The State of Monte Carlo Neutron Transport: The Role of GPUs and Portable Performance Abstractions

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Abstract—Since near the beginning of electronic computing Monte Carlo neutron transport has been a fundamental approach to solving nuclear physics problems. Over the past few decades Monte Carlo transport applications have seen significant increase in their capabilities and decreases in time to solution. Research efforts have been focused on areas such as MPI scalability, load balance with domain decomposition, and variance reduction techniques. In the last few years however the landscape has been changing. Due to the inherently parallel nature of these applications Monte Carlo transport applications are often used in the super-computing environment. Supercomputers are changing, becoming increasingly more parallel on node with GPGPUs and/or Xeon Phi co-processors powering the bulk of the compute capabilities. In order to fully utilize the new machines capabilities it is becoming ever more important to migrate to a many-core perspective of any computing algorithms. Monte Carlo transport applications, like many others, have the potentially difficult task of figuring out how to effectively utilize this new hardware. Many groups have taken the initial steps to look into this problem or have focused their efforts on a sub-problem, such as continuous energy lookups. In other fields a promising approach is displayed in the use of portable performance abstractions in order to specify what is parallel. These abstractions provide the foundations for applications to write code once and run on any supported platform. This paper describes the state of the art in Monte Carlo neutron transport, with a special emphasis on the affects of upcoming architectures.

Contents

I. Introduction

Today's Supercomputer landscape is in flux. Supercomputer architectures are making more extreme changes then they have undergone in 20 years. One big driving factor for this change are the concerns about energy usage as we scale to larger and larger machines. A metric, FLOPS/Watt is often used to describe this relationship. In order to maximize the FLOPS/Watt metric, architectures are shifting away from fast and complex multi-core CPUs and adding in much larger numbers of much slower simpler processors. The amount of parallelism available on any given node in a supercomputer is growing but factors of hundreds or thousands because of this change. This change brings new and interesting challenges that need to be overcome.

In addition to the increase in node level parallelism, it is unclear which architecture choice will prove to be a winning design. Currently there are many different architectures to choose from when designing a supercomputer and there is no obvious choice to place one design above the others, or if any of these designs are going to end up above the others. NVIDIA provides General Purpose Graphics Processing Units (GPGPUs) which are a highly parallel throughput optimized devices. Intel provides their Many Integrated Core (MIC) co-processor which provides large vector lanes and many threads. Other groups are turning to Field Programmable Gate Arrays (FPGAs) for a solution. Across the Department of Energy (DOE) National Labs both the NVIDIA and Intel approaches are being pursued in their newest procurements [1], [2].

Application developers now face a complex and unclear path forward. There is additional levels of complexity and potentially large application changes that will need to be made in order to effectively utilize this increase in parallelism. In addition, an application programmer cannot simply begin a cycle of porting to a new hardware architecture. Instead, applications need to address the issue of portability as well as performance or they run the risk of becoming outdated or unusable very quickly. This problem is especially challenging when optimization choices for one architecture can contradict with optimization choices on another architecture.

There are a large number of physics and multi-physics applications that exist today that must figure out how to navigate this complex and challenging landscape. Simple ports to new architectures are often not enough to guarantee performance, and will still require applications to be ported multiple times to multiple architectures. This paper will explore these concerns and today's current efforts for portable performance solutions in the scope of one of these physics applications, Monte Carlo Neutron Transport.

II. WHAT IS MONTE CARLO NEUTRON TRANSPORT?

"The first thoughts and attempts I made to practice [the Monte Carlo method] were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaire. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays. This was already possible to envisage with the beginning of the new era of fast computers, and I immediately thought of problems of neutron diffusion and other questions of mathematical physics, and more generally how to change processes described by certain differential equations into an equivalent form interpretable as a succession of random operations. Later... [in 1946, I] described the idea to John von Neumann and we began to plan actual calculations."

- Stan Ulam 1983 [3]

John von Neumann became interested in Stan Ulams idea and was outlined in detail how to solve the neutron diffusion and multiplication problems in fission devices. Since this time Monte Carlo methods have continued to be a primary way for solving many questions in Neutron transport. [3]

A. Definition

E. E. Lewis and W. F. Miller Jr. in Computational Methods of Neuron Transport describes Monte Carlo transport as a simulation of some number of particle histories by using a random number generator. For each particle history that is calculated, random numbers are generated and used to sample from probability distributions describing the different physical events a particle can undergo, such as scattering angles or the length between collisions. Ivan Lux and Laslo Koblinger further this definition in their book Monte Carlo Particle Transport Methods: Neutron and Photon Calculations:

"In all applications of the Monte Carlo method a stochastic model is constructed in which the expected value of a certain random variable (or of a combination of several variables) is equivalent to the value of a physical quantity to be determined. This expectation value is then estimated by the averaging of several independent samples representing the random variable introduced above. For the construction of the series of independent samples, random numbers following the distributions of the variable to be estimated are used." [4]

Estimating this type of quantity takes on this mathmatical form:

$$\hat{x} = \frac{1}{N} \sum_{n=1}^{N} x_n,$$

where x_n represents the contribution of the nth history for that quantity. And so for the Monte Carlo method we tally the x_n from each particle history in order to compute the expected value $\hat{x}$. [5]

