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DGX-1 User Training

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Converge to the Cloud

Agenda

- DGX-1 Overview
- NVIDIA GPU Cloud (NGC)
- Virtual Machine vs. Container
- What's Docker?
- Why NVIDIA Docker?
- NVIDIA Docker Sub-Commands
- Running Docker Containers
- Docker on HPC Systems
- Singularity: A Container Engine for HPC
- Running with Singularity
- SLURM Overview and Architecture
- SLURM Commands for the User
- Containers (Singularity) with SLURM Sample Script

NVIDIA DGX-1



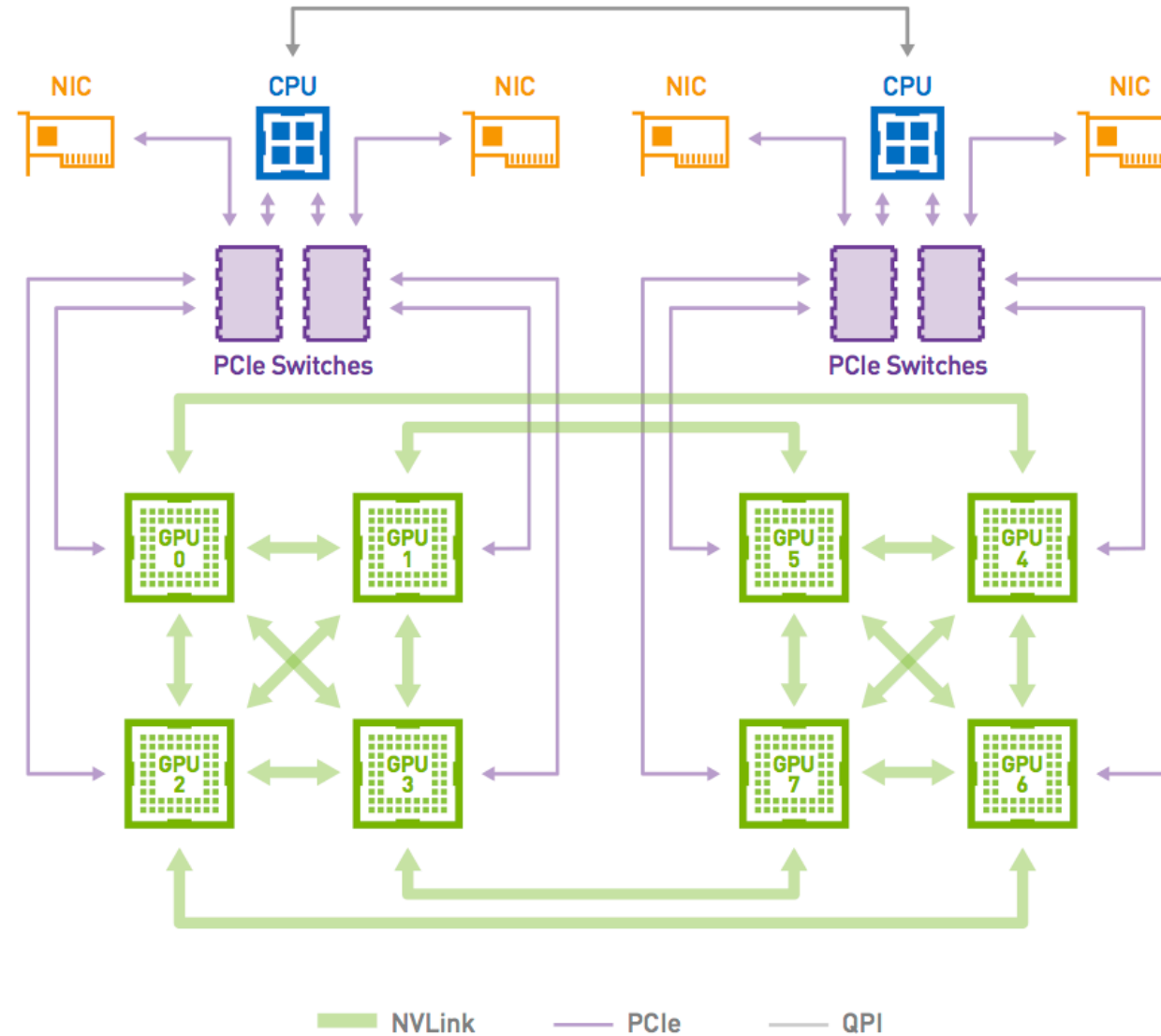
DGX-1 Overview



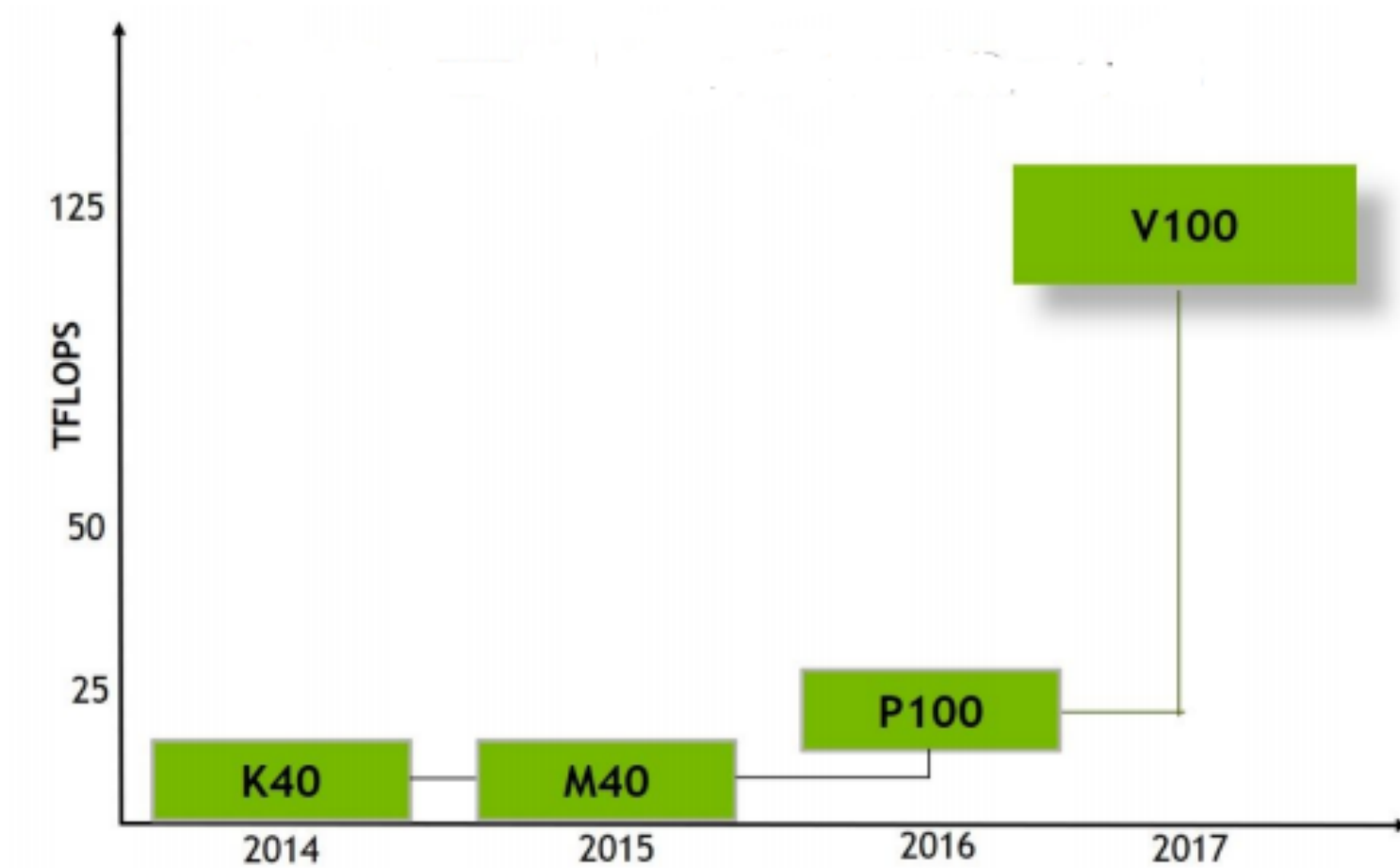
System Specifications

GPUs	8xTesla V100
GPU Memory	256 GB (32 GB/GPU)
CPU	Dual 20-core Intel Xeon E5-2698 v4 2.2 GHz
NVIDIA CUDA Cores	40,960
NVIDIA Tensor Cores (on V100 based systems)	5,120
