Compiling and running on ThetaGPU

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Outline

- https://www.alcf.anl.gov/user-guides
- Compiling and Running on ThetaGPU (DGX A100)
  - System Overview
  - Queuing and running jobs with `qsub` & `mpirun`
  - Software & Lmod Environment Modules
  - Building your code
  - Key tips throughout
- **JaeHyuk Kwack**: Performance Profiling Tools
- **Corey Adams**: AI and Frameworks
- Q&A

See also: Chris Knight's "Getting Started on ThetaGPU" talk from ALCF Computational Performance Workshop 2021-05-04
https://www.alcf.anl.gov/events/2021-alcf-computational-performance-workshop

Getting Started on ALCF Resources

- General documentation
  - ThetaKNL: https://www.alcf.anl.gov/support-center/theta/theta-thetagpu-overview
  - ThetaGPU: https://www.alcf.anl.gov/support-center/theta-gpu-nodes
  - Polaris: https://www.alcf.anl.gov/polaris
  - AI-Testbed: https://ai.alcf.anl.gov/

- Cobalt job scheduler documentation: https://www.alcf.anl.gov/support-center/theta/running-jobs-and-submission-scripts
- `qsub` is the primary Cobalt command for job submission
  - `-q [job-queue]` is either `single-gpu` or `full-node`
  - `-A [project]` is the allocation on ThetaGPU that the job is charged to
  - `-t [wallclock time]` sets the time limit for the job
  - `-n [nodecount]` specifies the number of nodes for the job

```
qsub -t 60 -n 1 -q single-gpu -A allocation -M user@anl.gov -I
```

HPC wire

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Argonne Augments Theta Supercomputer with GPUs to Accelerate Coronavirus Research

December 3, 2020

Dec. 3, 2020 — Earlier this year, the U.S. Department of Energy's (DOE) Argonne National Laboratory unveiled an upgrade to its high-performance computing (HPC) resource Theta. The new hardware stands to substantially improve the performance and capability of the Theta supercomputer, an Intel-HPE/Cray XC40 system housed at the Argonne Leadership Computing Facility (ALCF). The ALCF is a U.S. DOE Office of Science User Facility.

Deployed rapidly in response to the global pandemic, the Theta upgrade and its supporting systems are currently being leveraged in the fight against the coronavirus and associated COVID-19 disease. Funding for the hardware was provided by the Coronavirus Aid, Relief and Economic Security (CARES) Act, signed into law in March.

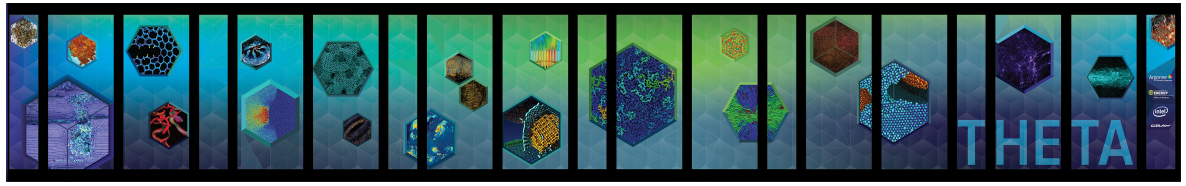
With a core that combines both graphics processing unit (GPU) and central processing unit (CPU) capabilities, the augmented Theta architecture adds 24 NVIDIA DGX A100 nodes to the existing system. Each DGX A100 node comprises eight NVIDIA A100 Tensor Core GPUs and two AMD Rome CPUs that provide 320 gigabytes (7680 GB aggregately) of GPU memory for training artificial intelligence (AI) datasets, while also enabling GPU-specific and GPU-enhanced HPC applications for modeling and simulation.

For system documentation, visit the Theta User Guide

To be considered for an allocation award, please submit your request using the ALCF's Discretionary Allocation Request form.

ALCF staff members augment Theta with the installation of NVIDIA DGX A100 nodes. (Image: Argonne National Laboratory)

ThetaGPU



- https://www.alcf.anl.gov/support-center/theta/theta-thetagpu-overview
- **ThetaGPU** = expansion of Theta originally to support coronavirus research (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 240 GB/s throughput (`/lus/theta-fs0/projects/`)
  - Eagle (`/lus/eagle/projects/`): 100 PB Lustre with 650 GB/s throughput
  - Grand (`/lus/grand/projects/`): 100 PB Lustre with 650 GB/s throughput

NVIDIA DGX versions (per node)

- DGX-1 (April 2016)
  - —8x P100 or V100 (first gen 16 GB) GPUs
  - —2x 20-core Intel Xeon E5-2698 v4 CPUs

- DGX-2 (May 2018)
  - —16x V100 (second gen 32 GB) GPUs
  - —2x 24-core Intel Xeon 8168 CPUs

- DGX A100 (May 2020)
  - —8x A100 (40 GB) GPUs
  - —2x 64-core AMD Rome 7742 CPUs