One very important question to answer with any statistical answer is just how good is our estimated value $\hat{x}$ when we compare to the true value $\bar{x}$. It turns out that the uncertainty in $\hat{x}$ decreases with increasing numbers of particle histories, and generally falls of asymptotically proportionate to $N^{-1/2}$. [5]

B. The Equation

The equation being solved by the neutron transport problem, shown below, displays each of the pieces that makes up a full Monte Carlo transport algorithm. This equation is known as the Linearized Boltzmann transport equation for neutrons:

$$\frac{1}{\nu}\frac{\partial \Psi(\vec{r}, E, \Omega, t)}{\partial t} + (\nabla \cdot \Omega)\Psi(\vec{r}, E, \Omega, t) + \Sigma_a(\vec{r}, E)\Psi(\vec{r}, E, \Omega, t)$$
$$=$$
$$\int_{E'} \int_{\Omega'} \Sigma_s(\vec{r}, E', \Omega' \to E, \Omega)\Psi(\vec{r}, E, \Omega, t)d\Omega'dE' +$$
$$\chi(E) \int_{E'} \nu(E')\Sigma_f(\vec{r}, E') \int_{\Omega'} \Psi(\vec{r}, E, \Omega, t)d\Omega'dE' +$$
$$S_ext(\vec{r}, E, \Omega, t)$$

[6] where $\Psi(\vec{r}, E, \Omega, t)$ is angular flux, $\Sigma_a(\vec{r}, E)$ is the macroscopic cross section for particle absorption, $\Sigma_s(\vec{r}, E', \Omega' \to E, \Omega)$ is the macroscopic cross section for particle scattering, $\Sigma_f(\vec{r}, E')$ is the macroscopic cross section for particle production from a fission collision source, $\chi(E)$ is a secondary particle spectrum from he fission process, $\nu(E)$ is the average number of particles emitted per fission, $S_ext(\vec{r}, E, \Omega, t)$ represents an external source, $\vec{r}$ is the spacial coordinates, E is the energy, Ω is angular direction, and t is the term for time. [6]

C. Algorithm Approach

While there are many ways people can solve this problem generally people consider tracking particle histories and the algorithm that follows is often called the history based approach because of this. Algorithm 1 shows the history based approach for a simple research code [7] but has the same properties we can use to describe the method. Algorithm 2 shows the outer most scope of a Monte Carlo Problem for referencing where different optimizations or stages occur. For example in Algorithm 1 this takes place inside the Cycle Loop and shows only the steps for Cycle Tracking.

Algorithm 1: History based Monte Carlo algorithm

---
1 **foreach** *particle history* **do**
2   **while** *particle not escaped or absorbed* **do**
3   sample distance to collision in material
4   sample distance to material interface
5   compute distance to cell boundary
6   select minimum distance, move particle, and perform event
7   **if** *particle escaped spatial domain* **then**
8   update leakage tally
9   end particle history
10   **if** *particle absorbed* **then**
11   update absorption tally
12   end particle history

Algorithm 2: Monte Carlo Method

---
1 Parse Inputs
2 **foreach** *Cycle* **do**
3   Cycle Initialize
4   Cycle Tracking
5   Cycle Finalize
6 Gather Tallies

III. STATE OF THE ART RESEARCH

In order to understand the state of the art research in Monte Carlo transport, it is important to have some perspective on what has been done in the field already. There is a long history of research and improvements for Monte Carlo transport problems and understanding this path and the machines that that research was designed for can help guide analysis of more recent efforts. In the field of Monte Carlo transport most research in the last 5 years has been related to GPGPU computing or has been physics based as apposed to computer science based research. We will review and discuss the GPU research in a later section. In this section we will look at the significant areas of interest when dealing with Monte Carlo transport applications that do not pertain to GPUs, namely Parallel performance on different architectures, load balancing,

optimizations in nuclear data look-ups, and research dealing with variance reductions.

A. Parallel Performance

In this section we will see the parallel performance of a number of different Monte Carlo particle transport applications on different architectures ranging from the vector machines of the 80's to multi-core compute clusters.

Shared Memory Performance

Shared memory systems refer to machines or models where all processors can access the same memory space. Taking this a step further the unified memory architecture (UMA) shared memory systems not only do all processors have access to the same memory but they also have access to all memory in the same time [8]. One type of shared memory system that was popular in the 1970's and 1980's was the vector machine. Vector machines took the shared memory system and added additional synchronicity to the system by making all of the processors issue the same instruction [9].

Vector Machine Performance

In the 1980's Monte Carlo transport algorithms began adapting "event-based" methods in order to vectorize their algorithms for use on a vector machine. These new algorithms were used because the traditional history based approach has complete independence of particle histories. But in order to effectively utilize the vector architecture particles must be computed on the same code paths. By changing the algorithm to follow events instead of histories the Monte Carlo method could be used in a vector based approach. [10]

One common element when reviewing the work done in this area is to see that the vector approach is often related to stacks, and properly organizing particles into the right stack so that calculations can be preformed [11], [12]. Another approach is to try to use only one main stack and pull off only the minimum information needed to compute the events into sub-stacks [10]. With each of these approaches particle events determine how the particles are organized or what information is needed for processing. The main drawback to the event based approach is the added time processing data movement or sorting.

