N-Body Simulation

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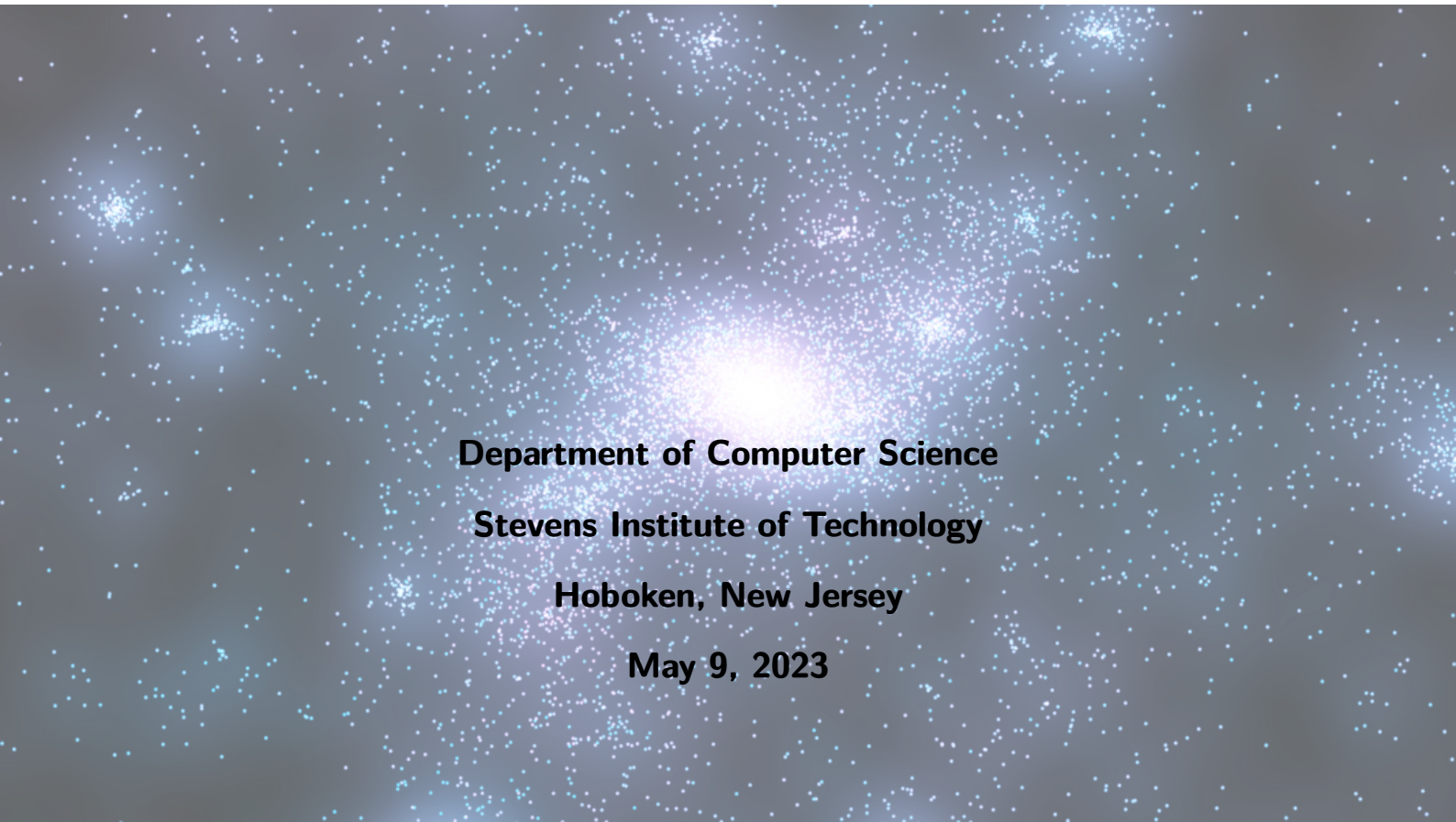
CS677: Final Project Report

Professor Mordohai



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1 | Introduction

For my project, I implemented a parallel brute force N-Body Simulation which runs in $O(n^2)$ time. The brute force approach is often times called the "all-pairs N-body simulation" as it simulates the interaction between all the pairs of bodies in the simulation, while other methods, such as the Barnes-Hut simulation, achieve better performance by approximating the interaction by reducing the number of interactions based on the distance between two bodies.