ThetaGPU - Logging in and navigating

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

- First, access ThetaKNL login nodes

  $ ssh user@theta.alcf.anl.gov

- **ThetaKNL**: launch job on service nodes, then run on compute nodes

  $ qsub -I -n 4 -t 60 -q debug-cache-quad -A …

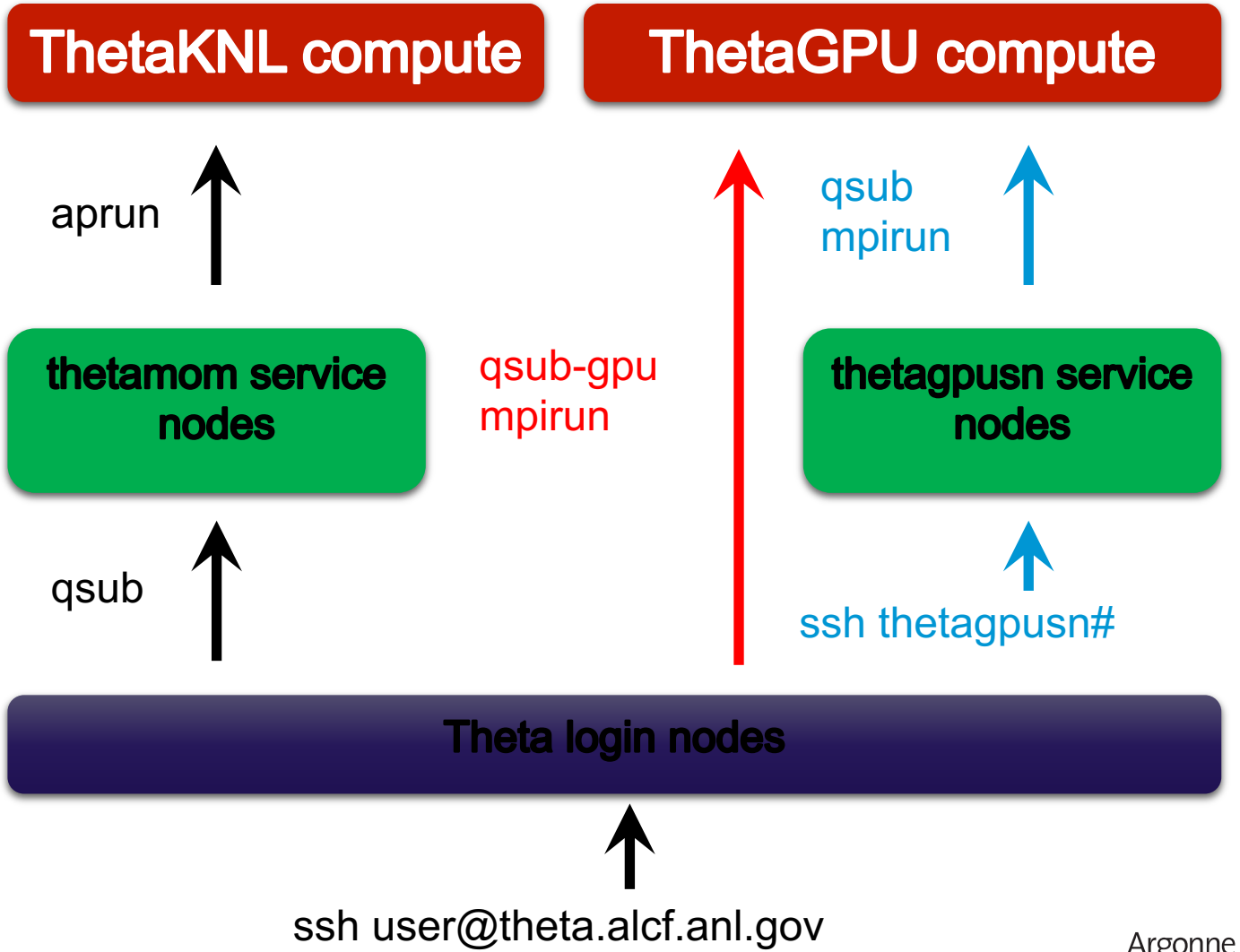
  $ aprun -n 4096 –N 32 –d 4 –j 2 -cc depth …

- **ThetaGPU**: login to service nodes, then build and run on compute nodes

  $ ssh thetagpusn1

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

  $ mpirun …



Theta - Logging in and navigating

- Alternatively, you can stay on ThetaKNL login node and load/unload ThetaGPU scheduler as needed:

```
$ module load cobalt/cobalt-gpu
```

`hostname` is your friend!

SSH onto the same Theta login node each time (e.g. for running a persistent `tmux` server)

On your laptop, `~/.ssh/config`:

```
Host theta
HostName thetaloginX.alcf.anl.gov
User username
ControlMaster auto
ControlPath ~/.ssh/cm_socket/%r@%h:%p
ControlPersist 10m
```

Where X is in [1, 6]. Then

```
ssh theta
```

ThetaGPU - Submitting Script Jobs

- https://www.alcf.anl.gov/support-center/theta-gpu-nodes/running-jobs-thetagpu
- Executable is invoked within script (bash, csh, …)

- mpirun is used to launch executables on compute nodes
- `> cat myscript.sh`
- `#!bin/sh`
- `#COBALT -n 2 -t 15 -q full-node -A <project_name>`
- `#COBALT --attrs pubnet`
- `echo “Starting Cobalt job script”`
- `mpirun -hostfile ${COBALT_NODEFILE} –n 16 -N 8 <app> <app_args>`

Cobalt Options

MPI Ranks

Ranks per node

- `> qsub ./myscript.sh`
  `123456`

ThetaGPU - mpirun Overview

- https://www.alcf.anl.gov/support-center/theta-gpu-nodes/running-jobs-thetagpu
- mpirun options
  - Total number of MPI ranks: –n <total_number_ranks>
  - Number of MPI ranks per node: –N <number_ranks_per_node>
  - Environment variables: –x <VAR1=1> –x <VAR2=1>
  - Display MPI process map: -display-map
  - Display detected resource allocation: -display-allocation
  - Process binding: --bind-to <hwthread|core|socket|…>
- Environment settings you may need
  - -x OMP_NUM_THREADS=<num_threads>
- See also man mpirun

ThetaGPU - Queues

- https://www.alcf.anl.gov/support-center/theta-gpu-nodes/queue-policy-thetagpu
- Two queues currently available with simple First-In First-Out (FIFO) policy
  - full-node: request entire node
  - single-gpu: request single gpu; node resources shared by other users
    - analogous to debug queue to build applications and debug

queue	full-node	single-gpu
MinTime	5 minutes	5 minutes
MaxTime	12 hours	1 hour
MaxQueued	20 jobs	1 job
MaxRunning	10 jobs	1 job

- Check website for current policies

ThetaGPU - qsub attributes and networking quirks

- HTTP/S networking disabled by default on compute nodes; use a proxy

```
export http_proxy=theta-proxy.tmi.alcf.anl.gov:3128
export https_proxy=theta-proxy.tmi.alcf.anl.gov:3128
```

