GPU in Physics Computation: Case Geant4 Navigation

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Abstract. General purpose computing on graphic processing units (GPU) is a potential method of speeding up scientific computation with low cost and high energy efficiency. We experimented with the particle physics simulation toolkit Geant4 used at CERN to benchmark its geometry navigation functionality on a GPU. The goal was to find out whether Geant4 physics simulations could benefit from GPU acceleration and how difficult it is to modify Geant4 code to run in a GPU.

We ported selected parts of Geant4 code to C99 & CUDA and implemented a simple γ-physics simulation utilizing this code to measure efficiency. The performance of the program was tested by running it on two different platforms: NVIDIA GeForce 470 GTX GPU and a 12-core AMD CPU system. Our conclusion was that GPUs can be a competitive alternate for multi-core computers but porting existing software in an efficient way is challenging.

1 Introduction

Graphic processing units (GPUs), also known as graphic adapters, or 3D cards, were originally expansion cards for personal computers. The purpose of these devices is to externalize graphics related computing from the main processor (CPU) and to increase the speed of these calculations with specialized hardware. The main driving force of GPU technology development has been the demand for fast 3D graphics in computer games. Polygon-based rendering is an ideal application for specialized parallel co-processor architectures. Subsequently, more complex and customizable computation capabilities have been added, and recently, GPUs have developed into fully programmable general purpose parallel computers [13].

The modern GPUs can achieve high computation speeds, measured in floating point operations per second (FLOPS), compared to their size, cost and energy consumption. This makes them attractive for use also outside the computer game industry. These devices, and similar GPU-derived accelerators with no graphic processing capabilities, have recently developed interest in many fields of scientific computing and have been successfully used to speed up vari-
ous applications. The high computing performance on GPUs is based on massive parallelism and is generally achievable only if the computation can be split into a large number of parallel tasks that require little global communication. GPU programming can be done using relatively high-level languages and toolkits with varying level of portability. Alternatives include NVIDIA’s CUDA and the newer cross-platform OpenCL by Khronos group.

In the current work we study whether GPUs are beneficial for particle physics simulations and how existing physics software can be ported to GPUs. The motivation for our research is the Large Hadron Collider particle accelerator that started running at CERN during in late 2009 and it is now producing data for physics experiments. The purpose of this accelerator is to provide new information on the basic structure of matter. From computing and data storage point of view, LHC experiments produce over 15 petabytes of data annually.

2 Background

2.1 Monte Carlo Simulations in Particle Physics

Particle physics simulations have an essential role in contemporary experimental nuclear and particle physics. They are used in designing and calibrating particle detectors and generating detectable signatures for hypothesized physics phenomena. Modern particle physics experiments require increasingly large amounts of Monte Carlo data from complex and computationally intensive simulations. Examples of physics experiments requiring extensive Monte Carlo simulations include CMS and ATLAS experiments related to the Large Hadron Collider (LHC) at CERN, Geneva, Switzerland.

Monte Carlo particle physics simulations are also important in other fields, such as medical physics, where an example application is the planning of maximally safe and accurate radiotherapy treatments.

2.2 Geant4

Geant4 is “a toolkit for simulating the passage of particles through matter”. It can simulate a comprehensive set of different physical processes over a wide range of particle energies for a variety of long-lived particles. It is designed to offer a comprehensive set of functionalities needed to construct a (Monte Carlo) particle physics simulation program for a specific setup. It is a large object oriented system implemented in C++.

The Geant4 toolkit is used in many contemporary particle physics experiments, such as CMS and ATLAS at CERN and BaBar at SLAC. It is also utilized in medical applications, for example in radio therapy planning.


2.3 The NVIDIA Fermi GPU Architecture

This is a brief description of the hardware architecture (NVIDIA “Fermi”) of the GPU used in our experiments. Its differences compared to contemporary multi-core CPU architectures are a key factor determining the performance of GPU programs.

In the Fermi architecture [1], a device (e.g. one GPU) consists of several (e.g. 16 on the Tesla GPUs) streaming multiprocessors and each multiprocessor has a number (32) of cores. Each core executes a warp of threads (32 threads) in a manner called Single-Instruction, Multiple-Thread (SIMT) by NVIDIA. In SIMT, the threads in one warp always execute a common instruction with different data. If the instruction paths of the threads diverge on a data-dependent branch instruction, the divergent branches are executed sequentially, that is, threads in one branch wait for the threads in the other branch to execute. SIMT can be viewed as a special case of the SIMD (Single-Instruction, Multiple-Data) architecture.

