Welcome to Nvidia HPC SDK Training

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Jan 12-13, 2022
Introduction

- NVIDIA HPC SDK is a Comprehensive Suite of Fortran, C, and C++ Development Tools and Libraries
  - NVIDIA compiler is default and recommended compiler for Perlmutter GPU
- Hands-on training provided by NVIDIA to NERSC/OLCF/ALCF users
  - Thanks Jeff Larkin, Brent Leback, Max Katz, Matt Stack, Robert Searles
- Topics include:
  - GPU architecture and HPC SW developer considerations
  - Standard Language Acceleration and Libraries
  - OpenACC
  - OpenMP offload
  - CUDA
  - Profiling tools
Some Logistics (1)

- Muted upon joining Zoom due to large number of attendees
- Please change your name in Zoom session as “first_name last_name”
  - Click “Participants”, then “More” next to your name to rename
- Live “Captions” and “View Full Transcripts” are enabled
- Please ask your questions in Slack (preferred) instead of Zoom chat
  - [https://tinyurl.com/nvhpc-jan2022-slack](https://tinyurl.com/nvhpc-jan2022-slack)
Some Logistics (2)

- Slides will be uploaded to the #presentations in Slack
- Videos will be available at a later date
- Hands-on exercises
  - git clone https://github.com/olcf/NVHPC2022
  - NERSC users: use Perlmutter
  - OLCF users: use Summit
  - Other users: use NERSC training account on Perlmutter
- Please help us with answering the survey afterwards
  - https://tinyurl.com/nvhpc-jan2022-survey
## Agenda (1)

**Day 1, 9:00 am - 12:30 pm (Pacific time), January 12, Wednesday**

<table>
<thead>
<tr>
<th>Time (PDT)</th>
<th>Topic</th>
<th>Presenters</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00 am</td>
<td>Introduction (10 min)</td>
<td>NERSC/OLCF/ALCF</td>
</tr>
<tr>
<td>9:10 am</td>
<td>Introduction and Updates to NVHPC SDK (55 min)</td>
<td>Jeff Larkin</td>
</tr>
<tr>
<td>10:05 am</td>
<td>GPU Architecture and HPC SW Developer Considerations (25 min)</td>
<td>Brent Leback / Max Katz</td>
</tr>
<tr>
<td>10:30 am</td>
<td>Break (15 min)</td>
<td></td>
</tr>
<tr>
<td>10:45 am</td>
<td>NVHPC Standard Language Acceleration, Libraries (30 min)</td>
<td>Brent Leback / Max Katz / Matt Stack</td>
</tr>
<tr>
<td>11:15 am</td>
<td>Introduction to Nsight Systems and Nsight Compute (30 min)</td>
<td>Max Katz</td>
</tr>
<tr>
<td>11:45 am</td>
<td>Break + Lab + Demo: stdpar, profiling (45 min)</td>
<td>Brent Leback / Max Katz / Matt Stack/ Robert Searles</td>
</tr>
<tr>
<td>12:30 pm</td>
<td>End of Day 1</td>
<td></td>
</tr>
</tbody>
</table>
# Agenda (2)

Day 2, 9:00 am - 12:30 pm (Pacific time), January 13, Thursday

<table>
<thead>
<tr>
<th>Time (PDT)</th>
<th>Topic</th>
<th>Presenters</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00 am</td>
<td>NVHPC OpenACC (45 min)</td>
<td>Brent Leback</td>
</tr>
<tr>
<td>9:45 am</td>
<td>NVHPC OpenMP (45 min)</td>
<td>Brent Leback</td>
</tr>
<tr>
<td>10:30 am</td>
<td>Break (15 min)</td>
<td></td>
</tr>
<tr>
<td>10:45 am</td>
<td>Introduction to CUDA (30 min)</td>
<td>Max Katz</td>
</tr>
<tr>
<td>11:15 am</td>
<td>Putting it Together (15 min)</td>
<td>Brent Leback</td>
</tr>
<tr>
<td>11:30 am</td>
<td>Break + Lab + Demo: OpenACC, OpenMP, and more (60 min)</td>
<td>Brent Leback / Max Katz / Matt Stack / Robert Searles</td>
</tr>
<tr>
<td>12:30 pm</td>
<td>End of Day 2</td>
<td></td>
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</tbody>
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NERSC Perlmutter Usage Info

- NERSC users are added to the `ntrain4` project
- Training account expires Jan 18
- Perlmutter Compute node reservations. To access, use:
  - Jan 12, 10:30-13:30: `#SBATCH --reservation=nvhpc_day1 -A ntrain4_g`
  - Jan 13, 10:30-13:30: `#SBATCH --reservation=nvhpc_day2 -A ntrain4_g`
- Outside of reservations, use:
  - `#SBATCH --reservation=nvhpc_day1 -A ntrain4_g` or `#SBATCH --reservation=nvhpc_day2 -A ntrain4_g`
- Perlmutter documentation is here
  - [https://docs.nersc.gov/systems/perlmutter/](https://docs.nersc.gov/systems/perlmutter/)
NVHPC on Perlmutter Cheat sheet