Brown reported theoretical speedups of 20x-85x for his consideration and deemed this approach well worth the efforts required to change codes around in order to use this approach [11]. Martin saw speedups randing from 5x to 12x depending on the problem and the machine he was running on by using the single big stack, sub-stack approach [10]. Bobrowicz explicit stack approach reaches speedups of around 8x - 10x compared with the original history-based approach [12]. Finally Burns in using a LANL Benchmark code GAMTEB showed he could acheive similar performance to Bobrowics by following a similar approached as that laid out by Brown [13].

TABLE I
PARALLEL PERFORMANCE ON THE MTA USING MULTITHREADING

Procs	Time (sec)	Speedup	Efficiency
Parallelization by zones only			
1	764	1.00	1.00
2	400	1.91	0.95
4	227	3.37	0.84
8	167	4.58	0.57
Parallelization by zones and energies			
1	745	1.00	1.00
2	370	2.01	1.01
4	187	3.98	0.99
8	94	7.92	0.99

Multi-Threaded Architecture Performance

Other shared memory systems, separate from vector machines, where tried in this time. One such machine was the Tera Multi-Threaded Architecture (MTA). This approach focused on the use of incredibly parallel processors, hardware threading, and a simple shared memory, no cache, design. The idea was by focusing on threading they could mask away memory latency [14], [15].

One Photon transport application tried two methods of parallelizing their application on the Tera MTA. For their problem the zones and energies of the region needed to be looped over and photons falling in those ranges where then computed. So for their application they chose to parallelize over zones and also over zones and energies at once through loop unrolling. Table I shows that the parallelization on the MTA over zones and energies maintains incredible efficiency giving their application good speedups here, while parallelizing over only zones does not expose enough parallel work to hide memory latency and so efficiency drops of quickly.

More modern systems utilize shared memory ideas as well, with a majority of the scientific efforts utilizing openMP threading models for shared memory processing. Often this model is overlooked in preference of distributed computing via MPI but that is not always the case. Given an all particle method, openMP codes tend to scale incredibly well with the only draw backs having to do with those few areas requiring atomic operations. With, in my experience, an nearly perfect efficiency on a node, in the case of no atomic operations and plenty of work.

Distributed Memory Performance

One of the major transitions in supercomputing came with the shift from vector computing to distributed memory computing. This type of computing is most often done with MPI and has, for the last 20 years, been a primary method of achieving parallel performance on clusters and supercomputers alike. In the message passing model of parallelism, independent processes work together through the use of messages to pass data between processors. In this model, parallel efficiency is generally improved by spending more time working independently and is negatively affected by time spent sending messages [16].

The Monte Carlo particle transport history-based approach lends itself to the distributed model very well. Since each particle history is independent of any other particle histories and can be easily split up over processors [16]. The only complications we normally see when we move to the distributed memory systems is that we often use domain decomposition which increases the complexity and use of the message passing interface. We will discuss the domain decomposition challenges in the load balance section under state of the art research.

Given the embarrassingly parallel nature of the Monte Carlo transport problem, the performance of this model produces results as suspected. As we increase MPI processes we continue to get a nearly liner speedup. Majumdar shows that with 16 nodes and 8 MPI tasks per node, his biggest run, he was still able to achieve a 88% efficiency [14] in his code that was parallel over zones and energies. In an all particle code, Mercury at LLNL, we can see parallel efficiencies of 80-90% when using MPI parallelism [17].

Distributed + Shared Memory Performance

Given the heterogenous nature of todays computing environment, and even in the fairly homogenous environment we are leaving, it is a common next step to consider combining distributed and shared memory parallel schemes. It seems an obvious extension to either of these models to add the other. Shared memory parallelism exists on a node or on one of the new accelerator devices. Distributed memory parallelism provides the opportunity for scaling to large supercomputers or clusters, giving you many nodes to work with. Given the nature of these two models it is surprising how often the additional extension of combining them is not done as most often shared memory models are overlooked in favor of distributed models, and since the distributed model works "well enough" even with in a node, it is often not worth the effort to try to combine these two methods. This is no longer going to be true when we start adding accelerators and many people have found benefits of combining these models anyways.

The combined distributed-shared model is often referred to as MPI+X [18]. The X in this description being replaced with whichever shared memory system is preferred. The most common implementation of MPI+X to date is the MPI + OpenMP model. Utilizing MPI for node to node communication and OpenMP for on node parallelism [18].

Yang has recently shown that the MPI+OpenMP model has benefits of achieving the nearly perfect parallel efficiency one would expect as well as significantly decreasing the memory overhead to an equivalent MPI only implementation. He was able to show 82-84% parallel efficiencies and a decrease in memory cost from $\tilde{1}.4GB$ to $\tilde{2}00MB$ for 8 processors [16]. Majumdar shows that with 16 nodes and 8 OpenMP threads per node, he was able to achieve a 95% parallel efficiency which is an improvement over the his MPI only methods 88% parallel efficiency [14].