The device has a large global memory with unsynchronized read-write access from the multiprocessors. There is also cached read-only memory, constant memory and special texture memory with automatic interpolation. Each multiprocessor has a smaller amount of shared memory that can be used manually for local synchronization or automatically as L1 cache for the global memory. In addition, each multiprocessor has a set of 32-bit registers. The Fermi GPUs are capable of native 32-bit and 64-bit IEEE-compliant floating point calculations.

In order to efficiently exploit the full potential of a Fermi GPU, one must be able to parallelize the computational problem to thousands of threads that require little global synchronization. One multiprocessor can execute $32 \times 32 = 1024$ threads concurrently and to hide latencies from global memory access with context switching, there should be multiple warps of suspended threads waiting on each multiprocessor. There are also other constraints, such as the limited number of registers on each multiprocessor.

Because of these constraints and the nature of SIMT architecture, algorithms that can be implemented efficiently on parallel MIMD (Multiple-Instruction, Multiple-Data) machines, such as multi-core CPUs, do not necessarily execute efficiently on NVIDIA GPUs.

3 Methods

We study a minimalistic Monte Carlo physics simulation program for calculating where $\gamma$-particles interact with matter. A similar program could, in theory, be used as an GPU accelerated part of a more complex physics framework. The most computationally intensive parts of this program are the geometry navigation calculations (see section [3.2]), that are done using Geant4 code.
Algorithm 1 Monte Carlo simulation for free path lengths of particles

1. Generate $W \sim \text{Uniform}((0, 1])$
2. Set $Y = -\log W$ (now $Y$'s have distribution $\text{Exp}(1)$)
3. Calculate $T = G^{-1}_{x_0, \omega}(Y)$ as follows:
   - Set $S_0 = 0$, $t_0 = 0$, $j \leftarrow 0$
   - While $S_j < Y$, do
     - Set $j \leftarrow j + 1$
     - Compute the next intersection $t_j > t_{j-1}$ and get $\mu_j$ using Geant4.
     - Set $S_j = S_{j-1} + (t_j - t_{j-1})\mu_j$ (may be $\infty$)
   - Set $T = t_{j-1} + \frac{Y - S_{j-1}}{\mu_j}$

3.1 The Simple Particle Physics Simulation

Suppose a beam of $N(0)$ particles moves through matter. The number of particles left after distance $x$ can be modeled with the differential equation
\[
\frac{dN(x)}{dx} = -N(x)\mu(x),
\] (1)
where $\mu = \sigma \rho N_A/A$ is the mean free path in a material with density $\rho$, atomic weight $A$ and a total cross section of $\sigma$. The solution of (1) is
\[
N(x) = N(0)e^{-\int_0^x \mu(y)dy} =: N(0)e^{-G(x)}
\] (2)
and the probability of a single particle interacting before traveling distance $x$ is therefore
\[
\mathbb{P}(X < x) = 1 - \frac{N(x)}{N(0)} = 1 - e^{-G(x)},
\] (3)
where $X$ is a random variable representing the free path length of the particle. Assuming $G$ is invertible, we can generate random variables $Z$ with this distribution from $\text{Exp}(1)$-distributed variables $Y$ as
\[
Z = G^{-1}(Y).
\] (4)

Suppose we have a geometry of objects defining an attenuation coefficient $\mu(x)$ in a point $x \in \mathbb{R}^3$, and a particle with starting point $x_0$ and a unit direction $\omega$. The probability of the particle interacting before distance $t \geq 0$ is
\[
\mathbb{P}(T < t) = 1 - e^{-\int_0^t \mu(x_0 + y\omega)dy} =: 1 - e^{-G_{x_0, \omega}(t)}.
\] (5)
To generate random variables $T$ with the correct distribution, one must be able to compute $G^{-1}_{x_0, \omega}(t)$. Suppose the geometry is composed of a finite amount of
different materials that define regions with piecewise smooth boundaries. Then
we may calculate the integral as

\[ G_{x_0, \omega}(t) = \sum_{i=1}^{M} (t_i - t_{i-1}) \mu_i + (t - t_M) \mu_{M+1} =: S_M + (t - t_M) \mu_{M+1} \]  

(6)

and

\[ G_{x_0, \omega}^{-1}(z) = t_M + \frac{z - \sum_{i=1}^{M} (t_i - t_{i-1}) \mu_i}{\mu_{M+1}} = t_M + \frac{z - S_M}{\mu_{M+1}} \]  

(7)

where \( 0 = t_0 < t_1 < \ldots < t_M < t \) are the distances to the different material
boundaries in the path of the particle and \( \mu_i \) are the mass attenuation coefficients
of the corresponding materials:

\[ \mu(x_0 + t \omega) = \mu_i \] for all \( t \in (t_{i-1}, t_i) \).  

