

Benchmarking different hardware architectures using a parallel implementation of the N-Body Simulation algorithm

Jan MRÁZEK, mrazeja7@ksu.edu

Abstract—This is a write-up paper which describes my efforts when working on a course project for the Advanced Computer Architecture Experiments course at Kansas State University during the Fall 2017 semester.

First, the N-Body Simulation problem is described. As there are multiple ways of simulating a system of large amounts of space bodies, two different algorithms are presented and their pros, cons, accuracy, time complexity and implementation difficulty are compared.

One of the algorithms is then implemented in a simple, naive way and then optimized, parallelized and custom-tuned to run on computer chips of very different architectures.

This optimization is done in multiple iterations, each time with explanations as to the relative speedups and overall performance.

Finally, multiple different versions of the algorithm are run on computer hardware of different architectures, and the resulting data is analyzed and commented on. Performance is measured in the amount of billions of floating-point operations per second, and the efficiency of each computer chip is addressed. An overall conclusion is drawn which compares the results gathered during the benchmarking phase of the project.

I. PROJECT PROPOSAL

In my course project, I explored the ins and outs of efficient parallel design and better cache-friendliness when it comes to programming techniques when applied on different CPU architectures. After briefly describing the N-Body simulation and two different algorithms which can be used to solve it, I chose one and implemented it in the C++ language. I then fine-tuned the source code to better suit each CPU architecture that was tested. Then I benchmarked all of the different implementations that I created and commented on the (sometimes vast) performance differences and speedup yields between them.

II. PROBLEM DEFINITION

The N-Body simulation

The N-body simulation is a way to simulate the continuous gravitational interactions among potentially very large amounts of galactic bodies, solar systems and similar particles, where every body influences the positions and velocity vectors of all other bodies. It is a tool that is used widely and frequently in the fields of astronomy and astrophysics to help researchers reach a better understanding of the evolution of a large-scale structure of the universe.[1]

III. PROBLEM BACKGROUND AND SCOPE

There are many ways to go about the problem of implementing a suitable algorithm for the simulation of galactic particle movements.

The first thing that we have to think about when it comes to making a choice in this matter is the trade-off between a relatively reasonable time-complexity of the algorithm and the scientific accuracy of the algorithm according to the laws of physics that is required.

If we needed to run a truly massive number (hundreds of millions to billions of space bodies) N-Body movement simulation for a high amount of iterations, it would be best to choose the Barnes-Hut algorithm. If instead we prioritize complete accuracy of all computations above all and don't really mind extremely long running times on the same amount of bodies for the same amount of iterations, it is best to stick with an algorithm that solves the simulation in a brute-force manner.



Figure 1: An illustration of an orbital timelapse in *Universe Sandbox*²

[2]

Brute-Force algorithm

The most obvious and most accurate algorithm of solving the N-body simulation is simply a brute-force approach. This algorithm makes sure to compute the forces that are being applied between all pairs of space particles within a given system, thus ensuring scientifically correct movements. This algorithm is also sometimes called "the all-pairs N-Body simulation algorithm."

In the computation of each iteration, or time step, we calculate the force vectors \mathbf{f}_{ij} , which signifies the force that is

point operations per second) that they deliver.[7] This is especially true for the brute-force (or all-pairs) N-Body algorithm, as it responds fairly positively to parallelization efforts.

There have been discussions whether the *FLOP/s* metric is even useful in the comparison of these algorithms, or whether the "amount of science done" should somehow be considered instead. Other algorithms, such as the Barnes-Hut algorithm, may be less efficient theoretically, but they can deliver more "information" in the same amount of computation time.

Nowadays, it is possible to simulate dynamic systems with as many as 10^{11} space particles. In 2010, a team of programmers at Nagasaki University in Japan created a parallel implementation of the N-body problem using NVIDIA's CUDA technology. When the massively parallel implementation was ran on a supercomputer containing a total of 576 *GT200* (Tesla 2.0 architecture) GPUs, they measured a performance of 190.5 *TFLOP/s*. [8]

The theoretical processing power of such a supercomputer should be in the neighborhood of about 580 *TFLOP/s*, as one *GT200* chip can perform as many as (depending on core configuration and clock speeds) 1010 *GFLOP/s*. [9]

The resulting 190.5 *TFLOP/s* is a very respectable number, especially since the code that was used to run the computation used the Barnes-Hut algorithm, instead of the "faster" (*FLOP/s*- or performance-wise) brute-force method.