System Memory	512 GB 2,133 MHz DDR4 LRDIMM
Storage	Data: 4x1.92 TB SSD RAID-0 OS: 1x1.92 TB SSD
Network	Dual 10 GbE, 4 IB EDR

Hybrid Cube Mesh Architecture



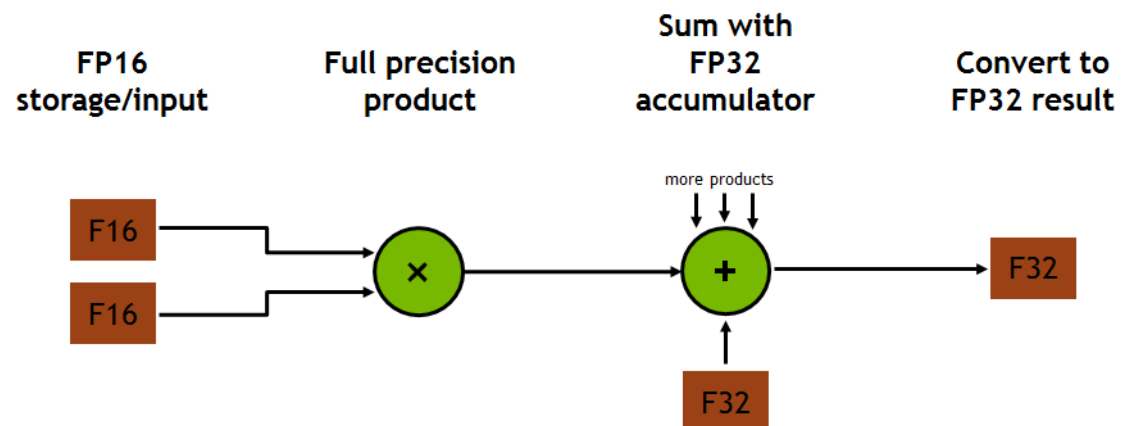
PERFORMANCE FOR AI AND HPC



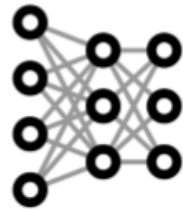
Tensor Cores

$$\mathbf{D} = \begin{pmatrix} A_{0,0} & A_{0,1} & A_{0,2} & A_{0,3} \\ A_{1,0} & A_{1,1} & A_{1,2} & A_{1,3} \\ A_{2,0} & A_{2,1} & A_{2,2} & A_{2,3} \\ A_{3,0} & A_{3,1} & A_{3,2} & A_{3,3} \end{pmatrix} \begin{pmatrix} B_{0,0} & B_{0,1} & B_{0,2} & B_{0,3} \\ B_{1,0} & B_{1,1} & B_{1,2} & B_{1,3} \\ B_{2,0} & B_{2,1} & B_{2,2} & B_{2,3} \\ B_{3,0} & B_{3,1} & B_{3,2} & B_{3,3} \end{pmatrix} + \begin{pmatrix} C_{0,0} & C_{0,1} & C_{0,2} & C_{0,3} \\ C_{1,0} & C_{1,1} & C_{1,2} & C_{1,3} \\ C_{2,0} & C_{2,1} & C_{2,2} & C_{2,3} \\ C_{3,0} & C_{3,1} & C_{3,2} & C_{3,3} \end{pmatrix}$$