- SSH port 22 blocked on both service and compute nodes

  → cannot clone Git repos over SSH

- Enable Multi-Instance GPU (MIG) mode (**currently disabled and waiting for response from NVIDIA)**

```
--attrs mig-mode=True
```

- Enable high performance networking on compute nodes (typically over ESNet)

```
--attrs=pubnet
```

Clone/push/pull via Git SSH URLs on `thetaloginX`

e.g. `tmux` running on `thetaloginX` with windows:

1. on `thetaloginX` for networking over SSH
2. on `thetagpusn1` for launching jobs, inspecting modules
3. on `thetagpuY` (compute node) for running job

ThetaGPU – Lmod Modules

https://lmod.readthedocs.io/en/latest/

- A tool for managing a user's environment
  - Sets your PATH, LD_LIBRARY_PATH, shell functions, etc. to access desired front-end tools
  - Your TensorFlow, PyTorch, Horovod, MPI library, compiler version, etc. 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 swap <mod_old> <mod_new>
  - List information about module: module show <mod>
  - Include additional modules: module use <path_to_extra_modules>

```
➜  ~ module avail

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

-------------------------- /lus/theta-fs0/software/environment/thetagpu/lmod/modulefiles --------------------------
   Core/StdEnv       (L,D)    hpctoolkit/2021.04.30-gpu           nvhpc-nompi/21.3
   aocl/blis-3.0              hypre/2.22.0                        nvhpc-nompi/21.7                          (D)
   cmake/3.19.5               llvm/main-20210811                  nvhpc/20.9
   conda/pytorch              nccl/nccl-v2.8.4-1_CUDA11           nvhpc/21.2
   conda/tensorflow           nccl/nccl-v2.9.9-1_CUDA11.3         nvhpc/21.3
   conda/2021-06-26  (D)      nccl/nccl-v2.11.4-1_CUDA11.4 (D)    nvhpc/21.7                                (D)
   conda/2021-06-28           netcdf/c-4.8.0-fortran-4.5.3        openmpi/openmpi-4.0.5_ucx-1.10.0_nvhpc-21.7
   conda/2021-09-22           nvhpc-byo-compiler/20.9             openmpi/openmpi-4.0.5                     (L)
   conda/2021-11-30           nvhpc-byo-compiler/21.2             openmpi/openmpi-4.1.0_ucx-1.10.0
   darshan/3.3.0              nvhpc-byo-compiler/21.3             openmpi/openmpi-4.1.0_ucx-1.11.0_gcc-9.3.0
   hdf5/1.8.13                nvhpc-byo-compiler/21.7      (D)    openmpi/openmpi-4.1.0
   hdf5/1.8.22                nvhpc-mpi/21.7                      openmpi/openmpi-4.1.1_ucx-1.10.1_gcc-9.3.0
   hdf5/1.12.0       (D)      nvhpc-nompi/20.9                    openmpi/openmpi-4.1.1_ucx-1.11.2_gcc-9.3.0  (D)
   hdf5/1.12.1-nvhpc          nvhpc-nompi/21.2

------------------- /lus/theta-fs0/software/spack/share/spack/modules/linux-ubuntu20.04-x86_64 --------------------
   autoconf-2.69-gcc-9.3.0-qz4d4gi          libtool-2.4.6-gcc-9.3.0-uh3mpsu
   berkeley-db-18.1.40-gcc-9.3.0-pn2cxag    m4-1.4.18-gcc-9.3.0-eixehd4
   bison-3.7.6-gcc-9.3.0-b3ikzdr            m4-1.4.19-gcc-9.3.0-7fztfyz
   bison-3.7.6-gcc-9.3.0-d4ucav2            ncurses-6.2-gcc-9.3.0-n5vhymf
   clingo-bootstrap-spack-gcc-9.3.0-gbsyvaq openssl-1.1.1k-gcc-9.3.0-rvjrbxt
   clingo-bootstrap-spack-gcc-9.3.0-uwnqfyx perl-5.32.1-gcc-9.3.0-ylpdpx6
   cmake-3.20.2-gcc-9.3.0-r5aseli           perl-5.34.0-gcc-9.3.0-aa6w4wx
   cmake-3.20.3-gcc-9.3.0-57eqw4f           pkgconf-1.7.4-gcc-9.3.0-newgzwq
   diffutils-3.7-gcc-9.3.0-2eqr3yc          re2c-1.2.1-gcc-9.3.0-drh4oxu
   gdbm-1.19-gcc-9.3.0-g4xrv3g              readline-8.1-gcc-9.3.0-fvag4vk
   libiconv-1.16-gcc-9.3.0-w6zptbc          zlib-1.2.11-gcc-9.3.0-p7dmb5p
   libsigsegv-2.13-gcc-9.3.0-2fxv3ky

  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".
```

Current CUDA driver (2022-01-26)

- CUDA 11.4 is default toolkit/runtime and device driver version

```
➜  ~ nvidia-smi
Wed Jan 26 00:17:51 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 470.82.01    Driver Version: 470.82.01    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   22C    P0    51W / 400W |      0MiB / 40536MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
```

- CUDA 11.3 and 11.0 libraries still available (https://docs.nvidia.com/deploy/cuda-compatibility/)

```
➜  local hostname
thetagpu11
➜  local pwd
/usr/local
➜  local ll
total 56K
drwxr-xr-x  2 root root 4.0K Jan 18 16:32 bin/
lrwxrwxrwx  1 root root   22 Aug  9 09:58 cuda -> /etc/alternatives/cuda/
lrwxrwxrwx  1 root root   25 Jun 24  2021 cuda-11 -> /etc/alternatives/cuda-11/
drwxr-xr-x 15 root root 4.0K Jul 12  2021 cuda-11.0/
drwxr-xr-x 15 root root 4.0K Jun 24  2021 cuda-11.3/
drwxr-xr-x 16 root root 4.0K Nov  8 15:11 cuda-11.4/
drwxr-xr-x  4 root root 4.0K Nov  8 14:39 dcgm/
```