V. METHODS AND FACILITIES USED

Before I started working on this semestral project, I planned to first implement a naive version of the brute-force N-Body simulation algorithm. Then I wanted to work iteratively in an effort to optimize the source code in order to take better advantage of a computer's memory hierarchy, more specifically the CPU's caches.

I decided to use the C++ programming language to write all of my source code where applicable, and for the CUDA part of my implementation, I would use NVIDIA's CUDA-C language, which is actually just C/C++ with a little bit of extra functionality. I also took advantage of C++'s C++11 standard, which brings a lot of new features into the language compared to its previous versions. In order to get very accurate timing results during my benchmarking efforts, I used C++11's `<chrono>` library. I could have used other, older libraries to do this task, but I wanted to try a new approach, even when it comes to an area that probably doesn't offer much improvement anymore.

Then I wanted to transform the code using the OpenMP parallel programming interface, and finally, if time permitted, create an implementation that would use NVIDIA's CUDA technology.

I planned on testing and benchmarking the computing performance of all of these proposed versions on the following hardware:

- a typical personal computer CPU architecture, i.e. Intel's x86-64. I planned to use Kansas State University's Beocat supercomputer to run the tests on this architecture.
- an ARM-architecture based computer. I wanted to use my own OrangePi One micro-computer, which had been

setup as a media center in my home. This micro-computer uses a single Allwinner H3 SoC (system-on-chip) with a quad-core processor and an integrated GPU. The CPU's clock speed is 1200 MHz. I planned to install a fresh distribution of the ARMbian OS on it and run all of my tests that way.

- a computer equipped with Intel's Xeon Phi coprocessor card. I hoped to confirm my theoretical knowledge I have about this coprocessor card – that it is extremely suitable for simple, embarrassingly parallel computations and vector computing. I hoped to see a significant speedup compared to Intel's x86-64 architecture. I planned to run my tests on a Xeon Phi-equipped computer at my home university (Czech Technical University in Prague, Czech Republic).
- I also wanted to run a CUDA implementation on a computer equipped with an NVIDIA graphics processor. I hoped to run these benchmarks on nodes that are part of Beocat and have dedicated GPUs just for this purpose.

VI. BREAKDOWN OF TASKS, TIME AND WORK SCHEDULE

The first step needed to take is the implementation of a really simple, unoptimized, sequential N-body simulation algorithm.

The next task on my plan was the integration of some sort of graphical interface that I would use to better understand the exact happenings during my calculations, and to possibly help debug the algorithm's implementation. Another good side that I thought it would bring to the project is the fact that it would look

After obtaining a working naive sequential implementation of the project, I planned to start my work on redesigning the algorithm in a more efficient manner. I wanted to try to apply my knowledge that I gained during the semester in CIS 750 in order to maximize the usage of all system resources, which of course includes the usage of a parallel interface, which was also a step that I needed to take. I planned to integrate the OpenMP parallel programming interface into the code, as well as directives used to run programs on the Xeon Phi coprocessor card (with the use of Intel's C++ compiler).

Of course, I also planned to create a parallel version of my implementation using NVIDIA's CUDA technology.

I would then test and measure running times with a variable amount of cores used for the computation and a variable amount of bodies. I wanted to ideally try to collect a large amount of data to get a better grasp on the overall performance of the algorithm when used on different machines and chips.

The last step in my course project would be the analysis of data was to be gathered.

To put my proposed work schedule into perspective, you can take a look at the Gantt chart in figure 3.

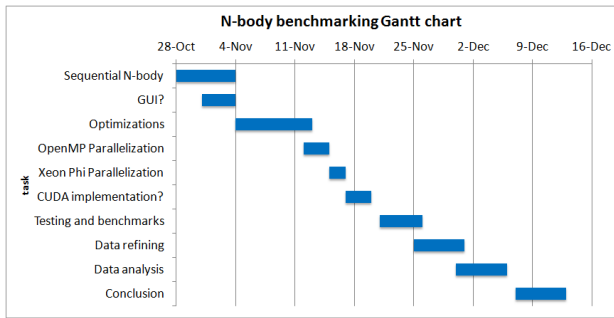


Figure 3: Gantt chart of the proposed estimated project work schedule

VII. PROJECT PROGRESS: NAIVE IMPLEMENTATION

The first task on my plan was the implementation of a naive version of the brute-force N-Body simulation algorithm.