FP16 or FP32 FP16 FP16 FP16 or FP32



FASTEST PATH TO DEEP LEARNING



Fully-integrated and pre-optimized
Insights in hours instead of weeks

EFFORTLESS PRODUCTIVITY



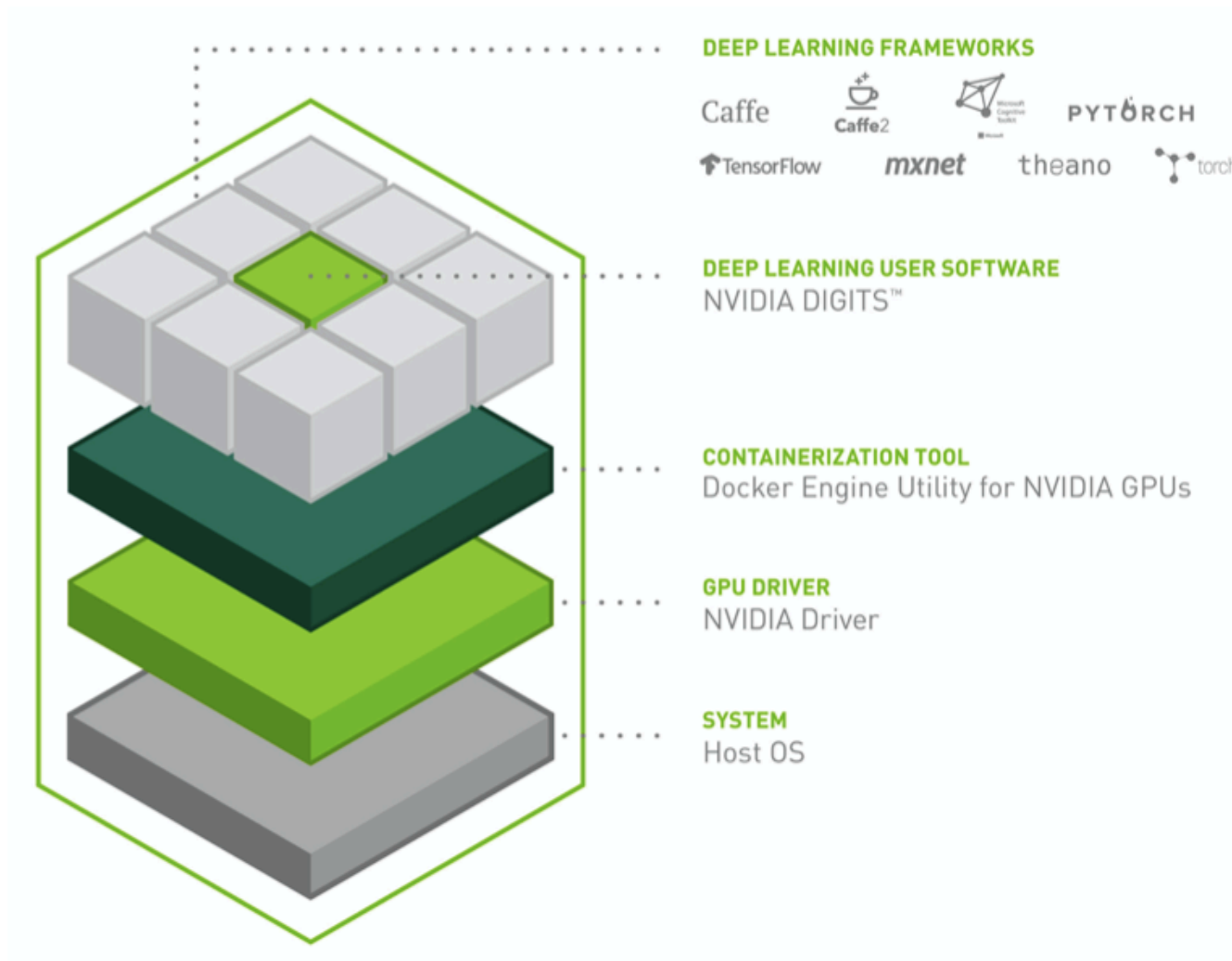
Optimized frameworks and cloud
managed for faster insights