Monitor your running job's GPU utilization with `nvidia-smi`

```
qstat –u username –f
# find compute node name thetagpuX
ssh thetagpuX
watch –n 1 nvidia-smi
```

ThetaGPU - GPU Assignment

- https://www.alcf.anl.gov/support-center/theta-gpu-nodes/gpu-monitoring
- Map processes to GPUs on each node

- Programming model and framework semantics (CUDA, Tensorflow, etc…)
- MPI_Comm_rank(MPI_COMM_WORLD, &me)
- cudaGetDeviceCount(&num_devices);
- cudaSetDevice(me % num_devices);

- Environment variables (e.g. in helper scripts)

```
export CUDA_VISIBLE_DEVICES=4
```

ThetaGPU - GNU Compilers

- https://www.alcf.anl.gov/support-center/theta-gpu-nodes/compiling-and-linking-thetagpu
- GCC w/ OpenMPI
  - Default environment
  - GPU Programming Models: CUDA, OpenCL
  - Use C/C++ wrappers: mpicxx, mpicc
  - Fortran is not supported (gfortran not installed)

ThetaGPU - NVIDIA Compilers

- https://www.alcf.anl.gov/support-center/theta-gpu-nodes/compiling-and-linking-thetagpu
- NVIDIA HPC SDK
  - Load module

```
$ module use /lus/theta-fs0/software/environment/thetagpu/lmod/tmp
$ module swap openmpi openmpi-4.1.0_nvhpc-21.3
$ module list
Currently Loaded Modules:
1) Core/StdEnv   2) nvhpc-nompi/21.3   3) openmpi-4.1.0_nvhpc-21.3
```

  - GPU Programming Models: CUDA, OpenCL, OpenACC, OpenMP
  - Use pgc++, pgcc, pgf90, etc…
  - Use mpicxx, mpicxx, mpif90, etc…

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

ThetaGPU - NVIDIA Compilers

- https://www.alcf.anl.gov/support-center/theta-gpu-nodes/compiling-and-linking-thetagpu
- NVIDIA HPC SDK modules
  - Adds NVIDIA SDK compilers, libraries, and tools to paths

```
ftware/environment/thetagpu/lmod/modulefiles ----------------------------------------
   llvm/release-12.0.0       (D)    nvhpc-nompi/21.3
   nccl/nccl-v2.8.4-1_CUDA11        nvhpc/20.9                        (D)
   nvhpc-byo-compiler/20.9   (D)    nvhpc/21.2
   nvhpc-byo-compiler/21.2          nvhpc/21.3
   nvhpc-byo-compiler/21.3          openmpi/openmpi-4.0.5             (L)
   nvhpc-nompi/20.9          (D)    openmpi/openmpi-4.1.0_ucx-1.10.0
   nvhpc-nompi/21.2                 openmpi/openmpi-4.1.0             (D)
```

- nvhpc: adds all NVIDIA SDK compilers, libraries, and tools to paths
- nvhpc-byo-compiler: identical to nvhpc, but doesn't set compiler environment variables
- nvhpc-nompi: excludes MPI libraries
  - Preferred module
  - Important to use ALCF provided OpenMPI modules for multi-node runs

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, OpenCL, OpenMP
  - Use clang, clang++
  - Use mpicxx, mpicxx

Build your software on a compute node (e.g. a `single-gpu` allocation), not on a service node!

Thank you!

Performance Profiling Tools

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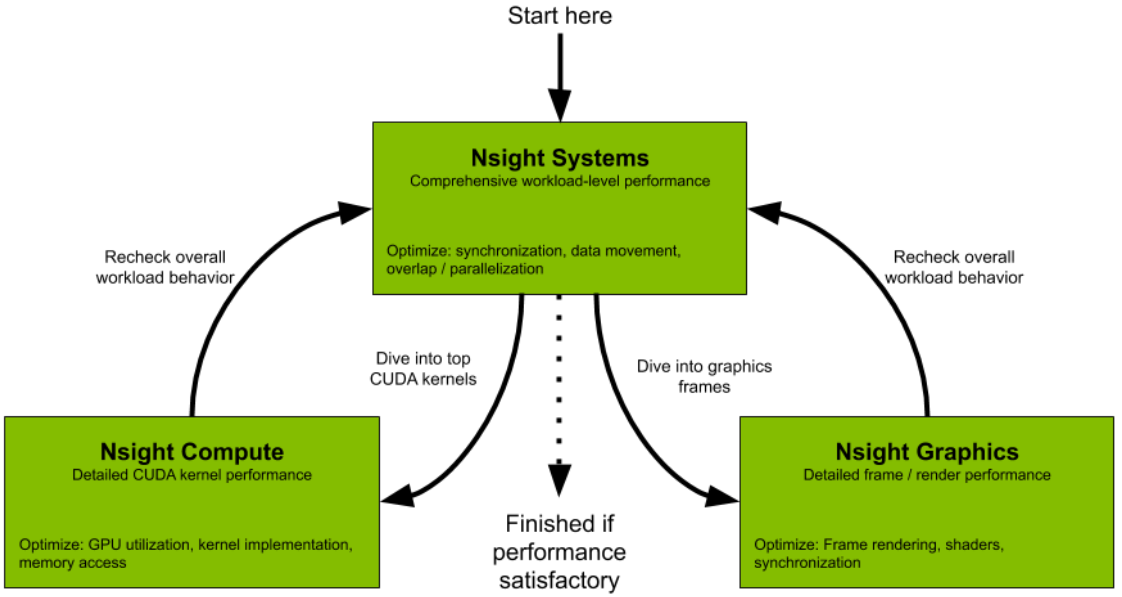
NVIDIA Tools overview

- Nsight Systems
  - —A system-wide visualization of an application performance
  - —To optimize bottlenecks to scale efficiently across CPUs and GPUs on ThetaGPU
- Nsight Compute
  - —An interactive kernel profiler for applications
  - —Providing detailed performance metrics and API debugging via a user interface and command line tool
  - —Providing customizable and data-driven user interface and metric collection that can be extended with analysis scripts for post-processing results
- Nsight Graphics
  - —A stand-alone tool for graphics applications