I chose to write the naive version in such a way that it would be very easily readable and simple to understand. I created a `Body` class that represents each individual body object and all of its properties (those being the position vector, velocity vector and mass). This class also contains an `updatePhysics()` method, which essentially calculates the \mathbf{f}_{ij} force vector for any body j that is passed to the method as an argument. The whole system used in the simulation is contained in the `Simulation` class. It contains a vector of all bodies in a given system, as well as additional properties used for the simulation, such as the number of iterations that have passed since the beginning, or a method that takes care of randomly generating a given number of bodies.

I quickly benchmarked this early version of the implementation and found out that it produces a computing performance of about 5 GFLOPs/s when run on a single core on K-State's Beocat supercomputer.

GIF animations

A utility that I also used a lot of the time when creating and debugging the naive implementation was the GIF-making library for C/C++ created by Charlie Tangora. [10] Using this library, I could see the results of any edits I made in the source code almost immediately. I integrated the library in such a way that it is very simple to generate an animated image in .gif format with given dimensions and number of frames. The background of this animated image is always black, with all bodies being represented as green dots. The shade of green of these dots is also customized to reflect the mass of each body in the system.

VIII. PROJECT PROGRESS: STRUCTURE OF ARRAYS

After having completed the naive implementation, I took a look at redesigning pretty much the whole source code in order to take advantage of the CPU's cache.

I thought about the concept of spatial locality of data in the cache, and decided to ditch the object-oriented design of my simulation. I ended up changing my whole approach to storing data in memory. Instead of keeping on using an "array

of structures" kind of design that is easy to understand at a glance, I rewrote the code to represent a "structure of arrays" approach. In reality, I got rid of nearly the entire class structure of the code, and instead used dynamically allocated arrays to store the attributes of all bodies. I implemented different arrays that each stored one of the parameters for all bodies within the system. This way, the spatial locality concept of the cache can be taken advantage of during the force vector calculations.

Resulting speedup

After running some very quick benchmarks and comparing the results, I found out that this improved version of my simulation boasts an approximately 10% higher performance when compared to the previous object-oriented approach depending on the simulation size (i.e. body count and number of iterations).

You can see the differences in the performance of these two designs in figure 4.

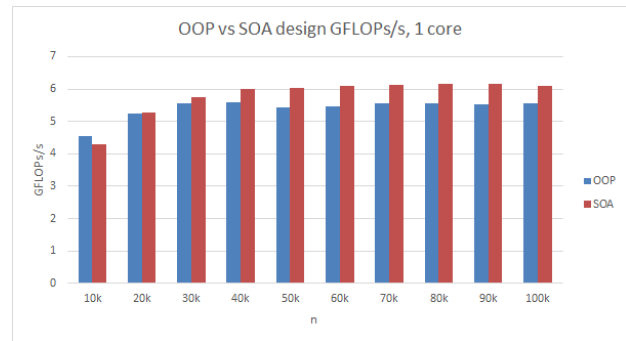


Figure 4: Performance comparison of OOP vs SOA approaches

IX. PROJECT PROGRESS: PARALLELIZATION WITH OPENMP

After redesigning the application to make better use of the CPU's cache, I took a look at parallelizing the code.

As the machines I would use to benchmark the program contain multiple processors each with a significant amount of computing cores, not taking advantage of them would mean a loss of a huge amount of performance.

With help from the OpenMP parallel programming interface, I changed the code in a way that the force vector calculations could be performed almost completely independently in different CPU threads. To make this possible, I used the `#pragma omp parallel for` directive, which automatically parallelizes a `for` loop. Using the `schedule(dynamic)` clause, I told the compiler to schedule each iteration of the `for` loop dynamically. From running some quick tests, I found that this approach was slightly more efficient (a speedup of about 3%) than static or any other form of scheduling. I also used the `#pragma omp simd reduction` clause to take advantage of some of the vector instructions that all modern x86 CPUs have. Using this directive also further helps the compiler vectorize `for` loops.

Resulting speedup

To benchmark and verify the speedup and effectiveness of my efforts to try to parallelize the application using OpenMP, I ran a multitude of benchmarks, all on Beocat.

I mainly ran benchmarks that measured the simulation's speedup depending on the number of threads being used. I also ran all of these tests with variable numbers of bodies in the simulation. You can see a graph of some of my results in figure 5.