B. Load Balance and Domain Decomposition Algorithms

In order to achieve high levels of parallelism in transport problems with many geometries or zones different parallel execution models are used. Two primary models used are domain decomposition and replication. Domain decomposition involves spatial decomposition of the geometry into domains, and then the assigning of processors to work on specific domains. Replication involves storing the geometry information redundantly on each processor and assigning each processor a different set of particles. [19] [17]

Load balance is often discussed in conjunction with domain decomposition since particles often migrate between different regions of a problem and so not all spatial domains will require the same amount of computational work. In many applications there is at least one portion of the calculation that must be completed by all processors before all the processors can move forward with the calculation. If one processor has more work than any other all of the others must wait for that processor to complete its work [19] [17]. This load-imbalance can cause significant issues with scalability as paralleism is increased from hundreds to millions of processors [20].

When to Load balance: One key consideration when wanting to preform a load balance calculation is to understand the cost of preforming that calculation as well. If too much time is spent making sure the problem is always perfectly load balanced then computational resources are being wasted on a non-essential calculation resulting is overall slower performance. However, if too little resources are devoted to load-balancing than the problem will suffer from load-imbalance and the negative effects that entails. One solution is to preform load balance at the start of each cycle or iteration of a Monte Carlo transport calculation but only when that load balance will result in a faster overall calculation [19] [17].

An algorithm to determine when to load balance was explained in references [19] [17] where the following criterion could be checked inexpensively each cycle to determine if a load-balance operation should take place. First, is to compute a speedup factor by comparing current parallel efficiency (ε_C) to what parallel efficiency would be if processors were to redistribute their load (ε_{LB}). Second, is to predict the run time by using the time to execute the previous cycle(τ_{Phys}), the speedup factor(S), and finally the time to compute the load balance itself(τ_{LB}). Finally ,is to compare the predicted run with and without load balancing to determine if the operation is worth while. [19] [17]

$$S = \frac{\varepsilon_C}{\varepsilon_{LB}} \tag{1}$$

$$\tau^{'} = \tau_{Phys} \cdot S + \tau_{LB} \tag{2}$$

$$\tau = \tau_{Phys} \tag{3}$$

$$if\ (\tau^{'} < 0.9 \cdot \tau\ )\ DynamicLoadBalance(); \tag{4}$$

Extended Domain Decomposition: As an extension to the domain decomposition of meshes, O'Brien and Joy demonstrated an algorithm to domain decompose Constructive Solid Geometry (CSG) in a Monte Carlo transport code. One key difference between mesh and CSG geometries is that mesh geometries contain a description of cell connectivity where as cells defined though CSG do not. In order to domain decompose these CSG cells each cell was given a bounding box and since each domain is also a box a test for if a cell belongs inside a domain becomes an axis-aligned box-box intersection test. [21]

In addition to pure mesh and pure CSG problems other combinations might be useful, such as the combination of mesh and CSG problems where there are large-scale heterogeneous and homogeneous regions. In this method a mesh region is embedded inside a CSG region allowing for the use of each in whichever region one or the other is more optimal. [22]

Load Balance at Scale: When load balancing massively parallel computers it is unscalable to need to examine the workload of every processor. O'Brien, Brantley and Joy present their scalable load balancing algorithm that runs in $\Theta(log(N))$ by using iterative processor-pair-wise balancing steps that will ultimitely lead to a balanced workload. Their algorithm shows remarkable ability to load balance and is demonstrated up to 2 million processors on the Sequoia supercomputer at Lawrence Livermore National Laboratory. [20]

The pair-wise load balancing scheme maintained a high efficiency; with the load-balanced runs maintaining efficiencies of 95% at 2 million processors when the not load-balanced runs continuously drops to around 68% efficiency at 2 million processors. In addition the load-balanced version is able to maintain near perfect scaling up to 2 million processors. By dispersing the workload over processors effectively it also decreases the overall tracking time. [20]

Algorithms that interact with the particles and geometries can also be revisited after domain decomposition is added. Specifically a Global Particle Find algorithm, a test for done, and domain neighbor replication. The global particle find can be solved with a simple tree search; even though building the tree is not a scalable algorithm it is fast. By using MPI_I allreduce() for the global test for done in place of a complex hand coded algorithm scalability and ease of maintenance is achieved. Lastly, the domain neighbor replication algorithm ended up being very important or scalability and achieved 100% load balance and reduced memory usage by using a recursive Euclidean GCD algorithm to build a bipartite graph between adjacent domains. [23]

C. Nuclear Data

A large part of many Monte Carlo transport calculations is the process of looking up nuclear data information. Both microscopic and macroscopic cross section information is needed in order to understand what reactions a particle undergoing a collision will do. Depending on the problem and the choices made to solve it, time spent looking up nuclear data can often be between 10% and 85% of the over all runtime. The problems that spend more time looking up cross section data are often using what is known as the continuous energy model where energy value are stored as a large sequence of points

and exact values are found through interpolation. The second method that is used which makes cross section lookups faster but less accurate is multi-group cross sections, where cross section data is stores in some number of bins and all energies that land in the bin are given the same value. This can often reduce the search many orders of magnitude.

