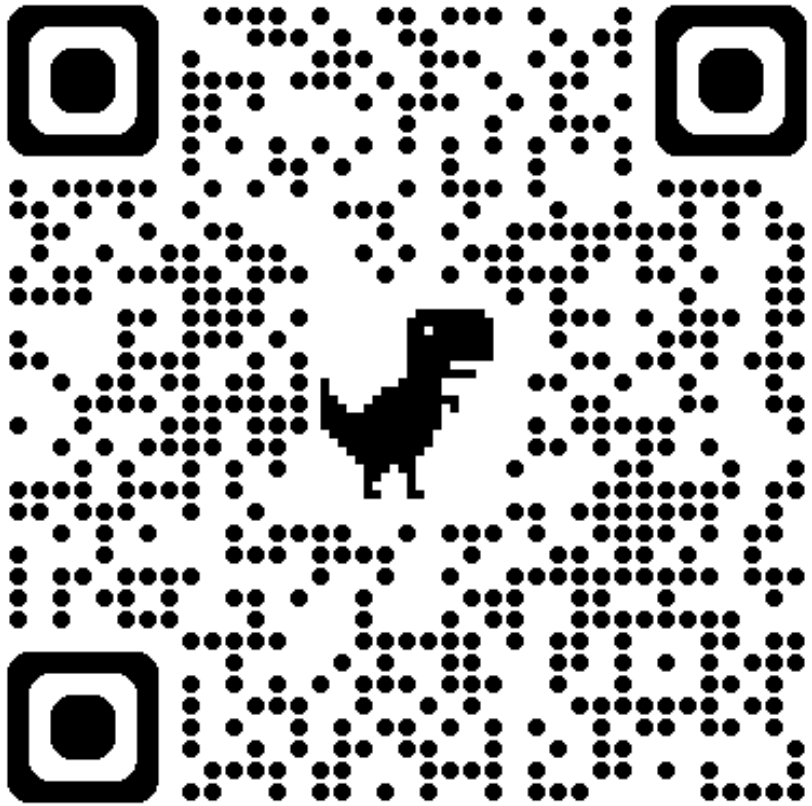
Introduction to GPU Acceleration

View the Slides



https://github.com/ResearchComputing/Intro_GPU_Acceleration

Meet the User Support Team

Layla Freeborn

Brandon Reyes

Andy Monaghan

Michael Schneider

