

# GPU Intro and Python AI + GPU

## High-Performance Computing

Summer 2021 at GIST

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Saint Louis University



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— EST. 1818 —

# Jupyter Notebook

- <https://jupyter.org/>

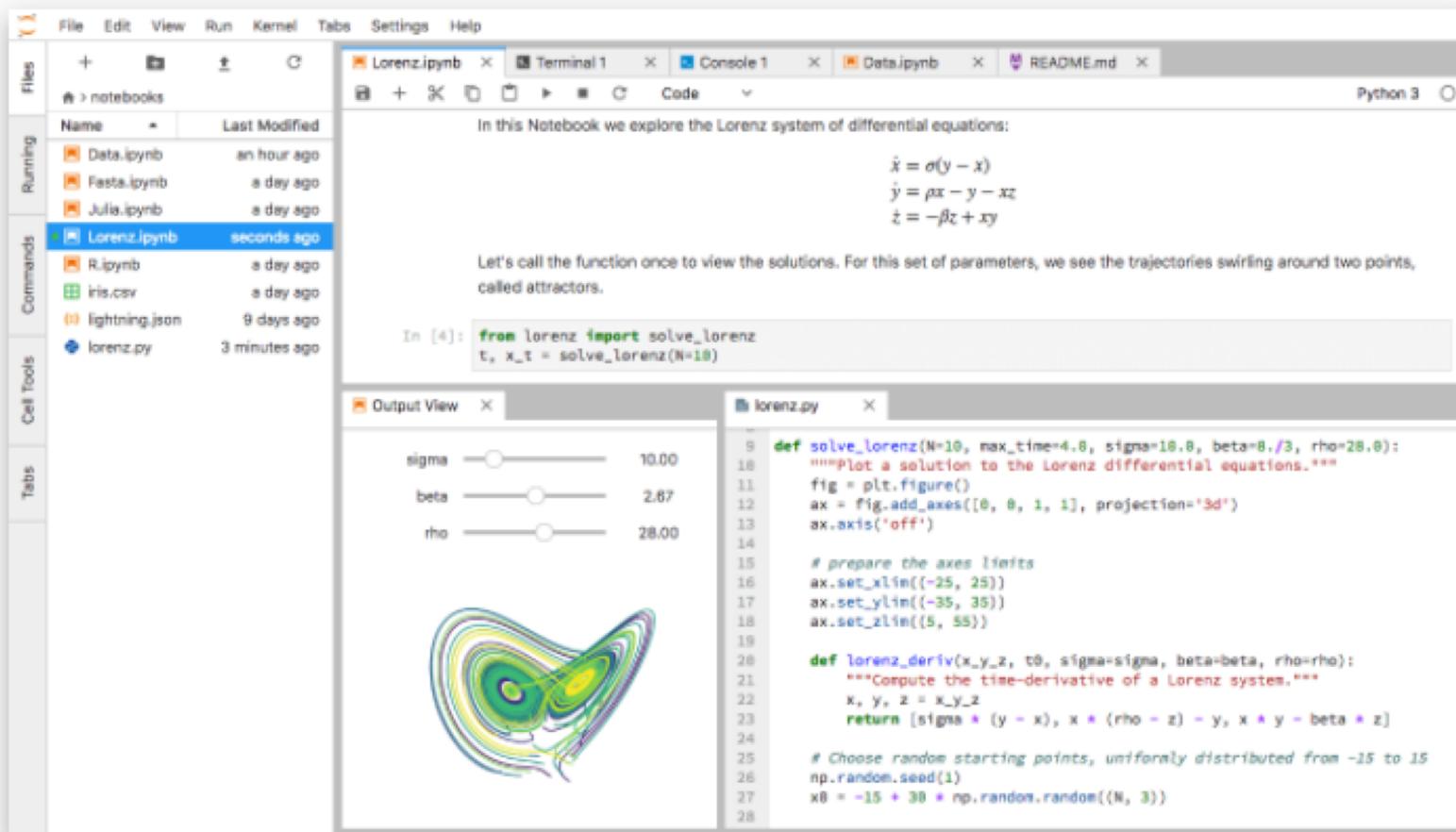


Project Jupyter exists to develop open-source software, open-standards, and services for interactive computing across dozens of programming languages.

# Jupyter Lab

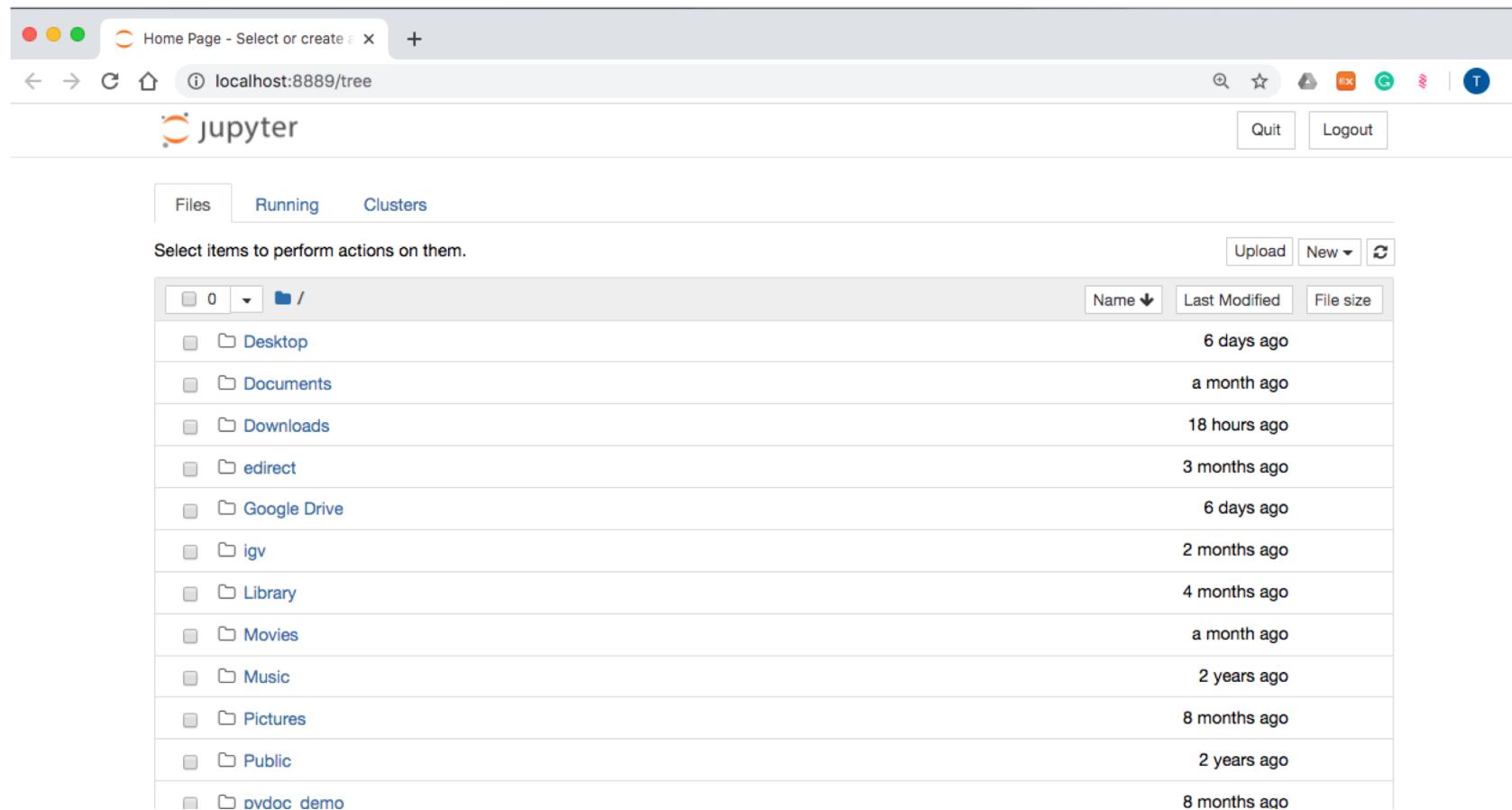
- <https://jupyterlab.readthedocs.io/en/stable/>

JupyterLab is the next-generation web-based user interface for Project Jupyter. Try it on Binder.  
JupyterLab follows the Jupyter Community Guides.



# Run Jupyter Notebook (Jupyter Lab)

- Install and run
  - Jupyter notebook: just type “jupyter notebook” and it will open a default web browser



# How to run the program on GIST VM via Jupyter Notebook?

- <https://techtalktome.wordpress.com/2017/03/28/running-jupyter-notebooks-on-a-remote-server-via-ssh/>
- Remote (Server: our case is GIST VM):
  - \$ jupyter notebook password
  - \$ jupyter notebook --no-browser --port=8887
    - Be careful: Each user will use a unique port. If someone is using the port, change the 8887 to something else.
- Local (Mac or Windows):
  - \$ ssh -N -L localhost:8888:localhost:8887 YourAccount@210.125.85.148
  - Open a browser and type localhost:8888

# How to run a program on GIST VM via Jupyter Notebook?

jupyter

Quit Logout

Files Running Clusters

Select items to perform actions on them.

Upload New ↘

<input type="checkbox"/> 0	▼	📁 /	Name ↓	Last Modified	File size
<input type="checkbox"/>	📁	Assignments		40 minutes ago	
<input type="checkbox"/>	📁	Lab		2 hours ago	
<input type="checkbox"/>	📄 !			7 days ago	843 B

# GPU

- GPU: Graphics Processing Unit
  - Designed for real-time graphics
  - Present in almost every PC
  - Increasing realism and complexity



# What is GPU?

- It is a processor optimized for 2D/3D graphics, video, visual computing, and display.
- It is highly parallel, highly multithreaded multiprocessor optimized for visual computing.
- It provides real-time visual interaction with computed objects via graphics images, and video.
- It serves as both a programmable graphics processor and a scalable parallel computing platform.
- Heterogeneous Systems: combine a GPU with a CPU

# Nvidia GPU

## The Best Budget Graphics Cards in 2021

**Featured**



**NVIDIA GEFORCE RTX 3070**

› Cooling System: Fan  
› Boost Clock Speed: 1.73 GHz  
› GPU Memory Size: 8 GB

**\$499.99**

[CHECK AVAILABILITY](#)

[+ Compare](#)

**Featured**



**NVIDIA GEFORCE RTX 3060 Ti**

› Cooling System: Fan  
› Boost Clock Speed: 1.67 GHz  
› GPU Memory Size: 8 GB

**\$399.99**

[CHECK AVAILABILITY](#)

[+ Compare](#)

---



**NVIDIA GEFORCE RTX 3080**

› Cooling System: Fan  
› Boost Clock Speed: 1.71 GHz  
› GPU Memory Size: 10 GB

**\$699.99**

[CHECK AVAILABILITY](#)

[+ Compare](#)

# RTX 3080

## GEFORCE RTX 3080

### THE ULTIMATE PLAY

The GeForce RTX™ 3080 delivers the ultra performance that gamers crave, powered by Ampere—NVIDIA's 2nd gen RTX architecture. It's built with enhanced RT Cores and Tensor Cores, new streaming multiprocessors, and superfast G6X memory for an amazing gaming experience.

