

# Software Tools for Machine Learning & Deep Learning

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# Hardware

- CPU
  - Speed (GHz) – General ML
  - # of Cores – Parallel computing
- RAM – General ML
  - Size (GB) – Image Processing
  - Speed (MHz) – Loading speed
- GPU – DL
  - Buffer (Memory) – Crucial: model scale, input/batch size ( $\geq 6\text{GB}$ )
  - CUDA Cores – Speed

## GEFORCE GTX 1080 Ti

GPU Engine Specs:

NVIDIA CUDA® Cores	<b>3584</b>
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Boost Clock (MHz)	<b>1582</b>
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Memory Specs:

Memory Speed	<b>11 Gbps</b>
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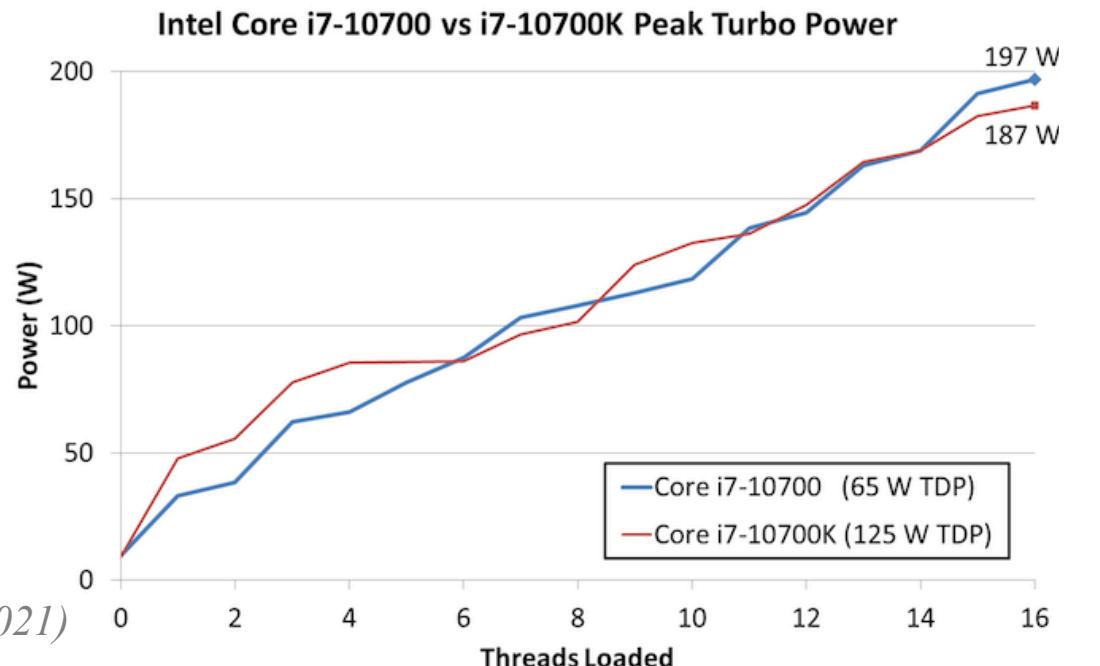
Standard Memory Config	<b>11 GB GDDR5X</b>
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Memory Interface Width	<b>352-bit</b>
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**Out of  
memory (OOM)  
issues**

# Hardware (Cont.)

- Solid-state disk (SSD) – read/write data fast
  - Speed (MB/s)
  - Size (GB) – by needs
  - \*Tips: SSD (512GB) + HDD (2TB)
- Cooling system, power supply
  - Multi-CPU
  - Multi-GPU
  - High-speed RAM/SSD

