Machine Learning
[Understanding the Environment]

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Outline

❑ **Overview**

❑ Package Management Tools

❑ GPU

❑ Docker

❑ Conclusion

Overview

❑ To run a machine learning (ML) model

➢ You have to set up an environment

➢ **Using virtualization or package management tools is a good practice**

- You can migrate the code and reproduce the result easily
- Different applications will not affect each other

❑ In this tutorial

➢ We will provide some guidelines for setting up the environment

- The examples are executed in Linux
- For Windows users, we recommend using Windows Subsystem for Linux

➢ We will help you understand the environment

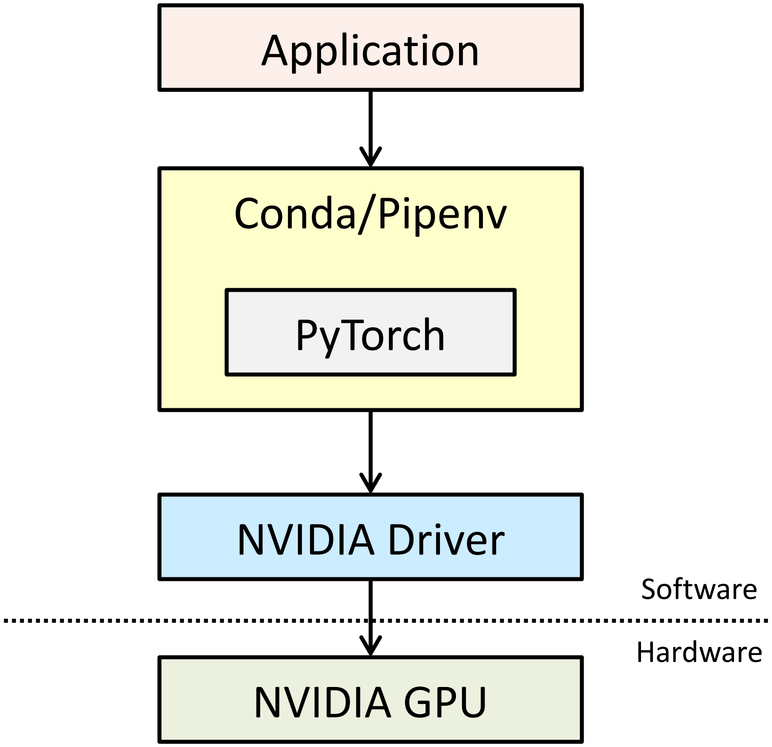
- The software stack
- NVIDIA GPUs

Outline

- ❑ Overview
- ❑ **Package Management Tools**
  - ➢ Prerequisites
  - ➢ Conda
  - ➢ Pipenv
  - ➢ Summary
- ❑ GPU
- ❑ Docker
- ❑ Conclusion

Prerequisites

- ❑ Package management tools
  - ➢ Help you manage the environment
  - ➢ Do not manage the GPU driver
- ❑ To utilize GPUs, make sure the GPU driver is intalled



Conda

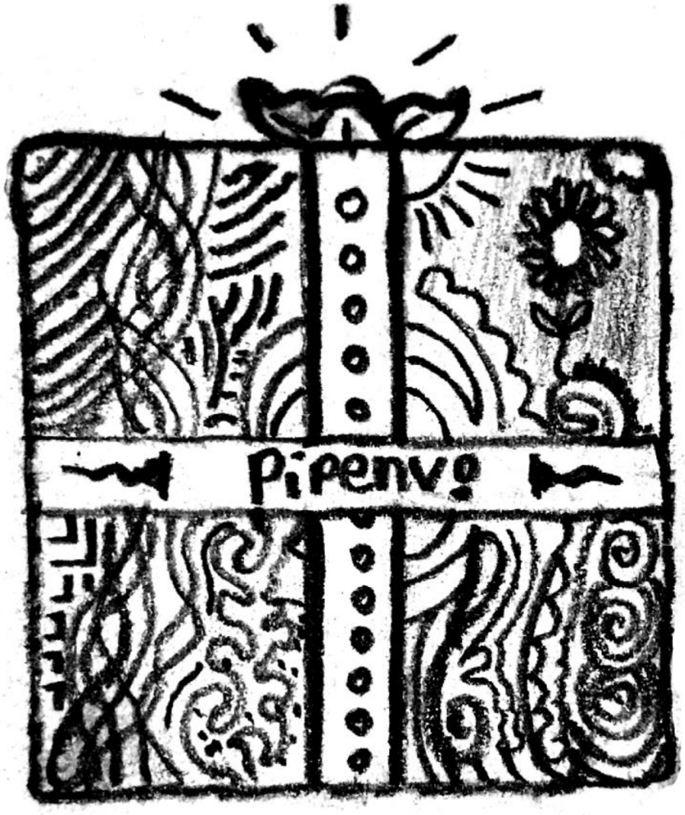
- ❑ Conda
  - ➢ An open source package and environment management system
  - ➢ Supports Windows, MacOS, and Linux
- ❑ We take Anaconda as an example