REVOLUTIONARY AI PERFORMANCE

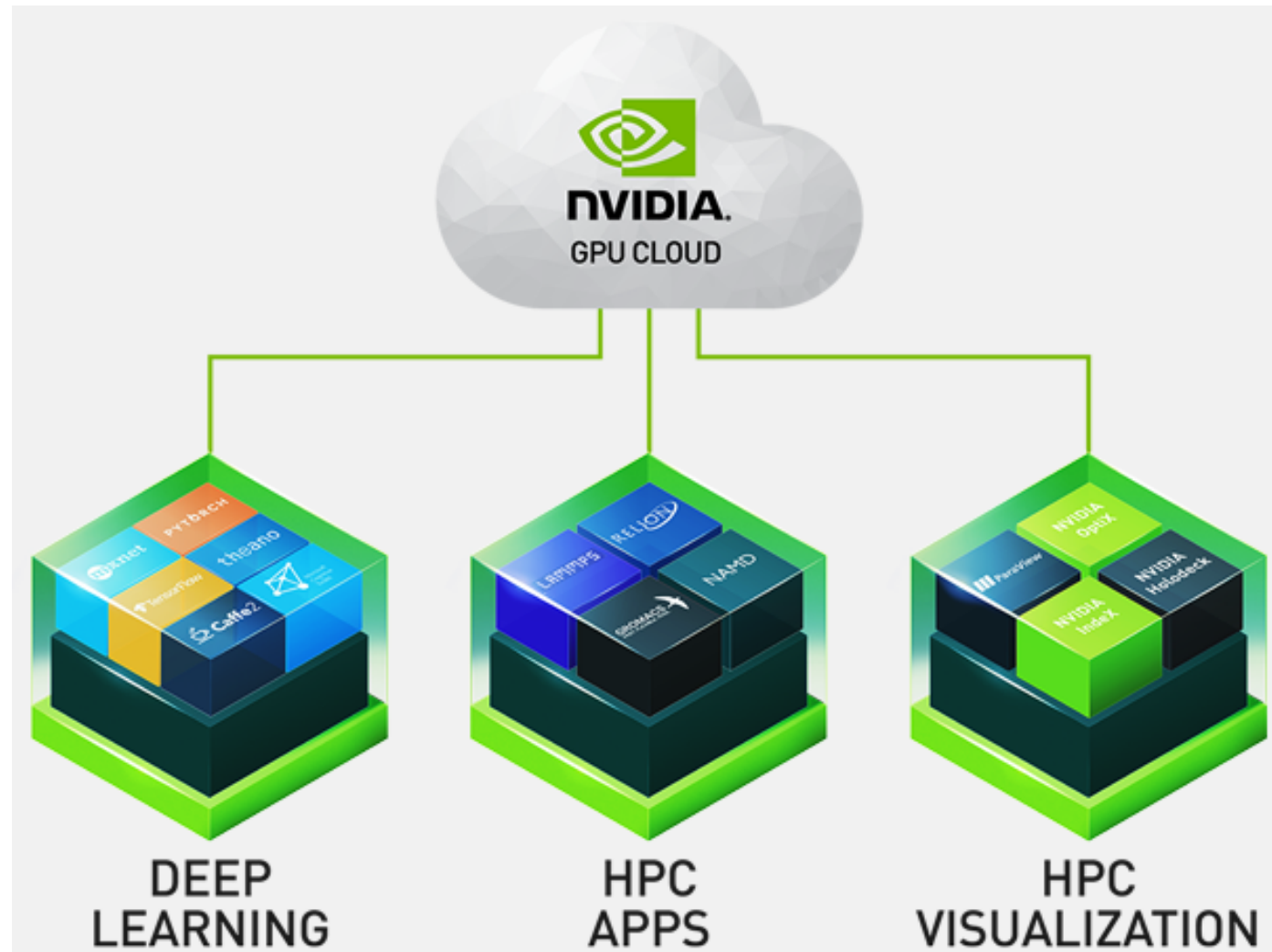


DGX software stack for fastest GPU
performance in the industry

The DGX-1 Deep Learning Software Stack

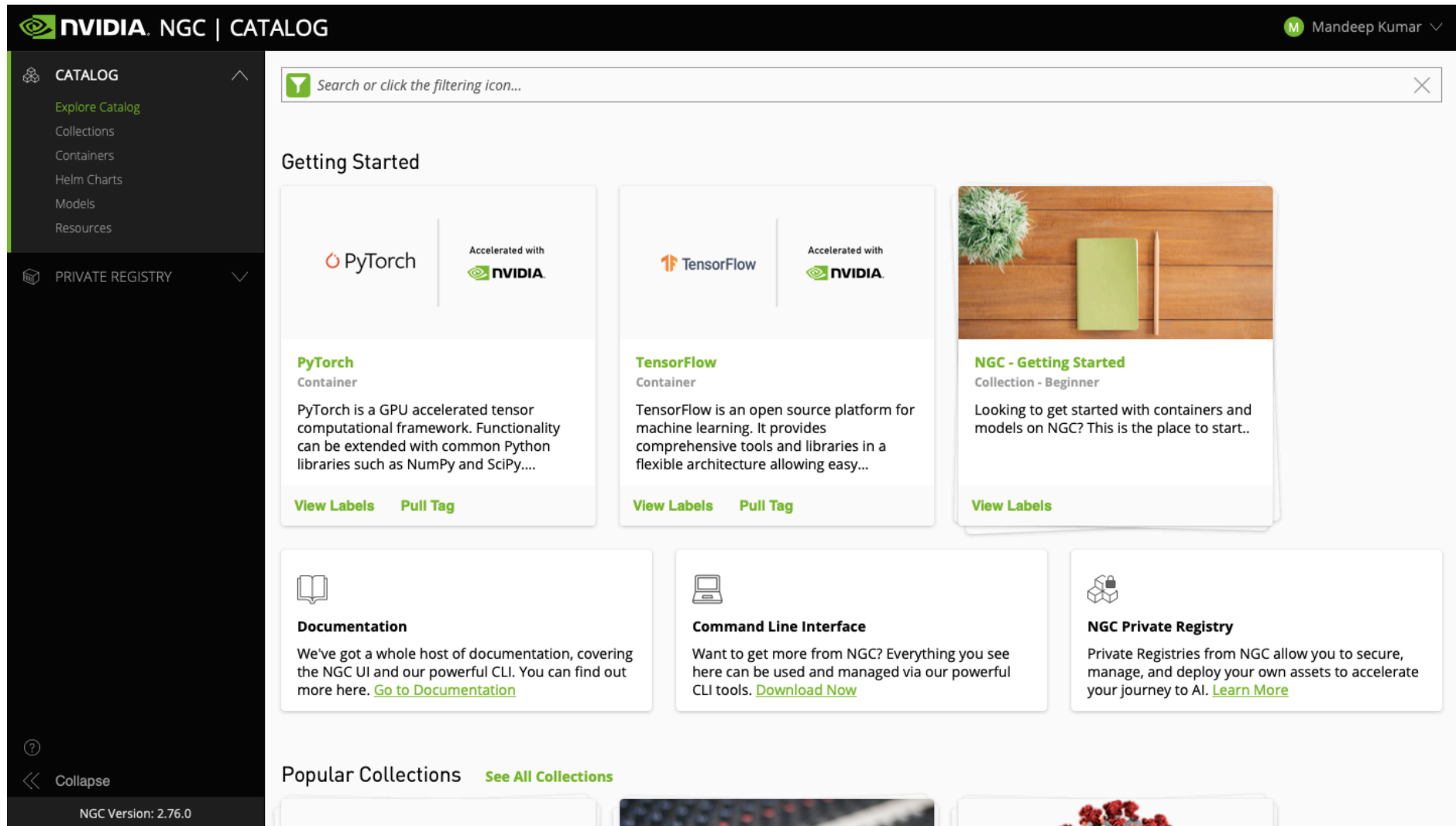


NVIDIA GPU Cloud (NGC)



NVIDIA GPU Cloud (NGC)

<https://ngc.nvidia.com/catalog>



The screenshot shows the NVIDIA NGC Catalog interface. At the top, the header reads "NVIDIA NGC | CATALOG" with a user profile "Mandeep Kumar" on the right. A left sidebar contains navigation links: "CATALOG" (with sub-links: Explore Catalog, Collections, Containers, Helm Charts, Models, Resources) and "PRIVATE REGISTRY". The main content area features a search bar and a "Getting Started" section with three cards: "PyTorch Container" (described as a GPU accelerated tensor computational framework), "TensorFlow Container" (described as an open source platform for machine learning), and "NGC - Getting Started Collection - Beginner" (described as a place to get started with containers and models). Below these are three more cards: "Documentation", "Command Line Interface", and "NGC Private Registry". At the bottom, there is a "Popular Collections" section with a "See All Collections" link. The footer indicates "NGC Version: 2.76.0".


NVIDIA NGC | CATALOG Mandeep Kumar


CATALOG Explore Catalog Collections Containers Helm Charts Models Resources


PRIVATE REGISTRY


Search or click the filtering icon...


Getting Started


 Accelerated with NVIDIA
PyTorch
Container
PyTorch is a GPU accelerated tensor computational framework. Functionality can be extended with common Python libraries such as NumPy and SciPy....
[View Labels](#) [Pull Tag](#)

 Accelerated with NVIDIA
TensorFlow
Container
TensorFlow is an open source platform for machine learning. It provides comprehensive tools and libraries in a flexible architecture allowing easy...
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NGC - Getting Started
Collection - Beginner
Looking to get started with containers and models on NGC? This is the place to start..
[View Labels](#)


Documentation
We've got a whole host of documentation, covering the NGC UI and our powerful CLI. You can find out more here. [Go to Documentation](#)


Command Line Interface
Want to get more from NGC? Everything you see here can be used and managed via our powerful CLI tools. [Download Now](#)

