-7.5.0-otkkten                m4-1.4.18-gcc-7.5.0-mkc3u4x          pkgconf-1.7.3-gcc-10.2.0-4aysapw
   gcc-10.2.0-gcc-7.5.0-jj2fh4j                   mpc-1.1.0-gcc-7.5.0-pj4yncj          pkgconf-1.7.3-gcc-7.5.0-4sh6pym

  Where:
   L:  Module is loaded
   D:  Default Module

Use "module spider" to find all possible modules and extensions.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".
```

ThetaGPU - NVIDIA Compilers

https://www.alcf.anl.gov/support-center/theta-gpu-nodes/compiling-and-linking-thetagpu

- NVIDIA HPC SDK
  - Load module, single node

```
$ module load nvhpc
$ module list
Currently Loaded Modules:
1) Core/StdEnv  2) nvhpc/21.3  3) openmpi-4.1.0_nvhpc-21.3
```

  - GPU Programming Models: CUDA, OpenMP

  - Use nvc++, nvc, nvfortran
  - For OpenMP offload: -mp=gpu -gpu=cc80
  - Use mpicxx, mpicxx, mpif90, etc…

https://developer.nvidia.com/hpc-sdk

ThetaGPU - LLVM Compilers

https://www.alcf.anl.gov/support-center/theta-gpu-nodes/compiling-and-linking-thetagpu

- LLVM w/ OpenMP offload
  - Load module

```
$ module load llvm
$ module list
Currently Loaded Modules:
 1) openmpi/openmpi-4.0.5   2) Core/StdEnv   3) llvm/release-12.0.0
```

  - GPU Programming Models: CUDA, OpenMP

  - Use clang++, clang
  - For OpenMP offload: -fopenmp -fopenmp-targets=nvptx64
  - Use MPI wrappers: mpicxx, mpicc, etc…

ThetaGPU – Running a Job

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

```
ssh user@theta.alcf.anl.gov
module load cobalt/cobalt-gpu
# submit to the reservation, using two possible queues:
# ecp_openmp_hackathon queue (full node, 8 GPUs):
# limits are currently set at 1hr max walltime, 1 job max running, and 5 jobs max queued
qsub -I -q ecp_openmp_hackathon -t 60 -n 1 -A ecp_omp2021

# single-gpu queue (1 GPU):
# limits are currently set at 1hr max walltime, 1 job max running, and 1 jobs max queued
qsub -I -q single-gpu -t 60 -n 1 -A ecp_omp2021

# Examples for OpenMP offload are here:
https://github.com/argonne-lcf/CompPerfWorkshop-2021/tree/main/01_openmp/demo
```


ANY QUESTIONS?