Quick Start - Anaconda

Steps	Linux Command
Install Anaconda with the installer (Check the document for details)	`bash Anaconda3-2021.11-Linux-x86_64.sh`
Create an environment (You can replace `test_env` with your desired environment name)	`conda create -n test_env`
Install packages (You can find the command in the PyTorch official website)	`conda install -n test_env pytorch torchvision torchaudio cudatoolkit=11.3 -c pytorch`
Activate the environment	`conda activate test_env`
Run your application	`python ml.py`
Leave the environment	`conda deactivate`

Pipenv

- ❑ Pipenv
  - ➢ A tool that creates and manages a virtualenv



Quick Start - Pipenv

❑ To know more about Pipenv, please check the document

Steps	Linux Command
Install Pipenv with pip3	`pip3 install pipenv`
Install packages	`pipenv install numpy torchvision torch --index https://download.pytorch.org/whl/cu113`
Activate the environment	`pipenv shell`
Run your application	`python ml.py`
Leave the environment	`Ctrl + D`

Summary

- To utilize GPU, you must install driver on your host machine

- Using Conda or Pipenv to build environments is recommended
  - Programs become portable
  - Results can be reproduced easily
  - Applications do not affect each other

- You can stop here if you just want to finish the homework

GPU Not Detected

- Sometimes, you may find that the GPU is not detected
  - There are many possible reasons

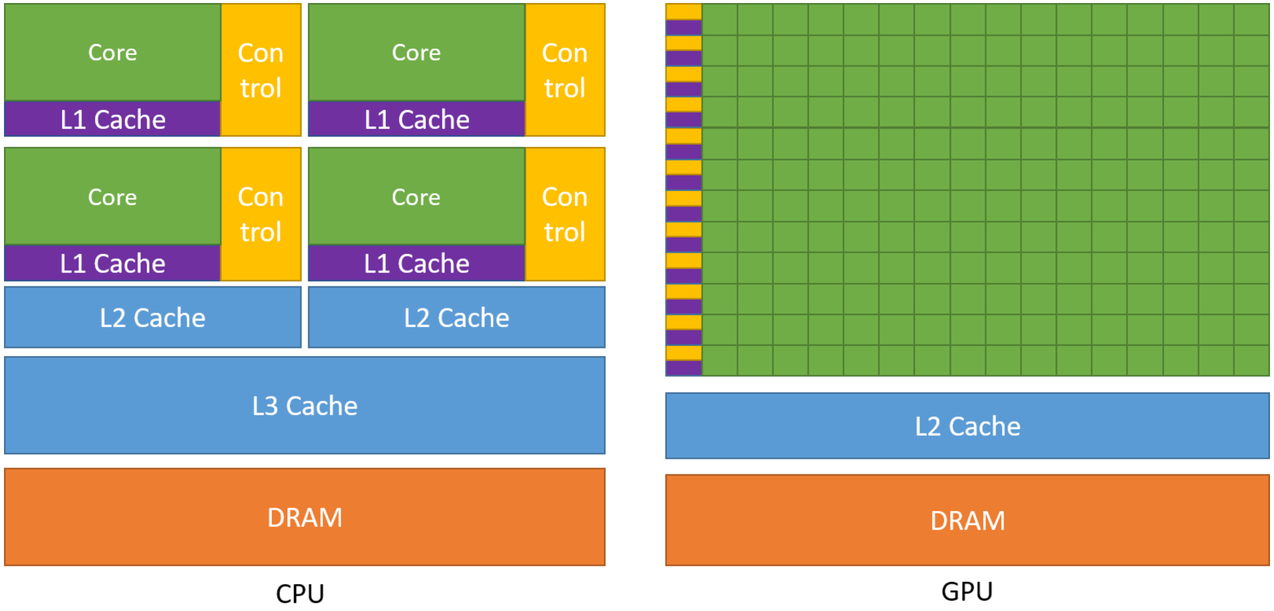
- In order for the GPU to work properly, we need to have some basic understanding of the GPU and its related software
  - We only focus on NVIDIA GPUs