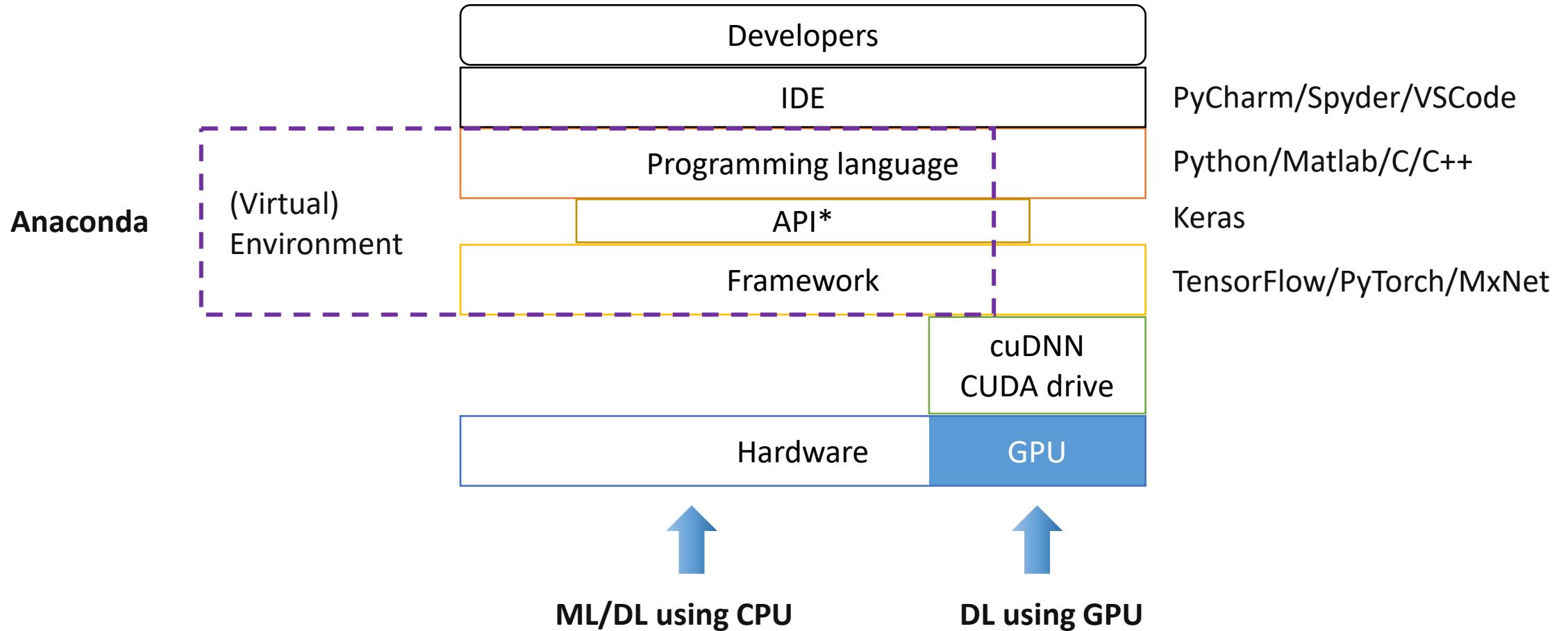


# Hardware: Tips

- Develop/test on PC, running on workstation
  - Smaller input/batch sizes
  - Smaller model scales
  - Smaller loops
  - ...
- HPC at GWU (*discuss details later*)
- Cloud Computing resources
  - AWS
  - Google Cloud
  - ...



# Software overview



# Languages for general ML

- MATLAB
  - **Advantages:** quick to get started and easy to use; visualization; detailed official help documentation; high credibility
  - **Disadvantages:** need to buy; slow official updates; lower flexibility; not many users in the DL field
- Python
  - **Advantages:** free; fast community-based update; higher flexibility; widely used in the NLP/DL field; rich packages
  - **Disadvantages:** difficult to get started; not intuitive enough; mixed help information; may not reliable



# Languages/tools for general ML

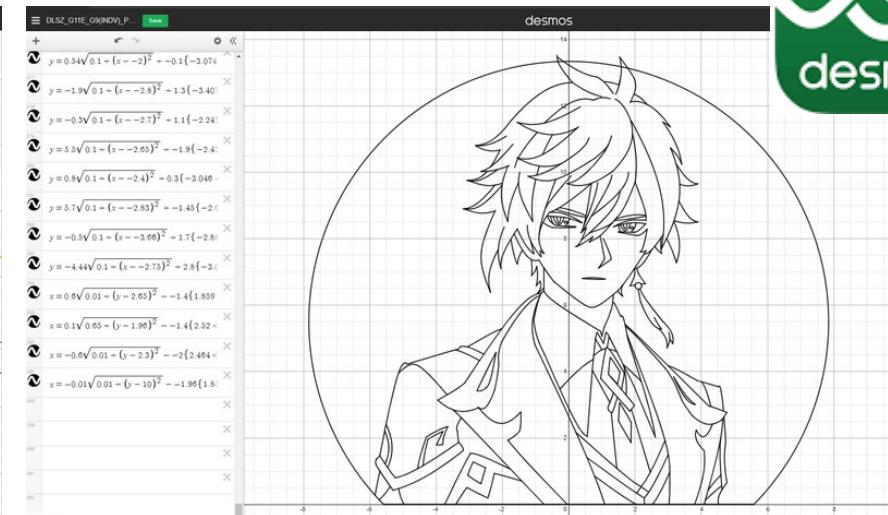
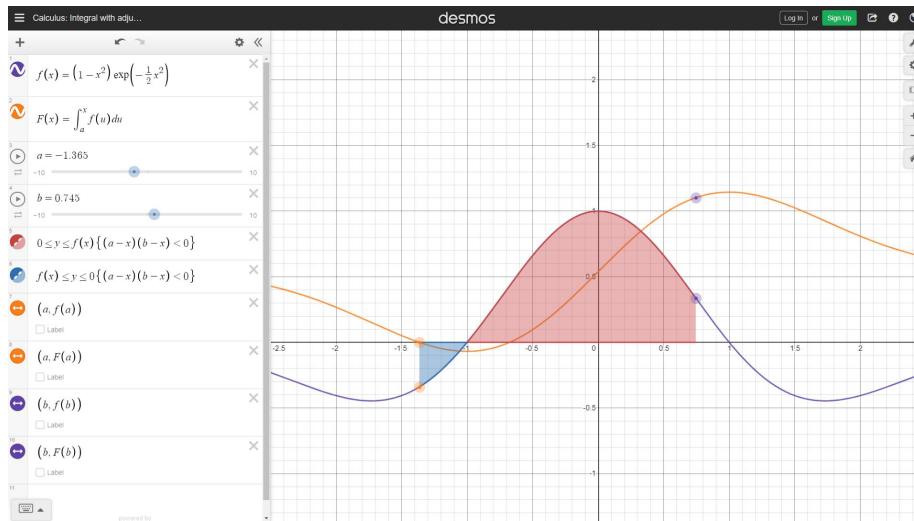
- Other tools
  - **Wolfram Mathematica**: symbolic & numeric computations

```
In[3]:= DSolve[y''[x] + y[x] == Exp[x], y, x]
```

```
Out[3]= \{y \rightarrow Function[\{x\}, c_1 \text{Cos}[x] + c_2 \text{Sin}[x] + \frac{1}{2} e^x (\text{Cos}[x]^2 + \text{Sin}[x]^2)]\}
```



