CPU PySpark GPU CUDA **Gravity Simulator**

Our Team: Group 1



Pranay Angiya Janarthanan



Aditya Sharma

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Objectives Why Compare?





Supercomputer stations are becoming extremely popular with multi-cluster systems working together

GPU Computational Advantage



Can perform thousands of calculations at once



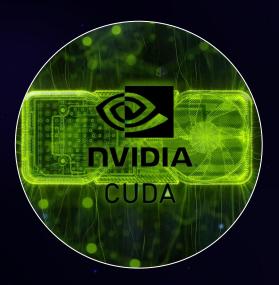
Easy to collect and integrate



High demand for AI and other ML based calculations



Which is Better?



GPU-Based (CUDA)



Cluster-Based (PySpark)

02 Background

What is CUDA and Pyspark?



CUDA



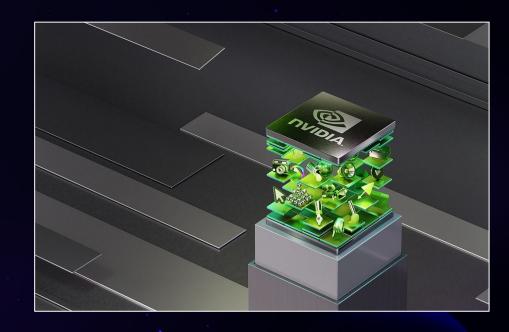
Parallel Computing Platform developed by NVIDIA



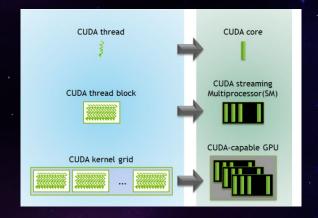
Traditionally used for graphics rendering



Utilizes thousands of GPU Cores to run parallel computational tasks for AI, data processing, etc



Computing Architecture





Threads

Handles a set of computations (Traditionally single computations per thread)



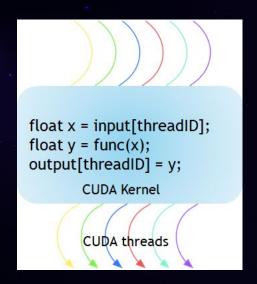
Thread Blocks

Collects a block of threads that often share some small and fast memory (Chosen in multiples of 32)

Kernel Grid

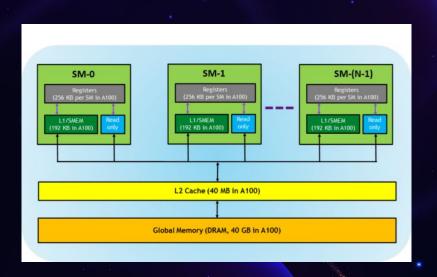
A stack or grid of Blocks used to organize dimensions (1D for vectors, 2D or 3D for multidimensional problems)

Kernels and Memory Management



Functions on GPUs

Functions launched from CPU (host) to run onto GPU (Device) (Requires memory allocated variables)



Memory Levels

Threads have registers. Streaming Multiprocessors have shared memory for threads in blocks. Grids have L2 and DRAM

PySpark

Fault Tolerance

Distributed Computing

Local and Cluster Based

Parallel Data Processing



O3 Methodology

What are we comparing?



Gravity Simulator



Large amount of vector calculations for each body

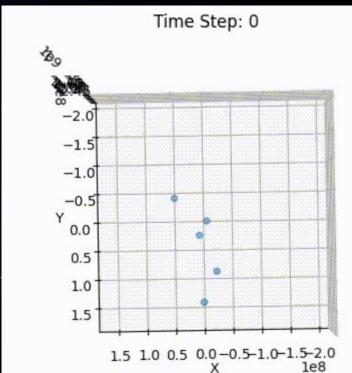
$$F_g = G \frac{m_1 m_2}{r^2}$$



Scalable Problem for Size N



Places stress on resources like CPU, GPU, and memory



System Setup

PySpark (Local)



- 4 Intel i7 Cores per Worker Node
 - 6 GB RAM per Session
 - 1 Worker Node
 - 8 Threads

CUDA (Google Colab)



- Tesla T4
- 2560 CUDA Cores
- 15 GB GPU Ram

CUDA Code

```
Body *d bodies;
float3 *d acc;
cudaMalloc(&d bodies, n*sizeof(Body));
                                           // Allocate Memory in GPU for Bodies
cudaMalloc(&d acc, n*sizeof(float3));
                                           // Allocate Memory in GPU for Accelerations
cudaMemcpy(d_bodies, h_bodies, n*sizeof(Body), cudaMemcpyHostToDevice); // Copy data from CPU to GPU
// Setup CUDA launch parameters
int blockSize = 64;  // Number of threads per block
int gridSize = 2;  // Number of blocks
// Benchmark simulation
auto start_sim = std::chrono::high_resolution_clock::now();
for (int s = 0; s < steps; s++) {
                                                                                  // Run kernal to compute accelerations
   compute_accelerations<<<qridSize, blockSize>>>(d_bodies, d_acc, n, G, eps2);
   update_bodies<<<gridSize, blockSize>>>(d_bodies, d_acc, n, dt);
                                                                                  // Run kernal to update bodies
   cudaDeviceSynchronize();
auto end_sim = std::chrono::high_resolution_clock::now();
double sim time = std::chrono::duration<double>(end sim - start sim).count();
cudaMemcpy(h bodies, d bodies, n*sizeof(Body), cudaMemcpyDeviceToHost);
                                                                                  // Copy data from GPU back to CPU
```