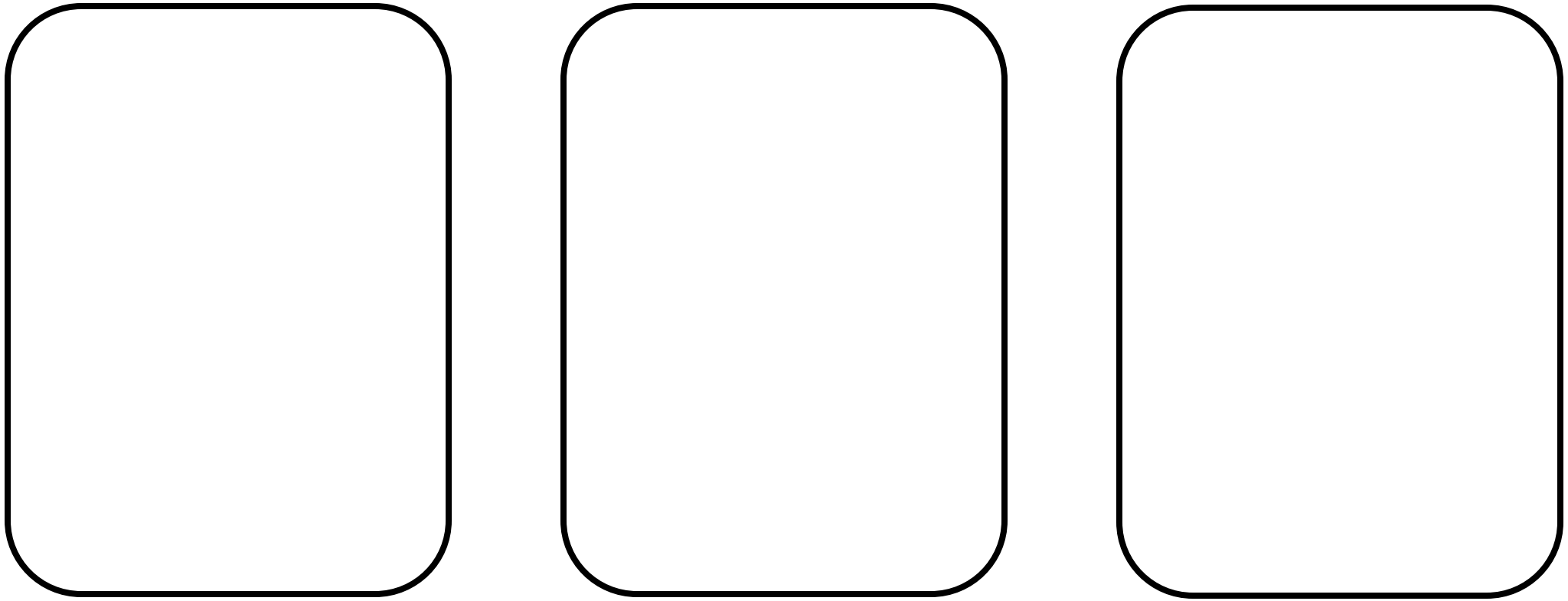
John Reiland

Dylan Gottlieb

Mohal Khandelwal

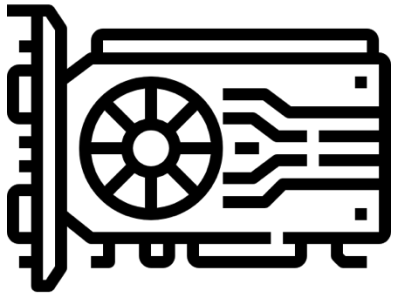
Ragan Lee

Session Overview



GPU Icon

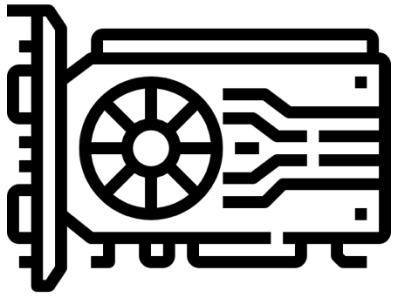
Session Overview



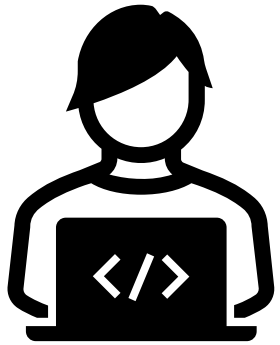