- **Desmos**: graphing calculator, FREE



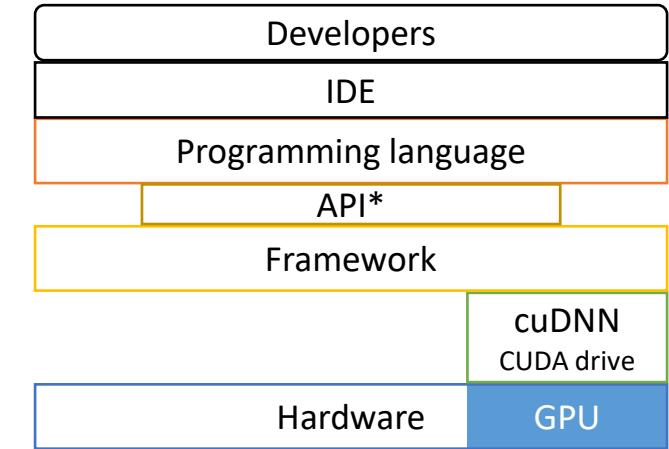
# Tools for DL

## Examples:

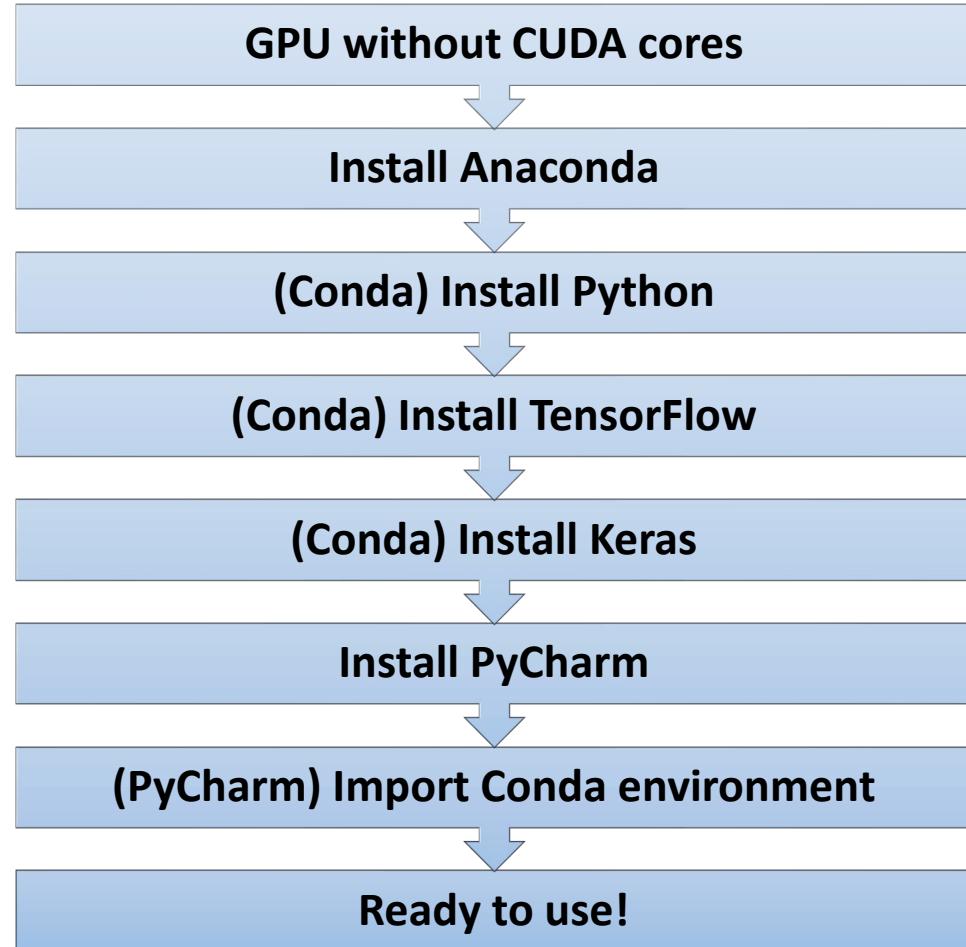
- TensorFlow + Keras + Python + PyCharm
- PyTorch + Python + VSCode/PyCharm