Research that deals with nuclear data lookups is often concerned with speeding up the search for a given cross section at a given energy. This search problem is the main bottleneck in the cross section lookup algorithms. Linear searches, binary searches, and Hash based searches are often employed for this. In addition combining isotopes into a unionized grid is a common method for reducing the total number of searched required, though it greatly increases the memory needed to store the cross section data.

Each of the common competing continuous algorithms is well defined and compared by Wang et. al. and are described as follows [24]:

Hashing: Each material's whole energy range is divided up into N equal intervals, and for every individual isotope inside the material an extra table is established to store isotopic bounding indexes of each interval [25]. The new search intervals are thus largely narrowed with respect to the original range and can be reached by a single float division. The hashing can be performed on a linear or logarithmic scale; the search inside each interval can be performed by a binary search or linear search. In the original paper [25], a logarithmic hashing was chosen with $N \simeq 8000$ as the best compramize between performance and memory usage. Another variant is to perform the hashing at the isotope level.

Unionized grid: A global unionized table gathers all possible energy points in the simulation and seconds table provides their corresponding indexes in each isotope energy grid [26]. Every time an energy lookup is performed, only one search is required in the unionized gris and the isotope index are directly provided by the secondary index table. Timing resutls show that this method has a significant speedup over the conventional binary search but can require up to a $36\times$ more memory space [27].

Fractional cascading: This is a technique to speedup search operations for the same value in a series of related data sets [27]. The basic idea is to build a unified grid for the first and second isotopes, then for seconds and third, etc. When using the mapping technique, once we find the energy index in the first energy grid all the following indexes can be read directly from the extra index teables without further computations. Compared to the global unionized methods, the fractional cascading technique greatly reduces memory usage.

We will discuss recent work done in the area of nuclear data lookups when we discuss many-core based Monte Carlo research as much of the results are targeted at NVIDA GPGPUs or the Intel XEON Phi many-core coprocessor.

D. Variance Reduction Techniques

Variance reduction is a key concept in Monte Carlo transport problems. Often without some use of variance reduction certain problems would take an incredible amount of time and computing power to begin finding a solution. The idea behind variance reduction is to increase the efficiency of Monte Carlo calculations and permit the the reduction of the sample size in order to achieve a fixed level of accuracy or increase accuracy at a fixed sample size [28]. Some commonly used variance reduction techniques are common random numbers, antithetic variates, control variates, importance sampling and stratified sampling, although most used in Monte Carlo transport is some form of importance sampling.

Common Random Numbers:: This method of variance reduction involves comparing two or more alternative configurations instead of only a single configuration. Variance reduction is achieved by introducing an element of positive correlation between the sets. [29]

Antithetic Variates: This method of variance reduction involves taking the antithetic path for each path sampled — so for a given path $\{\varepsilon_1, ..., \varepsilon_M\}$ one would also take the path $\{-\varepsilon_1, ..., -\varepsilon_M\}$. This method reduces the number of samples needed and reduces the variance of the sampled paths. [30]

Control Variates: This method of variance reduction involves creating a correlation coefficient by using information about a known quantity to reduce the error in an unknown quantity. This method is equivalent to solving a least squares system and so is often called regression sampling. [31]

Importance Sampling: This method of variance reduction involves estimating properties of a particular distribution, while only having samples generated from a different distribution than the distribution of interest. This method emphasizes important values by sampling them more frequently and sampling un important values less frequently [32]. This is often achieved through methods known as splitting or Russian roulette. In splitting and Russian roulette particles are each given a weight and if particles enter an area of higher importance they are split into more particles with less weight giving a larger sample size. If particles travel in a region that is not important they undergo Russian roulette where some particles are killed off and others are given a heavier weight to account for those removed. [33]

Stratified Sampling: This method of variance reduction is accomplished by separating members of a population into homogeneous groups before sampling. Sampling each stratum reduces sampling error and can produce weighted means that have less variability than the arithmetic mean of a simple sampling of the population. [34]

Modern research in the area of variance reduction techniques often includes a specific problem that requires a more focused study to utilize one of these previously described patterns. For example in the problem of atmospheric radiative transfer modeling Iwabuchi recently published work describing their proposal of some variance reduction techniques that they can use to help solve the problem of solar radiance calculations. They describe four methods that are developed directly from their problem. The first is to use a type of Russian roulette on values that will contribute small or meaningless amounts to the overall calculation within some

threshold. Other methods include approximation methods for sharply peaked regions of the phase space, forcing collisions in under sampled regions, and numerical diffusion to smooth out noise. [35]

IV. STATE OF THE ART: GPU RESEARCH

In this section we will be looking at the recent advances in Monte Carlo research on GPU architectures. We will first look at different approaches people have taken to get onto the GPU. We will then look at Monte Carlo transport from the medical transport perspective in order compare approaches from the different communities. Then we will look at uses of ray tracing within a monte carlo transport application. Finally we will look at new algorithms choices through event based Monte Carlo transport.