**STARTING AT \$699.00**

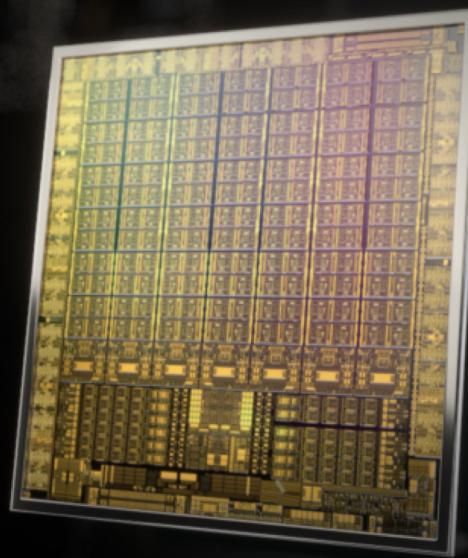
2ND GENERATION  
RT CORES

2X THROUGHPUT

3RD GENERATION  
TENSOR CORES

UP TO 2X THROUGHPUT

NEW  
SM  
2X FP32 THROUGHPUT



# RTX 3080

- Specs (<https://www.nvidia.com/en-us/geforce/graphics-cards/30-series/rtx-3080/>)

GEFORCE RTX 3080		
<b>GPU Engine Specs:</b>	NVIDIA CUDA® Cores	8704
	Boost Clock (GHz)	1.71
	Base Clock (GHz)	1.44
<b>Memory Specs:</b>	Standard Memory Config	10 GB GDDR6X
	Memory Interface Width	320-bit
<b>Technology Support:</b>	Ray Tracing Cores	2nd Generation
	Tensor Cores	3rd Generation
	NVIDIA Architecture	Ampere
	Microsoft DirectX® 12 Ultimate	Yes

## What is RTX?

- RTX stands for Ray Tracing Texel eXtreme and is also a variant under GeForce.
- The RTX cards were specially designed to support real-time ray tracing which made the video looked more beautiful.
- They were first announced in 2018 and uses Turing architecture.
- These cards support the DXR extension in Microsoft's DirectX12 and also DLSS (Deep Learning Super Sampling).

NVIDIA's Ampere architecture is an evolution of Turing, which powered the RTX 20 series. The new architecture includes huge gains in three key areas: streaming multiprocessors (SM) with double the throughput of their predecessors, second-gen RT cores that deliver significantly better performance, and third-gen Tensor cores that offer sizable gains in AI-based tasks.

<https://www.windowscentral.com/nvidia-geforce-rtx-3080-review>

# RTX 3080

Graphics Card	RTX 3080 FE
Architecture	GA102
Process (nm)	Samsung 8N
Transistors (Billion)	28.3
Die size (mm <sup>2</sup> )	628.4
GPCs	6
SMs	68
FP32 CUDA Cores	8704
Tensor Cores	272
RT Cores	68
Boost Clock (MHz)	1710
VRAM Speed (Gbps)	19
VRAM (GB)	10
VRAM Bus Width	320
ROPs	96
TPCs	34



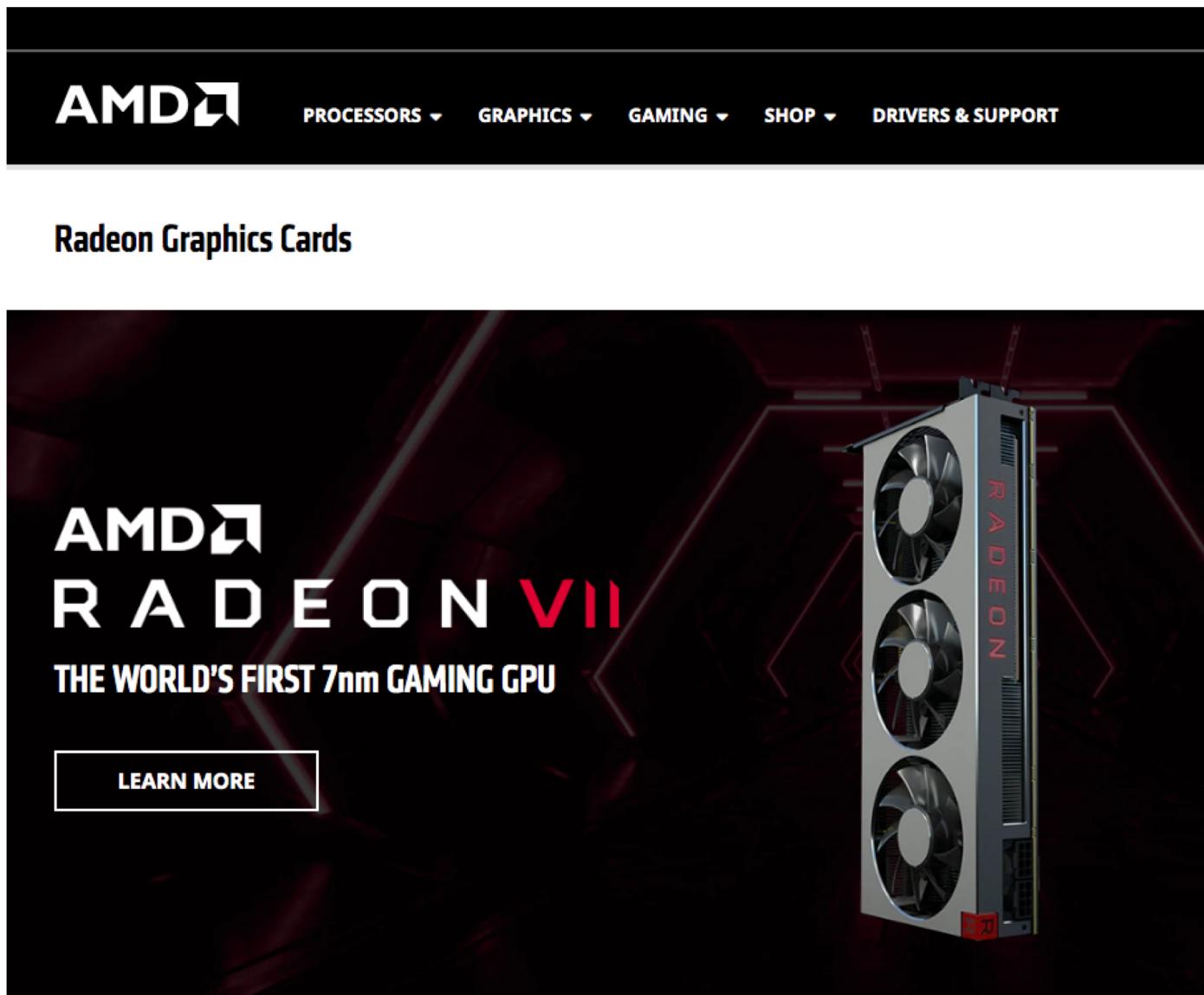
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RT Cores	68
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VRAM (GB)	10
VRAM Bus Width	320
ROPs	96
TPCs	34



- Nvidia GPUs consist of several GPCs (Graphics Processing Clusters), each of which has some number of SMs (Streaming Multiprocessors). Nvidia splits each SM into four partitions that can operate on separate sets of data. With Ampere, each SM partition now has 16 FP32 CUDA cores, 16 FP32/INT CUDA cores, a third-gen Tensor core, load/store units, and a special function unit. The whole SM has access to shared L1 cache and memory, and there's a single second-gen RT core. In total, that means 64 FP32 cores and 64 FP32/INT cores, four Turing cores, and one RT core.
- <https://www.tomshardware.com/reviews/nvidia-geforce-rtx-3080-review>

# AMD Radeon



The image shows a screenshot of the AMD Radeon website. At the top, there is a black navigation bar with the AMD logo and links for PROCESSORS, GRAPHICS, GAMING, SHOP, and DRIVERS & SUPPORT. Below the navigation bar, the text "Radeon Graphics Cards" is displayed. On the left side of the main content area, the text "AMD RADIATOR VII" is shown, followed by "THE WORLD'S FIRST 7nm GAMING GPU". A "LEARN MORE" button is located at the bottom left. On the right side, there is a large image of the AMD Radeon VII graphics card, which has three large fans and a red "RADEON" logo.

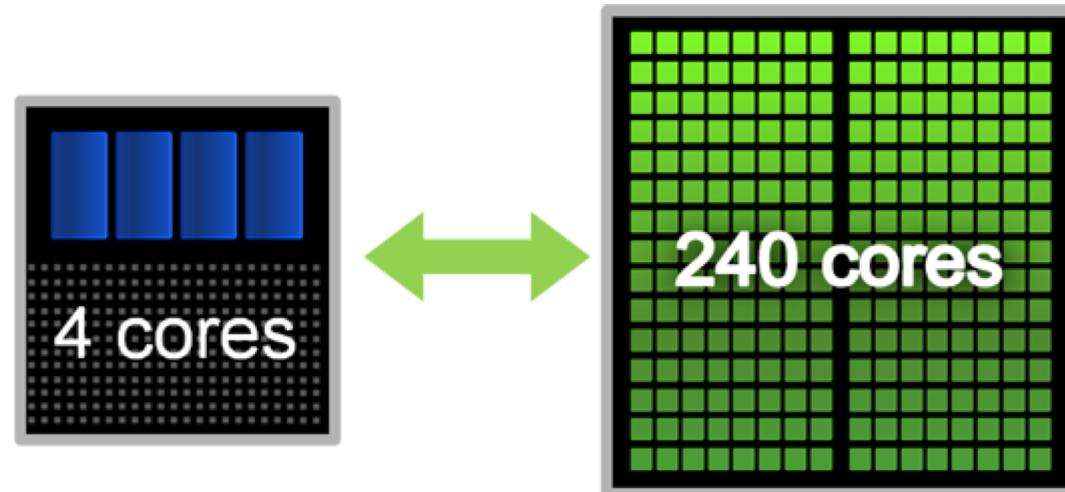
- My MacBook Pro has Radeon Pro 560



The image shows a screenshot of the macOS High Sierra System Report. At the top, it says "macOS High Sierra Version 10.13.6". Below that, it lists system specifications: "MacBook Pro (15-inch, 2017)", "Processor 2.9 GHz Intel Core i7", "Memory 16 GB 2133 MHz LPDDR3", "Graphics Radeon Pro 560 4096 MB Intel HD Graphics 630 1536 MB", and "Serial Number C02WH0NFHTDF". At the bottom, there are two buttons: "System Report..." and "Software Update...".