## Recommend: Anaconda

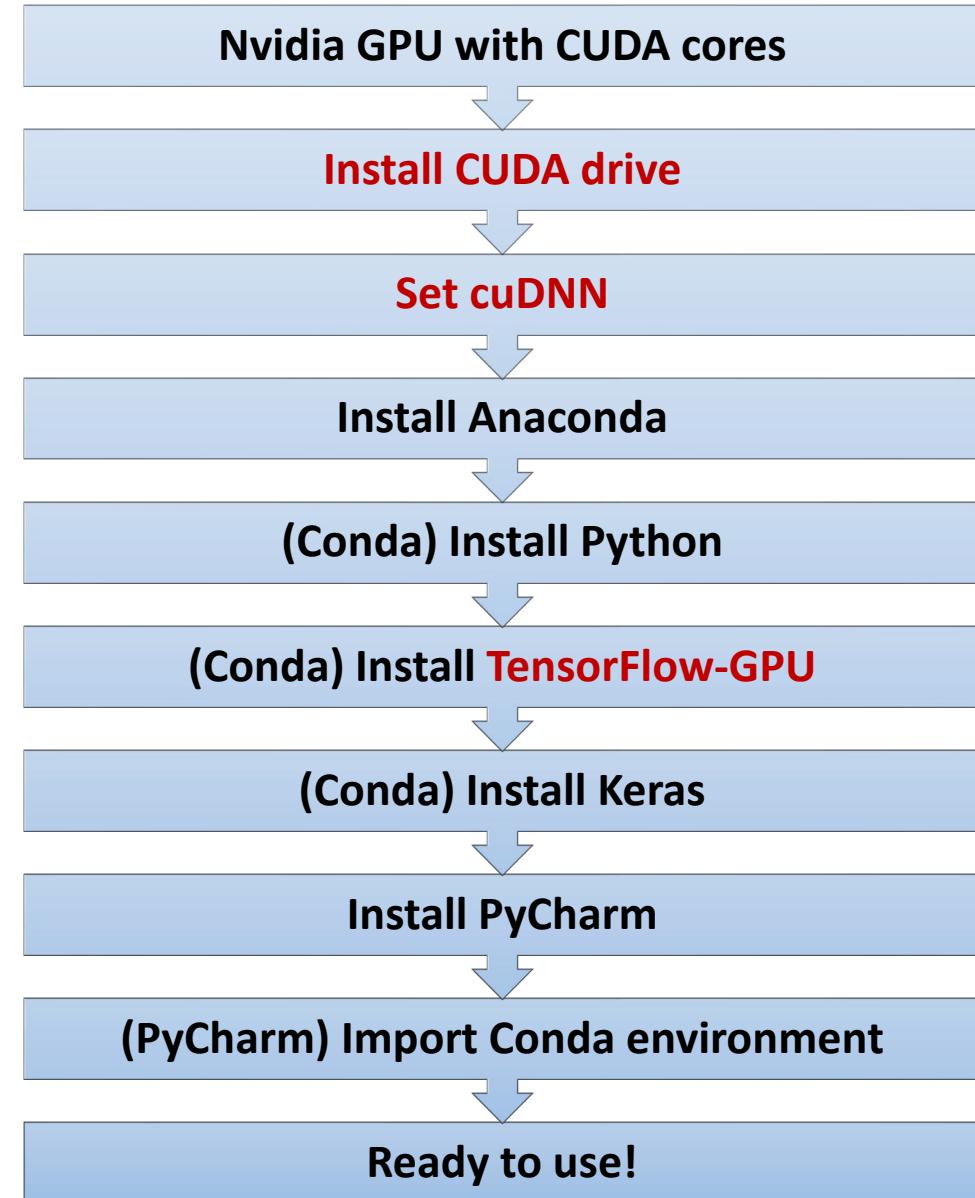
- Virtual environments for development
- Includes/controls: Frameworks + APIs + Languages