A. CPU Versus GPU

"A simple way to understand the difference between a CPU and GPU is to compare how they process tasks. A CPU consists of a few cores optimized for sequential serial processing while a GPU has a massively parallel architecture consisting of thousands of smaller, more efficient cores designed for handling multiple tasks simultaneously." [36]
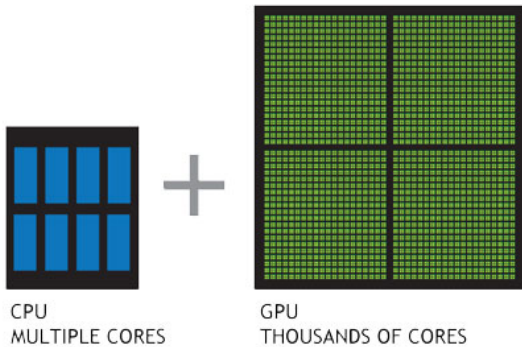
[36]

A CPU has been developed from the beginning to optimize the performance of a single task. In order to accomplish this CPUs have been latency optimized, meaning that the time to complete one task, including gathering the necessary memory, has been reduced in any way possible. GPUs on the other-hand have been throughput optimized in order to complete as many tasks as possible in a given amount of time. This means that the time to complete a single task is most likely significantly longer than in a CPU but in a fixed amount of time the GPU will be able to accomplish many more tasks. So given a large enough number of tasks that can be accomplished in parallel the GPU can complete all of them faster.

B. First Pass at GPU Computing

In this section we will analyze the different approaches that people have taken to get their Monte Carlo transport codes working for GPUs. By comparing and contrasting these different approaches we can see for a variety of problems if any approaches were more successful and which approaches struggled to get desired levels of performance out of the hardware. It is important to note that the actual runtimes and

speedups are less important then the theoretical speedups compared to the achieved speedups as hardware has been changing very quickly over the last ten years for these comparisons.

Accuracy:

One of the first considerations the scientific community has when being introduced to a new computing platform is what levels of accuracy can they achieve with their simulation codes. It was common that in early GPU computing when double floating point precision was not supported or supported well that people started thinking about GPU computing as not being accurate enough for their needs. Many early attempts at GPU computing includes discussions of accuracy in order to validate the correctness of their results. While modern GPGPUs support double precision much better than before making much of the worry irrelevant, it is still important to consider the accuracy of a method that runs on a new hardware and may use a new algorithm.

Nelson discussed accuracy in his thesis work [37], stating that during the time of his work the floating-point arithmetic accuracy was not fully IEEE-754 compliant which opens the question of accuracy without a more fully featured test. Additionally, since NVIDIA as complete control over the implementation of floating point calculations on their GPUs their may be differences between generations that mitigate the usefulness of an accuracy study on one generation of hardware. Current generations of the NVIDIA GPU hardware are IEE-754 compliant. In order to address issues of floating point accuracy they have even included a detailed description of the standard and the way CUDA follows the standard showing that at least while floating point accuracy is still a concern it is no more a concern than it was on a CPU implementation. [38] Nelson's other primary accuracy consideration was the difference in computation time between double and single precision. In older GPU hardware there was no support for double precision in the hardware and so in order to achieve double precision significantly more calculations were needed. In modern GPU hardware double precision is becoming increasingly better supported and in the gpgpu cards there are dedicated double precision units and all of the necessary hardware changes required to include them.

Others also wanted to consider the accuracy of their initial gpu conversions. Jia et. al [39] showed that in their development of a Mont Carlo dose calculation code they could achieve speedups of 5 to 6.6 times their CPU version while maintaining within 1% of the dosing for more then 98% of the calculation points. They considered this adequate accuracy to consider using GPUs for doing these computations. Yepes et. al [40] also considered accuracy in their assessment of their GPU implementation. They concluded that in term of accuracy there was a good agreement between the dose distributions calculated with each version they ran, the largest discrepencies being only ∼3%, and so they could run the GPU version as accurately as any general-purpose Monte Carlo program.

Performance:

A second factor that is important to people making their first pass at GPU Monte Carlo is performance. Most early GPU studies emphasize the speedups between CPU and GPU as the primary advantage for moving over to the GPU hardware. Given the change in supercomputing designs these comparisons have become increasingly more important.

Badal and Badano [41] present work on photon transport in a voxelized geometry showing results around $27\times$ over a single core CPU. Their work emphasizes simply using GPUs instead of CPUs and the advanatage as GPUs continue to increase in performance faster than CPUs.

Nelsons work presented in his thesis [37] shows a variety of models and considerations for his performance results. His work solving neutron transport considered multiple models for running the problem and optimizing for the GPU. The model that produced his best results shows $19.37\times$ from a 49,152 neutrons per batch run for single precision. The same model shows $23.91\times$ when using single precision and fast math, For double precision performance the model labeled model four had the fastest speedups with $11.21\times$ and $12.66\times$ with fast math.

Work presented by Tickner [42] on X-ray and gamma ray transport uses a slightly modified scheme from the others by launching particles on a per block basis. In this way he hoped to remove the instruction level dependancies between particles running on the GPU hardware. In this work he showed he was capable of producing speedups of up to $35\times$ over those running the old algorithm.