Credit: NVIDIA (https://developer.nvidia.com/tools-overview)

Step-by-step guide on ThetaGPU (1/2)

- Common part on ThetaGPU
  - Build your application for ThetaGPU
  - Submit your job script to ThetaGPU or start an interactive job mode on ThetaGPU as follows:

```
$ module load cobalt/cobalt-gpu
$ qsub -I -n 1 -t 30 -q full-node -A {your_project}
```

- Nsight Systems
  - Run your application with Nsight Systems as follows:

```
$ nsys profile -o {output_filename} --stats=true ./{your_application}
```

- Nsight Compute
  - Run your application with Nsight Compute

```
$ ncu --set detailed -k {kernel_name} -o {output_filename} ./{your_application}
```

  - Remark: W/o -o option, Nsight Compute provides performance data as a standard output

Step-by-step guide on ThetaGPU (2/2)

- Post-processing the profiled data
  - —Post-processing via CLI

```
$ nsys stats {output_filename}.qdrep
$ ncu -i {output_filename}.ncu-rep
```

  - —Post-processing on your local system via GUI
    - Install NVIDIA Nsight Systems and NVIDIA Nsight Compute after downloading both of them from the NVIDIA Developer Zone.
    - Download nsys output files (i.e., ending with .qdrep and . sqlite) to your local system, and then open them with NVIDIA Nsight Systems on your local system.
    - Download ncu output files (i.e., ending with .ncu-rep) to your local system, and then open them with NVIDIA Nsight Compute on your local system.

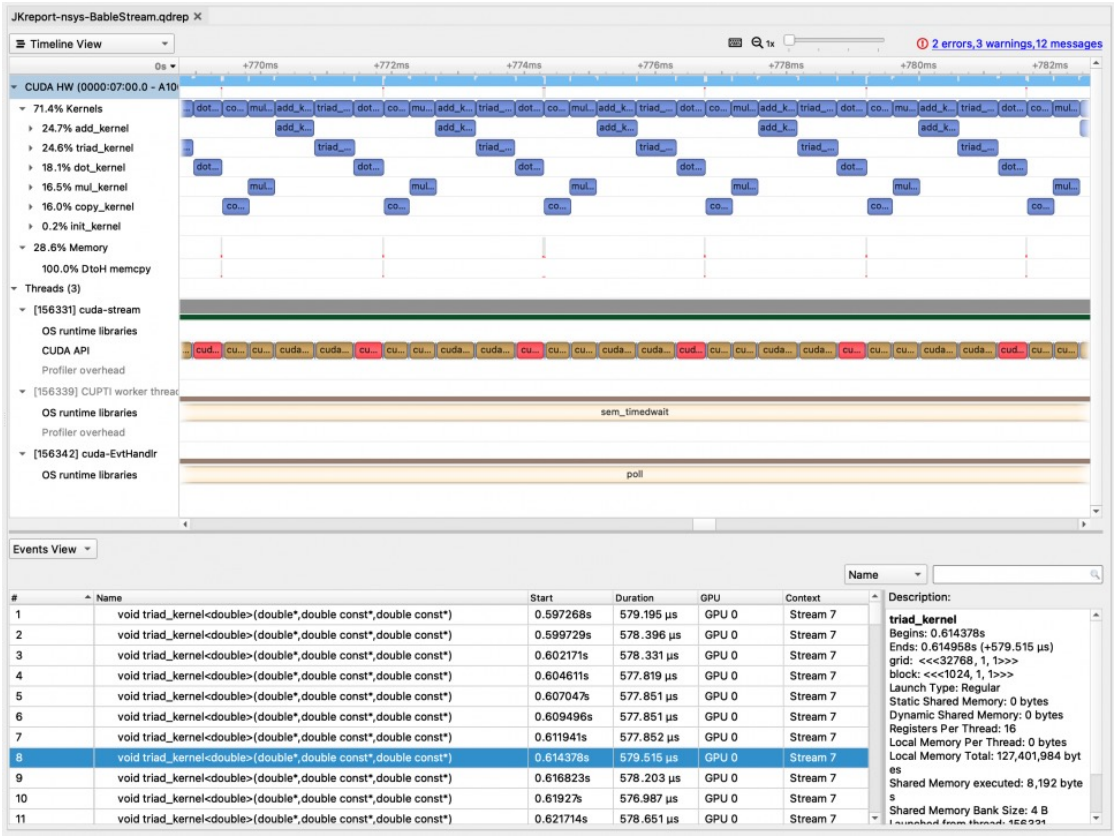
  - —More options for performance analysis with Nsight Systems and Nsight Compute

```
$ nsys --help
$ ncu --help
```

Nsight Systems Demo with a simple example

```
jkwack@thetagpu18:~/HPC_benchmarks/BabelStream/JK_thetaGPU$ nsys profile -o JKreport-nsys-BableStream --stats=true ./cuda-stream
…
Generating CUDA API Statistics...
CUDA API Statistics (nanoseconds)
Time(%)      Total Time       Calls         Average         Minimum         Maximum  Name
-------  --------------  ----------  --------------  --------------  --------------  ----------------------------------------------------------------------------------
   44.8       280504347           4      70126086.8         1050249       276881346  cudaMalloc
   31.4       196878210         401        490968.1          381542          600948  cudaDeviceSynchronize
   22.4       140280462         103       1361946.2          436597        32339232  cudaMemcpy
    1.0         6263864           4       1565966.0         1236542         1884610  cudaFree
    0.4         2729558         501          5448.2            4970           36269  cudaLaunchKernel

Generating CUDA Kernel Statistics...
CUDA Kernel Statistics (nanoseconds)
Time(%)      Total Time   Instances         Average         Minimum         Maximum  Name
-------  --------------  ----------  --------------  --------------  --------------  ------------------------------------------------------------------
   24.7        58518170         100        585181.7          580347          594395  void add_kernel<double>(double const*, double const*, double*)
   24.6        58312184         100        583121.8          576987          595067  void triad_kernel<double>(double*, double const*, double const*)
   18.1        42942748         100        429427.5          419548          438333  void dot_kernel<double>(double const*, double const*, double*, int)
   16.5        39062588         100        390625.9          388733          392125  void mul_kernel<double>(double*, double const*)
   16.0        37980930         100        379809.3          376541          392925  void copy_kernel<double>(double const*, double*)
    0.2          521628           1        521628.0          521628          521628  void init_kernel<double>(double*, double*, double*, double, double, double)
…
Report file moved to "/gpfs/mira-home/jkwack/HPC_benchmarks/BabelStream/JK_thetaGPU/JKreport-nsys-BableStream.qdrep"
Report file moved to "/gpfs/mira-home/jkwack/HPC_benchmarks/BabelStream/JK_thetaGPU/JKreport-nsys-BableStream.sqlite"
```