Basics Of GPUs

GPU Icon

Session Overview



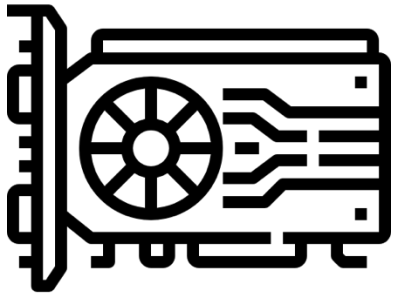
Basics Of GPUs



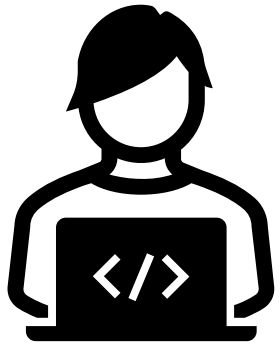
Code Optimization

GPU Icon

Session Overview



Basics Of GPUs

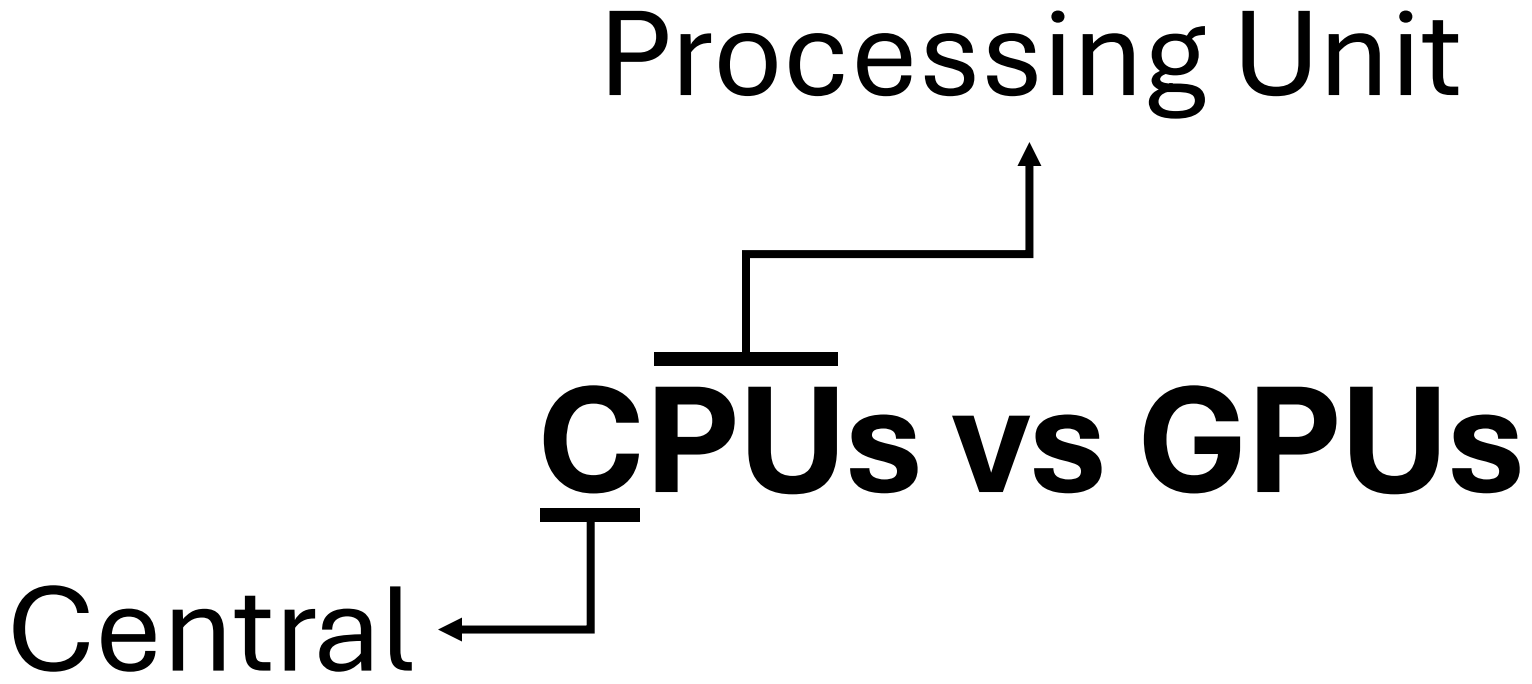