# Configuration



DL using CPU



DL using GPU

# Version problems

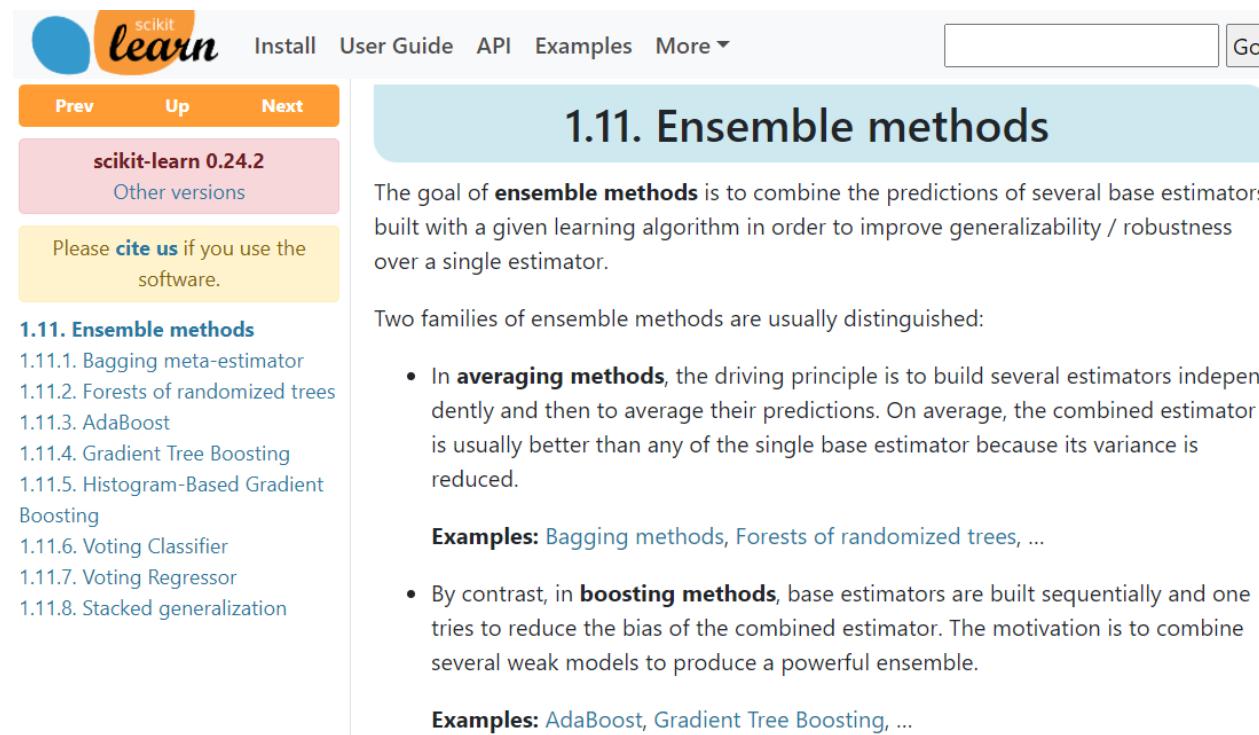
- OS (Win, Linux, macOS)
- CPU/GPU
- CUDA, cuDNN, framework, programming language,...

Version	Python version	cuDNN	CUDA
tensorflow_gpu-2.3.0	3.5-3.8	7.6	10.1
tensorflow_gpu-2.2.0	3.5-3.8	7.6	10.1
tensorflow_gpu-2.1.0	3.5-3.7	7.6	10.1
tensorflow_gpu-2.0.0	3.5-3.7	7.4	10
tensorflow_gpu-1.15.0	3.5-3.7	7.4	10
tensorflow_gpu-1.14.0	3.5-3.7	7.4	10
tensorflow_gpu-1.13.0	3.5-3.7	7.4	10
tensorflow_gpu-1.12.0	3.5-3.6	7	9
tensorflow_gpu-1.11.0	3.5-3.6	7	9
tensorflow_gpu-1.10.0	3.5-3.6	7	9
tensorflow_gpu-1.9.0	3.5-3.6	7	9
tensorflow_gpu-1.8.0	3.5-3.6	7	9
tensorflow_gpu-1.7.0	3.5-3.6	7	9
tensorflow_gpu-1.6.0	3.5-3.6	7	9
tensorflow_gpu-1.5.0	3.5-3.6	7	9
tensorflow_gpu-1.4.0	3.5-3.6	6	8
tensorflow_gpu-1.3.0	3.5-3.6	6	10.8

Windows GPU

# Packages for ML/DL in Python

- **NumPy**: basic functions for math and matrix
- **SciPy**: scientific computing
- **Scikit-learn**: machine learning library
- **Matplotlib**: plotting library
- **OpenCV**: computer vision
- **Pandas**: data manipulation and analysis
- ...



The screenshot shows a section of the scikit-learn documentation titled "1.11. Ensemble methods". The page header includes the scikit-learn logo, navigation links for "Install", "User Guide", "API", "Examples", and "More", and a search bar with a "Go" button. A sidebar on the left lists sub-sections: "1.11. Ensemble methods", "1.11.1. Bagging meta-estimator", "1.11.2. Forests of randomized trees", "1.11.3. AdaBoost", "1.11.4. Gradient Tree Boosting", "1.11.5. Histogram-Based Gradient Boosting", "1.11.6. Voting Classifier", "1.11.7. Voting Regressor", and "1.11.8. Stacked generalization". The main content area starts with a paragraph about ensemble methods: "The goal of **ensemble methods** is to combine the predictions of several base estimators built with a given learning algorithm in order to improve generalizability / robustness over a single estimator." It then describes two families of ensemble methods: averaging methods and boosting methods, each with examples.

