Introduction to GPU Acceleration on Alpine

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Research Computing at CU Boulder

Computing and Data Beyond the Desktop

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- high-speed data transfer
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RMACC Cyber Infrastructure

https://ask.cyberinfrastructure.org/c/rmacc/65

- Provides opportunity for RMACC members to converse amongst themselves and with the larger research computing community
- The "go to" general Q&A platform for the global research computing community - researchers, facilitators, research software engineers, CI engineers, sys admins and others.

Overview

- Intro to Alpine's Heterogeneous Architecture
- Criteria for GPU Acceleration
- Factors Affecting GPU Speedup
- GPU Programming Tools
- Requesting GPUs on Alpine with Slurm
- GPU Monitoring on Alpine
- Hands-on Example: matmul with TensorFlow



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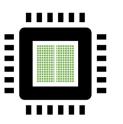
CPUs vs GPUs

Central Processing Unit



- General workhorse
- Contains dozens of cores
- Good for serial processing and handling multiple

Graphics Processing Unit



- Specialized
- Contains thousands of cores
- Good for parallel processing and handling specific tasks quickly

Alpine's Heterogeneous Architecture

A100 GPU



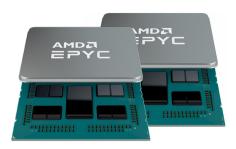
8 nodes x 3 GPUs /node

MI100 GPU



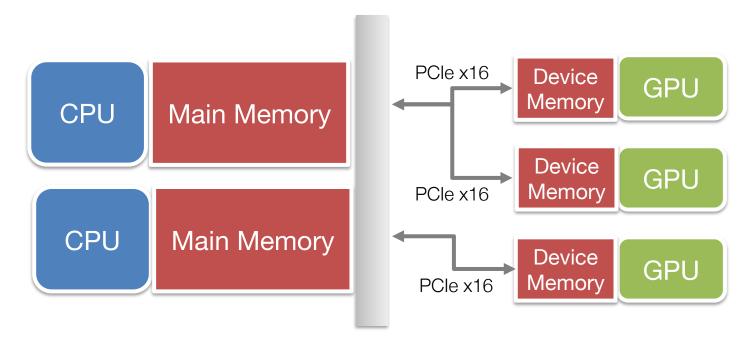
8 nodes x 3 GPUs /node

Milan CPU



64 nodes with64 cores per node

Alpine's Heterogeneous Architecture



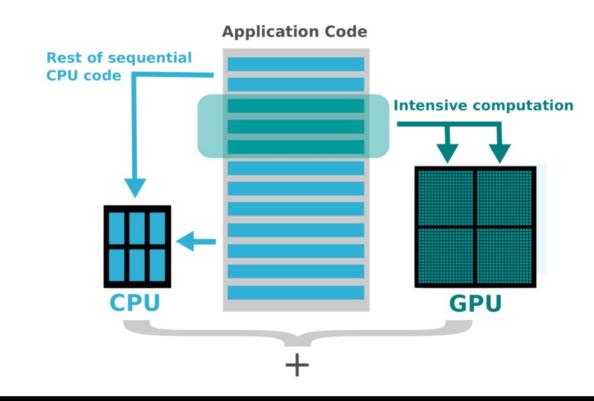
Combines main processors and accelerators, e.g., CPUs and GPUs



GPU-Accelerated Code

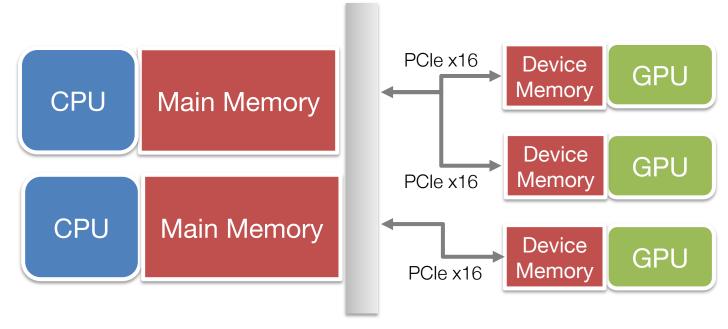
Offloading model

 Increased speed can be achieved by porting computationally intensive parts of code to GPU(s)





GPU-Accelerated Code



Data needs to be copied from CPU to GPU, computation is performed on the GPU, then output is transferred back to CPU.