(8)

We may therefore generate random variables \( T \) with distribution [5] using an
uniform random number generator and Geant4 as described in algorithm [1].

3.2 Geant4 navigation

In Geant4 terminology navigation is the part of the toolkit that can solve the
following simply-stated, interrelated, geometrical problems:

- If a particle is in point \( A \), inside which geometrical objects, volumes, is it?
- Will the particle hit a volume boundary, that is, will it exit a volume or
  enter a new one on its way to point \( B \)? If so, where, and what is the
  normal of the boundary surface at that point?

These are subproblems for calculating the track of a particle that can interact
with the different materials it passes through. To solve these problems efficiently
to calculate the full track, one stores the navigation history of a particle. The
navigation history describes the volumes, inside which the particle currently is.
A general Geant4 geometry comprises a hierarchy of nested volumes and the
navigation history may indeed contain many levels. The full state, including the
navigation history, of the particle is stored in the navigator, which also has other
information, such as the normals of the last crossed surface boundaries.

3.3 Porting Geant4 Navigation to CUDA

The involved parts of Geant4 were first isolated from the full Geant4 code. They
were subsequently translated from C++ to C99 by replacing C++ classes with
C structs, their methods with functions with this-pointers as parameters and
replacing C++ standard library containers with C-arrays. C++ virtual function
were implemented using “fork” functions that call the appropriate implementation
based on the object type. This was because of the lack of function pointer
support in the CUDA version we used. The reason to translate the program to
C was to allow the program to be also compiled as OpenCL.
3.4 Benchmark Program

The basic operation principle of the benchmark program is listed as algorithm 2. The execution phase (5) is timed. All random numbers (in phase 3) are generated using the Mersenne Twister [14] pseudo-random number generator from the Boost C++ library. The CPU version of the program can be described as leaving out the transfer phases (4) and (6). The single-threaded CPU version of the program does phase (5) sequentially. A multi-threaded CPU version that uses OpenMP [7] to parallelize phase (5) is also implemented. The GPU version of the program uses CUDA.

Algorithm 2 Basic phases of the benchmark program

1. Load the geometry and transfer it to GPU memory.
2. Generate \( N \) particles: directions and initial positions \((\omega, x_0)_i, i = 1, \ldots, N\).
3. Generate an (exponentially distributed) “lifetime” number \( Y_i \) for each particle.
4. Transfer initial particle states and lifetimes to GPU memory.
5. Calculate the free path lengths \( T_i \) from \( Y_i, (\omega, x_0)_i \) as in algorithm 1 for each particle in parallel.
6. Transfer the free path length data \( T_i \) back to host memory.

In this program, the attenuation coefficients \( \mu \) are calculated from the densities \( \rho \) in the model geometry as

\[
\mu(x) = \rho(x)\mu_{\text{Al},E},
\]

where \( \mu_{\text{Al},E} \) is the mass attenuation coefficient of photons in aluminum for given photon energy \( E \). In our tests, all particles have the same energy, 1 MeV, that, according to [5], corresponds to a mass attenuation coefficient \( \mu_{\text{Al},E} = 0.06146 \text{ cm}^2/\text{g} \).

3.5 Test inputs

We use two different test geometries and two different particle distributions in order to demonstrate how the relative performances of CPU and GPU versions of the same code can have heavy input dependence. In both cases we have \( N = 100000 \) input particles.

In the Random particle setup the directions of the particles, \( \omega \), are uniformly distributed on the unit sphere \( S^2 \). The lifetimes of the particles are generated from the exponential distribution. The output of the program is a random sample from the distribution of the free path lengths of the particles. In the Regular
setup, the particles travel towards a regular 400×250 grid and are input to the program in column-major order. Instead of generating Exp(1) distributed lifetimes, all particles are assigned an equal lifetime of 1. In practice, the output in this case is a 400×250 volume raytraced bitmap image of the geometry.

The first test geometry, Spheres, consists of 8000 aluminium balls placed on a regular grid in a 5×5×5 meter vacuum cube. All particles start from the center of the geometry. The other, more complex, geometry, CMS, is based on a model of the CMS detector [6]. It is constructed by extracting all supported types of solids, namely boxes, tubes and cones, from the original model. The densities of the materials in the CMS model are also imported to the program.

4 Results

The GPU version of the program described in Section 3.4 was tested on a Linux desktop with an NVIDIA GeForce 470 GTX GPU. Both CPU programs, the single- and multi-threaded versions, were run on a 12-core AMD CPU system (2 × 6-Core AMD Opteron 2427). The execution times of the program in different test cases are shown in Table 1. In all test cases, the GPU was faster than a single CPU core. However, the speedup varied dramatically depending on the input. In the most beneficial example, the GPU was over 13 times faster than the single-threaded CPU version and 60% faster than the 12-core CPU system. In the most realistic example (CMS, Random), the GPU was only 60% faster than the single-threaded CPU version and the 12-core system performed 7 times better than this.