Outline

- ❑ Overview
- ❑ Package Management Tools
- ❑ <u>**GPU**</u>
  - ➢ NVIDIA GPUs
  - ➢ Software Stack
  - ➢ NVIDIA Driver
  - ➢ CUDA
- ❑ Docker
- ❑ Conclusion

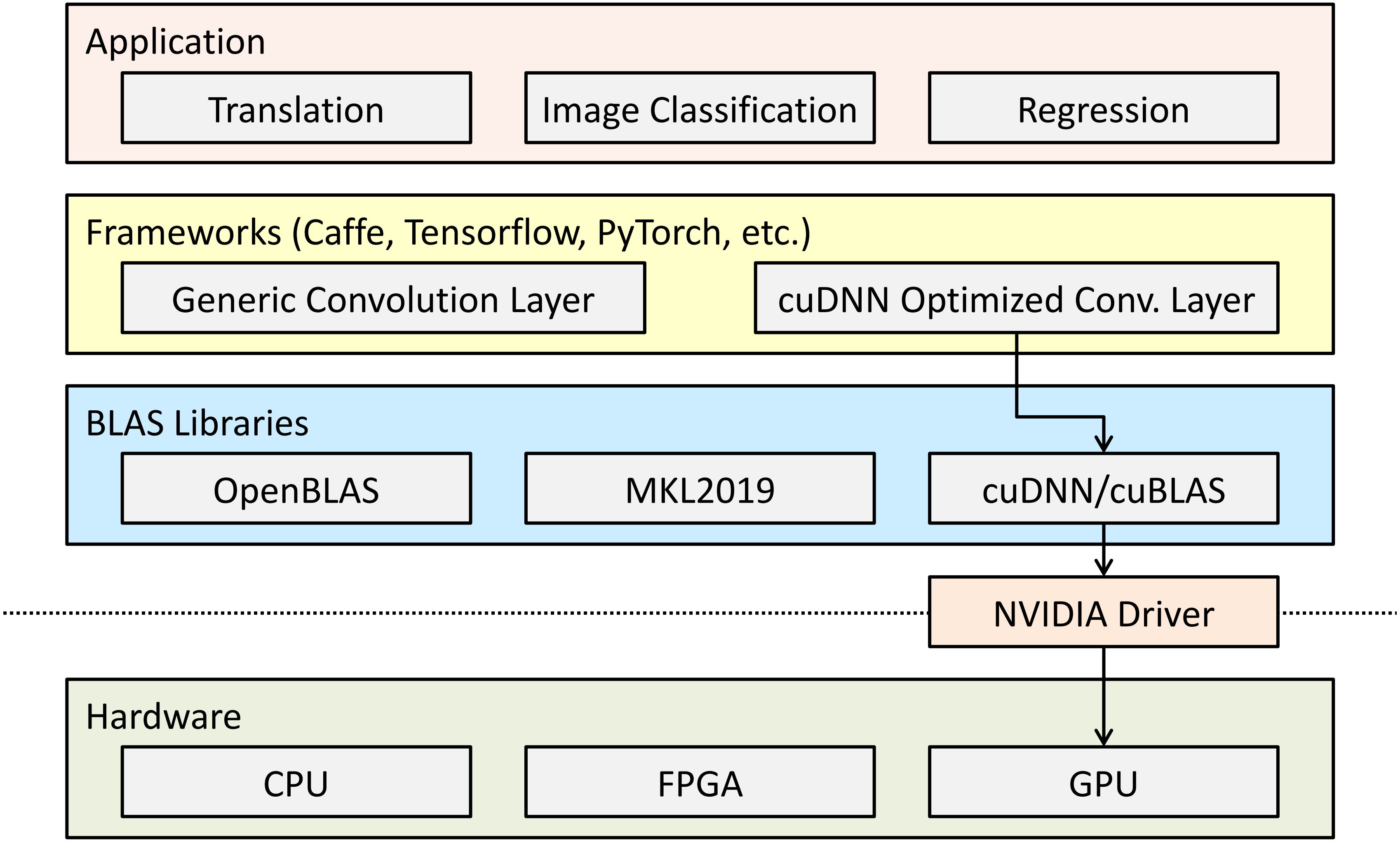
NVIDIA GPUs

- ❑ General Purpose Graphics Processing Units (GPGPU)
  - ➢ GPUs are originally designed for computer graphic applications
  - ➢ GPU is good at parallelizing "simple and repetitive" computations
    - E.g., matrix multiplication
  - ➢ There are massive matrix multiplication computations in ML models
    - We utilize GPUs to accelerate ML model training