Get Started on Alpine

Log in:

ssh <username>@login.rc.colorado.edu

Load the Alpine Slurm module:

module load slurm/alpine

Confirm the module is loaded:

module list



Overview

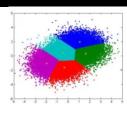
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Criteria for GPU Acceleration

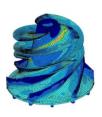
- 1. The time spent on computationally intensive parts of the workflow **exceeds** the time spent transferring data to and from GPU memory
- 2. Computations are massively parallel- the computations can be broken down into hundreds or thousands of independent units of work

- Floating-point operations
- Operations that involve running the exact same code on a huge number of different data points at once.



1. Dense Linear Algebra

vector and matrix operations, e.g. clustering algorithms, K-means



2. Sparse Linear Algebra

matrix multiplication matrices composed mostly of 0s, e.g. finite element analysis



3. Spectral Methods

solving differential equations, e.g. fluid dynamics, quantum mechanics, weather prediction



4. N-Body Methods

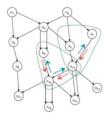
simulation of dynamical system of particles, e.g. astronomy, computational chemistry, physics





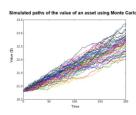
5. Structured Grids

computations that depend on neighbors in an irregular grid, e.g. image processing, physics simulations



6. Unstructured Grids

Grids with different elements that have a different number of neighbors, e.g. computational fluid dynamics



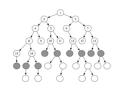
7. Map-Reduce & Monte Carlo

Each process runs completely independent from one another, e.g. Monte-Carlo, Distributed Searching

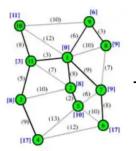


8. Combinational Logic

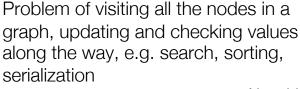
Usually involve performing simple operations on large amounts of data, e.g. hashing, encryption, checksums



9. Graph Traversal



10. Dynamic Programming

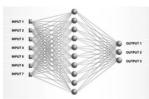


Algorithmic technique to compute solutions by solving overlapping subproblems, e.g. graph problems, sequence alignment



11. Backtracking

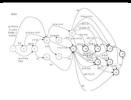
Build all possible solutions, usually branch-and-bound solution approach, e.g. puzzles, traveling salesman



12. Probabilistic Graphical Models

e.g. Bayesian networks, hidden Markov models, neural networks





13. Finite State Machines

Mathematical model of computation used to design computer programs and sequential logic circuits, e.g. data mining, video compression

Further Reading

- Geng et al. OpenCL and the 13 dwarfs: a work in progress
- Asanovic et al. The landscape of parallel computing research: A view from Berkeley
- Vincent Hindriksen's blog post The 13 application areas where OpenCL and CUDA can be used



Poll

What statement best describes your experience with GPU Acceleration?

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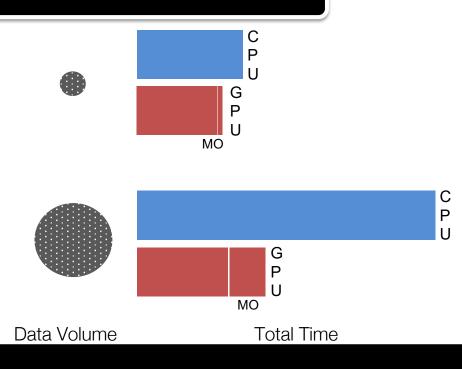


- 1 Data Volume
- 2 Data Dependency
- 3 Data Processing Order
- 4 Data Type
- 5 Code/Algorithmic Complexity
- 6 Computational Intensity



1 Data Volume

 The time spent transferring data to/from CPU to GPU is worthwhile for high data volumes





2 Data Dependency

- Processing a data point depends on previous data points.
 - This should be avoided!

```
for (i=1; i<1000; i++){
    sum = sum + a[i]; /* S1 */
}
```

```
for (i=1; i<1000; i++){
    a[i] = 2 + a[i]; /* S1 */
}
```



3 Data Processing Order

- Data should be written and read in a continuous order for maximum utilization of a GPU.
 - May require adjustments to algorithm

4 Data Type

- Operations on strings are slow unless they can be treated as numbers.
- Performance per GPU can vary quite a bit if workflows include 16-bit and 64-bit floats.