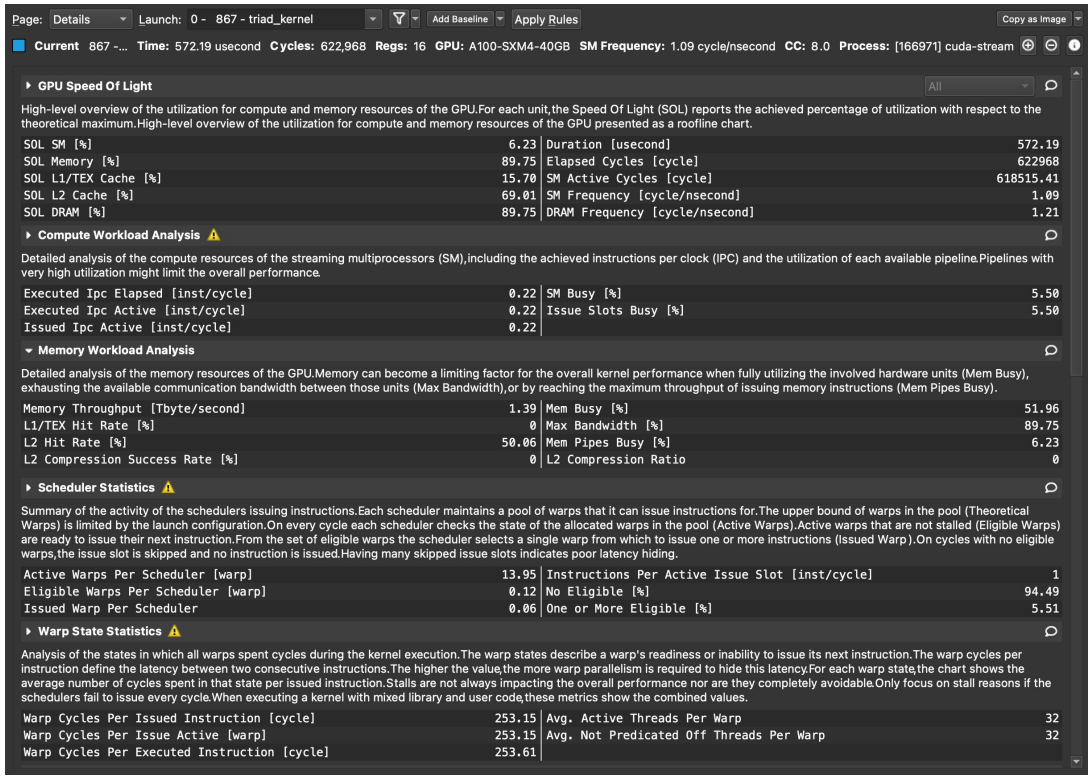
Nsight Systems Demo with a simple example