https://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html

Software Stack



Application

Translation

Image Classification

Regression

Frameworks (Caffe, Tensorflow, PyTorch, etc.)

Generic Convolution Layer

cuDNN Optimized Conv. Layer

BLAS Libraries

OpenBLAS

MKL2019

cuDNN/cuBLAS

NVIDIA Driver

Hardware

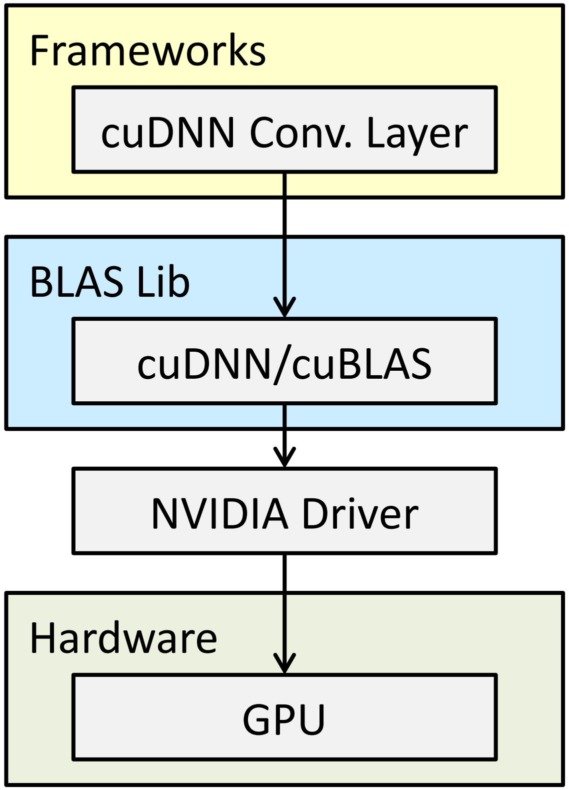
CPU

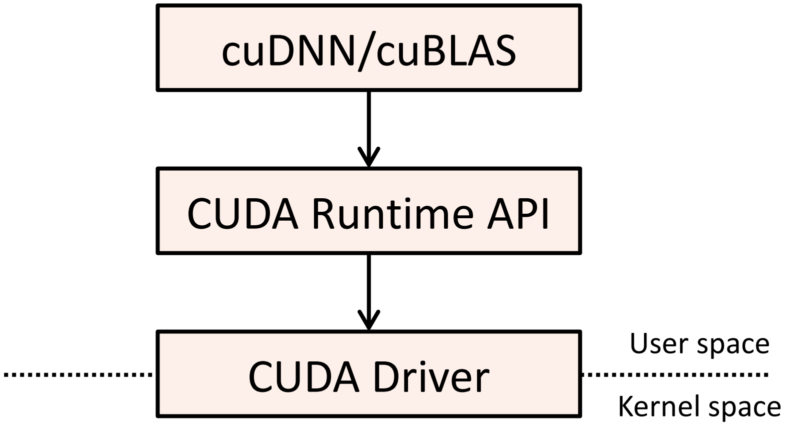
FPGA

GPU

NVIDIA Driver

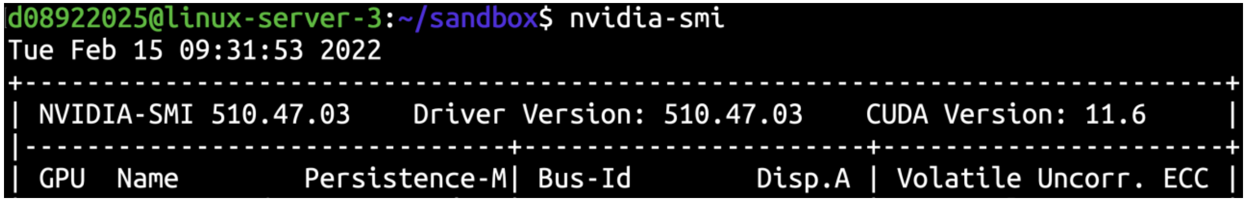
- NVIDIA driver
  - The software that allows operating systems (OS) to communicate with GPUs
  - Includes kernel modules