Jia et. al's work [39] in a dose calculation code for coupled electron photon transport follows a relatively straight forward algorithm. First they copy the necessary data to the GPU, then they launch with each thread independently computing the necessary work for their particle. Finally, when the correct number of particles has been simulated the results are brought back to the CPU and the program terminates. This method produced a modest performance increase of around 5 to 6.6 $\times$ their runs on a CPU when run on a GPU. The limitation of this speedup was attributed to the branching of the code and that effect it had on the GPU hardware.

In contrast to Jia et al's work Yepes et al [40] showed that a slightly different algorithm could greatly improve results. By converting a track-repeating algorithm instead of a full Monte Carlo Yepes et al gained around $75\times$ the performance on the GPU over the CPU. It is thought that the simpler logic of this algorithm generated threads which followed closer logic to that of the algorithm presented in Jia at al's work.

Throughout all of these examples one common theme can be seen. Performance can be gained doing Monte Carlo on the GPU. Performance can be more difficult to get due to the highly divergent nature of the full Monte Carlo application. Methods to deal with this divergence can show promising results that are worthy of further study. These outcomes are expected outcomes since Monte Carlo applications embarrassingly parallel (a good sign for GPUs) but also incredibly divergent (a bad sign for GPUs).

Approaches:

Monte Carlo transport applications tend to follow a simple model where each tracked particle is given its own thread and computations progress embarrassingly parallel. On a GPU this also makes sense as a starting point since particles are independent and this progression leads to a simple natural parallel approach. It is often pointed out however that due to the divergent nature of Monte Carlo this approach might not be the best way organize Monte Carlo codes on GPU hardware.

We mentioned in the previous section one persons approach at solving this dilemma and their performance gains by dealing with this issue. We will now look closer at the algorithm they used to better understand why if at all their approach should afford better performance than what was seen before.

We will first look at the particle-per-block tracking algorithm described by Tickner [42]. First each tracked particle or quantum of radiation is given to a block of threads. Then calculations are performed for one particle on each block of threads. For example the particle intersection tests with the background geometry can be preformed in parallel on those threads for each piece of geometry that particle might be able to collide with. Areas where these parallel instructions can be utilized within a particles calculation are then used by the threads in a block computing for that particle.

This particle-per-block technique has shows promise as an effective way to counter act the divergence issue. Positives, as they also described, particles often diverge quite quickly from one another in the code paths they follow. This means that threads in a block are not always able to travel in lock step and can cause some serialization of the parallel regions. By using only one particle per block the divergence problem is nearly entirely removed from the equation. Additionally this method introduces new areas of parallelism that are not otherwise being taken advantage of, instruction level parallelism in the particles calculations.

This method however, does not take full advantage of the parallelism in the hardware like those methods that do not mind the divergence do. Many threads can execute simultaneously at once within a block and only groupings of 32 threads are held in a WARP forced into the lockstep pattern that causes potential slowdowns. By running only one particle per block you are sacrificing some parallelism as not all tasks to calculate a particles path are parallel operations. Additionally, since warps are scheduled out of thread blocks any particle operations that are not done in parallel among the threads of a block are serializing themselves in a similar manner as to those algorithms that run one thread per particle waiting while divergent particles have a turn.

In summary I think that this method has some merit if it can find enough parallel work in the thread block to execute additional parallel tasks that would otherwise be stalled if following a simpler method. I also think that this method might end up showing the same characteristics of the simpler particle-per-thread model if the extra parallelism is not found, and instead loose out on the parallelism provided by particles

that are not divergent from one another.

A second possibly more obvious method to escape the divergence issue is to switch particle tracking algorithms more dramatically from a history based version to an event based version. We will have a discussion of this further in the Section on event based algorithms later in this paper. Event based approaches require much more work then simply transforming an existing code to use the history based version on the GPU. And as Du et al discovered in their attempt at a event based Monte Carlo version of the Archer code [43] [44] getting any speedups with that method is a whole new host of challenges to overcome.

Abstracts:

The Following Text Is not complete... it is abstracts and summaries to be made into a complete story. : The history of Monte Carlo methods is closely linked to that of computers: The first known Monte Carlo rogram was written in 1947 for the EN lAC; a pre-release of the first Fortran compiler was used for Mon e Carlo In 1957; Monte Carlo codes were adapted to vector computers in the I 980s, clusters and parallel computers In the 199.0s, and teraflop systems in the 2000s. Recent advances include hierarchical parallelism, combini.ng threaded calculatIOns on multicore processors with message-passing among different nodes. WIth. the advances In computmg, Monte Carlo codes have evolved with new capabilities and new ways of use. ProductIon codes such as MCNP, MYP, MONK, TRIPOLI and SCALE are now 20-30 years old (or more) and are very rich in advanced featUres. The former "method 'Of last resort" has now become the first choice for many applications. Calculations are now routmely performed on office computers, not just on supercomputers. Current research and development efforts re investigating the use of Monte Carlo methods on FPGAs. GPUs, and many-core processors. Other far-reachmg research is exploring ways to adapt Monte Carlo methods to future exaflop systems that may have 1 M or more concurrent computational processes. [45]