N-Body Simulations can be used to model the interaction between many different things, such as planets, galaxies, and particles. My simulation models the interaction between bodies exerting a gravitational force on one another, with a very large and dense mass being in the middle that also exerts a force on every body in the simulation.

The acceleration of a body due to the gravitational force exerted on it by another body can be modeled by the following equation:

$$a_i \approx G \cdot \sum_{j=1}^{N} \frac{m_j \cdot \vec{r_{ij}}}{(\|\vec{r_{ij}}\|^2 + \epsilon^2)^{\frac{3}{2}}} \tag{1.1}$$

The ϵ is known as a softening factor and is set to 1×10^{-8} in order to prevent division by zero and not have particles collide, but rather pass through each other. My simulation uses this equation to update the velocity of each particle over a small time-step $dt = 0.01$ by multiplying the result a_i by the time-step dt.

I have tested multiple different implementations of the brute-force algorithm. They include sequential CPU code, OpenMP parallelized CPU code, basic CUDA code (this is just a direct port of the sequential CPU code to a CUDA kernel), and optimized CUDA code using shared memory and loop unrolling. Both of the CUDA versions use structures of arrays, `float4`s, and a compiler flag that flushes denormal numbers to zero (more on this later) to achieve the most optimal speed.

Times were recorded in milliseconds using the `high_resolution_clock` from the `<chrono>` library from the `C++` STL. For the CPU implementation, the timer was started before the function that handled the simulation was called and was ended as soon as the function returned. For the CUDA implementation, the timer was started before the kernel was called and was ended as soon as the kernel returned (before memory was copied from the device to the host). The time reported is the amount of time each function/kernel call took averaged over 10 total

calls, and the first CUDA kernel launch is ignored since it always takes significantly longer due to the overhead of setting up the device for the first call.

Each body's initial position and velocity was initialized randomly using the `<random>` library's `uniform_int_distribution<T>` class functionality.

The simulation, timing scripts, checkers, and LaTeXcode for this report in available on GitHub.

2 | Hardware Specifications

The simulation was run locally on my Windows 10 PC using WSL2. The specifications are the following:

- CPU: AMD Ryzen 5 5600X, 6-core, 12-Thread
- GPU: NVIDIA GeForce RTX 3070 Ti

These specifications are important as different CPUs will experience different speed-ups from OpenMP depending on how many threads are available. Along with that, different GPUs will also experience different speeds based on factors such as their streaming multiprocessor count.

3 | Suitability for GPU Acceleration - Amdahl's Law

Since the interaction between one pair of bodies is completely independent from the interaction between another pair of bodies, this problem is embarrassingly parallel. The entire computation can be parallelized on the GPU. Unlike the versions showed in class that updated each body's position vector on the CPU, the implementations discussed in this report have the entire computation on the GPU or in the OpenMP parallelized for-loop. With these implementations, we achieve 100% parallelism for simulating the interaction between all N bodies.

4 | CPU Implementations

The sequential implementation of the brute-force simulation is very simple. There are two for-loops with one nested in the other:

```
for (int i = 0; i < n; i++){
    float fx = 0.0f, fy = 0.0f, fz = 0.0f;
    for (int j = 0; j < n; j++){
```

```
float dx = b[j].x - b[i].x;
// code continues...
```

This sequential version of the code is very slow. Thanks to OpenMP, we can easily parallelize this by putting a `#pragma omp parallel for schedule(dynamic)` directive above the outer loop. This will spawn some number of threads, depending on how many are available on the CPU, and significantly speed up the simulation. By doing this, each thread calculates approximately `N/num_threads` interactions rather than a single thread calculating every interaction (as it did in the original code).

