Introducing RC's new NVIDIA Grace Hopper Superchip

Research Computing
UNIVERSITY OF COLORADO BOULDER

Introducing RC's new NVIDIA Grace Hopper Superchip

Instructor: Brandon Reyes

- Research Computing

- Website: www.rc.colorado.edu
- Documentation: https://curc.readthedocs.io
- Helpdesk: rc-help@colorado.edu
- Survey: http://tinyurl.com/curc-survey18

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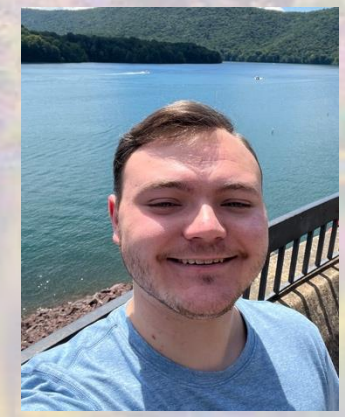
Meet the User Support Team

Layla
Freeborn

Brandon
Reyes

Andy
Monaghan

Michael
Schneider



John
Reiland

Dylan
Gottlieb

Mohal
Khandelwal

Ragan
Lee

Slides

https://github.com/ResearchComputing/introducing_rc_gh200_quick_byte

Session Overview

- GH200 architecture overview
  - Hardware specs
- What workflows will benefit from the GH200 architecture?
- RC's approach to software management
- Beta testing phase
- How can you run on the GH200s?

GH200 architecture overview

The Grace Hopper Superchip (GH200) is a newer chip provided by NVIDIA that allows the Grace CPU and Hopper GPU to concurrently and transparently access both the CPU and GPU memory