CUDA

- Compute Unified Device Architecture (CUDA)
  - "A parallel computing platform and application programming interface that allows software to use NVIDIA GPUs" [Wikipedia]
- CUDA Runtime API vs. CUDA Driver API
  - **The driver CUDA version must ≥ the runtime CUDA version**
  - Check the driver CUDA version



```
d08922025@linux-server-3:~/sandbox$ nvidia-smi
Tue Feb 15 09:31:53 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 510.47.03    Driver Version: 510.47.03    CUDA Version: 11.6     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
```

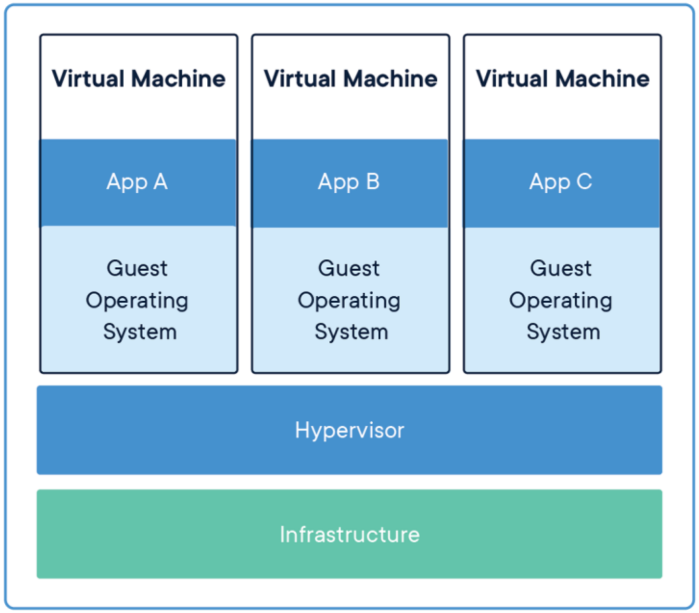
  - When we "install CUDA"
    - We **usually** refer to the CUDA runtime
    - You should check the framework compatibility
    - The version should not be greater than the driver CUDA version
    - You should choose the runtime CUDA version carefully

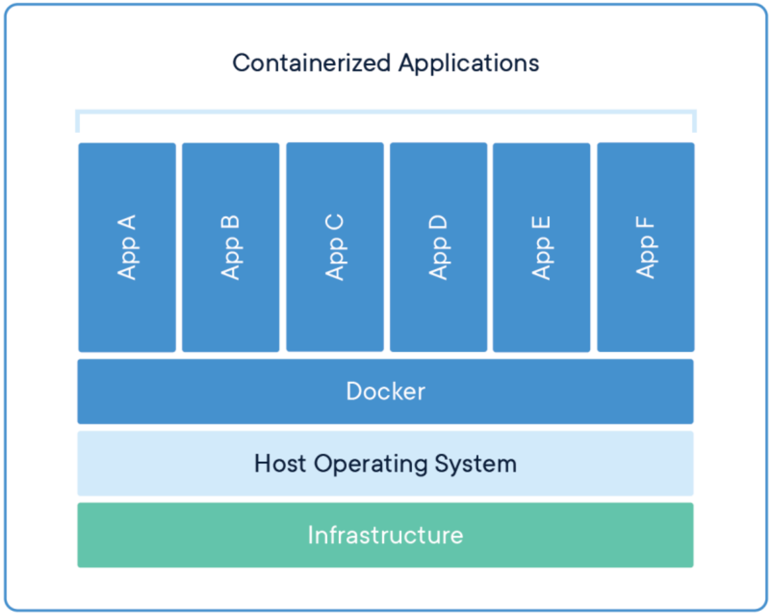
Outline

- Overview
- Package Management Tools
- GPU
- **Docker**
    - Virtualization
    - Why using Container?
    - Contanerization with Docker
    - Pulling Docker Images
    - NVIDIA Docker
- Conclusion

Virtualization

- ❑ Virtual machine (VM) and container





- ❑ You only have to know that
  - ➢ Containers only virtualize software layers above the OS level
    - It is a good choice if we only focus on specific hardware (e.g., NVIDIA GPUs)
  - ➢ Containers are relatively lightweight

https://www.docker.com/resources/what-container

Why using Container?