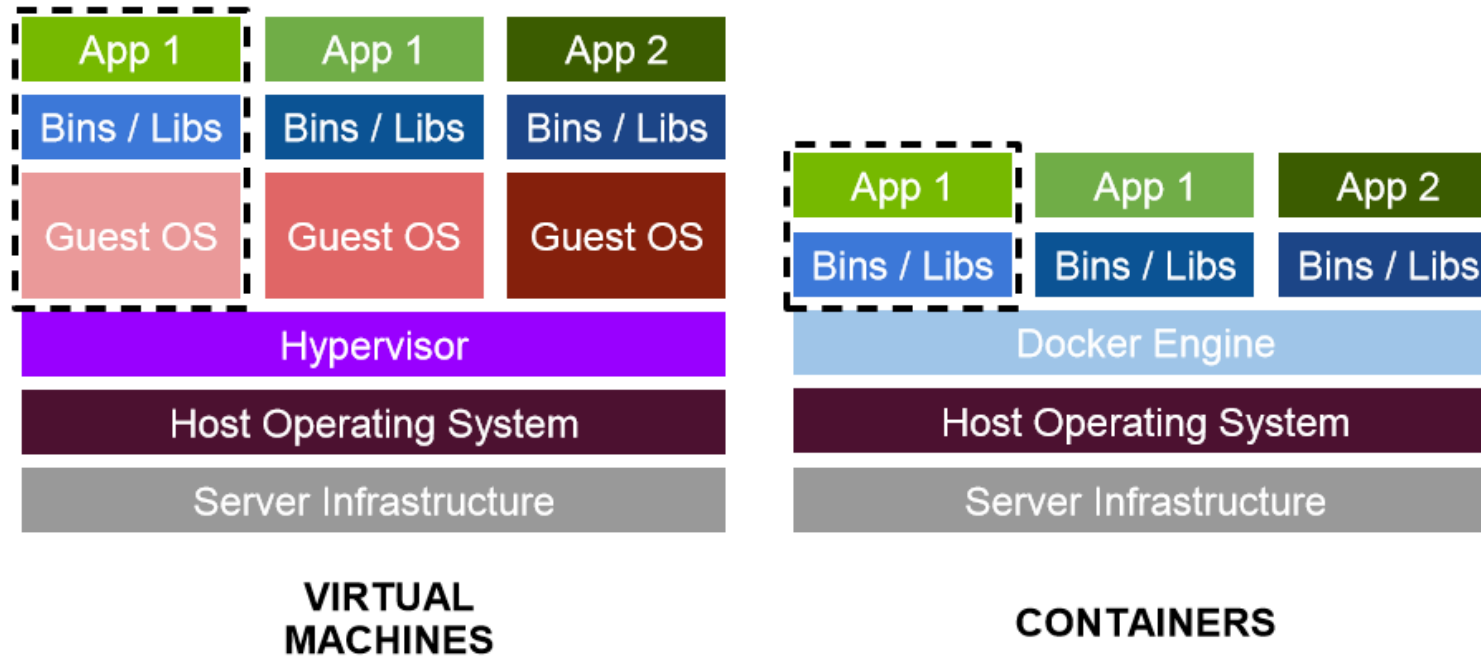

NGC Private Registry
Private Registries from NGC allow you to secure, manage, and deploy your own assets to accelerate your journey to AI. [Learn More](#)

Popular Collections [See All Collections](#)

NGC Version: 2.76.0

VIRTUAL MACHINE VS. CONTAINER

Not so similar



What's Docker?

“an open-source project that automates the deployment of software applications inside **containers** by providing an additional layer of abstraction and automation of **OS-level virtualization** on Linux.”

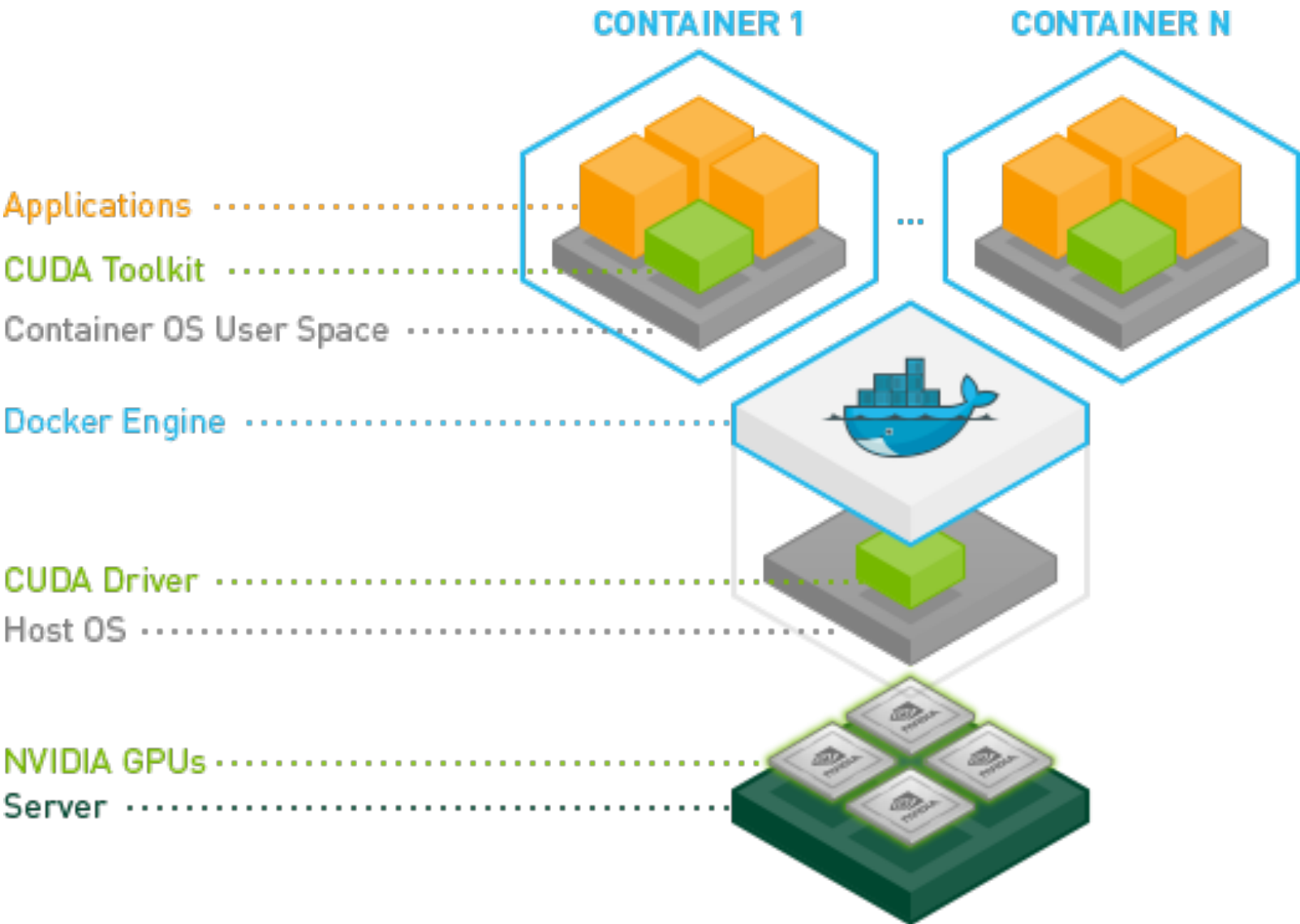
The key benefit of Docker:

- It allows users to **package an application with all of its dependencies into a standardized unit** for software development.

Why NVIDIA Docker?