The rest of the code is trivial and simply implements equation 1.1. It computes the Euclidean distance between the each pair of bodies and uses that to find the force of attraction between each pair. Each body's force vector is updated for every other body.

```
float dx = b[j].x - b[i].x;
float dy = b[j].y - b[i].y;
float dz = b[j].z - b[i].z;
float d = dx*dx + dy*dy + dz*dz + EPSILON * EPSILON;
float denom = 1.0f / sqrtf(d);
float denom_cubed = denom * denom * denom;

float m_j = b[j].m

fx += m_j * dx * denom_cubed;
fy += m_j * dy * denom_cubed;
fz += m_j * dz * denom_cubed;
```

Finally, the force of attraction between a body and the large, dense mass in the middle is computed. The code then integrates the force over the small time-step dt and multiplies by the gravitational constant ($G = 6.67 \times 10^{-11}$) to find the acceleration due to the force and adds this to the velocity vector. The velocity vector is then multiplied by dt and used to update the position vector.

```
// dx, dy, dz, and denom_cubed re-calculated for center mass...
m_c = center_obj.m
fx -= m_c * dx * denom_cubed;
fy -= m_c * dy * denom_cubed;
fz -= m_c * dz * denom_cubed;

b[i].vx += dt*fx*G;
b[i].vy += dt*fy*G;
b[i].vz += dt*fz*G;
```

```
b[i].x += dt * b[i].vx;
b[i].y += dt * b[i].vy;
b[i].z += dt * b[i].vz;
```

The code presented in class on May 3rd was very similar to this except I was updating the positions outside of the parallelized loop by using OpenMP's SIMD pragma directive (I simply added `#pragma omp simd` above a loop that iterated over every body and updated each body's position vector). This was because I was experiencing a bug when I would update the positions in parallel on the GPU, so decided to use SIMD for both implementations. After fixing that bug and moving the position update inside the parallelized loop I've noticed a slight increase in performance, but not too significant.

Something interesting I discovered prior to updating the positions in parallel was that compiling the `C++` code with the `-O3` flag to optimize the code as much as possible led to no difference when adding `#pragma omp simd`. Afer some research, I found out the loop I had originally was being automatically vectorized by the compiler due to the `-O3` flag turning on the `-ftree-vectorize` flag. I believe understanding more about how compilers optimize our code, oftentimes even better than any human could, is crucial to being a good programmer.

The figure below shows the time difference between the OpenMP implementation and the sequential implementation.

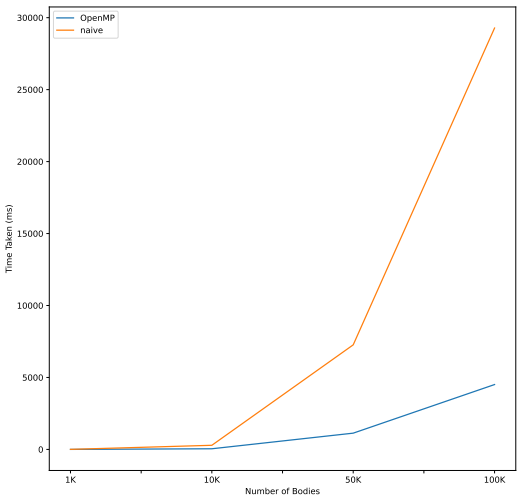


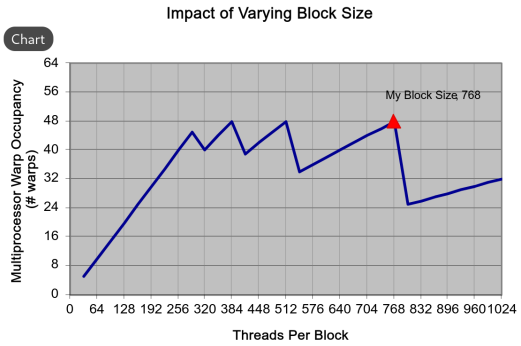
Figure 4.1: Time Difference When Using OpenMP

5 | CUDA Occupancy

Before discussing the GPU implementations, I feel it is important to discuss the CUDA Occupancy achieved in them. I use a total of 12,288 bytes of shared memory since each block utilizes a shared array of 768 (this is the block size) `float4`s, each having a size of 16 bytes. Using the CUDA Occupancy calculator [3] I was able to determine that my implementation is at 100% occupancy, as seen in the screenshots from the calculator below.