- Containers can virtualize more complex environments
  - Even if you "only want to train models"
    - You may use other frameworks that do not ship with CUDA and cuDNN
    - You may need NCCL to perform efficient parallel and distributed training
    - You may need to run an old version PyTorch, but the default CUDA version is too old to communicate with the latest powerful GPU

- Slurm and Kubernetes are popular server management tools in both academia and industry
  - Slurm supports singularity container
  - Kubernetes runs applications in Docker containers

slurm
workload manager

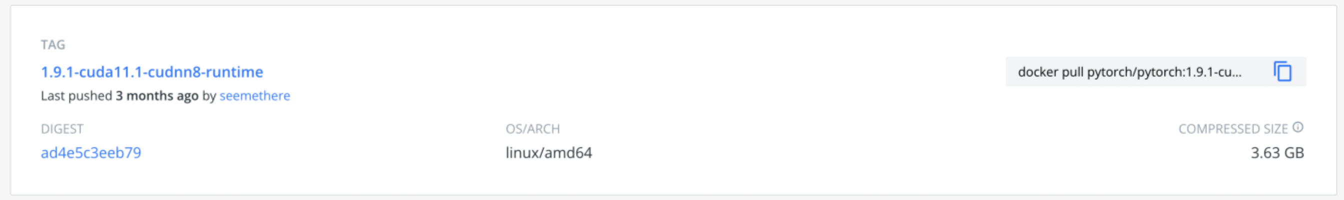
kubernetes

Containerization with Docker

- ❑ Docker
  - ➢ A platform for you to build and execute containers
  - ➢ Docker installation
    - Docker Desktop (for Mac and Windows) runs a VM
- ❑ Docker image
  - ➢ A set of instructions for creating a Docker container
- ❑ Steps of setting up environment with Docker
  - ➢ Install Docker
    - One-time effort
  - ➢ Build/pull an image
    - There are lots of built images
  - ➢ Run the container
  - ➢ Run your application

Pulling Docker Images

- ❑ Docker Hub
  - ➢ A place for finding and sharing Docker images
    - E.g., Docker Hub repository of PyTorch
- ❑ Check the Docker Hub and find the image tag
  - ➢ 1.9.1-cuda11.1-cudnn8-devel vs. 1.9.1-cuda11.1-cudnn8-runtime?

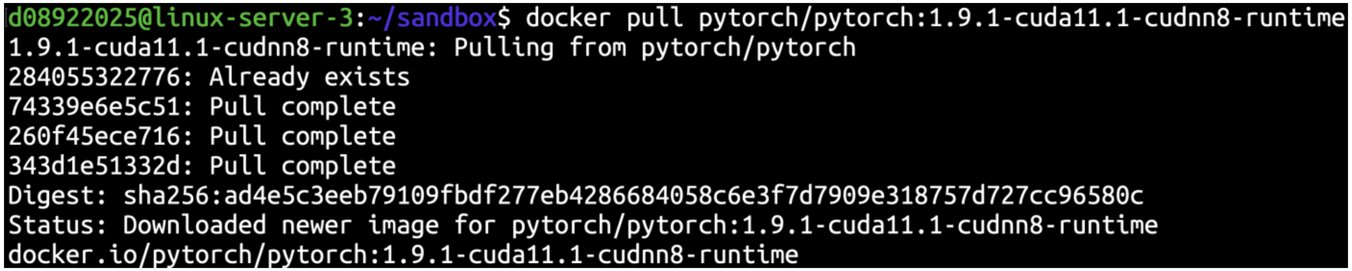


TAG
1.9.1-cuda11.1-cudnn8-runtime
Last pushed **3 months ago** by seemethere

docker pull pytorch/pytorch:1.9.1-cu...