# GPU and CPU

- Typically GPU and CPU coexist in a heterogeneous setting
- “Less” computationally intensive part runs on CPU (coarse-grained parallelism), and more intensive parts run on GPU (fine-grained parallelism)
- NVIDIA’s GPU architecture is called CUDA (Compute Unified Device Architecture) architecture, accompanied by CUDA programming model, and CUDA C/C++ language



# Difference among CPU, GPU, APU, FPGA, DSP, and Intel MIC?

- <https://www.quora.com/What-is-the-difference-among-CPU-GPU-APU-FPGA-DSP-and-Intel-MIC>

- CPU
  - CPU is a general purpose processor. General Purpose in the sense that it is designed to perform a number of operations but the way these operations are performed may not be best for all applications. Graphics or Video Processing is one such example. Although a CPU can perform these tasks (which involve repeated additions/multiplications which may be performed in parallel), the performance achieved is not good enough for modern applications.
- GPU
  - Graphics processing Unit or GPU is designed to accelerate creation of images for a computer display. A CPU consists of a few cores optimized for sequential serial processing while a GPU consists of thousands of smaller, more efficient cores designed for handling multiple tasks simultaneously. They are designed to perform functions such as texture mapping, image rotation, translation, shading, etc. They may also support operations such as motion compensation, calculation of inverse DCT, etc. for accelerated video decoding.
- Intel MIC
  - Intel Many Integrated Core or Intel MIC Architecture combines many Intel cores onto a single chip. Unlike its competitor in HPC market, NVidia TESLA GPU, it provides up to 61 cores. One of the key advantages that Intel MIC offers over NVidia GPUs is that it runs same instruction set as 64-bit Pentium. Standard C, C++ can be used for writing source codes to program these cores.
- APU
  - APU stands for Accelerated Processing Unit which refers to the main processor of system which has additional functionality for accelerating execution of certain operations. This additional capability may be provided by an on chip graphics processing unit. In simple terms APU is CPU + GPU on a single chip.
- DSP
  - Digital Signal Processor or DSP is optimized for high speed processing of numeric data representing the analog signals in real time. They are designed for quickly performing large number of numeric operations repeatedly on a series of data samples and are ideal for processing streaming digital signals. They provide functionalities that are helpful for DSP applications such as bit reverse addressing which is helpful for FFT computation, architectural support for very tight extremely low overhead loops, saturation arithmetic, etc.
- FPGA
  - An FPGA (Field Programmable Gate Array) is entirely different from CPU, GPU, DSP, etc. in the sense that it is not a processor in itself i.e. it does not run a program stored in the program memory. In layman's terms, an FPGA is nothing but a bulk of reconfigurable digital logic suspended in a sea of programmable inter-connects. A typical FPGA may also have dedicated memory blocks, digital clock manager, IO banks and several other features which vary across different vendors and models. Since they can be configured after manufacturing at customer's end, they can be used to implement any logic function (including but not limited to a processor core). This makes them ideal for re-configurable computing and application specific processing. Intel has recently announced a new range of Xeon Processors with integrated FPGA so that each chip can be configured at run type depending upon application needs.

# GIST AI-X Cluster System

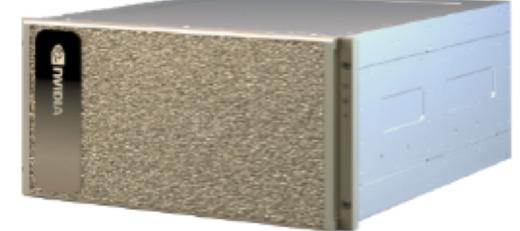


# Computing



## DGX A100

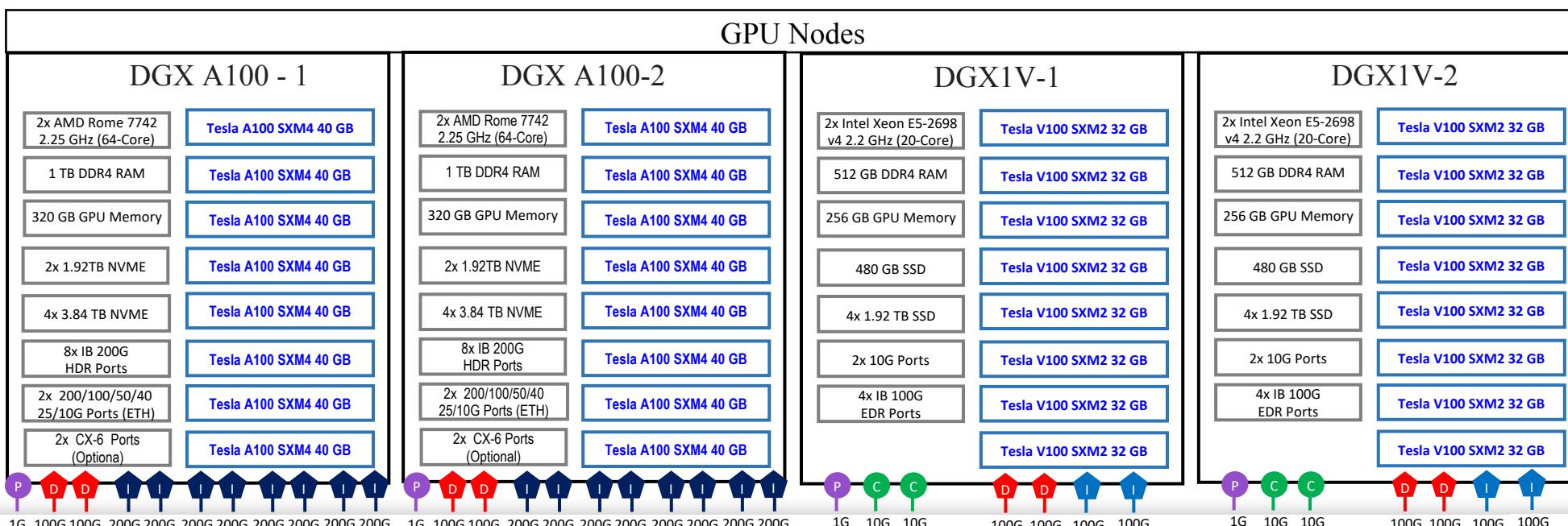
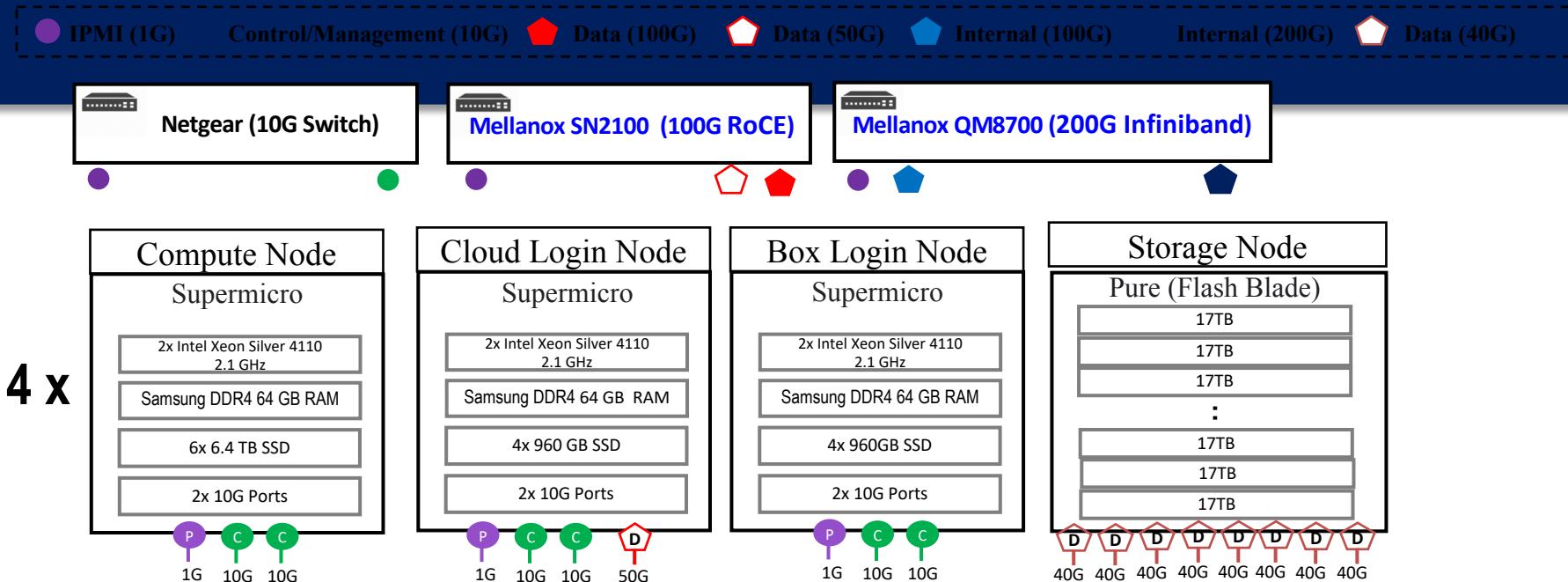
8x NVIDIA A100 GPUs  
320 GB GPU Memory  
1 TB System Memory  
Dual AMD Rome  
2.25 GHz (64-Core) CPU  
9x 200Gb/s NIC



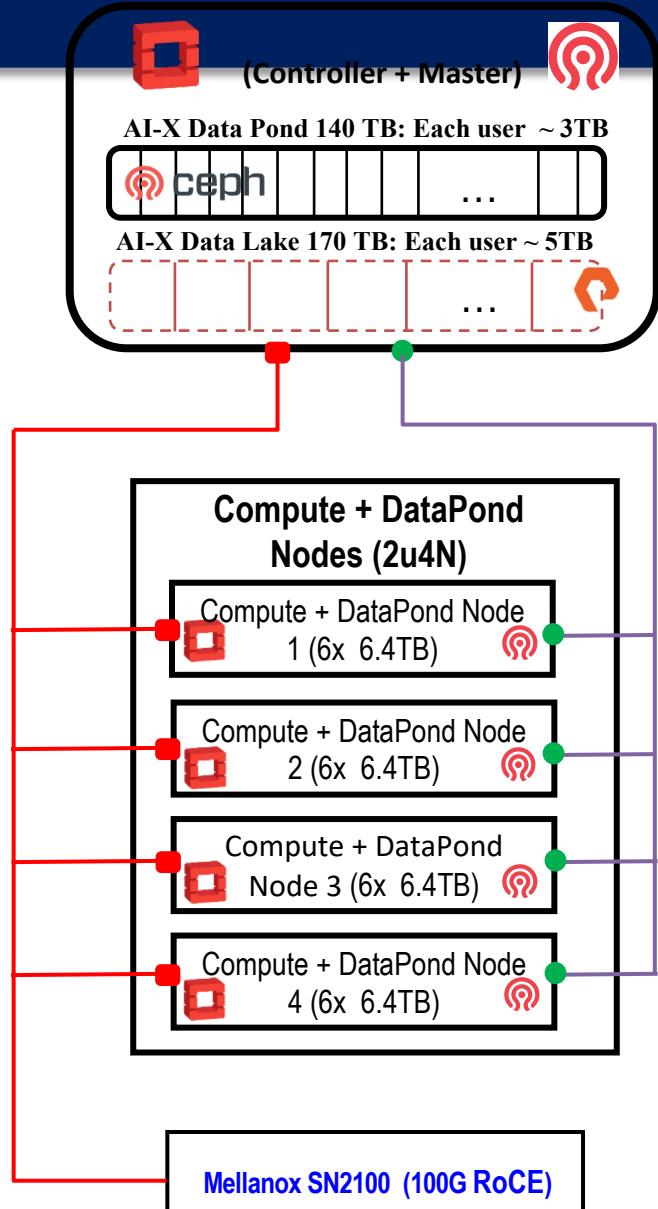
## DGX-1V

8x NVIDIA V100 GPUs  
256 GB GPU Memory  
512 GB System Memory  
Dual Intel Xeon E5-2698 v4  
2.2 GHz (20-Core) CPU  
4x 100Gb/s NIC