1.) Select Compute Capability (click):	8.6
1.b) Select Shared Memory Size Config (bytes)	65536
1.c) Select CUDA version	11.1
2.) Enter your resource usage:	
Threads Per Block	768
Registers Per Thread	32
User Shared Memory Per Block (bytes)	12288
(Don't edit anything below this line)	
3.) GPU Occupancy Data is displayed here and in the graphs:	
Active Threads per Multiprocessor	1536
Active Warps per Multiprocessor	48
Active Thread Blocks per Multiprocessor	2
Occupancy of each Multiprocessor	100%

(a) Calculator Showing 100% Occupancy Configuration



(b) Graph Of Best Number of Threads per Block

Figure 5.1: Results of the Occupancy Calculator [3]

I originally was using 1024 threads per block, which increased the shared memory size per block to be 16,384 bytes. However, using the occupancy calculator I discovered this was only utilizing 67% occupancy. After switching from 1024 threads per block to 768, I noticed a consistent 1 to 2 millisecond speed up when simulating 30,000 bodies. This speed up scaled appropriately while increasing the number of bodies, sometimes saving about a full second or two when N grew to 1 million bodies.

6 | GPU Implementations

There were two GPU implementations written for this project: one was a simple port of the inner loop from the CPU code to a CUDA kernel and the other was a more optimized algorithm that uses shared memory and loop unrolling. Since the simple version is very similar to the CPU code explained above, we will not discuss it here.

The kernel begins by determining the global thread ID. Then, the code iterates over every block in the grid using a for-loop and, for each block, populates an array in shared memory for

every thread in the current block to load in their corresponding body's information:

```
for (int t = 0; t < gridDim.x; t++)
    __shared__ float4 others[BLOCKSZ];
    float4 curr = p[t * blockDim.x + threadIdx.x];
    // load other threads' info into shared memory
    // the "w field" is used to store the mass
    others[threadIdx.x] = make_float4(curr.x, curr.y, curr.z, curr.w);
    __syncthreads();
```

The code then iterates over the array and calculates the interaction between the body corresponding to the thread running the code (determined by the global thread ID) and every body in the array. This is very similar to the inner loop to the CPU version except for a `#pragma unroll` placed above it so it will not be displayed here. One of the first thoughts I had was to launch another kernel from this one to parallelize this for-loop, but since each thread would be updating the same force I'd have to use atomic operations which would just slow it down anyway. Finally, something similar to the CPU code is done to calculate the ineraction between the current body and the large, dense center mass. The velocity vector is updated by calculating the acceleration from the force vector over dt and similarly the position vector is updated by calculating the displacement from the velocity vector over dt.

The figure below shows the difference in time between the optimized CUDA code and the basic code.

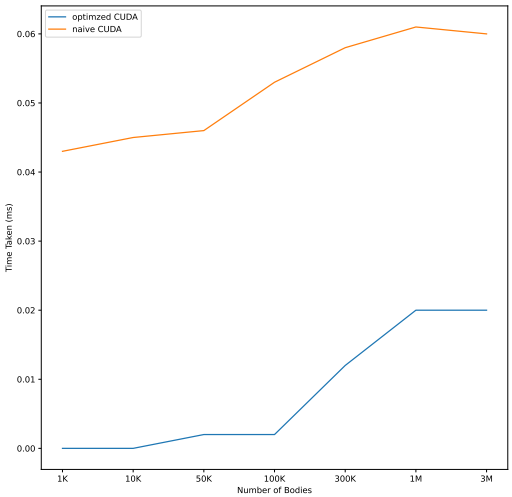


Figure 6.1: Time Difference Between CUDA Implementations

While I have not tested putting the bodies in constant memory, I believe my implementation

may provide similar speeds or even greater since it requires only one kernel launch and uses shared memory. Also, using constant memory wouldn't work once the number of bodies surpasses $N = 2,048$. This is because each body has two `float4`s to store its position, velocity, and mass which totals 32 bytes. Since constant memory is limited to 65,536 kilobytes, our number of bodies is also limited. This method, using a constant amount of shared memory per block (768 bodies $\times$ 16 bytes/body $=$ 12,288 bytes) allows us to simulate any number of bodies.