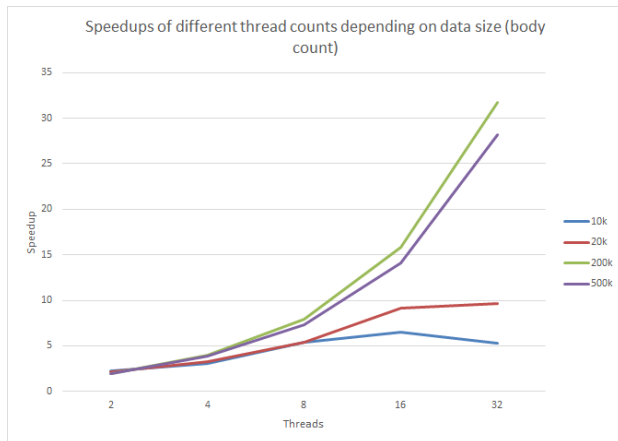


Figure 5: Parallel speedups when using OpenMP depending on number of threads and bodies

I decided to only pick a couple of data points - you can see the speedups when using 2 – 32 threads when compared to just a sequentially run application with either 10, 20, 100 or 500 thousand bodies, respectively. It is apparent that for large amounts of bodies, the speedups get even higher, reaching almost linear levels. The best speedup I measured when using 32 threads was 31.69, which is extremely good and can't really be improved much further.

The sometimes amazing speedups I measured are definitely due to the embarrassingly parallel nature of the brute-force N-Body simulation algorithm, but also due to the high efficiency of all compiler optimizations, vectorization and the OpenMP interface.

X. PROJECT PROGRESS: INTEL XEON PHI

After I was done with the implementation and benchmarking of the OpenMP parallel version of the N-Body simulation project, it was time to start rewriting the program once again for use on the Intel Xeon Phi coprocessor card.

The exact piece of hardware I used was a Xeon Phi 7120X. It is based on the Knight's Corner architecture, which was unveiled in 2013. It is indeed not the freshest piece of hardware, but it will do just fine. According to Intel's specifications page, ARK[11], this specific coprocessor card contains 61 independent CPU cores, each clocked at 1.24 to 1.33 GHz. It also features a different type of Hyper-Threading technology than Intel's typical CPUs, as each core takes care of up to 4 threads at once. This means that your program can effectively take up 244 threads in all. It also has 16 gigabytes of GDDR5 memory and a 512-bit memory bus. The theoretical

maximum floating-point performance of this particular Phi is 650.5 GFLOPs/s [12].

I ran all benchmarks that were using this device on a small computing cluster back at my home university, the Faculty of Electrical Engineering of the Czech Technical University.

Implementation specifics

Since the source code that I'd developed until this point was already pretty solid when it came to efficient memory usage, I didn't have to change the code too heavily in order to use the Xeon Phi coprocessor efficiently. As the Xeon Phi largely uses OpenMP, I was able to leave the parallelised code I had written earlier in with no modifications. I mainly added some additional directives that helped the device and Intel's compiler link the code. I opted to align all data arrays in order to help take advantage of vectorization; I used the `__attribute__((aligned(256)))` clause when defining each property array to let the compiler know that the corresponding data is properly aligned and can be safely vectorized.

Resulting results and speedups

Benchmarking the Xeon Phi-friendly code was pretty straightforward. I mostly recycled all of the benchmarking scripts that I used in my previous tests.

I used dataset sizes that were identical to all of my previous benchmarks, and after I measured all running times and calculated the resulting performance in GFLOPs/s, I made the chart you can see in figure ?? In it, I made a simple bar graph that illustrates the difference in performance between the Xeon Phi version of my simulation and the previous OpenMP implementation running on 32 threads on a typical x86-64 architecture.

Even though the Xeon Phi uses nearly 8 times the number of threads, it only managed to be approximately 2.3 times as fast as the regular CPU. This is definitely caused by the whole nature of this architecture; instead of a relatively small number of very complex CPU cores, the Xeon Phi relies on a bigger number of very simple cores which operate over a shared memory. It also runs at a much slower clock rate, about a third to a half of that of the regular Xeon CPUs that I used for my previous tests. Its microarchitecture is also quite a bit older than the CPUs I used, which also causes a non-insignificant performance difference.

When taking into consideration the device's maximum floating-point performance of 650.5 GFLOPs/s, my maximum achieved performance of 393 GFLOPs/s is really good. It only reaffirmed the fact that the brute-force N-Body simulation algorithm is computationally not very complex and quite embarrassingly parallel.