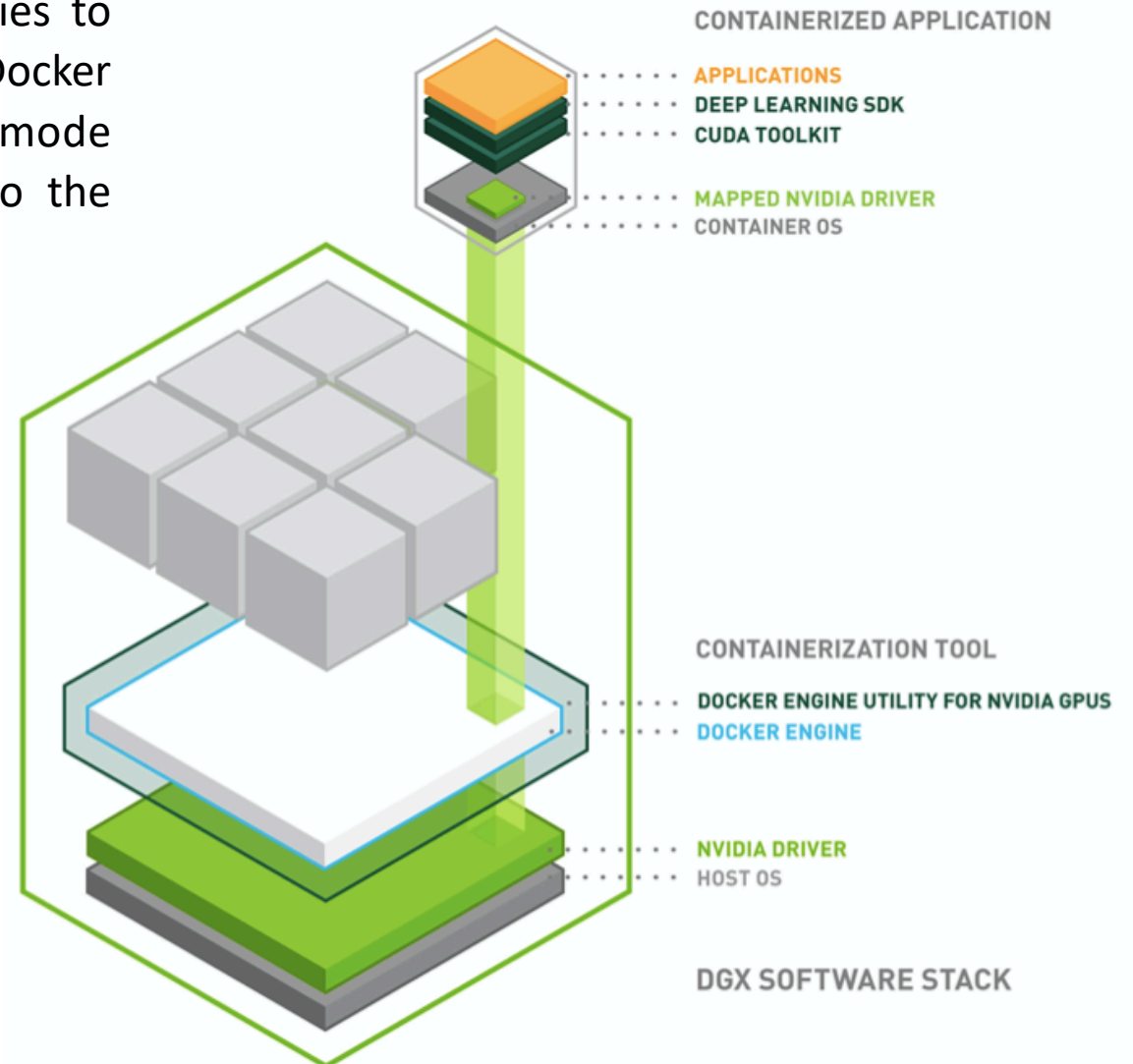
- Docker containers are hardware-agnostic and platform-agnostic
- NVIDIA GPUs are specialized hardware that require the NVIDIA driver
- Docker does not natively supported NVIDIA GPUs with containers
- nvidia-docker makes the images agnostic of the NVIDIA driver

NVIDIA Docker



NVIDIA Docker

Docker containers encapsulate application dependencies to provide reproducible and reliable execution. The Docker Engine Utility for NVIDIA GPUs maps the user-mode components of the NVIDIA driver and the GPUs into the Docker container at launch.



NVIDIA Docker Sub-Commands

nvidia-docker pull

nvidia-docker images

nvidia-docker run

nvidia-docker ps

nvidia-docker exec

nvidia-docker commit

nvidia-docker logs

Running Containers

```
nvidia-docker run -it --rm --name <container_name> -u $(id -u):$(id -g) -p 8080:8888 --net=host  
-v local_dir:container_dir nvcr.io/nvidia/<framework_name>:<xx.xx>
```

Docker run Options:

- **--rm** remove the container after it exits
- **-i -t** or **-it** interactive, and connect a “tty”
- **--name** give the container a name
- **-u \$(id -u):\$(id -g)** set the ID of the user in the container
- **-p 8080:8888** port map from host to container
- **--net=host** networking stack in the container
- **-v ~/data:/data** map storage volume from host to container (bind mount) i.e. bind the ~data directory in your home directory to /data in the container

Docker on HPC Systems

- HPC systems are shared resources
- Docker's security model is designed to support trusted users running trusted containers; e.g., users can escalate to root.
- Docker not designed to support batch-based workflows.
- Docker not designed to support tightly-coupled, highly distributed parallel applications (MPI).
- No native support with open source workload managers like SLURM.