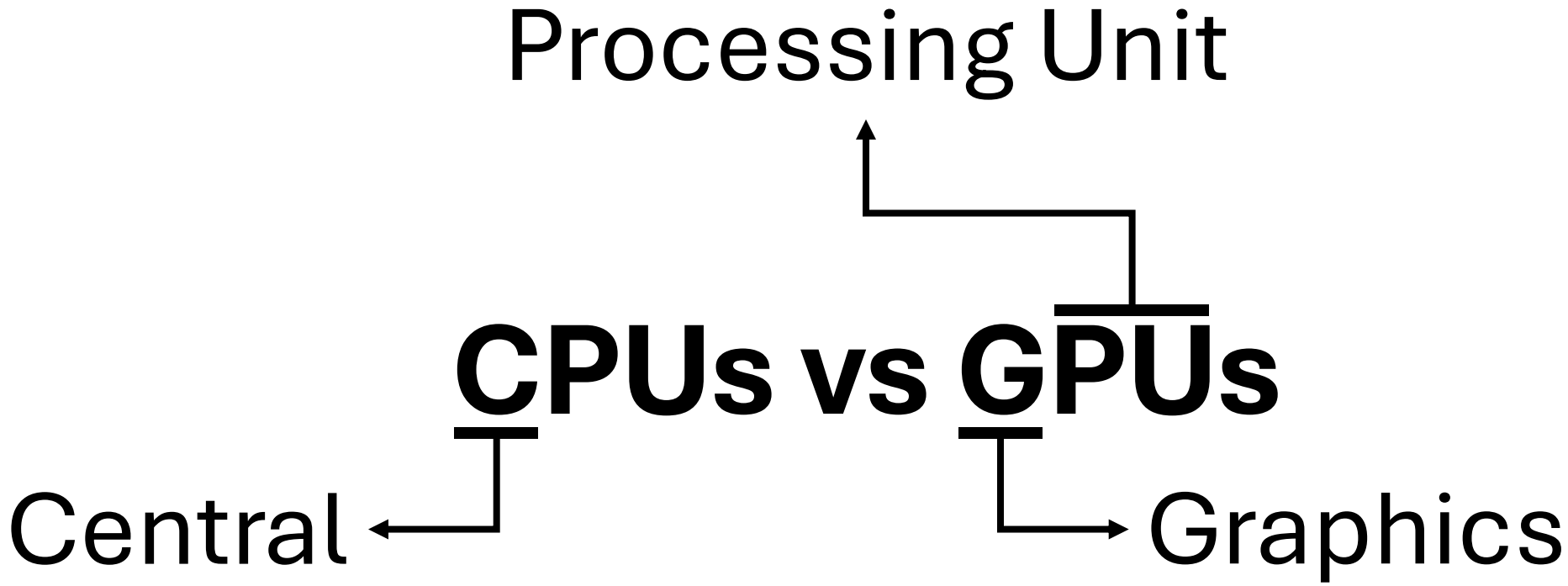
Code Optimization

Monitoring GPU Usage

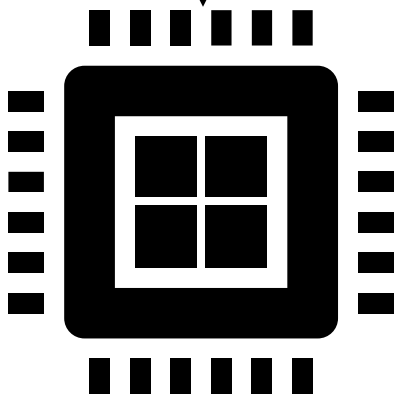
GPU Icon

CPUs vs GPUs


Processing Unit
CPUs vs GPUs
Central


Processing Unit
CPUs vs GPUs
Central
Graphics