7 | GPU Optimizations

There are three more optimizations I used to make the CUDA code as efficient as possible in both versions and they include the `-ftz=True` compiler flag, using `float4`s rather than regular floats, and using a structure of arrays.

The CPU code uses an array of structures to represent the simulation, where each structure represents a body and has float fields for the body's x, y, z position and velocity and a field for its mass. The GPU code uses a single structure of arrays that represents the entire simulation. This structure has two `float4` arrays, where the first array of `float4`s stores each body's x, y, z position and mass, and the other stores each body's velocity. Using the structure of arrays enables greater memory coalescing and uses bandwidth more efficiently.

`Float4`s achieve better performance on the GPU because they utilize vectorized memory accesses [2]. Experiments have shown that using `float4`s rather than regular floats can increase speeds by up to 25% [5]. The reason for this is twofold: "multi-word vector memory accesses only require a single instruction to be issued, so the bytes per instruction ratio is higher", and "vector sized transaction request from a warp results in a larger net memory throughput per transaction" [4]. Therefore, by using `float4`s I achieve significant speed-ups on top of using a structure of arrays.

The `-ftz=true` flag flushes what are known as "denormal values" to zero. This is by far the most interesting optimization I learned about while doing research for this project. Denormal values are floating point numbers where the mantissa is normalized and the leading zeros from it are moved into the exponent, resulting in an exponent that is too small and cannot be represented [1]. These numbers can slow down computation time significantly, especially for functions like `sqrtf()` and `rsqrtf()`. Since these numbers are so small, flushing them to zero does not affect accuracy at all. Using the `-ftz=true` flag will flush all denormalized numbers to be flushed to

zero, which doesn't have a performance impact on adds or multiplies but it does for functions like `rsqrtf()` which map to hardware instructions, sometimes providing a 20% speed increase [1]. I did not see this significant of a speed increase, but saw a small one nonetheless as shown in the figure below.

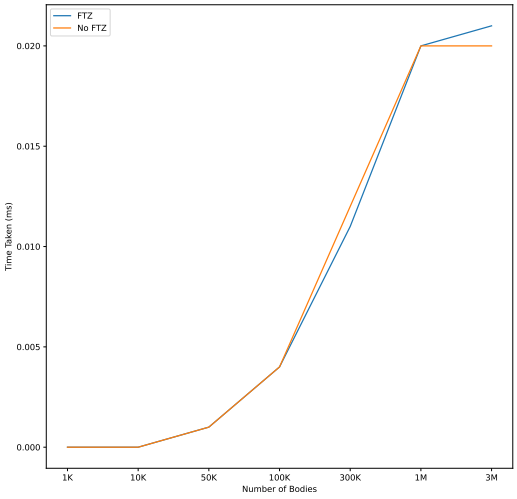
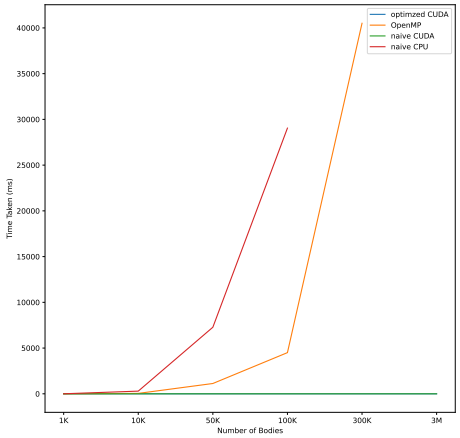