O4 Analysis

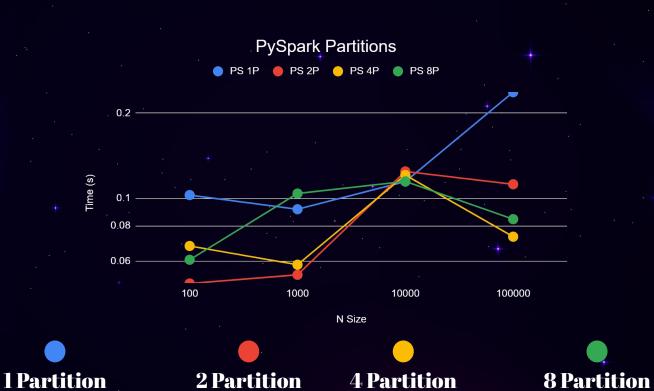
How did each perform?



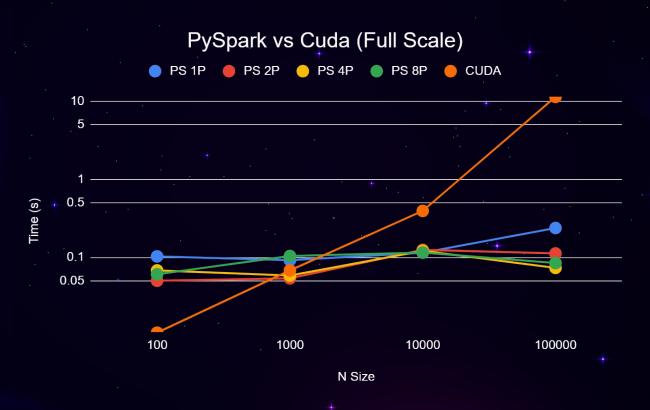
Results

N	PySpark 1	PySpark 2	PySpark 4	PySpark 8	CUDA
100	0.1026408672	0.049995422	0.0678431988	0.06061911583	0.010807
1000	0.09149217606	0.0536363125	0.05823016167	0.1039690971	0:067764
10,000	0.114677023	0.1244206429	0.1207845211	0.1145432327	0.392621
100,000	0.2371878624	0.1120731831	0.07315087318	0.0843768120	11.347148

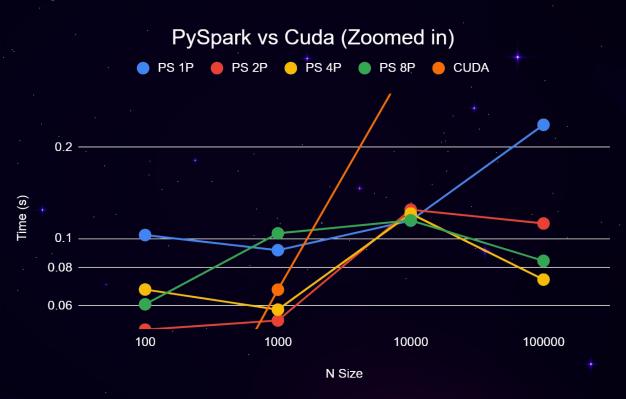
PySpark Partitions



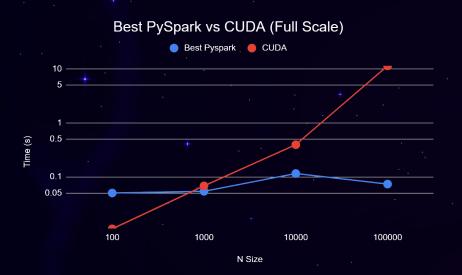
PySpark vs CUDA (Full Scale)

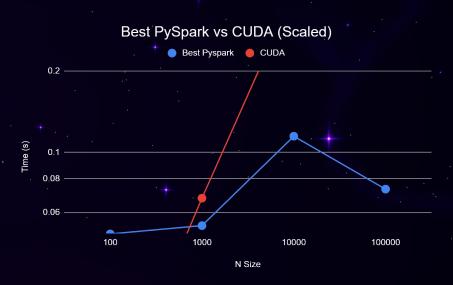


PySpark vs CUDA (Zoomed in)



Best PySpark vs CUDA





O5 Conclusions

What did we find?

PySpark vs CUDA



Low N performance for CUDA

- Given low values for N, CUDA performs better
- Limited by Block Size to 1024
 - Scaling issue with data past 1000



PySpark Scalability with partitions

- Ability to add Partitions and choose optimal value for performance
- Requires either large dataset or increased partitions and resources



Specialized Use Cases

- CUDA specialized in Neural Networks and Large Parallelization
- PySpark excels with large data manipulation

Thanks

Do you have any questions?

as4108@rutgers.edu pa446@rutgers.edu