Overcome these Issues with Singularity

Singularity: A Container Engine for HPC

- Reproducible, portable, sharable, and distributable containers
- No trust security model: untrusted users running untrusted containers
- No user contextual changes or root escalation allowed; user inside container is always the same user who started the container
- It automatically derived user's home directory; user can also bind other directories at runtime

Running with Singularity

Save the NGC container as a local Singularity image file:

```
singularity build <framework_name>.sif docker://nvcr.io/nvidia/<framework_name>:<xx.xx>
```

e.g,

```
singularity build tensorflow_21.07-tf2-py3.sif docker://nvcr.io/nvidia/tensorflow:21.07-tf2-py3
```

Run Singularity image file on NVIDIA GPU:

```
singularity run --nv --bind local_dir:container_dir <framework_name>.sif <Container-Name>
```

e.g,

```
singularity run --nv /opt/apps/sif/tensorflow_21.07-tf2-py3.sif yourcode.py
```

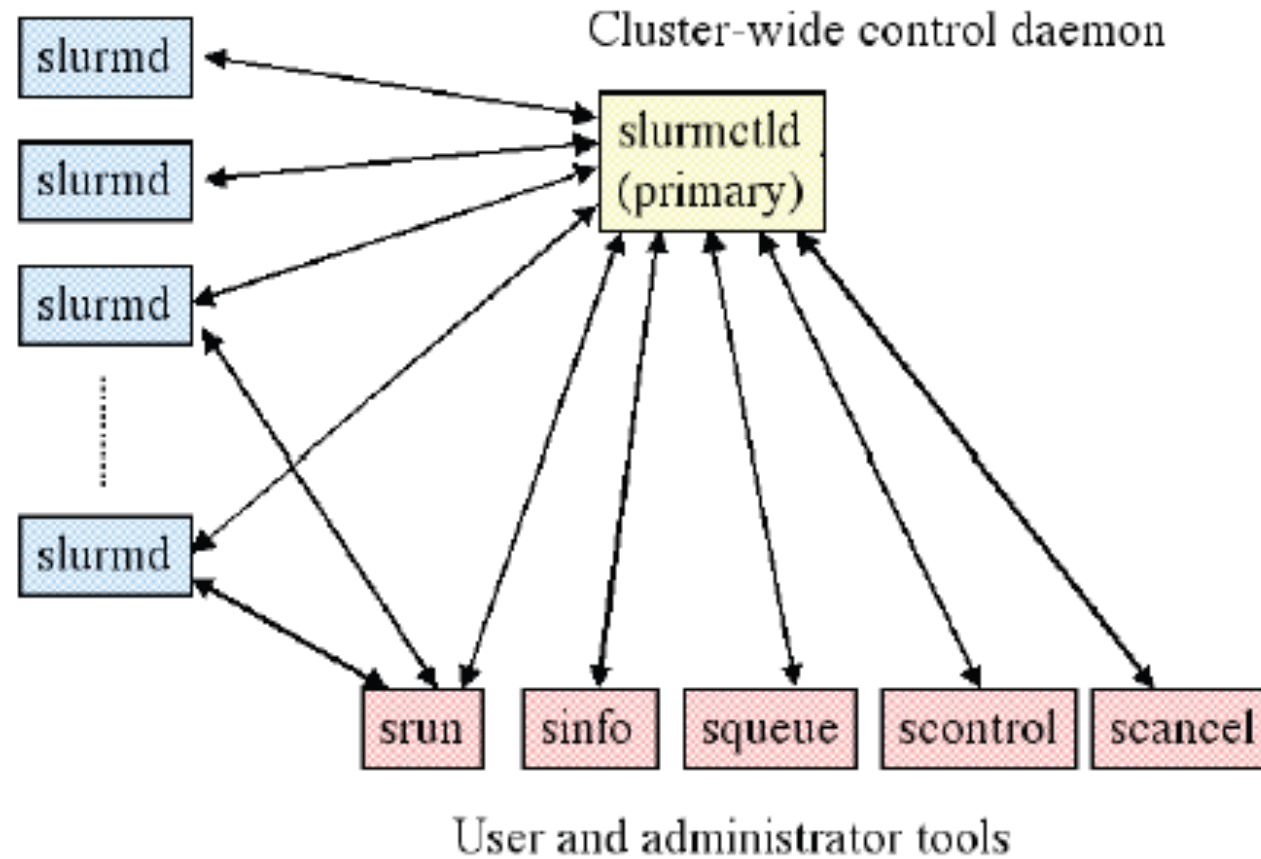
SLURM (Simple Linux Utility for Resource Management) is a highly configurable open source workload and resource manager.

It provides three key functions:

- It allocates exclusive and/or non-exclusive access to resources to users for some duration of time so they can perform work
- It provides a framework for starting, executing, and monitoring work on a set of allocated resources
- It arbitrates contention for resources by managing a queue of pending work

SLURM Architecture

One daemon per node



SLURM Commands for the User

- **sbatch**: Submit a batch script to SLURM.

sbatch <SCRIPT NAME>

- **squeue**: View information about jobs located in the SLURM scheduling queue.

squeue <JOB ID>

- **sinfo**: View information about SLURM nodes and partitions.

sinfo

- **scancel**: Used to signal or cancel a jobs or job steps that are under the control of SLURM.

scancel <JOB ID>

Containers (Singularity) with SLURM Sample Script

TensorFlow Container with SLURM Sample Script:

```
#!/bin/bash
#SBATCH --job-name=tf_test
#SBATCH --ntasks=8
#SBATCH --output=test_tf_%j.out
#SBATCH --gres=gpu:1
#SBATCH --partition=debug
singularity run --nv /opt/apps/sif/tensorflow_21.07-tf2-py3.sif python -c 'import tensorflow as tf; print(tf.__version__)'
```

PyTorch Container with SLURM Sample Script:

```
#!/bin/bash
#SBATCH --job-name=pytorch_test
#SBATCH --ntasks=8
#SBATCH --output=test_pytorch_%j.out
#SBATCH --gres=gpu:1
#SBATCH --partition=debug
singularity run --nv /opt/apps/sif/pytorch_21.07-py3.sif python -c 'import torch; print(torch.__version__)'
```

Thanks!