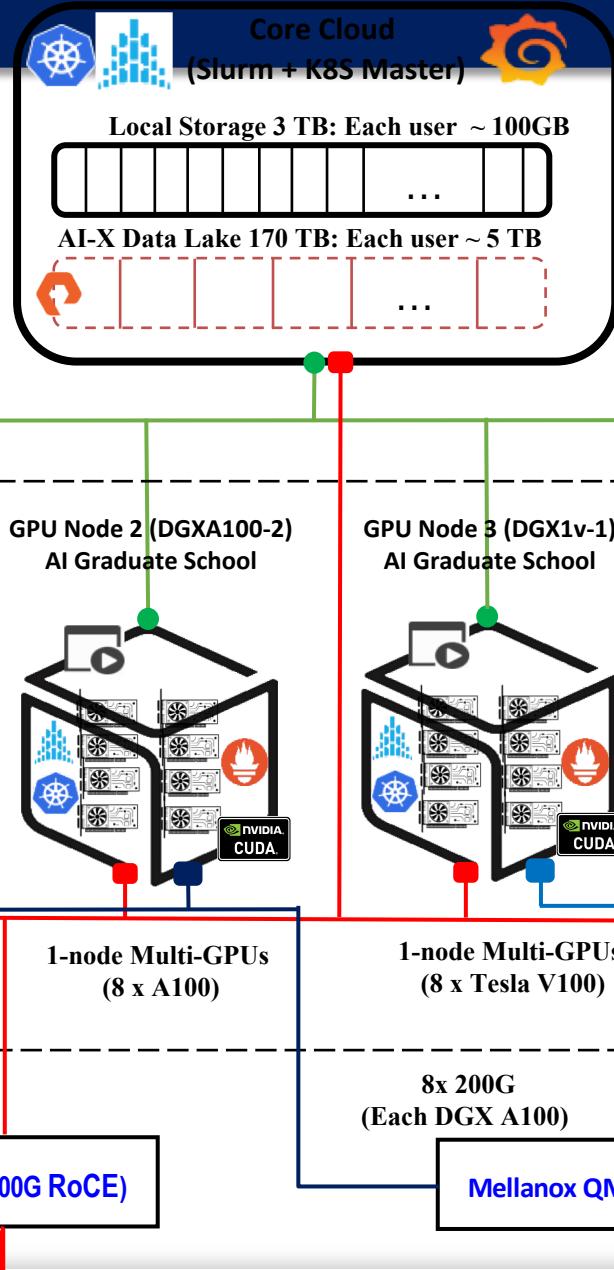




# Front Cluster



# Backend Cluster



- Management Network (10G)
- Data Network (100G RoCE)
- Internal Network (100G IB)
- Internal Network (200G IB)

# GPU Programming Option

## CUDA Versus OpenCL Versus OpenACC

 NVIDIA. ACCELERATED COMPUTING    Downloads    Training    Ecosystem    Forums    [Join](#)    [Login](#)

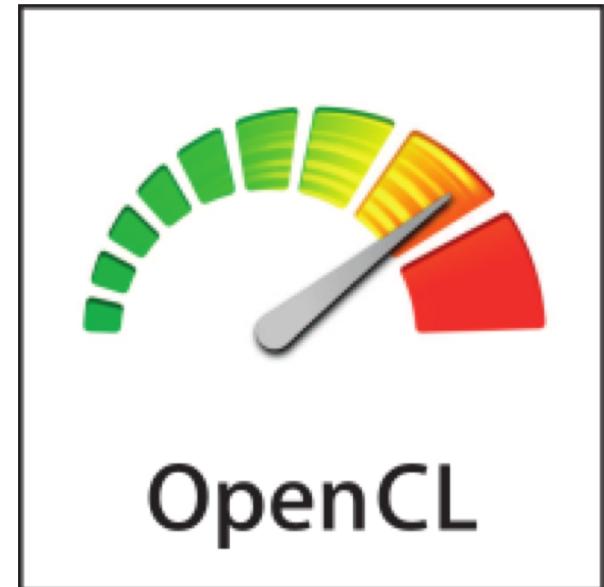
### CUDA Zone

CUDA® is a parallel computing platform and programming model developed by NVIDIA for general computing on graphical processing units [GPUs]. With CUDA, developers are able to dramatically speed up computing applications by harnessing the power of GPUs.

In GPU-accelerated applications, the sequential part of the workload runs on the CPU – which is optimized for single-threaded performance – while the compute intensive portion of the application runs on thousands of GPU cores in parallel. When using CUDA, developers program in popular languages such as C, C++, Fortran, Python and MATLAB and express parallelism through extensions in the form of a few basic keywords.

The [CUDA Toolkit](#) from NVIDIA provides everything you need to develop GPU-accelerated applications. The CUDA Toolkit includes GPU-accelerated libraries, a compiler, development tools and the CUDA runtime.

[Download Now >](#)



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### What is OpenACC?

OpenACC is a user-driven directive-based performance-portable parallel programming model designed for scientists and engineers interested in porting their codes to a wide-variety of heterogeneous HPC hardware platforms and architectures with significantly less programming effort than required with a low-level model.

[Get Started](#)   or [take the next steps](#)

```
#pragma acc data copy(A) create(Anew)
while ( error > tol && iter < iter_max ) {
    error = 0.0;
#pragma acc kernels {
#pragma acc loop independent collapse(2)
    for ( int j = 1; j < n-1; j++ ) {
        for ( int i = 1; i < m-1; i++ ) {
            Anew [j] [i] = 0.25 * ( A [j] [i+1] + A [j] [i-1] +
                                      A [j-1] [i] + A [j+1] [i]);
            error = max ( error, fabs (Anew [j] [i] - A [j] [i]));
        }
    }
}
```

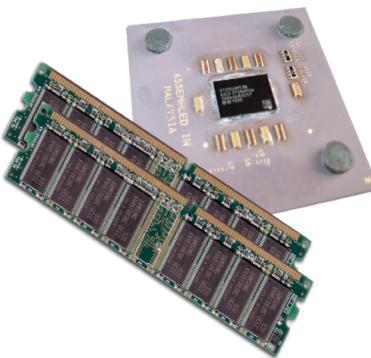
# What is CUDA?

- NVIDIA CUDA Architecture
  - Expose GPU computing for general purpose
  - Retain performance
- CUDA C/C++
  - Based on industry-standard C/C++
  - Small set of extensions to enable heterogeneous programming
  - Straightforward APIs to manage devices, memory etc.
- This session introduces CUDA C/C++

# Heterogeneous Computing

- Terminology:

- *Host* The CPU and its memory (host memory)
- *Device* The GPU and its memory (device memory)



Host



Device

<https://developer.nvidia.com/cuda-education>

© NVIDIA 2013

# Heterogeneous Computing

```
#include <iostream>
#include <algorithm>

using namespace std;

#define N          1024
#define RADIUS     3
#define BLOCK_SIZE 16

__global__ void stencil_1d(int *in, int *out) {
    __shared__ int temp[BLOCK_SIZE + 2 * RADIUS];
    int index = threadIdx.x + RADIUS;
    int gindex = threadIdx.x + blockDim.x * blockDim.x;
    int lindex = threadIdx.x + RADIUS;

    // Read input elements into shared memory
    temp[lindex] = in[gindex];
    if (threadIdx.x < RADIUS) {
        temp[lindex - RADIUS] = in[gindex - RADIUS];
        temp[lindex + BLOCK_SIZE] = in[gindex + BLOCK_SIZE];
    }

    // Synchronize (ensure all the data is available)
    __syncthreads();

    // Apply the stencil
    int result = 0;
    for (int offset = -RADIUS ; offset <= RADIUS ; offset++)
        result += temp[lindex + offset];

    // Store the result
    out[gindex] = result;
}

void fill_ints(int *x, int n) {
    fill_n(x, n, 1);
}

int main(void) {
    int *in, *out;           // host copies of a, b, c
    int *d_in, *d_out;       // device copies of a, b, c
    int size = (N + 2*RADIUS) * sizeof(int);

    // Alloc space for host copies and setup values
    in = (int *)malloc(size); fill_ints(in, N + 2*RADIUS);
    out = (int *)malloc(size); fill_ints(out, N + 2*RADIUS);

    // Alloc space for device copies
    cudaMalloc((void **)&d_in, size);
    cudaMalloc((void **)&d_out, size);

    // Copy to device
    cudaMemcpy(d_in, in, size, cudaMemcpyHostToDevice);
    cudaMemcpy(d_out, out, size, cudaMemcpyHostToDevice);

    // Launch stencil_1d() kernel on GPU
    stencil_1d<<<N/BLOCK_SIZE,BLOCK_SIZE>>>(d_in + RADIUS,
d_out + RADIUS);

    // Copy result back to host
    cudaMemcpy(out, d_out, size, cudaMemcpyDeviceToHost);

    // Cleanup
    free(in); free(out);
    cudaFree(d_in); cudaFree(d_out);
    return 0;
}
```