**1.11. Ensemble methods**

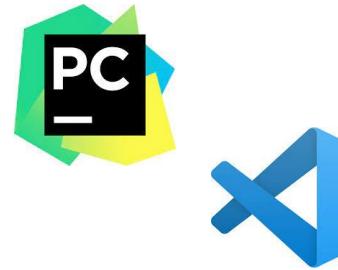
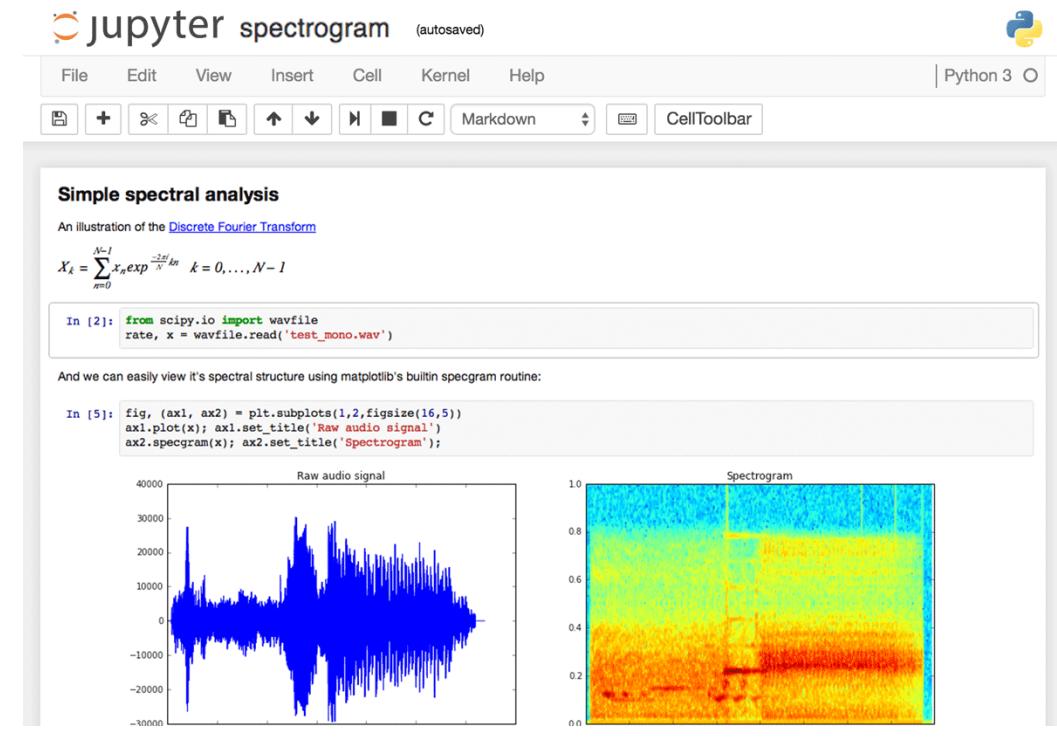
The goal of **ensemble methods** is to combine the predictions of several base estimators built with a given learning algorithm in order to improve generalizability / robustness over a single estimator.

Two families of ensemble methods are usually distinguished:

- In **averaging methods**, the driving principle is to build several estimators independently and then to average their predictions. On average, the combined estimator is usually better than any of the single base estimator because its variance is reduced.  
**Examples:** Bagging methods, Forests of randomized trees, ...
- By contrast, in **boosting methods**, base estimators are built sequentially and one tries to reduce the bias of the combined estimator. The motivation is to combine several weak models to produce a powerful ensemble.  
**Examples:** AdaBoost, Gradient Tree Boosting, ...

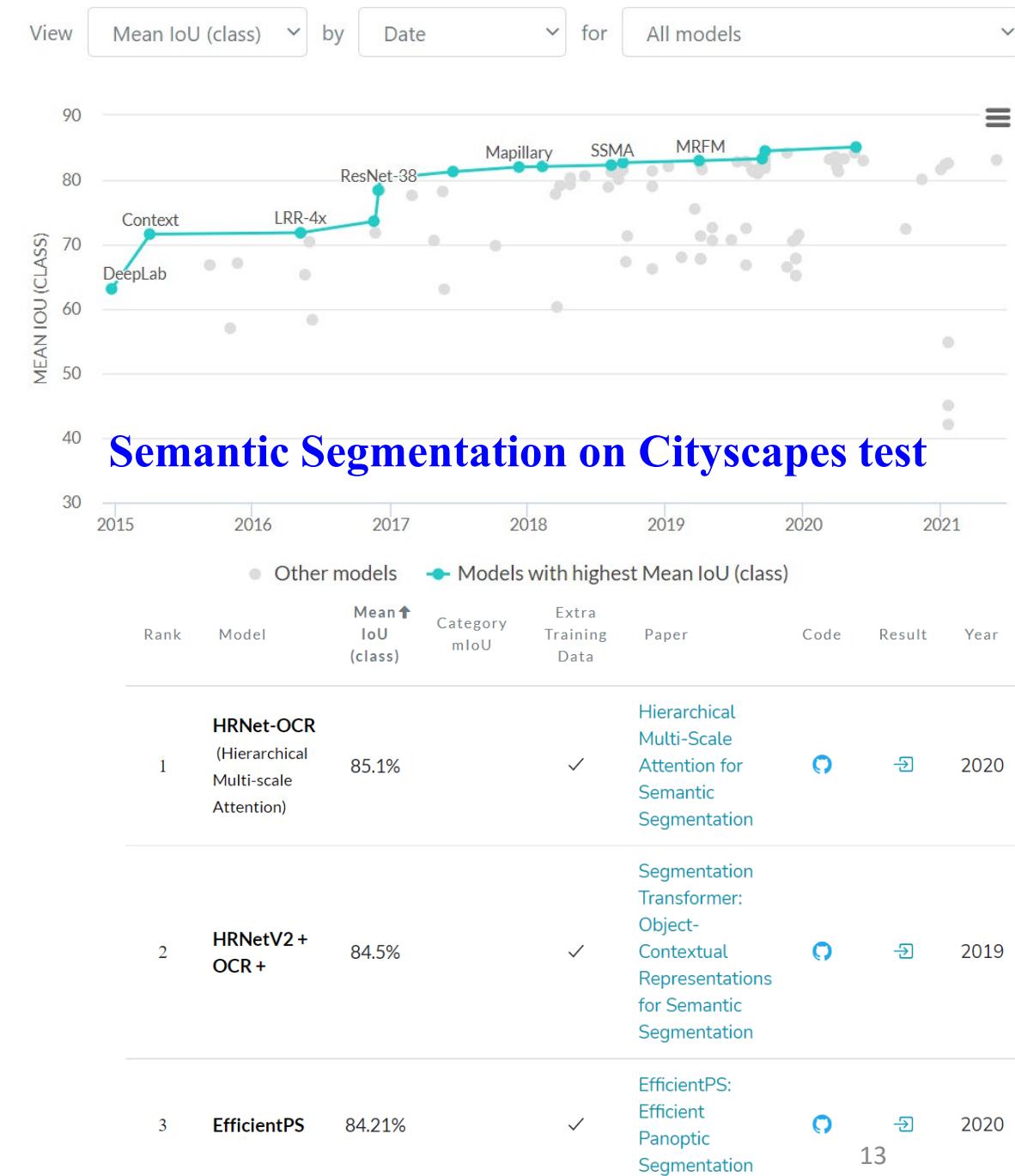
# Integrated development environment (IDE)