5 Code/Algorithmic Complexity

- 'Simple' code is better ported to GPUs
 - Deeply branched code and while-loops perform poorly on GPUs
 - Recursive functions need rewriting



6 Computational Intensity

 GPUs perform best when there is a lot of processing compared to loading and storing data (FLOP per Byte ratio)





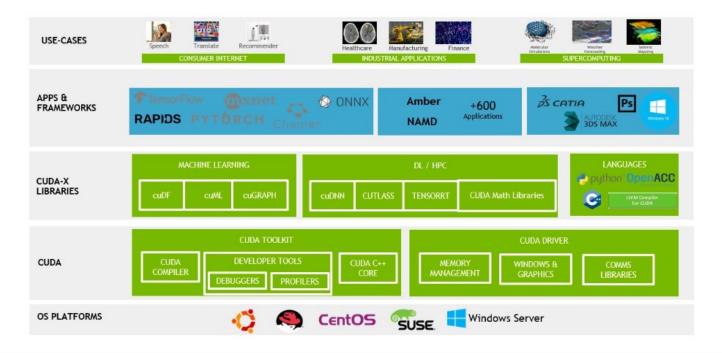
Performance increases from GPUs depend on several factors related to the data and algorithm.

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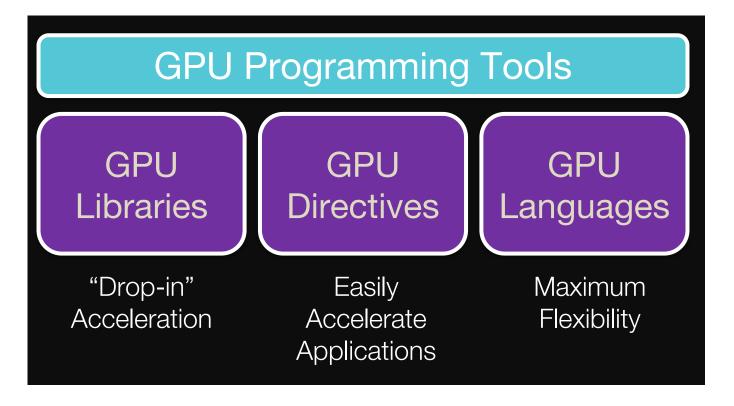


CUDA - a parallel computing platform and programming model





More than CUDA!





GPU Libraries

- Require little understanding of GPU hardware
- Usually involve minor changes to code
- Accelerated versions of many scientific libraries are available, e.g.
 - LAPACK → MAGMA, libFLAME
 - BLAS → cuBLAS, clBLAS
 - NumPy & SciPy → cuPy



DBSCAN on CPU

#create dataset with 100,000 points using make_circles function

from sklearn.datasets import make_circles

X, y = make_circles(n_samples=int(1e5), factor=.35, noise=.05)

#run DBSCAN clustering algorithm

from sklearn.cluster import DBSCAN

db = DBSCAN(eps=0.6, min samples=2)

 $y_db = db.fit_predict(X)$

DBSCAN with RAPIDS on GPU

#convert data to pandas.DataFrame then create cudf.DataFrame

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)

#use GPU-accelerated version of DBSCAN from cuML

from cuml import DBSCAN as cuml

DBSCANdb_gpu = cumlDBSCAN(eps=0.6, min_samples=2)

y_db_gpu = db_gpu.fit_predict(X_gpu)

GPU Directives

- Easier to learn and involve fewer changes to code that GPU programming languages
- Better portability among devices and platforms
- Compiler directives, e.g. OpenACC, are the most commonly used

GPU Directives

- Require little understanding of GPU hardware, but more than GPU libraries
 - Host- CPU
 - Device- GPU
 - Kernel- functions launched to the GPU

OpenACC

- A collection of compiler directives that specify loops and regions of code in standard C, C++, and Fortran to be offloaded from a host CPU to an attached parallel accelerator (developer.nvidia.com)
- Let compiler guess data allocation and movement or control it with directive clauses
- Can be used with GPU libraries, OpenMP

Basic Program Structure (C/C++)

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

Compiling (C/C++) for NVIDIA GPU

```
nvcc --acc -Minfo=accel your_program_acc.c pgcc -acc -ta=nvidia -c your_program_acc.c
```