parallel fn

serial code

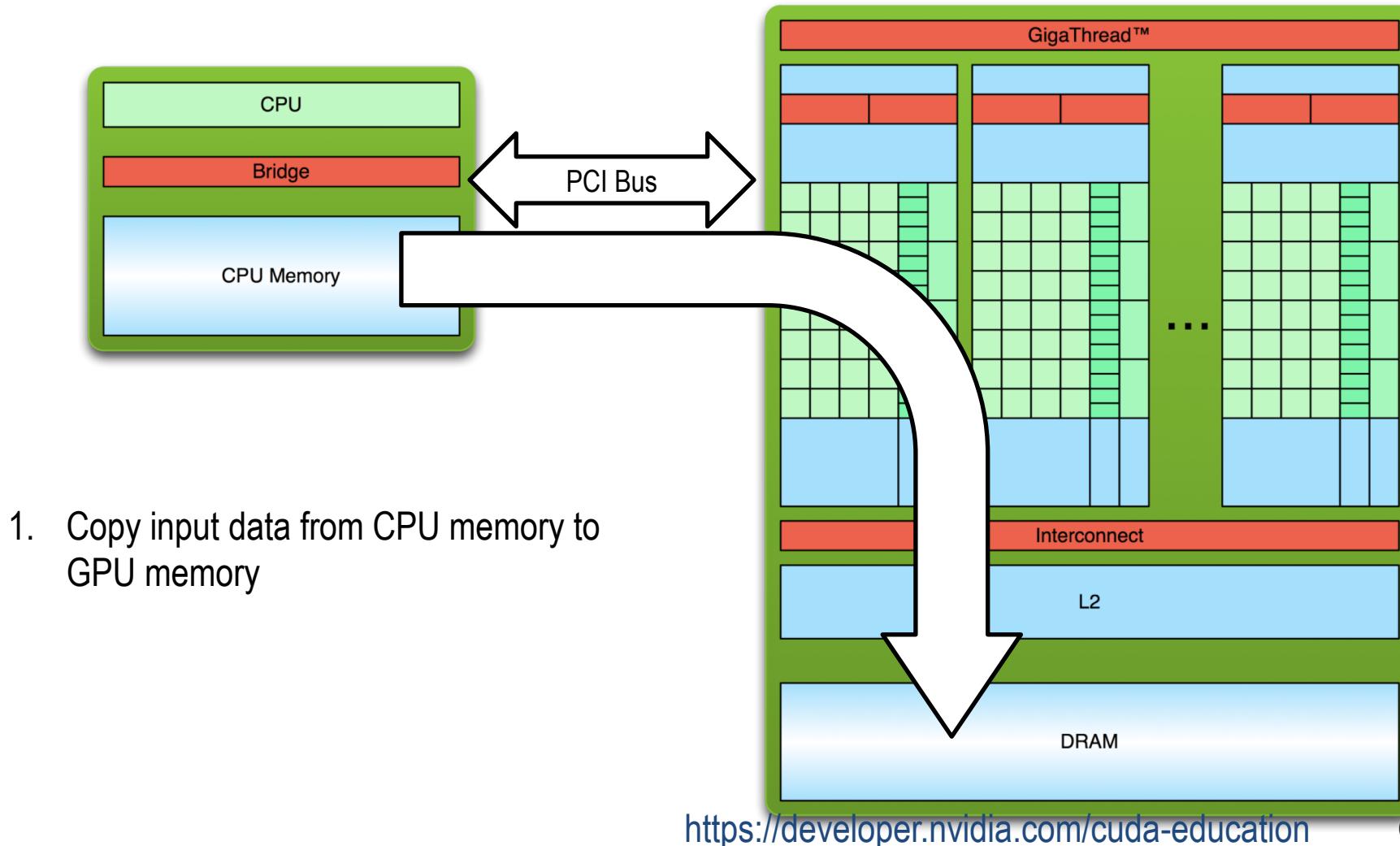
parallel code  
serial code

<https://developer.nvidia.com/cuda-education>

© NVIDIA 2013

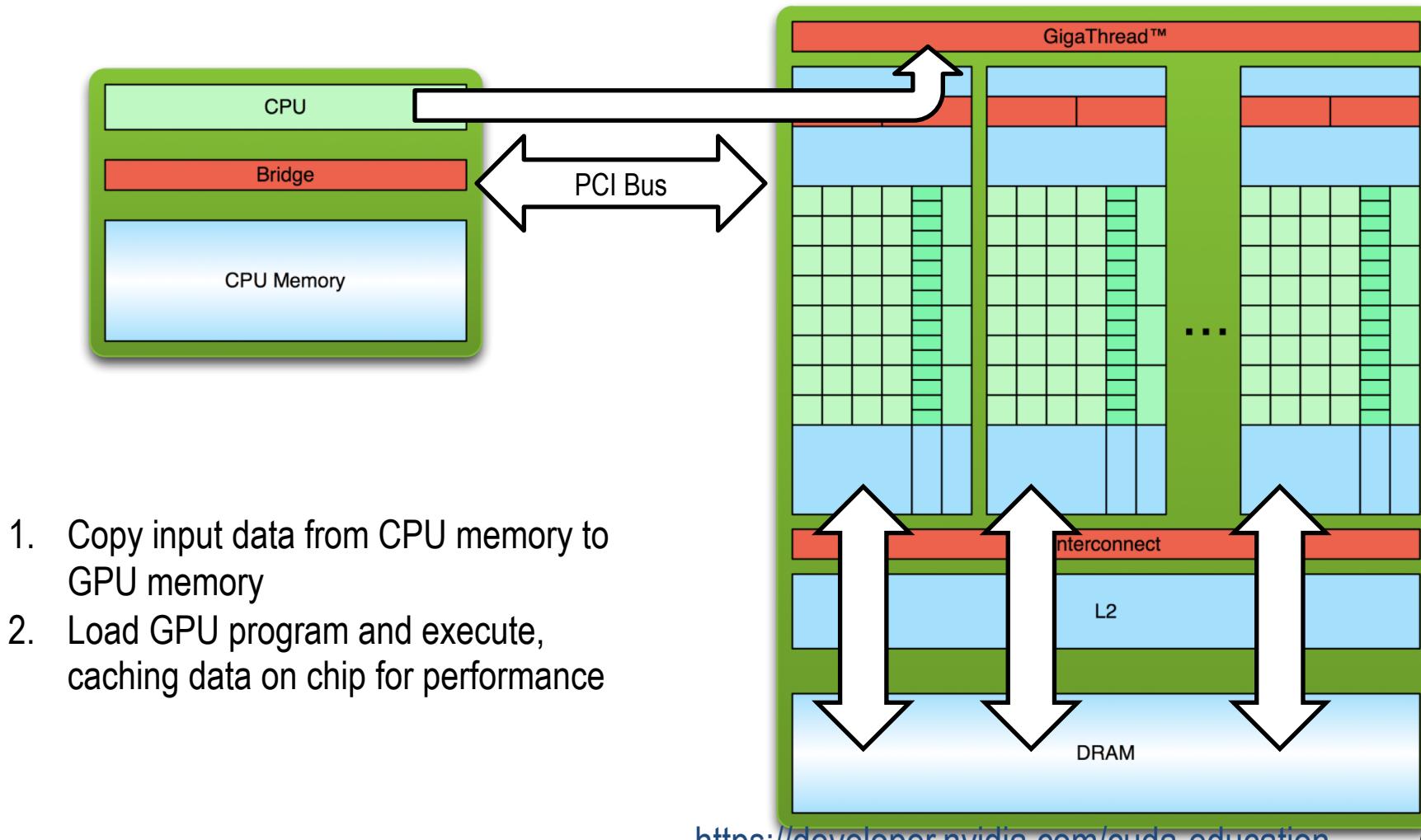


# Simple Processing Flow



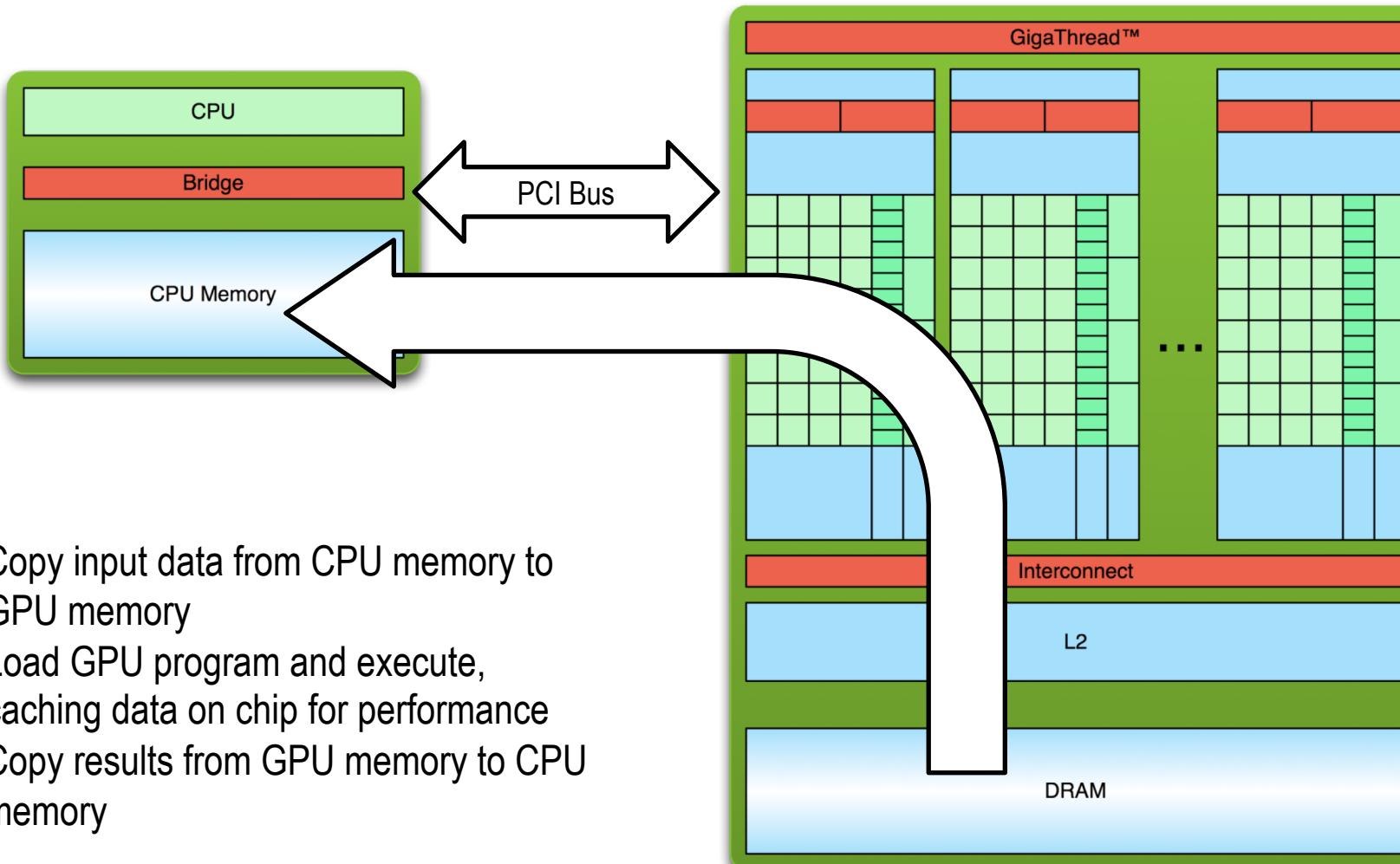
© NVIDIA 2013

# Simple Processing Flow



© NVIDIA 2013

# Simple Processing Flow



© NVIDIA 2013

# NVIDIA CUDA Toolkit

<https://developer.nvidia.com/cuda-toolkit>

## CUDA Toolkit

### Develop, Optimize and Deploy GPU-Accelerated Apps

The NVIDIA® CUDA® Toolkit provides a development environment for creating high performance GPU-accelerated applications. With the CUDA Toolkit, you can develop, optimize, and deploy your applications on GPU-accelerated embedded systems, desktop workstations, enterprise data centers, cloud-based platforms and HPC supercomputers. The toolkit includes GPU-accelerated libraries, debugging and optimization tools, a C/C++ compiler, and a runtime library to build and deploy your application on major architectures including x86, Arm and POWER.

Using built-in capabilities for distributing computations across multi-GPU configurations, scientists and researchers can develop applications that scale from single GPU workstations to cloud installations with thousands of GPUs.

Download Now

# A Quick Comparison between CUDA and C

C

```
void c_hello(){
    printf("Hello World!\n");
}

int main() {
    c_hello();
    return 0;
}
```

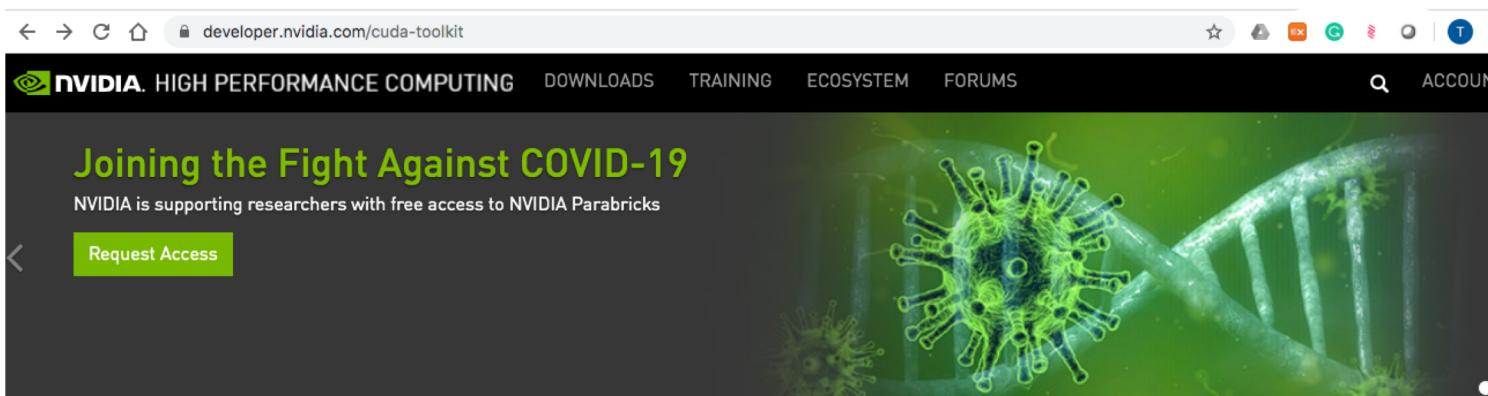
CUDA

```
__global__ void cuda_hello(){
    printf("Hello World from GPU!\n");
}

int main() {
    cuda_hello<<<1,1>>>();
    return 0;
}
```