To use NVHPC: 

```
module load nvidia/21.9  (loaded by default)
```

- Using native Nvidia compilers: 
  
  `nvfortran, nvc, nvc++, nvcc`

  or using Cray compiler wrappers: 
  
  `ftn, cc, CC`

  - Stdpar: `-stdpar -l<some_libs>`
  - OpenMP: `-mp=gpu -gpu=cc80`
  - OpenACC: `-acc=gpu -gpu=cc80`
  - CUDA: `-cuda` (or use nvcc to build)

- Add `-Minfo` flag when compile to show detailed information

- Set runtime environment variable `NVCOMPILER_ACC_NOTIFY` to
  
  - 1: Show kernel launches information
  - 2: Show data transfers between CPU and Devices
  - 3: Show both above

  works for OpenACC or OpenMP offload programs, not stdpar or CUDA

- Submit Slurm batch scripts with `sbatch my_batch_script`
Sample Compile and Run Batch Script

Stdpar code:
% nvc++ -stdpar=gpu -gpu=cc80 -Minfo -o code.exe code.cpp
or % CC -stdpar=gpu -gpu=cc80 -Minfo -o code.exe code.cpp

OpenMP offload code:
% nvfortran -mp=gpu -gpu=cc80 -Minfo -o code.exe code.f90
or % ftn -mp=gpu -gpu=cc80 -Minfo -o code.exe code.f90

- Compiling/Building software for Perlmutter
  ○ [https://docs.nersc.gov/systems/perlmutter/#compilingbuilding-software](https://docs.nersc.gov/systems/perlmutter/#compilingbuilding-software)
- Running Jobs on Perlmutter GPU
  ○ [https://docs.nersc.gov/systems/perlmutter/running-jobs/](https://docs.nersc.gov/systems/perlmutter/running-jobs/)

% cat my_batch_script
#!/bin/bash
#SBATCH -N 1
#SBATCH -C gpu
#SBATCH -G 1
#SBATCH -t 15
#SBATCH -c 128
#SBATCH -A ntrain4_g
#SBATCH --reservation=nvhpc_day1
#SBATCH --ntasks-per-node=1
#SBATCH --gpus-per-task=1
export NVCOMPILER_ACC_NOTIFY=3
srun ./code.exe

% sbatch my_batch_script
Hands-On NVHPC Perlmutter Tips

- Nsight-systems and nsight-compute profiling
  - [https://docs.nersc.gov/performance/readiness/#profiling-tools](https://docs.nersc.gov/performance/readiness/#profiling-tools)
  - run with `nsys profile --stats=true ./code.exe`

- Recommend to install NX (NoMachine)
  - Improves X-forwarding when using GUI tools
  - Instructions at: [https://docs.nersc.gov/connect/nx/](https://docs.nersc.gov/connect/nx/)
  - Good for the profiling tools hands-on with GUI
OLCF Summit Usage Info

- Summit reservations have been set up for this training. Users will need the follow in their batch scripts to access the reservation:
  
  On 1/12/22  #BSUB -U NVIDIA_SDK_1
  On 1/13/22  #BSUB -U NVIDIA_SDK_2

- Summit documentation is here
  
  https://docs.olcf.ornl.gov/systems/summit_user_guide.html
NVHPC on Summit Cheat sheet

To load NVHPC: `module load nvhpc/21.9`

- Compile with `nvfortran, nvc, nvc++`
  - Enable OpenMP: `-mp=gpu -gpu=cc70`
  - Enable OpenACC: `-acc=gpu -gpu=cc70`
  - Add `-Minfo` flag when compiling to show detailed information

- Compiler docs for Summit: [https://docs.olcf.ornl.gov/systems/summit_user_guide.html#compilers](https://docs.olcf.ornl.gov/systems/summit_user_guide.html#compilers)

Running Jobs

- Example Summit batch script:
  - [https://docs.olcf.ornl.gov/systems/summit_user_guide.html#batch-script](https://docs.olcf.ornl.gov/systems/summit_user_guide.html#batch-script)
    - Submit batch scripts with: `bsub your_batch_script.lsf`
Hands-On NVHPC Summit Tips

- Nsight-systems and nsight-compute profiling:
  https://docs.olcf.ornl.gov/systems/summit_user_guide.html?highlight=nsight#nvidia-nsight-compute
  - Make sure your write your profiles to GPFS
  - You cannot use the Nsight GUI on Summit, you will need to use scp or Globus to download your profile.
  - You will need to download the Nsight UI for your local machine to read the reports
  - Two ways to get it:
    - download the UI for your local system There are versions for Windows, Mac, and Linux (x86). You will need to register as an NVIDIA developer first.
Thank you!