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

Example Kernel Directive (C/C++)

```
//Hello_World_OpenACC.c
void Print_Hello_World()
{
#pragma acc kernels
    for(int i = 0; i < 5; i++)
        {
            printf("Hello World!\n");
        }
}</pre>
```

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

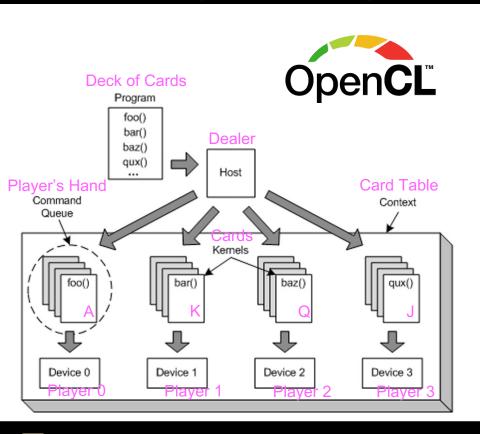
Example Data Directive (C/C++)

```
#pragma acc data copy(a)
{
    #pragma acc kernels
    {
        for(int i = 0; i < n; i++)
        {
            a[i] = 0.0
        }
    }
}</pre>
```

GPU Languages (Language Extensions)

- Require in-depth knowledge of hardware
- May involve substantial changes to code
- Code must be maintained to keep up with hardware changes & performance guidelines
- Alpine supports OpenCL (NVIDIA & AMD GPUs),
 HIP (NVIDIA & AMD), & CUDA (NVIDIA only)





Dealer distributes cards to players. Host distributes kernels to devices.

Player receives cards from dealer. Device receives kernels from host.

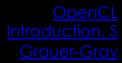
Dealer selects cards from a deck. Host selects kernels from a program

Each player receives cards as part of a hand. Each device receives kernels through the command queue.

Card table makes it possible for players to transfer cards to each other.

OpenCL Context allows devices to receive kernels and transfer data.





	Description	Code Example	OpenCL Introduction, S Grauer-Gray
1	Obtain OpenCL platform	clGetPlatformIDs(1, &platform, NULL)	
2	Obtain device id for at least one device (accelerator)	clGetDeviceIds(platform, CL_DEVICE_TYPE_GPU	U, 1, &device, NULL)
3	Create context for device	context = clCreateContext(NULL, 1, &device, NU	JLL, NULL, &err)
4	Create accelerator program from source code	program = clCreateProgramWithSource (contex &err)	kt, 1, (const char**) &program_buffer, &program_size,
5	Build the program	clBuildProgram(program, 0,)	
6	Create kernel(s) from program functions	kernel = clCreateKernel(program, "kernel_name	e", &err)
7	Create command queue for target device	queue = clCreateCommandQueue(context, dev	ice, 0, &err)
8	Allocate device memory / move input data to device memory	memObject = clCreateBuffer (context, NULL, SIZ clEnqueueWriteBuffer(command_queue, mem	
9	Associate arguments to kernel with kernel object	cl_int clSetKernelArg (kernel, arg_index, arg_siz	ze, *arg_value)
10	Deploy kernel for device execution	global_size = TOTAL_NUM_THREADS; local_size = WORKGROUP_SIZE; clEnqueueNDRangeKernel(command_queue, k NULL);	kernel, 1, NULL, &global_size, &local_size, 0, NULL,
11	Move output data to host memory	clEnqueueReadBuffer(command_queue, memono, NULL, NULL)	Object, blocking_read, offset, TOTAL_SIZE, hostPointer,
12	Release context/program/kernels/memory	clReleaseMemObject(memObject) / clReleaseK clReleaseContext(context)	ernel(kernel) / clReleaseProgram(program) /

GPU Frameworks

- Offer building blocks for designing, training, and validating workflows (like deep learning)
 - e.g. PyTorch, TensorFlow, Keras, Apache MXNet
- Rely on GPU-accelerated libraries