Even though the overall running times compared to a "regular" CPU architecture weren't as impressive as I had hoped, I am still glad I could measure the differences between these two wildly different architectures.

XI. ISSUE: ARM-BASED DEVICE

The next part of my project was the addition of results to be gathered from running benchmarks on a device equipped with an ARM-architecture based CPU. For this part of the project, I had picked an OrangePi One development board. This board has a quad-core Allwinner H3 SoC clocked at approximately 1.2 GHz, 512 megabytes of memory and a TDP of approximately 10 watts. I was looking forward to seeing just how much slower this architecture is to any other kind of contemporary architecture.

I ran into quite a big issue, though; the OrangePi device I owned and planned to use ended up not being reachable via `ssh`. After investigating further, it turns the power supply part of its circuitry had failed and thus it wouldn't run at all. I ended up not bothering trying to revive the device and just skip this part of the project altogether. Take these two paragraphs as a sort of an excuse for any results that are missing.

XII. PROJECT PROGRESS: CUDA IMPLEMENTATION

After I was done with all other benchmarks (excluding the ARM architecture for reasons mentioned earlier), I proceeded to create one last implementation of the brute-force N-Body simulation algorithm. This time, I used the CUDA-C language to make a version of the algorithm that could be run on NVIDIA GPUs.

Running any kind of scientific calculations on GPUs is incredibly time-efficient these days, especially so if the calculations are simple in nature and significantly parallel. That is why this algorithm was very suitable to receive a CUDA implementation.

Implementation specifics

The main thing to think about when designing a GPU-based application is the scheduling of threads, and memory management. It is usually a very good practice to chop the tasks that need to be processed into many very small parts and run them all in a massively parallel fashion.

I prepared all of the initial values for the given simulation system using the CPU and main memory, then I proceeded to copy all of those arrays into the graphics card's memory. After these initial steps were done, I simply created a thread for each of the bodies. Each of these threads then looped over all other $n - 1$ bodies in the system and calculated all resulting force vectors. Once this calculation was done, the thread simply updated the corresponding body's property arrays.

When running CUDA kernels on a GPU, it is important to select the right number of blocks and their corresponding size in number of threads. I chose a blocksize of 512, since this value is what I learned is probably the best from my previous homeworks in the CIS 750 course.

Resulting results and speedups

I originally wanted to run this CUDA code on one of Beocat's GPU-equipped nodes. These nodes feature a state-of-the-art NVIDIA GTX 1080 Ti graphics card, which is one of the fastest consumer-grade graphics cards available today.

However, after my benchmarking scripts had been waiting in Beocat's task queue for a week, I turned to benchmarking the application using other, more readily available GPUs.

XIII. CONCLUSION

In this course project for the CIS 750 - Advanced Computer Architecture Experiments course at Kansas State University, I tasked myself with implementing multiple versions of a brute-force or all-pairs algorithm that solves the N-Body simulation problem.

I implemented a naive and an optimized implementation of this algorithm at first, in both sequential and parallel versions, the latter ones using the OpenMP parallel programming interface. I then continued to create an implementation that could be run on the Intel Xeon Phi coprocessor (section X), and another implementation that could be run on NVIDIA's graphics processing units using CUDA technology (XII). I performed all of these implementations in either C++ or CUDA-C (CUDA implementation only). In section XI, I explained an issue I had with one of my proposed project parts and why I decided to skip a part of the project altogether.

For each of these implementations, I created test scripts and used those to benchmark the application on a vast variety of dataset sizes and thread counts. I measured the running times and overall computing performance of each version of the source code.

After the benchmarking was all done, I pooled all the resulting data that I gathered, analyzed it and commented on my findings. I largely confirmed my hypotheses that sacrificing code readability by using a Structure of Arrays kind of memory design would bring noticeable performance improvements, and that, as I showed in section X, using a Xeon Phi coprocessor would yield solid speedups, despite the exact model I used in my project being quite old and relatively slow.

I also found that using CUDA technology for this kind of simulation is indeed a very good idea and that its performance is very respectable.

I wish I could have tried to benchmark an ARM-architecture based device as well, but time management and an unexpected hardware failure forced me to not perform any tests on such a device.

In the future, I think it would be beneficial to repeat the project using the Barnes-Hut algorithm (that I briefly described in section III) and re-run all the benchmarks, just to see how much more efficient it really is, even if it's not as embarrassingly parallel as the brute-force algorithm.

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