Monte Carlo simulation is ideally suited for solving Boltzmann neutron transport equation in inhomogeneous media. However, routine applications require the computation time to be reduced to hours and even minutes in a desktop system. The interest in adopting GPUs for Monte Carlo acceleration is rapidly mounting, fueled partially by the parallelism afforded by the latest GPU technologies and the challenge to perform full-size reactor core analysis on a routine basis. In this study, Monte Carlo codes for a fixed-source neutron transport problem and an eigenvalue/criticality problem were developed for CPU and GPU environments, respectively, to evaluate issues associated with computational speedup afforded by the use of GPUs. The results suggest that a speedup factor of 30 in Monte Carlo radiation transport of neutrons is within reach using the state-of-the-art GPU technologies. However, for the eigenvalue/criticality problem, the speedup was 8.5. In comparison, for a task of voxelizing unstructured mesh geometry that is more parallel in nature, the speedup of 45 was obtained. It was observed that, to date, most attempts to adopt GPUs for Monte Carlo acceleration were based on nave implementations and have not yielded the level of anticipated gains. Successful implementation of Monte Carlo schemes for GPUs will likely require the development of an entirely new code. Given the prediction that future-generation GPU products will likely bring exponentially improved computing power and performances, innovative hardware and software solutions may make it possible to achieve full-core Monte Carlo calculation within one hour using a desktop computer system in a few years. [46]

An electron-photon coupled Monte Carlo code ARCHER - Accelerated Radiation-transport Computations in Heterogeneous Environments - is being developed at Rensselaer Polytechnic Institute as a software test bed for emerging heterogeneous high performance computers that utilize accelerators such as GPUs. In this paper, the preliminary results of code development and testing are presented. The electron transport in media was modeled using the class-II condensed history method. The electron energy considered ranges from a few hundred keV to 30 MeV. Moller scattering and bremsstrahlung processes above a preset energy were explicitly modeled. Energy loss below that threshold was accounted for using the Continuously Slowing Down Approximation (CSDA). Photon transport was dealt with using the delta tracking method. Photoelectric effect, Compton scattering and pair production were modeled. Voxelised geometry was supported. A serial ARHCHER-CPU was first written in C++. The code was then ported to the GPU platform using CUDA C. The hardware involved a desktop PC with an Intel Xeon X5660 CPU and six NVIDIA Tesla M2090 GPUs. ARHCHER was tested for a case of 20 MeV electron beam incident perpendicularly on a water-aluminum-water phantom. The depth and lateral dose profiles were found to agree with results obtained from well tested MC codes. Using six GPU cards, 6×10^6 histories of electrons were simulated within 2 seconds. In comparison, the same case running the EGSnrc and MCNPX codes required 1645 seconds and 9213 seconds, respectively, on a CPU with a single core used. [47]

Hardware accelerators are currently becoming increasingly important in boosting high performance computing systems. In this study, we tested the performance of two accelerator models, Nvidia Tesla M2090 GPU and Intel Xeon Phi 5110p coprocessor, using a new Monte Carlo photon transport package called ARCHER-CT we have developed for fast CT imaging dose calculation. The package contains three components, ARCHER-CTCPU, ARCHER-CTGPU and ARCHER-CTCOP designed to be run on the multi-core CPU, GPU and coprocessor architectures respectively. A detailed GE LightSpeed Multi-Detector Computed Tomography (MDCT) scanner model and a family of voxel patient phantoms are included in the code to calculate absorbed dose to radiosensitive organs under user-specified scan protocols. The results from ARCHER agree well with those from the production code Monte Carlo N-Particle eXtended (MCNPX). It is found that all the code components are significantly faster than the parallel MCNPX run on 12 MPI processes, and that

the GPU and coprocessor codes are 5.15?5.81 and 3.30?3.38 times faster than the parallel ARCHER-CTCPU, respectively. The M2090 GPU performs better than the 5110p coprocessor in our specific test. Besides, the heterogeneous computation mode in which the CPU and the hardware accelerator work concurrently can increase the overall performance by 13?18%. [48]

C. Monte Carlo and Medicine

A look at the GPU research being done in the medical field of monte carlo transport

D. Monte Carlo and Ray Tracking

a look at the combined efforts to put ray tracing techniques into monte carlo applications. MC and optix.

E. Event Based Techniques

A look at old and new event based approaches for mc applications.

V. WHAT IS PORTABLE PERFORMANCE

The term portable performance generally means the ability to achieve a high level of performance on a variety of architectures. In this case high performance is relative to each target system [49]. One important consideration then is what variety of systems are used that applications need to be portable for.

The top ranked machines in the world currently utilize technologies like general purpose graphics processing units (GPUs, e.g., NVIDIA Tesla in Titan), many-core coprocessors (e.g., Intel Xeon Phi in Tianhe-2), and large multi-core CPUs (e.g., IBM Power, Intel Xeon in Tianhe-2 and others) [49], [50], [51]. Further, future supercomputing designs may include low-power architectures (e.g., ARM), hybrid designs (e.g., AMD APU), or experimental designs (e.g., FPGA systems) [51]. Given this wide array of possible architectures the value of portable performance has never before been so high.

VI. MONTE CARLO AND PORTABLE PERFORMANCE

a look at monte carlo and pp abstractions. My alps work

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