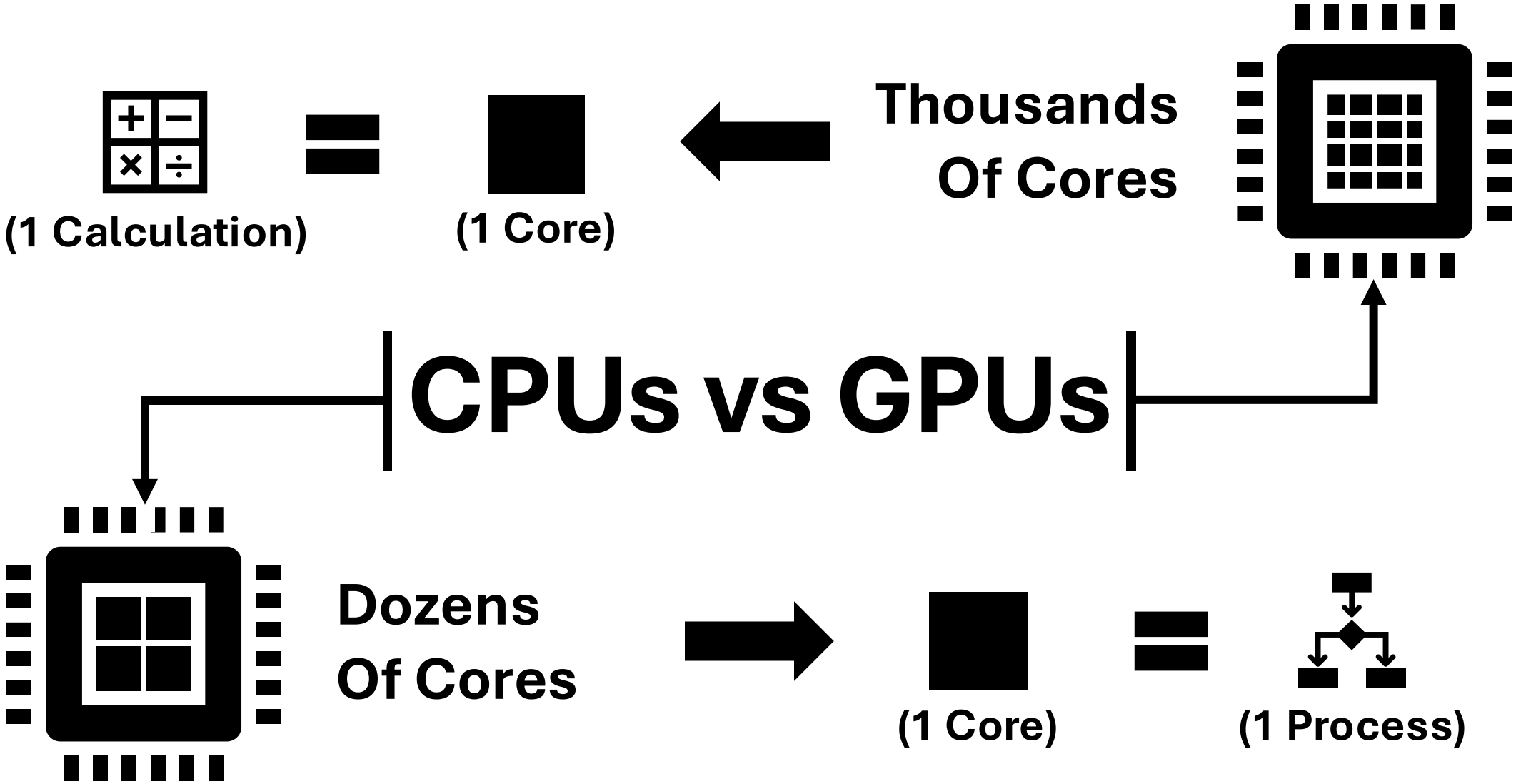
CPUs vs GPUs



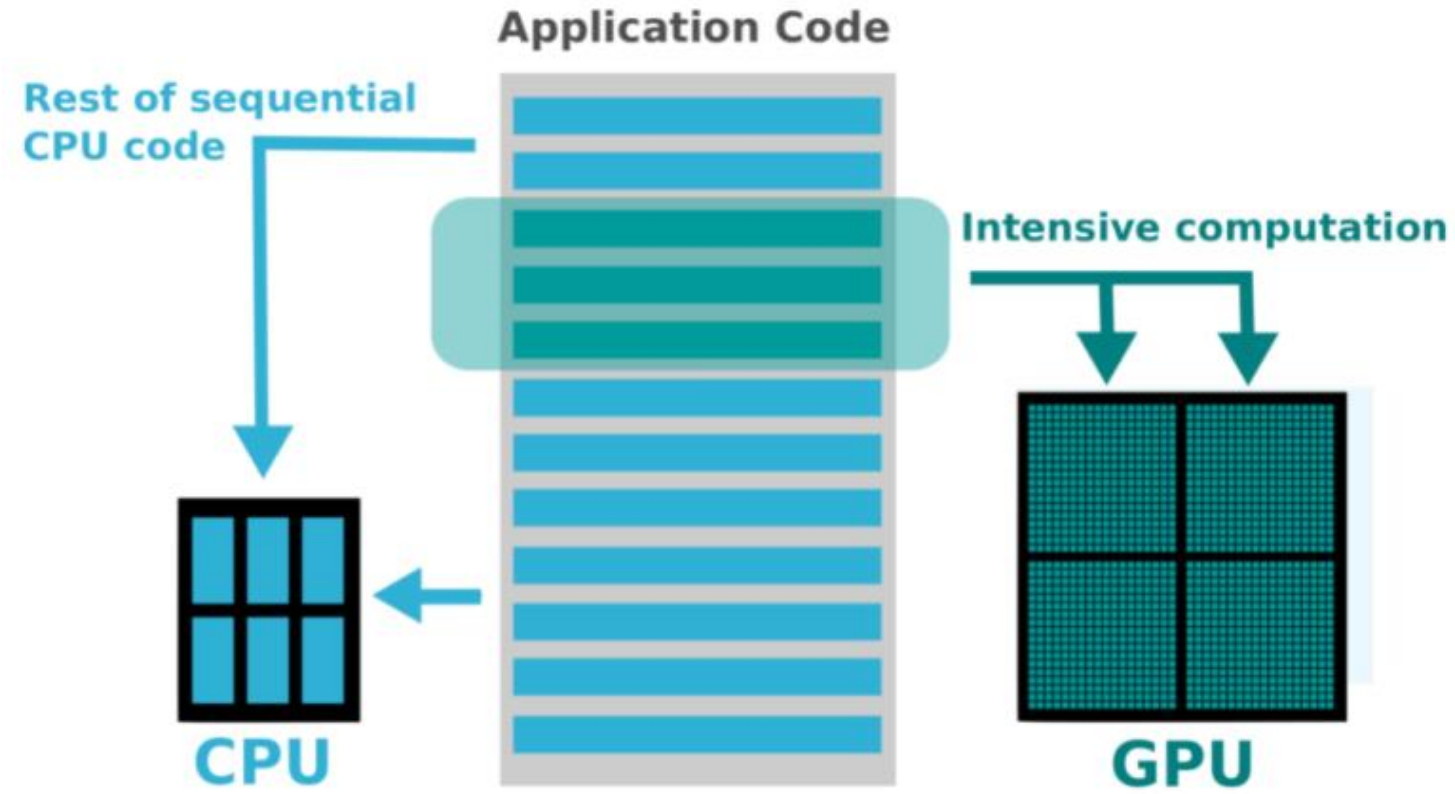
Dozens
Of Cores

(1 Core)

(1 Process)

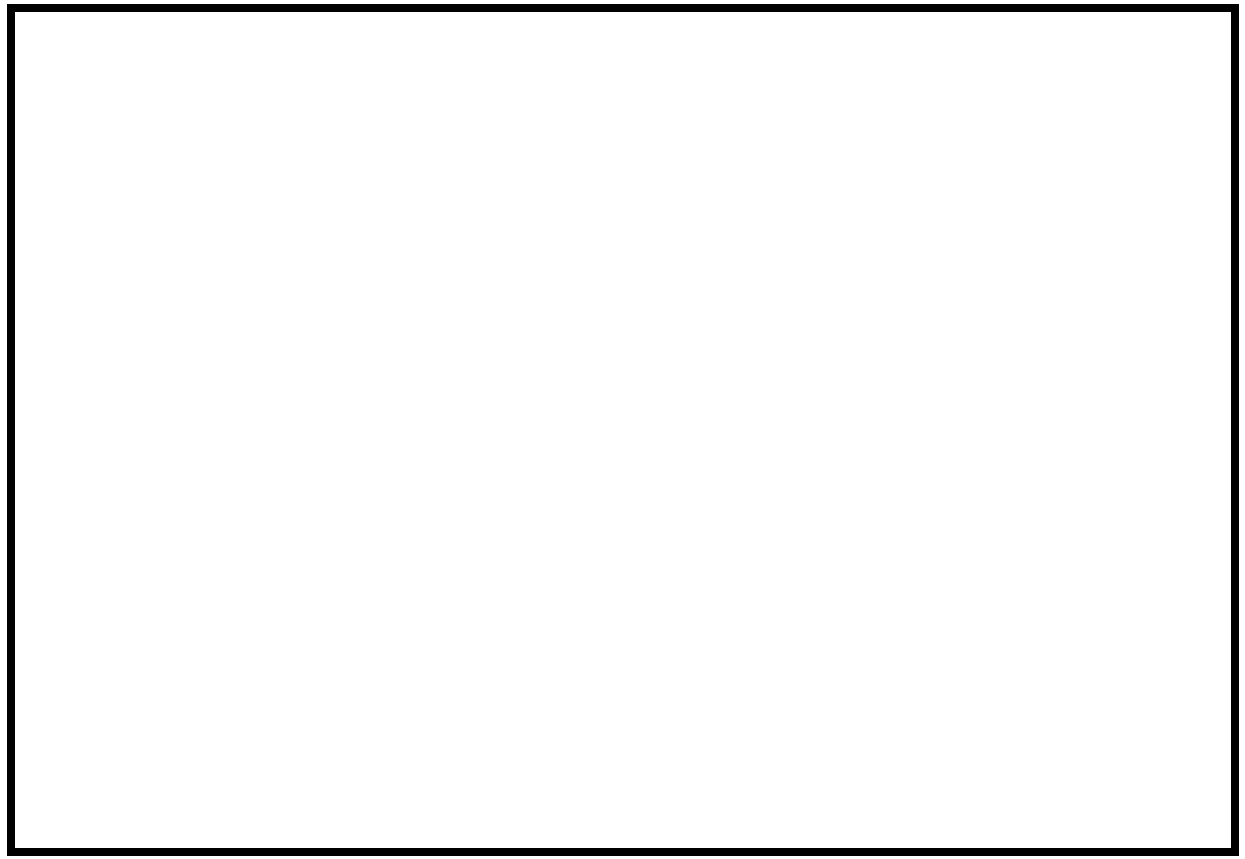

(1 Calculation)
(1 Core)
Thousands
Of Cores
CPUs vs GPUs
Dozens
Of Cores
(1 Core)
(1 Process)