# CUDA

- <https://developer.nvidia.com/cuda-toolkit>
- <https://devblogs.nvidia.com/even-easier-introduction-cuda/>
- <https://cuda-tutorial.readthedocs.io/en/latest/tutorials/tutorial01/>
- <https://www.nvidia.com/docs/IO/116711/sc11-cuda-c-basics.pdf>



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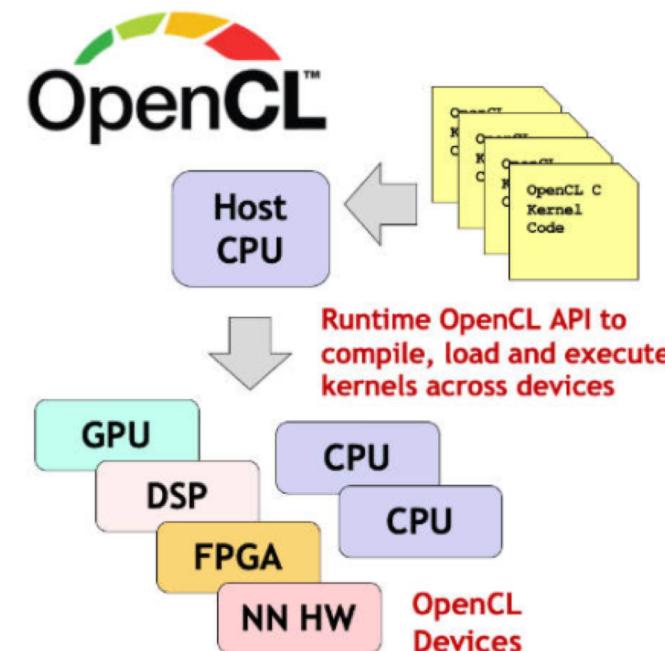
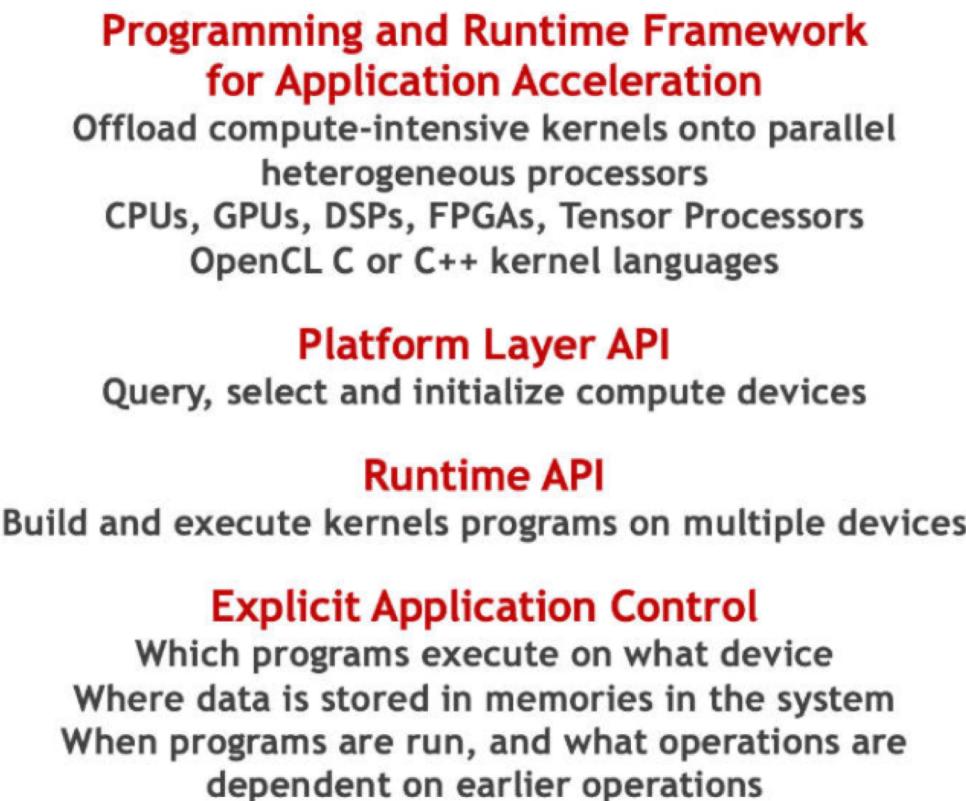
GPU-accelerated CUDA libraries enable drop-in acceleration across multiple domains such as linear algebra, image and video processing, deep learning and graph analytics. For developing custom algorithms, you can use available integrations with commonly used languages and numerical packages as well as well-published development APIs. Your CUDA applications can be deployed across all NVIDIA GPU families available on premise and on GPU instances in the cloud. Using built-in capabilities for distributing computations across multi-GPU configurations, scientists and researchers can develop applications that scale from single GPU workstations to cloud installations with thousands of GPUs.

# OpenCL

- <https://www.khronos.org/opencl/>

## OpenCL for Low-level Parallel Programming

OpenCL speeds applications by offloading their most computationally intensive code onto accelerator processors - or devices. OpenCL developers use C or C++-based kernel languages to code programs that are passed through a device compiler for parallel execution on accelerator devices.



**Complements GPU-only APIs**

- Simpler programming model
- Relatively lightweight run-time
- More language flexibility, e.g., pointers
- Rigorously defined numeric precision

# OpenACC

- <https://www.openacc.org/>

## What is OpenACC?

The OpenACC Organization is dedicated to helping the research and developer community advance science by expanding their accelerated and parallel computing skills. We have 3 areas of focus: participating in computing ecosystem development, providing training and education on programming models, resources and tools, and developing the OpenACC specification.

Get Started

or [take the next steps](#)

```
#pragma acc data copy(A) create(Anew)
while ( error > tol && iter < iter_max ) {
    error = 0.0;
#pragma acc kernels
{
#pragma acc loop independent collapse(2) reduction(max:error)
    for ( int j = 1; j < n-1; j++ ) {
        for ( int i = 1; i < m-1; i++ ) {
            Anew [j] [i] = 0.25 * ( A [j] [i+1] + A [j] [i-1] +
                A [j-1] [i] + A [j+1] [i]);
            error = max ( error, fabs (Anew [j] [i] - A [j] [i]));
        }
    }
    ...
}
```

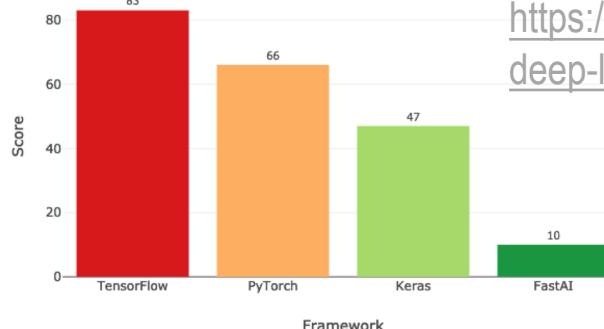
# Popular Deep Learning Framework



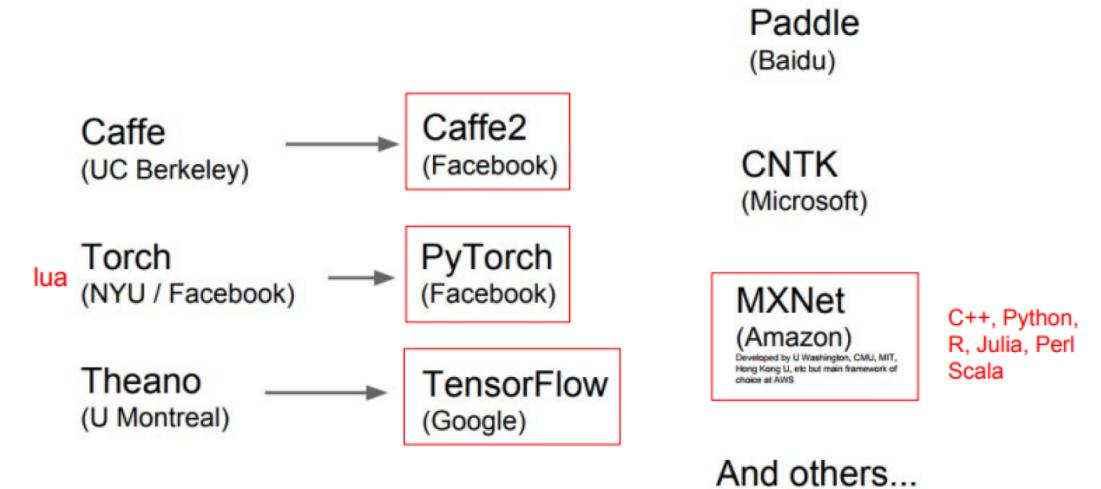
Deep Learning with Fast.Ai



Deep Learning Framework Six-Month Growth Scores 2019

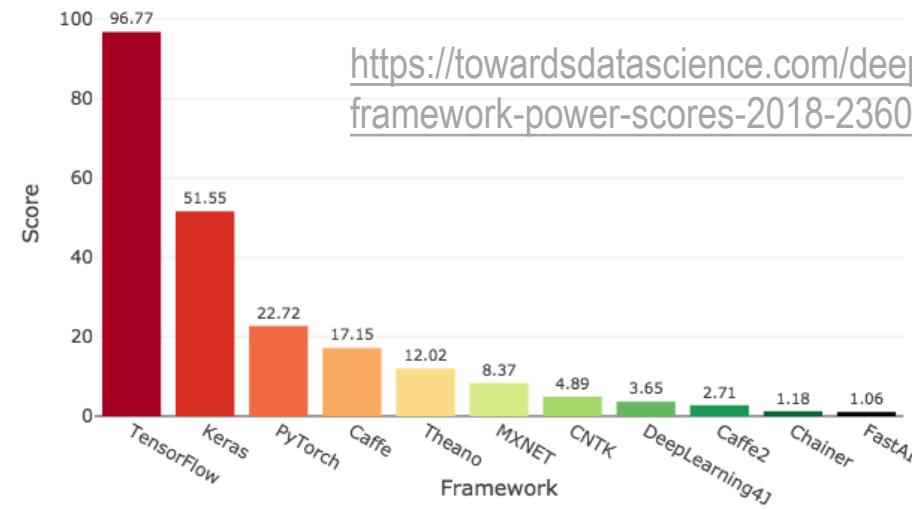


<https://www.kdnuggets.com/2019/05/which-deep-learning-framework-growing-fastest.html>



[https://web.cs.ucdavis.edu/~yjlee/teaching/ecs289g-winter2018/Pytorch\\_Tutorial.pdf](https://web.cs.ucdavis.edu/~yjlee/teaching/ecs289g-winter2018/Pytorch_Tutorial.pdf)

Deep Learning Framework Power Scores 2018



<https://towardsdatascience.com/deep-learning-framework-power-scores-2018-23607ddf297a>

# Machine/Deep Learning + GPU

TensorFlow

Install Learn API Resources Community Why TensorFlow

Search GitHub

## Install

Install TensorFlow

Packages pip Docker

Additional setup **GPU support**

Problems

Build from source Linux / macOS Windows Raspberry Pi

Language bindings Java C Go

Apply to speak at TensorFlow World. Deadline April 23rd. [Propose talk](#)

TensorFlow > Install 

## GPU support

TensorFlow GPU support requires an assortment of drivers and libraries. To simplify installation and avoid library conflicts, we recommend using a [TensorFlow Docker image with GPU support](#) (Linux only). This setup only requires the [NVIDIA® GPU drivers](#).