- **PyCharm:** comprehensive IDE, for large projects
- **VSCode:** light-weight IDE, support many languages
- **Jupyter Notebook:** interactive IDE, publish friendly
- **Spyder:** MATLAB-like, Anaconda built-in

A screenshot of the Spyder IDE interface. The main area shows Python code for generating data, performing calculations, and plotting. The variable explorer on the right lists variables like 'array\_int8', 'bars', 'df', 'filename', 'list\_test', 'nrows', 'r', 'radil', 'region', 'rgb', 'series', 'text\_none', and 'varible\_explorer'. Below the code editor are two plots: a 3D surface plot of a function over a grid and a polar plot with radial axes from 0 to 90 degrees and angular axes from 0 to 360 degrees. A Python console at the bottom shows some command-line interactions.

# Websites for ML/DL

- Guidebooks of each tools/software online – look-up books
- Github – without reinventing the wheel
- **Stack Overflow** – solve problems
- Kaggle – datasets
- **paperswithcode.com** – SOTA performance ranks with papers & codes
- Google – everything!
- ...



# HPC at GW



- One CPU node
  - Dual 20-Core 3.70GHz Intel Xeon processors
  - 192GB RAM
  - 800 GB SSD
- One GPU node
  - 2 NVIDIA **Tesla V100** GPU (4 for large nodes)
  - Dual 20-Core 3.70GHz Intel Xeon (18-Core Xeon for large nodes)
  - 192GB RAM (384GB for large nodes)
  - 800 GB SSD
- High throughput node, High memory node (3TB RAM!),(...)