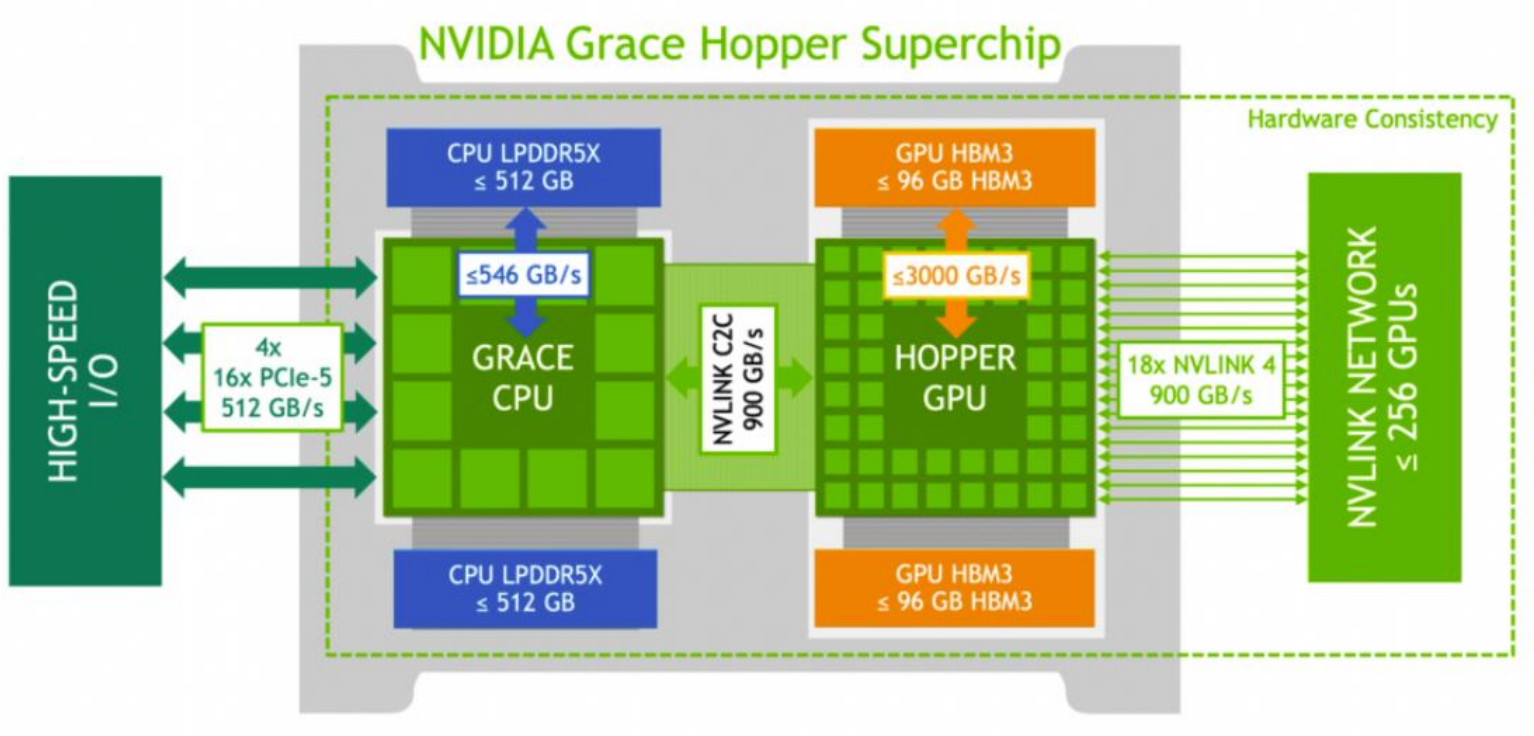


Image provided by https://resources.nvidia.com/en-us-grace-cpu/nvidia-grace-hopper

Specifications for our 2 GH200 nodes

- Grace CPU has 72 cores and roughly 480 GB of RAM
  - Arm based (Neoverse V2)
- Hopper GPU is an H100 and has roughly 100 GB of VRAM
- CPU and GPU are connected via NVIDIA NVLink-C2C
- FAST I/O speed (512 GB/s)
  - Top I/O speeds only apply to the SSD
- Roughly 1.7 TB of usable SSD on the node

Note: We have not enabled linking of multiple GH200 nodes

Benefits of GH200 architecture

- NVLink-C2C provides seamless memory management between the CPU and GPU
  - Allows GPU threads to access RAM, extending the GPU memory
- 1:1 GPU-to-CPU ratio
  - GPU and CPU have roughly the same processing power dedicated to them
  - Ideal for workloads that utilize the CPU and GPU to a high degree
- High-speed I/O to SSD and large SSD storage space
  - Allows users to store a large amount of their data locally on the node (while it is in use) and quickly access it

What workflows will benefit from the GH200 architecture?

- Heterogenous software that uses both the CPU and GPU
- Inference for Large Language Models
  - I was able to run Llama 3.1 405b (requires close to 300 GB of memory)
- Training large models and hyperparameter tuning
  - We have seen at least 2X speedup, some users reported 10X speedup
- NVIDIA also states that the following applications perform well on the GH200s:
  - Graph Neural Networks, ABINIT, OpenFOAM, GROMACS, FFTs, Multi-Grid Linear Solvers

RC's approach to software management

Due to the different architecture, there is a limited software stack. We currently provide:

- CUDA compilers through NVIDIA HPC SDK e.g. nvcc, nvc++
- CUDNN libraries
- Miniforge (mamba and conda)
  - If your specific library allows for aarch64 architecture with GPU capabilities, it will most likely work on the GH200s
- Apptainer
  - A large selection of compatible containers are available through NVIDIA's NGC catalog

We will work with you to install GH200 compatible software, in alignment with our software polices.

Beta testing phase

To identify issues and workflows that best run on the GH200s, we initiated a beta testing phase.

- This is directed towards users with established GPU workflows on either our A100 or MI100 GPUs
- An initial consultation is held to determine if the workflow is appropriate for the GH200s
- Once approved, we setup the software on the GH200s, onboard you to the nodes, and provide hands-on support for any issues encountered

How can you run on the GH200s?

- Submit a ticket to rc-help@colorado.edu
  - In subject include:
    - You are interested in running “X application” on the GH200s
  - In the email body:
    - Short description of what your workflow is trying to accomplish
    - Why you believe the GH200s would be beneficial to your workflow
    - Provide us Linux paths to the code you would like to run
    - If possible, any JobIDs of this workflow you have ran on a GPU node

Thank you!

Survey and feedback

http://tinyurl.com/curc-survey18

Slides

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