These install instructions are for the latest release of TensorFlow. See the [tested build configurations](#) for CUDA and cuDNN versions to use with older TensorFlow releases.

## Pip package

See the [pip install guide](#) for available packages, systems requirements, and instructions. To `pip` install a TensorFlow package with GPU support, choose a stable or development package:

```
$ pip install tensorflow-gpu # stable  
$ pip install tf-nightly-gpu # preview
```

Contents

- Pip package
  - TensorFlow 2.0
  - Alpha
- Hardware requirements
- Software requirements
- Linux setup
  - Install CUDA with apt
- Windows setup

- <https://www.amd.com/en/graphics/servers-radeon-instinct-deep-learning>

The screenshot shows the AMD Deep Learning Solutions page. At the top, there's a navigation bar with the AMD logo, menu items for PROCESSORS, GRAPHICS, GAMING, SHOP, and DRIVERS & SUPPORT, and a search bar. Below the navigation is a section titled "Deep Learning Solutions" with a "Share this page" button featuring icons for Facebook, Twitter, Pinterest, Email, and Print. A large, dark banner with a glowing blue network graph in the background contains the text "Unleash Deep Learning Discovery". Below this banner, a navigation menu includes links for OVERVIEW, SOLUTIONS, DEEP LEARNING FRAMEWORKS, and TECHNOLOGIES. A call-to-action box at the bottom left says "Ready-To-Deploy Deep Learning Solutions". On the right side, a sidebar provides information about cookie usage.

AMD

PROCESSORS ▾ GRAPHICS ▾ GAMING ▾ SHOP ▾ DRIVERS & SUPPORT

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Deep Learning Solutions

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# PyTorch + GPU

- <https://pytorch.org/>

The screenshot shows the official PyTorch website. At the top, there is a navigation bar with links: Get Started, Ecosystem, Mobile, Blog, Tutorials, Docs, Resources, GitHub, and a search icon. Below the navigation bar, the main title "FROM RESEARCH TO PRODUCTION" is displayed in large white text against a purple-to-orange gradient background. Underneath the title, a subtitle reads: "An open source machine learning framework that accelerates the path from research prototyping to production deployment." A prominent "Get Started" button is located below the subtitle. At the bottom of the page, there is a black banner containing three news items with arrows for navigation:

- PyTorch 1.5 released, new and updated APIs including C++ frontend API parity with Python.
- PyTorch library updates including new model serving library
- PyTorch 1.4 is now available - adds ability to do fine grain build level customization for PyTorch Mobile, updated domain libraries, and new experimenta...

# PyTorch and PyCUDA

- What is PyTorch?
  - <https://pytorch.org/>
  - Open source machine learning library
  - Developed by Facebook's AI Research lab
  - It leverages the power of GPUs
  - Automatic computation of gradients
  - Makes it easier to test and develop new ideas.
- What is PyCUDA?
  - <https://document.tician.de/pycuda/>
  - Pythonic access to Nvidia's CUDA parallel computation API.
  - Convenience. Abstractions like `pycuda.compiler.SourceModule` and `pycuda.gpuarray.GPUArray` make CUDA programming even more convenient than with Nvidia's C-based runtime.

Again, this course is not a Machine Learning, Deep Learning, or Natural Language Processing. course. If you are interested in ML/DL/NLP, consider to take the course coming soon.

# Multi-GPU Framework Comparison

Train+Val w/ data-loader + data-augmentation on real-data on SSD

DL Library	1xV100/CUDA 9/CuDNN 7	4xV100/CUDA 9/CuDNN 7
Pytorch	27min	10min
Keras(TF)	38min	18min
Tensorflow	33min	22min
Chainer	29min	8min
MXNet(Gluon)	29min	10min

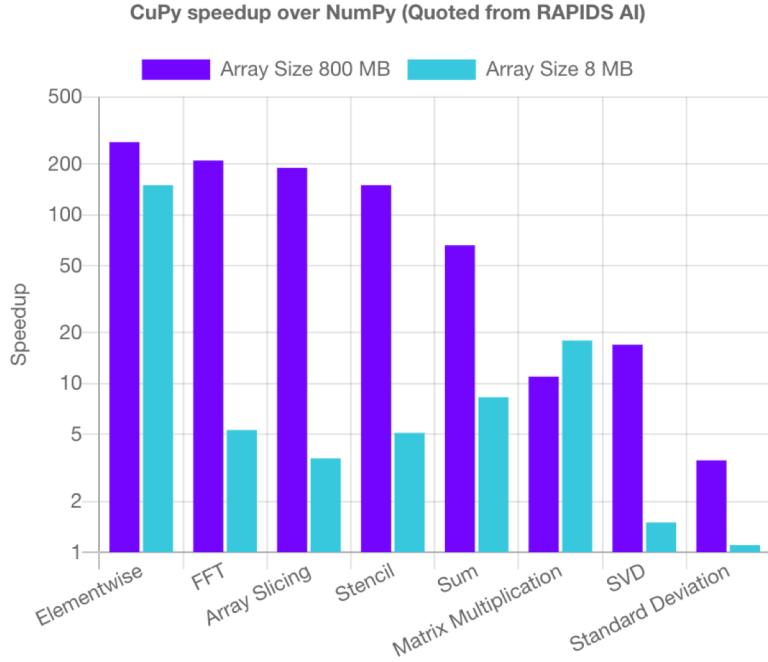
Train w/ synthetic-data in RAM

DL Library	1xV100/CUDA 9/CuDNN 7	4xV100/CUDA 9/CuDNN 7
Pytorch	25min	8min
Keras(TF)	36min	15min
Tensorflow	25min	14min
Chainer	27min	7min
MXNet(Gluon)	28min	8min

<https://medium.com/@iliakarmanov/multi-gpu-rosetta-stone-d4fa96162986>

# Numpy vs CuPy

- <https://cupy.dev/>



## HIGH PERFORMANCE WITH GPU

CuPy is an open-source array library for GPU-accelerated computing with Python. CuPy utilizes CUDA Toolkit libraries including cuBLAS, cuRAND, cuSOLVER, cuSPARSE, cuFFT, cuDNN and NCCL to make full use of the GPU architecture. The figure shows CuPy speedup over NumPy. Most operations perform well on a GPU using CuPy out of the box. CuPy speeds up some operations more than 100X. Read the original benchmark article [Single-GPU CuPy Speedups](#) on the RAPIDS AI Medium blog.



- <https://towardsdatascience.com/heres-how-to-use-cupy-to-make-numpy-700x-faster-4b920dda1f56>

**Here's How to Use CuPy to Make Numpy Over 10X Faster**

# Google Colab

## High-Performance Computing

Summer 2021 at GIST

Tae-Hyuk (Ted) Ahn

Department of Computer Science  
Program of Bioinformatics and Computational Biology  
Saint Louis University



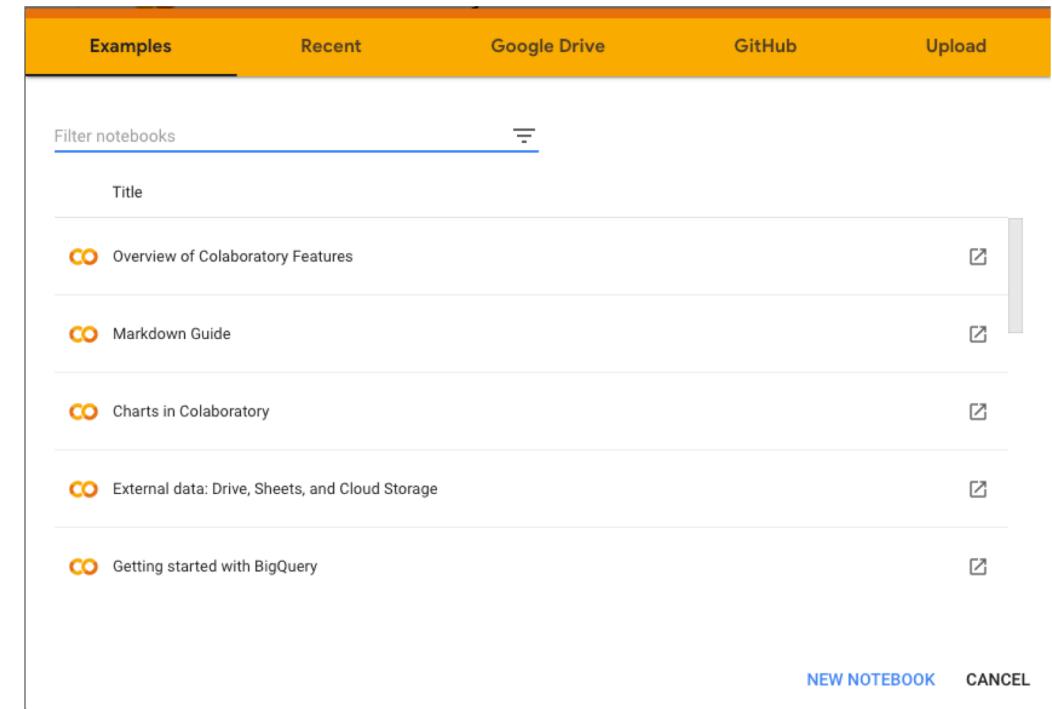
SAINT LOUIS  
UNIVERSITY™

— EST. 1818 —

# Google Colab

Colaboratory, or "Colab" for short, allows you to write and execute Python in your browser, with

- Zero configuration required
- Free access to GPUs
- Easy sharing
- Built on top of Jupyter Notebook
- Google Colab notebooks are stored on the drive



# Google Colab Let's Begin!

## Create a Colab Notebook

- 1. Open Google Colab.
- 2. Click on 'New Notebook'.

OR

1. Open Google Drive.
2. Create a new folder for the project.
3. Click on 'New' > 'More' > 'Colaboratory'.

I have below default Colab Notebooks directory. Check it on your Google Drive and create HPC\_Lab



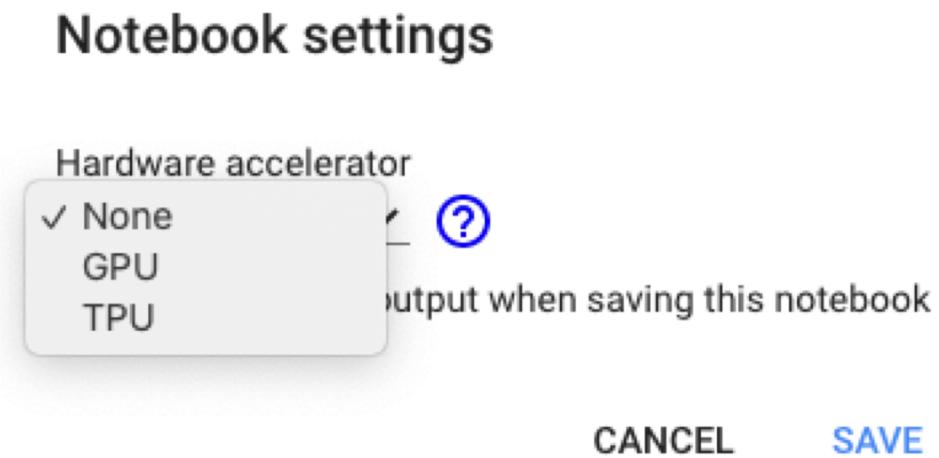
me

Feb 12, 2020

# Setting GPU Accelerator

The default hardware of Google Colab is CPU or it can be GPU.