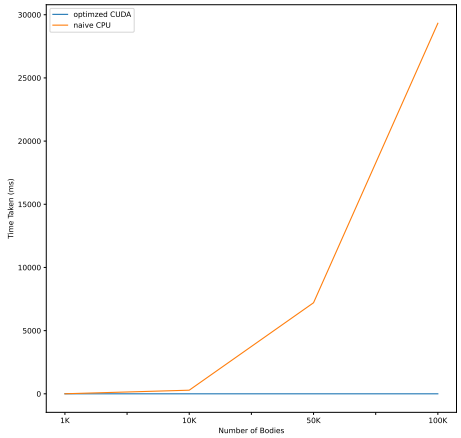
Figure 7.1: Time Difference When Using -ftz=true

8 | Other Time Experiments

I performed two more timing experiments. One plots the times between all of the implementations and the other plots the time comparison of the naive (sequential) CPU and the optimized CUDA code. The reason the graphs are cut off for the OpenMP and sequential CPU implementations are a certain point is because they began to take a very long time and plotting them would interfere with the readability of the graph. Considering the fact the simulation runs in $O(n^2)$ time we can imagine their graphs continuing in a nearly vertical fashion.



(a) Time Difference Between All Implementations



(b) Time Difference Between Sequential CPU and Optimized CUDA

Figure 8.1: More Comparisons
[3]

9 | Conclusion

This project demonstrates the benefit of parallelizing programs such as the N-Body simulation and the different performance gains based on how the code is parallelized. In an ideal world I would have an AMD Threadripper to see how fast the OpenMP version could run on 128 threads, but the 12 threads on my 5600X have done a good job at displaying the power of CPU parallelization. Clearly, the performance gains from using the GPU dwarf those of the parallel CPU code. Unfortunately, since this computation is I/O bound I could not test the GPU implementation for $N > 3,000,000$ as the memory transfers between the host and device started to take a very, very long time (upwards of a couple hours for multiple iterations) and I did not need my PC to reach the temperature of the Sun.

With this project, I learned a lot about CUDA programming, CUDA optimizations, OpenMP, hardware limitations, memory access patterns, and LaTeX.

10 | References

[1] Mark Harris. Cuda pro tip: Flush denormals with confidence, Jan 2013. URL: https://developer.nvidia.com/blog/cuda-pro-tip-flush-denormals-confidence/.

[2] Justin Luitjens. Cuda pro tip: Increase performance with vectorized memory access, Dec 2013. URL: https://developer.nvidia.com/blog/cuda-pro-tip-increase-performance-with-vectorized-memory-access/.

[3] Lei Mao. Cuda occupancy calculation, Jun 2022. URL: https://leimao.github.io/blog/CUDA-Occupancy-Calculation/.

[4] Maxim Milakov. Why are cuda vector types (int4, float4) faster?, Jul 2015. URL: https://stackoverflow.com/a/31449764.

[5] Vitality. Efficiency of cuda vector types (float2, float3, float4), Nov 2014. URL: https://stackoverflow.com/a/26702643.

A | Appendix

The appendix provides the raw data the graphs in the report were made from. I stored them as CSV files and constructed the graphs using the Pandas `DataFrame.plot` method.

OpenMP	Sequential CPU
0.537	2.799
44.927	286.363
1129.652	7265.756
4507.292	29280.727

Optimized CUDA	Basic CUDA
0.0	0.043
0.0	0.045
0.002	0.046
0.002	0.053
0.012	0.058
0.02	0.061
0.02	0.06

FTZ	No FTZ
0.0	0.0
0.0	0.0
0.001	0.001
0.004	0.004
0.011	0.012
0.02	0.02
0.021	0.02

CUDA	OpenMP	Basic CUDA	Sequential CPU
0.0	0.459	0.063	2.921
0.0	45.881	0.041	293.335
0.0	1126.822	0.042	7277.735
0.007	4501.621	0.051	29046.031
0.012	40508.699	0.055	
0.02		0.078	

Optimized CUDA	Sequential CPU
0.0	2.969
0.0	285.581
0.001	7206.065
0.003	29325.559