**Tesla V100 highlight**

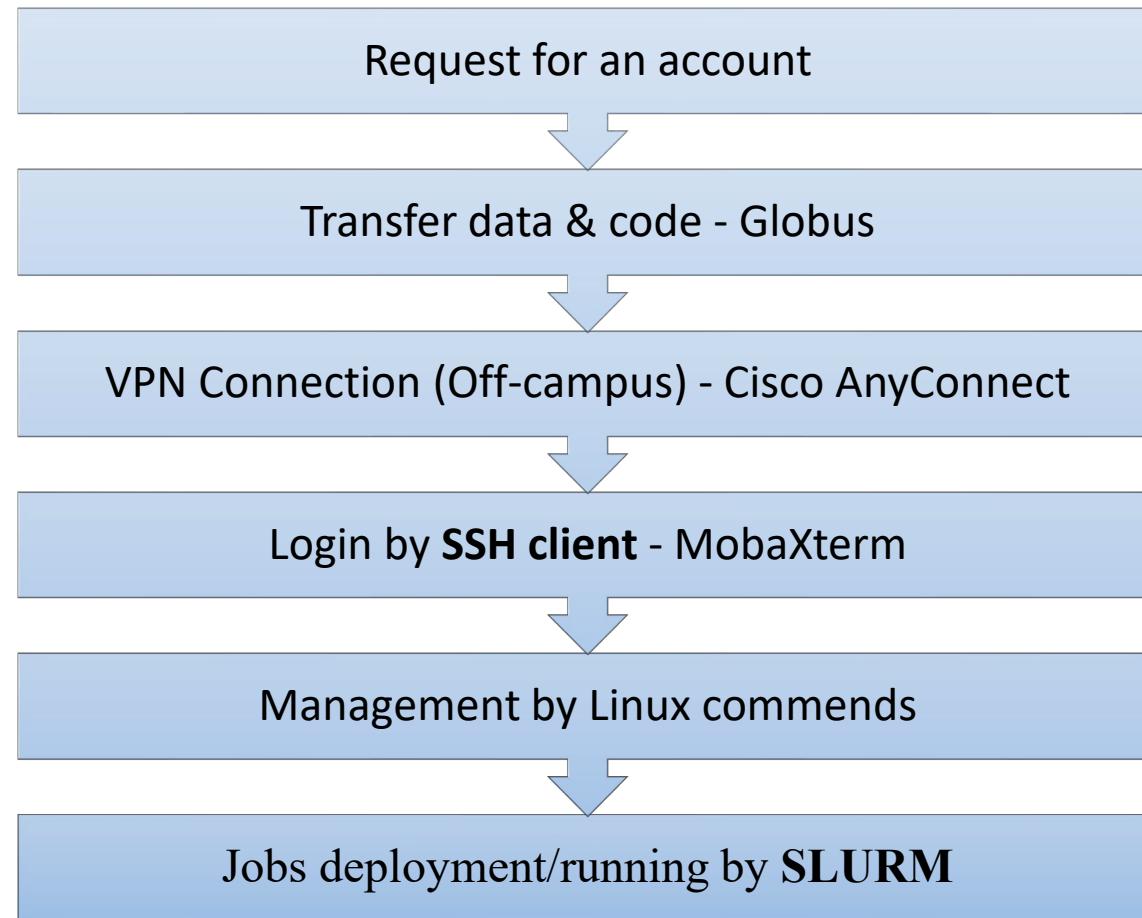
**640 Tensor Cores**

**5120 CUDA Cores**

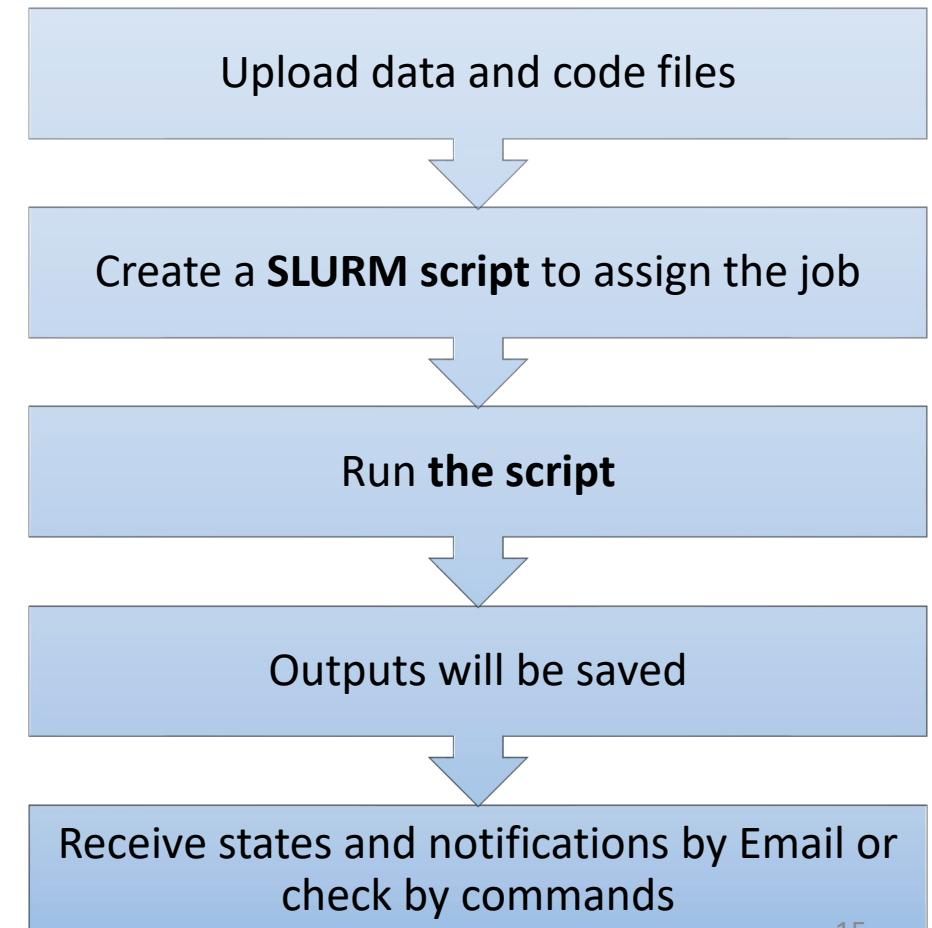
**16 GB Memory**

# How to use the HPC at GW

## Overview



## Workflow



# Epilogue

- The Medical Imaging & Image Analysis Laboratory

**SEH 5290**

W: [loewlab.seas.gwu.edu](http://loewlab.seas.gwu.edu)



- Detailed instruction of GWU HPC

[https://loewlab.seas.gwu.edu/files/2020/11/mia\\_GW\\_HPC\\_intro.pdf](https://loewlab.seas.gwu.edu/files/2020/11/mia_GW_HPC_intro.pdf)