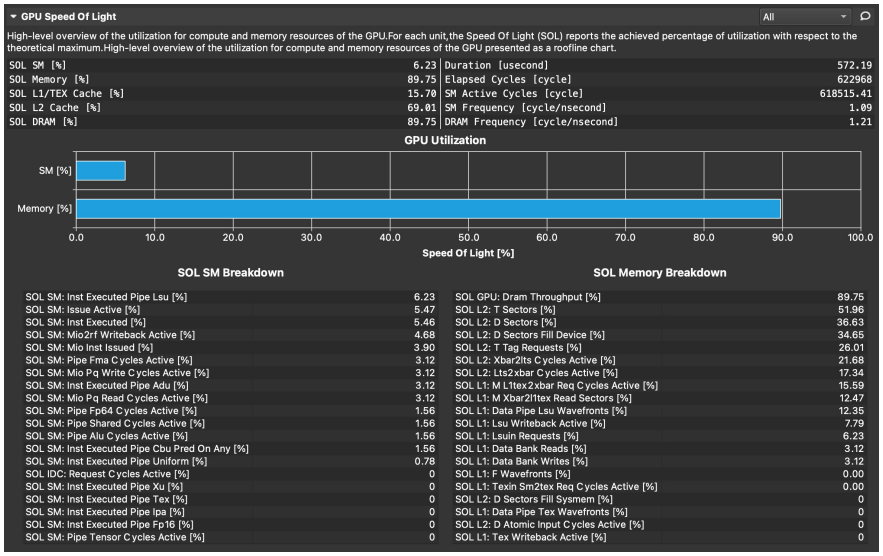


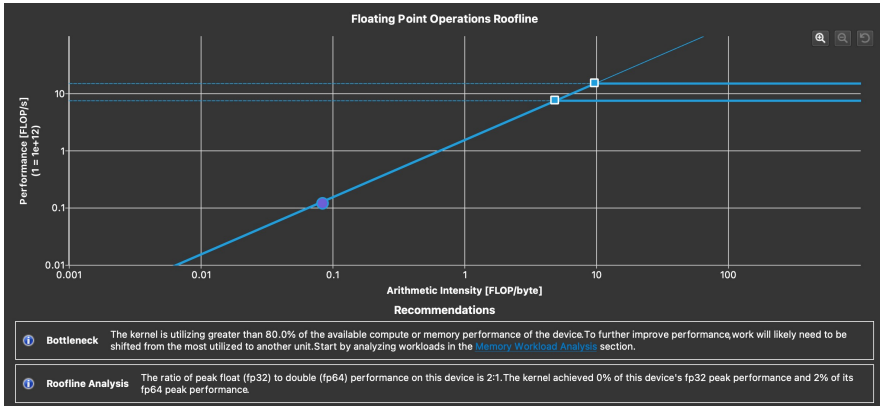
Nsight Compute Demo with a simple example

```
jkwack@thetagpu18:~/HPC_benchmarks/BabelStream/JK_thetaGPU$ ncu --set detailed -k triad_kernel -o JKreport-ncu_detailed-triad_kernel-BableStream ./cuda-stream
BabelStream
Version: 3.4
Implementation: CUDA
Running kernels 100 times
Precision: double
Array size: 268.4 MB (=0.3 GB)
Total size: 805.3 MB (=0.8 GB)
==PROF== Connected to process 166971 (/gpfs/mira-home/jkwack/HPC_benchmarks/BabelStream/JK_thetaGPU/cuda-stream)
Using CUDA device A100-SXM4-40GB
Driver: 11000
==PROF== Profiling "triad_kernel": 0%....50%....100% - 19 passes
==PROF== Profiling "triad_kernel": 0%....50%....100% - 19 passes
==PROF== Profiling "triad_kernel": 0%....50%....100% - 19 passes
…
==PROF== Profiling "triad_kernel": 0%....50%....100% - 19 passes

Function    MBytes/sec  Min (sec)   Max         Average
Copy        1336793.345 0.00040     0.00042     0.00041
Mul         1307948.274 0.00041     0.00043     0.00042
Add         1335561.797 0.00060     0.00062     0.00062
Triad       976.089     0.82503     1.00961     0.87930
Dot         1081921.148 0.00050     0.00055     0.00053

==PROF== Disconnected from process 166971
==PROF== Report: /gpfs/mira-home/jkwack/HPC_benchmarks/BabelStream/JK_thetaGPU/JKreport-ncu_detailed-triad_kernel-BableStream.ncu-rep
```