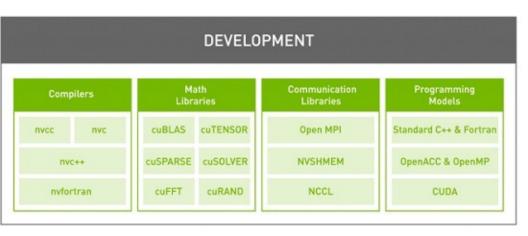


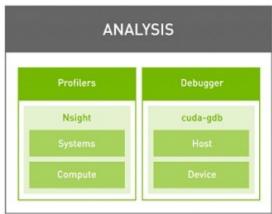




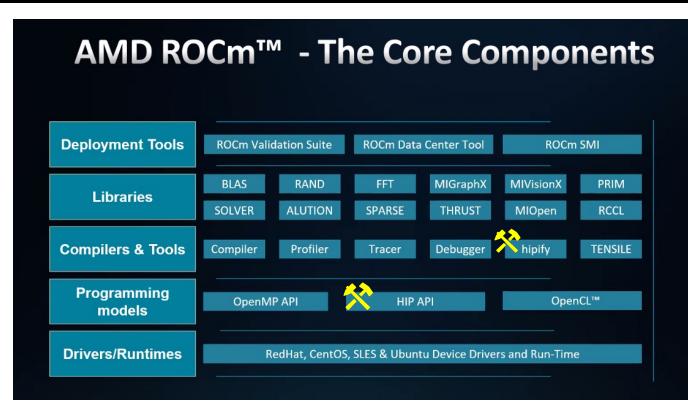
GPU programming tools vary in terms of ease of implementation, portability, and flexibility.

NVIDIA SDK









The Heterogeneous Computing Interface for Portability (HIP) is a vendor-neutral C++ programming model for implementing highly tuned workload for GPUs. HIP (like CUDA) is a dialect of C++ supporting templates, classes, lambdas, and other C++ constructs.

A "hipify" tool is provided to ease conversion of CUDA codes to HIP, enabling code compilation for either AMD or NVIDIA GPU (CUDA) environments. The ROCm™ HIP compiler is based on Clang, the LLVM compiler infrastructure, and the "libc++" C++ standard library.

Poll

Rank the GPU programming tools by how likely you are to use them, from most (1) to least likely (6).

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Requesting GPUs on Alpine with Slurm

Access Slurm job scheduler from login node

module load slurm/alpine

View Alpine GPU resources and configurations

sinfo --Format NodeList:30,Partition,Gres | grep gpu | grep -v "mi100|a100"

c3gpu-c2-u[1,3,5,7,9,11,13,15]aa100	gpu:a100:3
c3gpu-c2-u[1,3,5,7,9,11,13,15]aa100-ucb	gpu:a100:3
c3gpu-c2-u[1,3,5,7,9,11,13,15]aa100-csu	gpu:a100:3
c3gpu-c2-u[1,3,5,7,9,11,13,15]aa100-amc	gpu:a100:3
c3gpu-c2-u[17,19,21,23,25,27,2ami100	gpu:mi100·3
c3gpu-c2-u[17,19,21,23,25,27,2ami100-ucb	gpu:mi100:3
c3gpu-c2-u[17,19,21,23,25,27,2ami100-csu	gpu:mi100:3
c3gpu-c2-u[17,19,21,23,25,27,2ami100-amc	gpu:mi100:3
c3gpu-c2-u[17,19,21,23,25,27,2atesting	gpu:mi100:3
c3gpu-c2-u[1,3,5,7,9,11,13,15]atesting	gpu:a100:3

Nvidia A100s partition=aa100-<institution> e.g. partition=aa100-ucb

AMD A100s partition=ami100-<institution> e.g. partition=ami100-ucb

Requesting GPUs on Alpine with Slurm

Request a compile node

```
acompile --help
```

acompile --ntasks=4 --gpu=amdgpu --time=2:00:00

acompile --ntasks=4 --gpu=nvidia --time=2:00:00

Start an interactive job

sinteractive --ntasks=64 --gres=gpu:3 --partition=aa100-ucb --time=1:00:00

sinteractive --ntasks=20 --gres=gpu:1 --partition=ami100-ucb

sinteractive --gres=gpu:1 --partition=ami100-ucb --qos=long --time=7-00:00:00

sinteractive --gres=gpu:1 --nodes=2 --partition=ami100-ucb

Overview

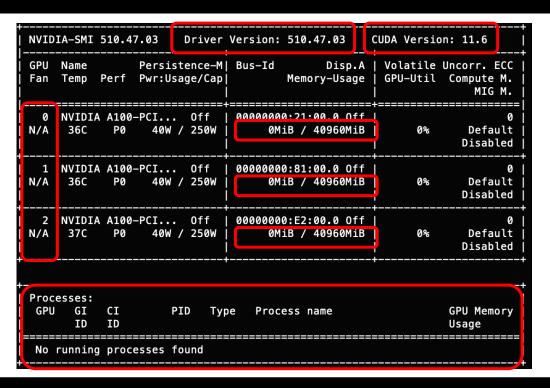
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nvidia-smi