DIGEST	OS/ARCH	COMPRESSED SIZE
ad4e5c3eeb79	linux/amd64	3.63 GB

  - ➢ Run "docker pull <image_tag>"



```
d08922025@linux-server-3:~/sandbox$ docker pull pytorch/pytorch:1.9.1-cuda11.1-cudnn8-runtime
1.9.1-cuda11.1-cudnn8-runtime: Pulling from pytorch/pytorch
284055322776: Already exists
74339e6e5c51: Pull complete
260f45ece716: Pull complete
343d1e51332d: Pull complete
Digest: sha256:ad4e5c3eeb79109fbdf277eb4286684058c6e3f7d7909e318757d727cc96580c
Status: Downloaded newer image for pytorch/pytorch:1.9.1-cuda11.1-cudnn8-runtime
docker.io/pytorch/pytorch:1.9.1-cuda11.1-cudnn8-runtime
```

NVIDIA Docker (1/2)

- ❑ Using GPUs in Docker container makes container less portable
  - Containers work in user space
    - Root privilege only means you can use some privileged system calls
  - Using NVIDIA GPUs requires kernel modules and user-level libraries
    - The CUDA version of the driver user-space modules must be exactly the same as the CUDA version of the driver kernel modules
    - The runtime CUDA version can be smaller than the driver CUDA version
  - The host driver must exactly match the version of the driver installed in the container

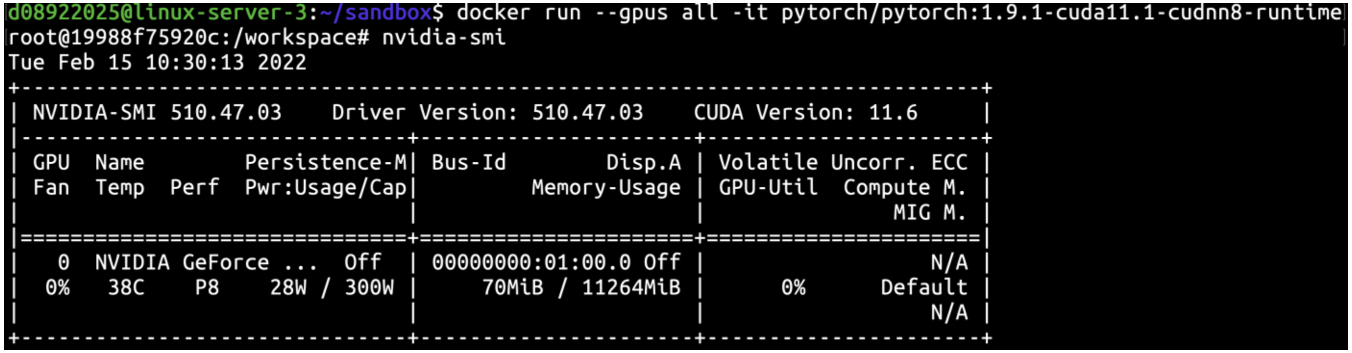
- ❑ We should use NVIDIA Docker
  - Install NVIDIA Docker
  - You do not have to install the NVIDIA driver in the container

https://github.com/NVIDIA/nvidia-docker

NVIDIA Docker (2/2)

❑ Steps

- ➢ Install the latest NVIDIA driver
  - One-time effort
- ➢ Install NVIDIA Docker
  - One-time effort
- ➢ Build/pull an image
- ➢ Run the container
- ➢ Run your application



```
d08922025@linux-server-3:~/sandbox$ docker run --gpus all -it pytorch/pytorch:1.9.1-cuda11.1-cudnn8-runtime
root@19988f75920c:/workspace# nvidia-smi
Tue Feb 15 10:30:13 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 510.47.03    Driver Version: 510.47.03    CUDA Version: 11.6     |
|-------------------------------+----------------------+----------------------+
| 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 GeForce ...  Off  | 00000000:01:00.0 Off |                  N/A |
|  0%   38C    P8    28W / 300W |     70MiB / 11264MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+
```

Outline

- ❑ Overview
- ❑ Package Management Tools
- ❑ GPU
- ❑ Docker
- ❑ **Conclusion**

Conclusion

- ❑ Whether or not you virtualize your environment
  - ➢ You must install the NVIDIA driver on the host to utilize NVIDIA GPUs
  - ➢ The runtime CUDA version must be less than or equal to the driver CUDA version

- ❑ If you want to use NVIDIA GPUs in containers
  - ➢ Using NVIDIA Docker makes your life easier
    - You do not need to install NVIDIA drivers in containers
    - Containers are more portable
  - ➢ You only have to pull the built Docker image from Docker Hub
    - You do not have to set up CUDA, cuDNN, and frameworks yourself
    - This is useful especially when the environment is complex

Q&A

Thank You!