Computational Offloading

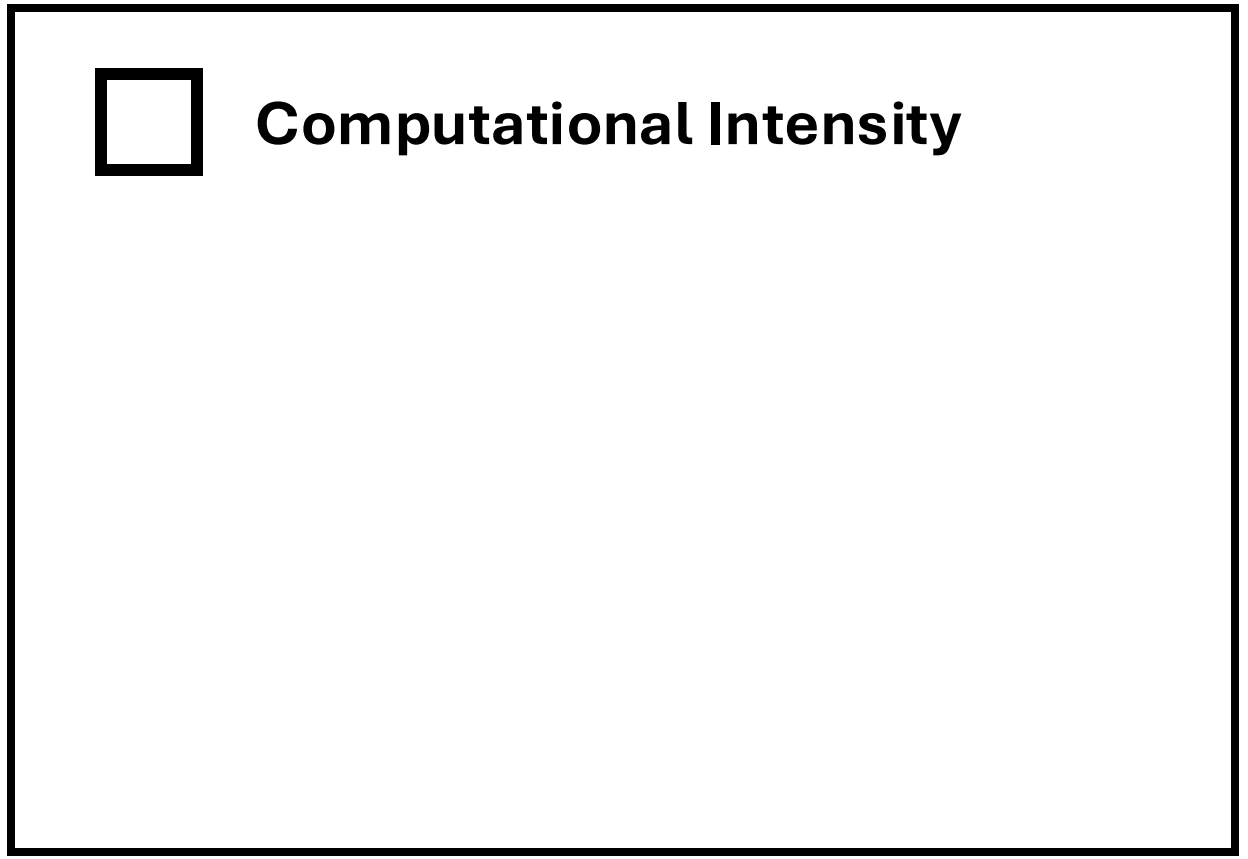


Graphic Source

GPU Acceleration Checklist



GPU Acceleration Checklist



GPU Acceleration Checklist

- ☐ **Computational Intensity**
- ☐ **Algorithmic Complexity**

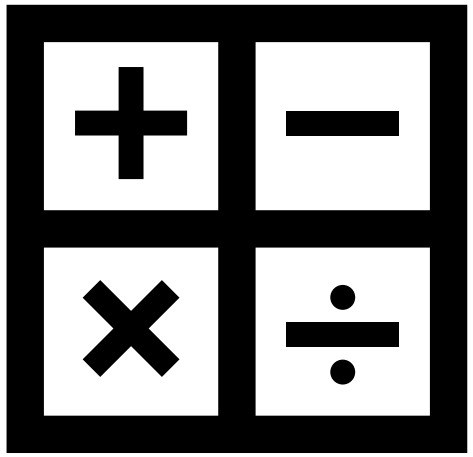
GPU Acceleration Checklist

- [ ] **Computational Intensity**
- [ ] **Algorithmic Complexity**
- [ ] **Data Type**