1. Click on ‘Edit’ > ‘Notebook Settings’ > ‘Hardware Accelerator’ > ‘GPU’.

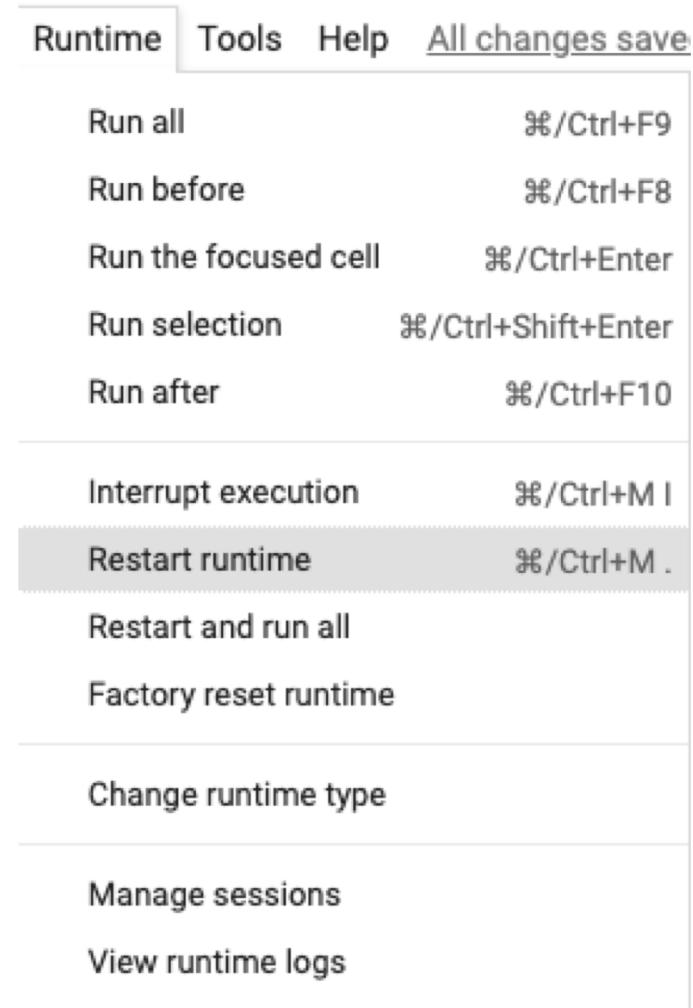


# Running a Cell

- Make sure the runtime is connected. The notebook shows a green check and ‘Connected’ on the top right corner.
- There are various runtime options in ‘Runtime’.

OR

- To run the current cell, press SHIFT + ENTER.



# Running a Cell

- Bash commands can be run by prefixing the command with '!'.

```
[1] !ls
```

```
sample_data
```



```
!ls sample_data/
```

anscombe.json	mnist_test.csv
california_housing_test.csv	mnist_train_small.csv
california_housing_train.csv	README.md

# Connect to your Google Drive

```
1 from google.colab import drive  
2 drive.mount('/content/drive/')
```

- When you run the code above, you should see a result like this:

The screenshot shows a Jupyter Notebook cell with the following code:

```
from google.colab import drive  
drive.mount('/content/drive/')
```

Below the code, there is a message: "Go to this URL in a browser: [https://accounts.google.com/o/oauth2/auth?client\\_id=947318989803-6bn6qk8qdgf4n4g3p](https://accounts.google.com/o/oauth2/auth?client_id=947318989803-6bn6qk8qdgf4n4g3p)".

There is also a text input field labeled "Enter your authorization code:" followed by a redacted text box.

- Click the link, copy verification code and paste it to text box. Then, it will be

```
[5] from google.colab import drive  
drive.mount('/content/drive/')
```

Mounted at /content/drive/

# Connect to your Google Drive

```
[6] !ls
```

```
drive sample_data
```

```
[8] !ls drive/MyDrive/
```

```
22.160P_A_Tilt_FPS26_Live5
23.160M_S_Automotive_Live5
'BCB-5250 Spring 2021 Survey.gform'
Career
'Colab Notebooks'
ColabTest
Commitment
'CSCI-2100 5002 Final Exam Schedule Voting.gform'
'CSCI-4850 5850 HPC Spring 2021 Survey.gform'
EBSCO
Kirmizis_2007_Sir2_wildtype_histone_H3.merge.bw
PersonalDocuments
Research
Software
Teaching
'-$summary.docx'
'Worksheet (1).gform'
Worksheet.gform
```

# Check CPU and RAM specifications



```
!cat /proc/cpuinfo  
!cat /proc/meminfo
```

```
CPU: processor : 0  
      vendor_id : GenuineIntel  
      cpu family : 6  
      model : 63  
      model name : Intel(R) Xeon(R) CPU @ 2.30GHz  
      stepping : 0  
      microcode : 0x1  
      cpu MHz : 2299.998  
      cache size : 46080 KB  
      physical id : 0  
      siblings : 2  
      core id : 0  
      cpu cores : 1  
      apicid : 0  
      initial apicid : 0  
      fpu : yes  
      fpu_exception : yes  
      cpuid level : 13  
      wp : yes  
      flags : fpu vme de pse tsc msr pae mce cx8  
      bugs : cpu_meltdown spectre_v1 spectre_v2  
      bogomips : 4599.99  
      clflush size : 64  
      cache_alignment : 64  
      address sizes : 46 bits physical, 48 bits virtual  
      power management:  
  
processor : 1  
vendor_id : GenuineIntel  
cpu family : 6  
model : 63
```

MemTotal:	13333564 kB
MemFree:	10529740 kB
MemAvailable:	12432924 kB
Buffers:	85436 kB
Cached:	1958172 kB
SwapCached:	0 kB
Active:	1025112 kB
Inactive:	1462468 kB
Active(anon):	409852 kB
Inactive(anon):	360 kB
Active(file):	615260 kB
Inactive(file):	1462108 kB
Unevictable:	0 kB
Mlocked:	0 kB
SwapTotal:	0 kB
SwapFree:	0 kB
Dirty:	372 kB
Writeback:	0 kB
AnonPages:	443960 kB
Mapped:	245996 kB
Shmem:	1012 kB
SLAB:	170772 kB

# Check GPU

```
!nvidia-smi
```

Thu Apr 29 13:36:22 2021

NVIDIA-SMI 465.19.01      Driver Version: 460.32.03      CUDA Version: 11.2							
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	Tesla P4	Off	00000000:00:04.0	Off			0
N/A	39C	P0	23W / 75W	199MiB / 7611MiB	0%	Default	N/A

Processes:

GPU	GI	CI	PID	Type	Process name	GPU Memory
ID						Usage

- <https://developer.nvidia.com/blog/nvidia-tesla-p4-gpus-available-now-on-the-google-cloud-platform/>

# Tesla P4 Specs

- <https://www.nvidia.com/content/dam/en-zz/Solutions/design-visualization/solutions/resources/documents1/Tesla-P4-Product-Brief.pdf>

Table 1. Product Specifications

Specification		Description
Product SKUs		PG414 SKU 200; NVPN: 699-2G414-0200-100 PG414 SKU 201; NVPN: 699-2G414-0201-100
Total board power		PG414 SKU 200: 75 Watts PG414 SKU 201: 50 Watts
GPU SKU		GP104-895-A1
PCI Device ID		0x1BB3
SSID		SKU 200: 0x11D8 SKU 201: 0x11E0
Board ID		0x10DE
NVIDIA® CUDA® cores		2560
GPU clocks	Base	885 MHz
	Maximum boost	1531 MHz (1113 MHz default)
	Idle	405 MHz
VBIOS	EEPROM size	4 Mbit
	UEFI	Supported
PCI Express interface		PCI Express 3.0 ×16 Lane and polarity reversal supported
Weight	Board	240 Grams
	Bracket with screws	9.7 Grams (low-profile bracket) 15.6 Grams (ATX bracket)

Table 2. Memory Specifications

Specification		Description
Memory clocks	Performance	2.8 GHz
	Idle	324 MHz
Memory size		8 GB
Memory bus width		256-bit
Memory configuration		8 pcs 256M × 32 GDDR5
Peak memory bandwidth		Up to 192 GBytes/s

# Need more powerful GPUs on Google Colab?



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### Faster GPUs

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### Longer runtimes

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### More memory

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#### What kinds of GPUs are available in Colab Pro?

With Colab Pro you get priority access to our fastest GPUs. For example, you may get access to T4 and P100 GPUs at times when non-subscribers get K80s. You also get priority access to TPUs. There are still usage limits in Colab Pro, though, and the types of GPUs and TPUs available in Colab Pro may vary over time.

In the free version of Colab there is very limited access to faster GPUs and to TPUs, and usage limits are much lower than they are in Colab Pro.

# Google Colab TPUs

- <https://colab.research.google.com/notebooks/tpu.ipynb>

## TPUs in Colab



In this example, we'll work through training a model to classify images of flowers on Google's lightning-fast Cloud TPUs. Our model will take as input a photo of a flower and return whether it is a daisy, dandelion, rose, sunflower, or tulip.

We use the Keras framework, new to TPUs in TF 2.1.0. Adapted from [this notebook](#) by [Martin Gorner](#).

# Tensorflow with GPU

- <https://colab.research.google.com/notebooks/gpu.ipynb>
- Open <https://colab.research.google.com/notebooks/gpu.ipynb> copy to your Drive and move it to your working directory!
- First, you'll need to enable GPUs for the notebook:
  - Navigate to Edit→Notebook Settings
  - select GPU from the Hardware Accelerator drop-down
- Next, we'll confirm that we can connect to the GPU with tensorflow:

```
%tensorflow_version 2.x
import tensorflow as tf
device_name = tf.test.gpu_device_name()
if device_name != '/device:GPU:0':
    raise SystemError('GPU device not found')
print('Found GPU at: {}'.format(device_name))
```

Found GPU at: /device:GPU:0

# Tensorflow with GPU

- Observe TensorFlow speedup on GPU relative to CPU

```
▶ %tensorflow_version 2.x
import tensorflow as tf
import timeit

device_name = tf.test.gpu_device_name()
if device_name != '/device:GPU:0':
    print(
        '\n\nThis error most likely means that this notebook is not '
        'configured to use a GPU. Change this in Notebook Settings via the '
        'command palette (cmd/ctrl-shift-P) or the Edit menu.\n\n')
    raise SystemError('GPU device not found')

def cpu():
    with tf.device('/cpu:0'):
        random_image_cpu = tf.random.normal((100, 100, 100, 3))
        net_cpu = tf.keras.layers.Conv2D(32, 7)(random_image_cpu)
        return tf.math.reduce_sum(net_cpu)

def gpu():
    with tf.device('/device:GPU:0'):
        random_image_gpu = tf.random.normal((100, 100, 100, 3))
        net_gpu = tf.keras.layers.Conv2D(32, 7)(random_image_gpu)
        return tf.math.reduce_sum(net_gpu)

# We run each op once to warm up; see: https://stackoverflow.com/a/45067900
cpu()
gpu()

# Run the op several times.
print('Time (s) to convolve 32x7x7x3 filter over random 100x100x100x3 images '
      '(batch x height x width x channel). Sum of ten runs.')
print('CPU (s):')
cpu_time = timeit.timeit('cpu()', number=10, setup="from __main__ import cpu")
print(cpu_time)
print('GPU (s):')
gpu_time = timeit.timeit('gpu()', number=10, setup="from __main__ import gpu")
print(gpu_time)
```

Time (s) to convolve 32x7x7x3 filter over random 100x100x100x3 images (batch x height x width x channel). Sum of ten runs.

CPU (s):

3.042170389000006

GPU (s):

0.04080971800001976

GPU speedup over CPU: 74x