- Command-line utility tool for monitoring NVIDIA GPUs
- Returns device- and process-level information
- Available on Alpine Nvidia nodes without loading any modules







rocm-smi

- Command-line utility tool for monitoring AMD GPUs
- Returns <u>extensive</u> information
- Available on Alpine AMD nodes without loading any modules



```
================== Concise Info ==================
      AvaPwr
          SCLK
               MCLK
                          PwrCap VRAM%
                                  GPU%
  Temp
  33.0c 39.0W
           300Mhz 1200Mhz
                       auto
                          290.0W
                                   0%
           300Mhz
              1200Mhz
                          290.0W
                       auto
                       auto
WARNING:
             One or more commands failed
```

More Information:

rocm-smi --help

Documentation available at

https://rocmdocs.amd.com/en/latest/ROCm_System_Managment/ROCm-SMI-CLI.html



Quiz

Quick Quiz!

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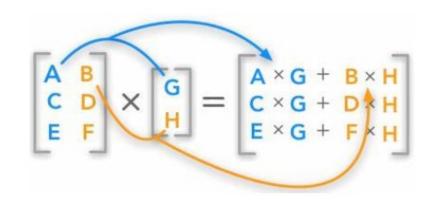


- A matrix is a rectangular array of numbers arranged in rows and columns.
- The order of a matrix is the number of rows and columns.

```
\begin{pmatrix} 6 & 2 & 4 \\ 2 & 1 & 6 \end{pmatrix}
```

Matrix multiplication is used in many ML algorithms.

We will use Tensorflow's tf.matmul function.







Navigate to your preferred working space (projects, scratch, etc.):

cd /projects/\$USER/

Git the repository:

git clone https://github.com/ResearchComputing/Intro_GPU_Acceleration.git

Make the scripts executable:

cd Intro_GPU_Acceleration chmod u+x tf*



tf.matmul-cpu.py

```
import os
import numpy as np
import tensorflow as tf
import time
os.environ['TF_CPP_MIN_LOG_LEVEL'] = '3'
os.environ['CUDA_VISIBLE_DEVICES'] = '-1'
if tf.test.gpu_device_name():
    print("GPU found")
else:
    print("Tensorflow is using only CPUs.")
numpy_start = time.time()
a = np.random.rand(10000,70000)
print("Numpy generated a random 10000x70000 matrix, matrix a")
b = np.random.rand(70000,10000)
print("Numpy generated a random 70000x10000 matrix, matrix b")
numpy_end = time.time()
print("It took numpy", numpy_end-numpy_start, "seconds to generate matrices a and b."
print("Tensorflow is beginning matrix multiplication."
tf start = time.time()
tf.matmul(a,b)
tf end=time.time()
print("Tensorflow multiplied matrices a and b in", tf_end-tf_start, "seconds.")
```

tf.matmul-gpu.py

```
import os
import numpy as np
import tensorflow as tf
import time
os.environ['CUDA_VISIBLE_DEVICES'] = '0'
os.environ['TF CPP MIN LOG LEVEL'] = '3'
numpy_start = time.time()
a = np.random.rand(10000,70000)
print("Numpy generated a random 10000x70000 matrix, matrix a")
b = np.random.rand(70000,10000)
print("Numpy generated a random 70000x10000 matrix, matrix b")
numpy_end = time.time()
print("It took numpy", numpy_end-numpy_start, "seconds to generate matrices a and b."
print("Tensorflow is beginning matrix multiplication."
tf start = time.time()
tf.matmul(a,b)
tf end=time.time()
print("Tensorflow multiplied matrices a and b in", tf_end-tf_start, "seconds.")
```

Start an interactive node on Alpine with 1 A100 as follows:

sinteractive --time=01:00:00 --ntasks=20 --gres=gpu:1 --partition=aa100-ucb --reservation=gpuclass

Activate the conda environment:

module load anaconda conda activate /curc/sw/conda_env/tf-gpu-cuda11.2



Run CPU-only script:

python tf.matmul-cpu.py

Tensorflow is using only CPUs.