GPU Acceleration Checklist

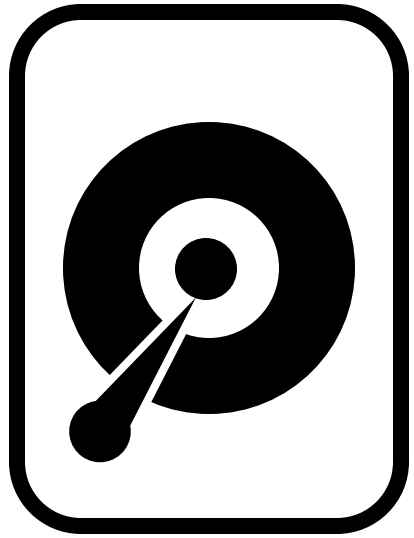
- [ ] **Computational Intensity**
- [ ] **Algorithmic Complexity**
- [ ] **Data Type**
- [ ] **Data Dependency**

Computational Intensity



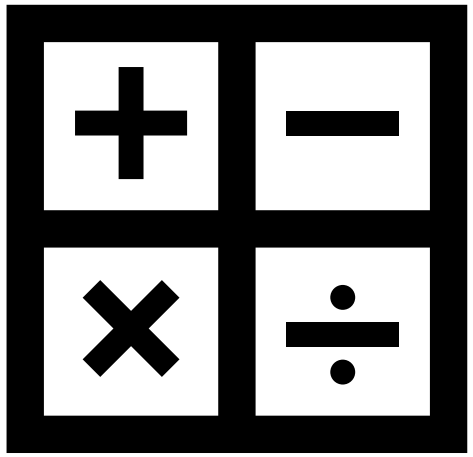
Calculations

VS



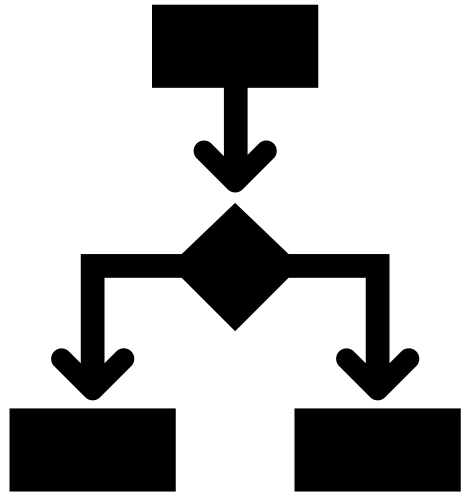
Data Access

Algorithmic Complexity



Calculations

VS



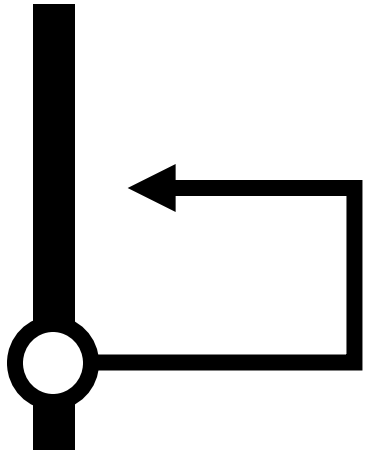
Branching Logic

Data Type

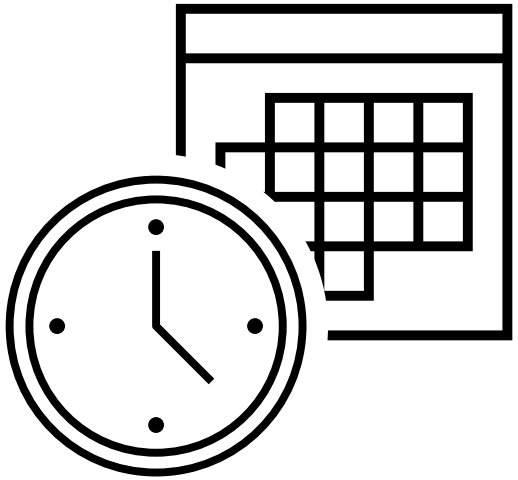
123 vs **“Text”**

Numeric **Complex Objects**

Data Dependency



Recursion



Temporal
Time / Dates

GPU Acceleration Checklist

- [ ] **Computational Intensity**
- [ ] **Algorithmic Complexity**
- [ ] **Data Type**
- [ ] **Data Dependency**

Alpine GPUs

	NVIDIA			AMD
Type	**A100**	**L40**	**GH200**	**MI100**
Cores	**7k**	**15K**	**17k**	**7.7k**
VRAM	**40 / 80**	**48**	**96**	**32**
Purpose	**General**	**Viz, AI Inference**	**AI Training, High Data I/O**	**Scientific**

Alpine GPUs

	NVIDIA			AMD
Type	**A100**	**L40**	**GH200**	**MI100**
Partition	**aa100**	**al40**	**gh200***	**ami100**
Nodes	**40 (8) / 80 (4)**	**3**	**2**	**2**
GPUs Per Node	**3**	**3**	**1**	**3**

Requesting GPUs

SLURM Directives:

--partition= < >

--gres=gpu:<#>

--ntasks=<#>

Requesting GPUs

SLURM Directives:

--partition= < >

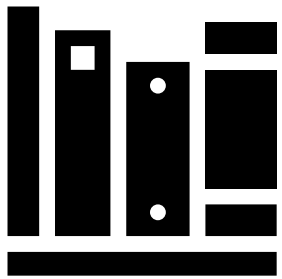
--gres=gpu:<#>

--ntasks=<#>

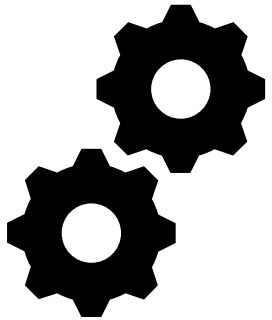
sinteractive --partition=ami100 --gres=gpu:2 --ntasks=20

#SBATCH <directive>

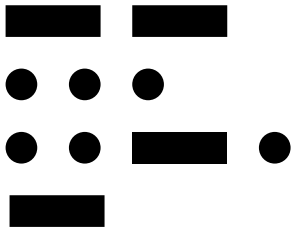
Code Optimization



Libraries



Directives



Languages

GPU Icon

Key Terms

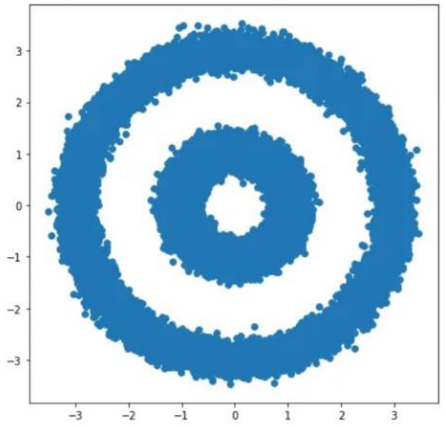
- Host == CPU
- Device == GPU
- Kernel == Functions launched on GPU

GPU Libraries – Drop in Replacement

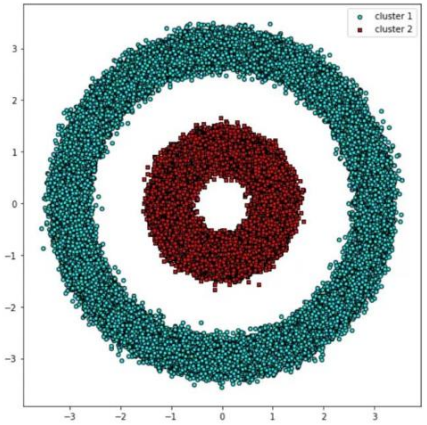
```
#create dataset with 100,000 points
from sklearn.datasets import make_circles
X, y = make_circles(n_samples=int(1e5), factor=.35, noice=.05)

#run DBSCAN clustering algorithm
from sklearn.cluster import DBSCAN
db = DBSCAN(eps=0.6, min_samples=2)
y_db = db.fit_predict(X)
```

Dataset



Clusters



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import pandas as pd
import cudf
X_df = pd.DataFrame({‘fea%d’%i: X[:,i] for i in range(X.shape[1])})
X_gpu = cudf.DataFrame.from_pandas(X_df)

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```

```
#run GPU-accelerated DBSCAN
from cuml import DBSCAN
```

GPU Libraries – Drop in Replacement

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1

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2

```
#run GPU-accelerated DBSCAN
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```

GPU-Enabled Frameworks

GPU Compiler Directives

Basic program structure

```
#include "openacc.h"
#pragma acc <directive>
[clauses [[,] clause]…] new-line
<code>
```

Kernel directives tell the compiler to generate parallel accelerator kernels for the loop nests following the directive.

Data directives tell the compiler to create code that performs specific data movements and provides hints about data usage.

Compile C code for NVIDIA GPU

```
pgcc –acc –ta=nvidia –c your_program_acc.c
```

Compile C++ code for NVIDIA GPU

```
nvcc --acc -Minfo=accel your_program_acc.c
```

Languages

- OpenCL (NVIDIA, AMD, & CPUs)
  - Flexible / portable option
- HIP (AMD -> NVIDIA)
  - AMD developed
  - Can convert CUDA code via `hippify`
- CUDA (NVIDIA only)
  - Most robust and largest developer community

Monitoring GPU Usage

- Nvidia-smi
- rocm-smi

```
+-----------------------------------------------------------------------------+
| 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 A100-PCI...  Off  | 00000000:21:00.0 Off |                    0 |
| N/A   36C    P0    40W / 250W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   1  NVIDIA A100-PCI...  Off  | 00000000:81:00.0 Off |                    0 |
| N/A   36C    P0    40W / 250W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   2  NVIDIA A100-PCI...  Off  | 00000000:E2:00.0 Off |                    0 |
| N/A   37C    P0    40W / 250W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

Troubleshooting GPU Workflows

- Is your application and/or code GPU accelerated?

  Confirm that you installed the GPU accelerated version!

- Does your application or code support **multi-**GPU acceleration?

- Is your application ROCM- or CUDA-aware?

  You can't run CUDA code on AMD GPUs. Not all applications are available for AMD GPUs.

- Can your application "see" the GPU?

- Did you request enough CPUs and RAM?

Documentation

https://curc.readthedocs.io/en/latest/

Survey and feedback

Survey: http://tinyurl.com/curc-survey18