In addition to the run times, we also measured energy usage of the test hardware. The results are shown in Figure 1. The idle power consumption of GPU is around 20 W that means around 25% increase. The peak power of GPU is around 165W that more than doubles the consumption of the desktop.

![Figure 1: Power usage of test hardware](image-url)
Table 1: Performance of the benchmark simulation

| Geometry | Particles | Platform        | Exec. time (ms) | Speedup factor |
|----------|----------|-----------------|-----------------|----------------|
| Spheres  | Regular  | CPU, 1-thread   | 442             | 1              |
|          |          | CPU, 12-thread  | 54              | 8.2            |
|          |          | GPU             | 33              | 13.3           |
|          | Random   | CPU, 1-thread   | 458             | 1              |
|          |          | CPU, 12-thread  | 56              | 8.2            |
|          |          | GPU             | 114             | 4.0            |
| CMS      | Regular  | CPU, 1-thread   | 22431           | 1              |
|          |          | CPU, 12-thread  | 1862            | 12.0           |
|          |          | GPU             | 8881            | 2.5            |
|          | Random   | CPU, 1-thread   | 15493           | 1              |
|          |          | CPU, 12-thread  | 1316            | 11.8           |
|          |          | GPU             | 9977            | 1.6            |

5 Discussion

Execution path divergence within a warp of threads is a key performance factor on the SIMT architecture [1]. In theory, heavy divergence can potentially slow down the program by up to a factor 32. The level of actual run-time divergences (that determines the performance) depends not only on the number of branching instructions in the program, but also on its input.

Geant4 Navigation code is complex and heavily branching and thus as such not optimal for the SIMT architecture. For regular enough input, however, the number level of divergence is low and the program performs well on the GPU. Our more realistic inputs do not exhibit such regularity and the corresponding GPU performance is poor. The performance is also be affected by other factors than branching, such as register space, memory access patterns and double precision floating point performance. CUDA profiler results showed that register space constraints were indeed a bottleneck factor limiting the performance of our application. This is probably due to the relatively large per-particle Geant4 navigator data structures required in our implementation.

We also tried more complex load balancing schemes on the GPU, such as using CUDPP[10] to periodically remove empty slots (of finished particles) from the warps with parallel stream compaction operations and refilling the GPU with new particles to maximize occupancy. Again, depending on the test case, this resulted to some speedup, but no dramatic performance increases were observed.

GPU implementations of Monte Carlo particle physics simulations have also been studied by [11] and [12]. Jahnke et.al. [11] have implemented a Geant4-based software for radiotherapy calculations on GPUs using CUDA. They report a 10–30 times speedup compared to a single core CPU when using an NVIDIA GTX 8800 graphics card. Jia et al. [12] have implemented a dose planning...
method package, also for radiotherapy, in CUDA, and report 5–7 times speedups when an NVIDIA Tesla C1060 GPU is compared against a 2.27GHz Intel Xeon CPU.

Our results are not that promising. Different test hardware can explain results a lot, but it also seems that efficient implementation of GPU algorithms is also essential. The problem in this approach for hardware benchmarking is that it is very difficult to compare the performance of different algorithms on different hardware.

It seems that an efficient GPU implementation of Geant4 in this context would indeed require rewriting the algorithms for the target GPU architecture, instead of porting code to CUDA as such. Especially, our results show, that it is not sufficient for an algorithm to be easily parallelizable on CPU (MIMD) architectures to yield an efficient GPU implementation.

6 Conclusions

We ported a piece of code from a large particle physics simulation toolkit to a general purpose GPU and compared its performance in a GPU and a 12 core CPU server.

The results indicated that the performance on the GPU may be heavily input-dependent. In our test cases, the GPU program, when compared to a single-threaded CPU version, was faster by a factor 1.6 – 13, depending on the test case. The corresponding speedup factor on the 12-core CPU system was 8–12 and it outperformed the GPU in most cases.

The algorithms were originally designed for CPUs and quite straightforwardly ported to GPU. Our results indicated that an efficient GPU implementation of Geant4 in the particle physics context would probably require rewriting the algorithms for the target GPU architecture.

Based on our case, we can say that GPU computing can be a cost-effective solution for simple enough problems but accelerating complex software packages efficiently using GPGPU is not necessarily a feasible alternative, even if the software was easily parallelizable on CPU systems.

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