Numpy generated a random 10000x70000 matrix, matrix a.

Numpy generated a random 70000x10000 matrix, matrix b.

It took numpy 6.565369129180908 seconds to generate matrices a and b.

Tensorflow is beginning matrix multiplication.

Tensorflow multiplied matrices a and b in 45.82650423049927 seconds.

Run GPU-accelerated script:

python tf.matmul-gpu.py

Numpy generated a random 10000x70000 matrix, matrix a.

Numpy generated a second random 70000x10000 matrix, matrix b.

It took numpy 6.620205402374268 seconds to generate the matrices.

Tensorflow is beginning matrix multiplication.

Tensorflow multiplied matrices a and b in 3.0970964431762695 seconds.



```
import numpy as np
import tensorflow as tf
import time
os.environ["CUDA_VISIBLE_DEVICES"]="0"
os.environ["TF CPP MIN LOG LEVEL"]="3"
numpy start=time.time()
a = np.random.rand(50000, 20000)
print("Numpy generated a random 50000x20000 matrix, matrix a.")
b = np.random.rand(20000, 50000)
numpy end=time.time()
print("Numpy generated a second random 20000x50000 matrix, matrix b.")
print("It took numpy", numpy end-numpy start, "seconds to generate the matrices.")
print("Tensorflow is beginning matrix multiplication.")
tf start = time.time()
c = tf.matmul(a,b)
tf_end = time.time()
print("Tensorflow multiplied matrices a and b in", tf_end-tf_start, "seconds.")
quit()
```

N	NVID	IA-SMI	510.47	7.03	Driver	Version:	510.47.03	CUI	DA Versi	on: 11.6
	Fan									Uncorr. ECC Compute M. MIG M.
=== N	0 N/A						0:21:00.0 iB / 40960		0%	0 Default Disabled
 N	1 N/A	NVIDIA 36C					0:81:00.0 iB / 40960		0%	0 Default Disabled
N	2 N/A			-PCI 40W /			0:E2:00.0 iB / 40960		0%	0 Default Disabled
+										
	Processes: GPU GI CI PID Type Process name ID ID								GPU Memory Usage	
	No running processes found									



```
import os
import numpy as np
import tensorflow as tf
import time
os.environ["CUDA VISIBLE DEVICES"]="0"
os.environ["TF CPP MIN LOG LEVEL"]="3"
numpy start=time.time()
a = np.random.rand(50000, 20000)
print("Numpy generated a random 50000x20000 matrix, matrix a.")
b = np.random.rand(20000, 50000)
numpy end=time.time()
print("Numpy generated a second random 20000x50000 matrix, matrix b.")
print("It took numpy", numpy_end-numpy_start, "seconds to generate the matrices.")
print("Tensorflow is beginning matrix multiplication.")
tf start = time.time()
c = tf.matmul(a,b)
tf end = time.time()
print("Tensorflow multiplied matrices a and b in", tf_end-tf_start, "seconds.")
quit()
```

```
NVTDTA-SMT 510.47.03
                        Driver Version: 510.47.03
                                                     CUDA Version: 11.6
GPU Name
                 Persistence-MI Bus-Id
                                             Disp.A
                                                       Volatile Uncorr. ECC
                                       Memory-Usage
Fan Temp Perf Pwr:Usage/Capl
                                                      GPU-Util Compute M.
                                                                     MIG M.
                                000000000:21:00.0 Off
                                 38819MiB / 40960MiB
                                                                    Default
                                                                   Disabled
    NVIDIA A100-PCI... Off
                                00000000:81:00.0 Off
N/A
     35C
                   40W / 250W
                                     0MiB / 40960MiB
                                                                    Default
                                                                   Disabled
    NVIDIA A100-PCI... Off
                                00000000:E2:00.0 Off
N/A
     37C
                   40W / 250W
                                     0MiB / 40960MiB
                                                                    Default
                                                                   Disabled
Processes:
      GΙ
           CI
                                   Process name
                                                                 GPU Memory
       ΙD
                                                                 Usage
                  3447060
                                   python
                                                                   38817MiB
```



- How could we speed this up even further?
- How would matrix size affect the observed speed up?

Thank you!

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

Alpine Documentation:

https://curc.readthedocs.io/en/latest/clusters/alpine/index.html

Ask for Help: colorado.edu/rc/userservices/contact

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