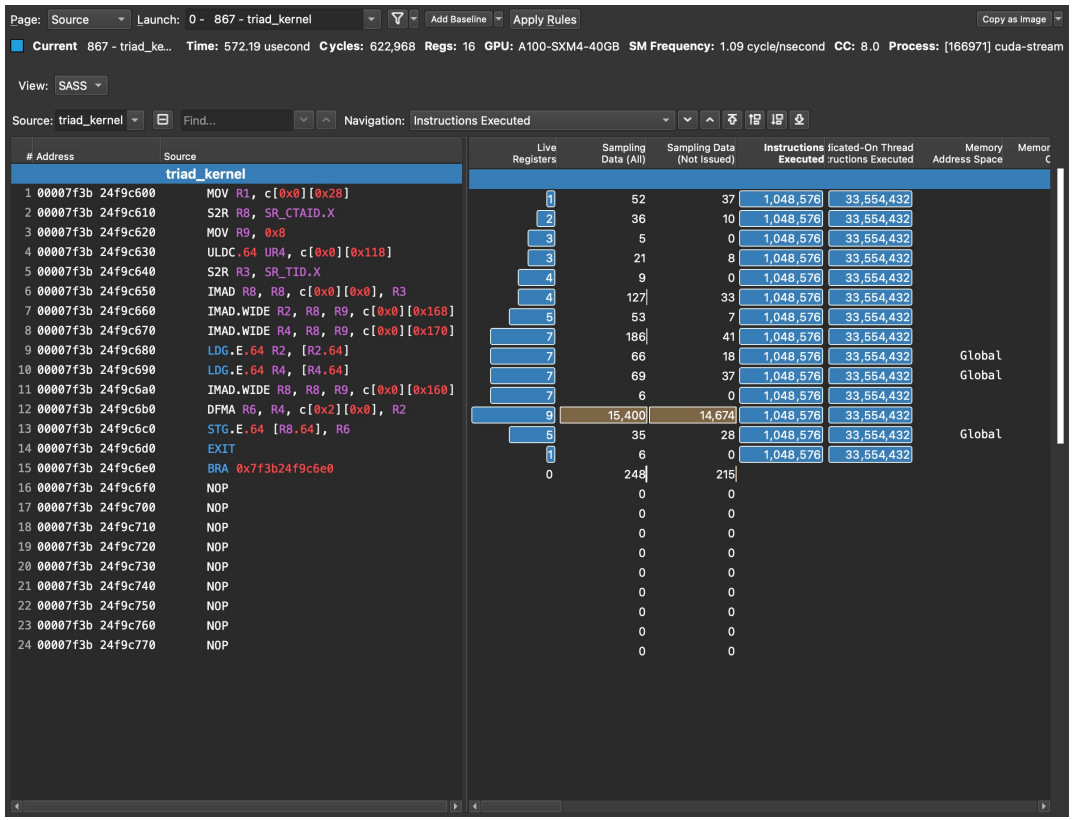
Nsight Compute Demo

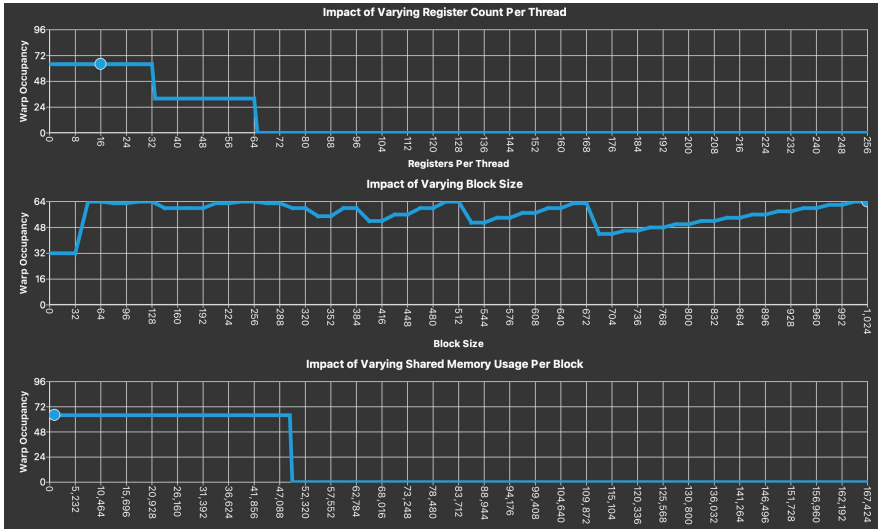


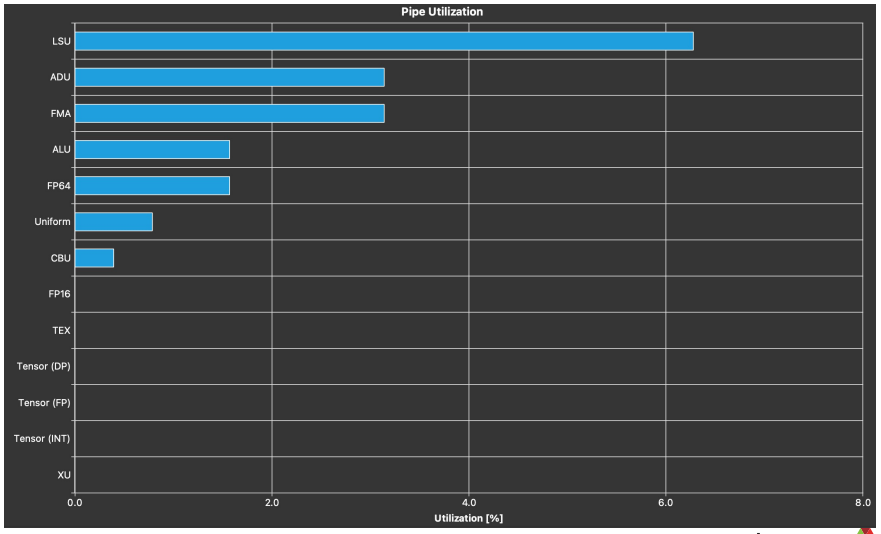




Nsight Compute Demo







Argonne NATIONAL LABORATORY

Thank you!

AI and Frameworks

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AI Frameworks

- ThetaGPU consists of high powered GPU accelerators that are prime for machine learning and deep learning applications.
- Here, I'll showcase the available tools and modules, as well as how to add your own tools, and links to further resources.

- We'll cover:
  - Modules;
  - Containers;
  - Scaling machine learning;
  - Investigating Machine learning performance.

Machine Learning Modules

- Modules on ThetaGPU are available for the most popular machine learning frameworks:
  - Use ‘module avail` to see all module options.
  - Machine Learning Frameworks are available with ‘**module load conda/${DATE}**`, where date can be:
    - 2021-11-30
    - 2021-09-22
    - 2021-06-28
    - 2021-06-26
  - Once the module is loaded, you still need to do `**conda activate**` to launch your conda environment.
- You can extend the conda environment with pip and virtualenv!
  - **python -m venv --system-site-packages ${LOCATION}**
  - **source ${LOCATION}/bin/activate**
  - **pip install [desired packages]**
- Conda modules include pytorch, tensorflow, horovod, and other packages, if something is missing please open a support ticket or contact us.

- *More info on modules is here: https://github.com/argonne-lcf/ai-science-training-series/blob/main/00_introToAlcf/02_howToSetupEnvironment.md*

Containers

- Containers are a great way to get the latest nvidia software in a portable way: you can use the same container on many systems, and run it in many locations.
- ALCF Systems support **singularity,** while many other locations support **docker.**
  - More info on singularity and docker are available here:
    - https://sylabs.io/guides/3.5/user-guide/introduction.html
    - https://www.docker.com/
- ALCF documentation pages have information about containers:
  - https://www.alcf.anl.gov/support-center/theta-gpu-nodes/nvidia-containers
- Significant tutorials and information about containers is available from the last computational performance workshop:
  - https://github.com/argonne-lcf/CompPerfWorkshop-2021/tree/main/03_containers
- Prebuilt containers for ThetaGPU are available here:
  - **/lus/theta-fs0/software/thetagpu/nvidia-containers/**

Scaling Deep Learning Software

- Scaling deep learning applications on ThetaGPU is easy with Horovod (TF and Pytorch) and DDP (Pytorch).
  - Documentation for the software is available online:
    - https://horovod.ai/
    - https://www.tensorflow.org/guide/distributed_training
    - https://pytorch.org/tutorials/intermediate/ddp_tutorial.html
- The Datascience team regularly updates and presents tutorials (with examples) for scaling deep learning applications on ThetaGPU. For examples, please see:
  - https://github.com/argonne-lcf/CompPerfWorkshop-2021/tree/main/05_scaling-DL
  - Tomorrow's AI for Science Tutorial will cover distributed deep learning in great detail!

Framework Performance

- In general, computations in python must be offloaded to the GPUs, with the deep learning frameworks or other tools, to achieve optimal performance.
- That said, it is easy to introduce bottlenecks into your python applications with one or two lines of poorly written code.
  - How do you find them? How do you improve it?
  - Significant information, including tutorials, examples, and guides for performance improvement, are available:
    - https://github.com/argonne-lcf/CompPerfWorkshop-2021/tree/main/09_profiling_frameworks
  - The deep learning frameworks also offer guides for performance measurements:
    - https://pytorch.org/tutorials/recipes/recipes/profiler_recipe.html
    - https://www.tensorflow.org/guide/profiler
- You should also pay attention to your data pipelines! Many deep learning applications stall out with data loading.
  - See this tutorial for tips and tricks: https://github.com/argonne-lcf/ai-science-training-series/tree/main/03_dataPipelines

Questions?

- Please ask here or send questions to:
  - support@alcf.anl.gov or
  - datascience@alcf.anl.gov

Thank you!!