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GPGPU-Enabled Physics Based Deformed Model Simulation

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B.S., Chihuahua Institute of Technology, 2011

THESIS

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Dedication

To both my parents, Enedino and Patricia for always being supportive of my dreams.

"UNIX is basically a simple operating system, but you have to be a genius to understand the simplicity" – Dennis M. Ritchie

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Abstract

Computer simulation techniques are widely adopted nowadays in many areas like manufacturing, engineering, graphics, animation, virtual reality and so on. However, the standard finite element based simulation is notorious for its expensive computation. To address this challenge, I present a GPU-based parallel implementation for simulating large elastic deformation. Classic modal analysis provides a set of orthonormal bases vectors, which span a spectral space encoding the dynamics of the elastic body. As each basis vector is orthogonal to each other, the computation is completely decoupled and can be well-fit into the modern GPGPU platform. We further explore the latest feature of NVIDIA CUDA so that the result of GPU computation can be directly used for upcoming rendering/visualization and a significant amount of overheads for transmitting data from client GPU and host CPU via the PCI-Express bus are avoided. Real-time simulation is made possible with this technique for many cases that otherwise is not possible.

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Glossary

ALU	Arithmetic Logic Unit.
API	Accelerated Programming Interface.
APU	Accelerated Processing Unit.
BLP	Bit Level Parallelism.
CISC	Complex Instruction Set Computer.
CPU	Compute Processing Unit.
DLP	Data Level Parallelism.
ENIAC	Electronic Numerical Integrator and Computer.
FEM	Finite Element Methods.
GPU	Graphics Processing Unit.
GPGPU	General Purpose Computing on Graphics Processing Units
GUI	Graphical User Interface.
ILP	Instruction Level Parallelism.
MIMD	Multiple Instruction Multiple Data.

Glossary

$MISD$	Multiple Instruction Single Data.
$RISC$	Reduced Instruction Set Computer.
$SIMD$	Single Instruction Multiple Data.
$SIMT$	Single Instruction Multiple Thread.
$SISD$	Single Instruction Single Data.
SP	Streaming Multiprocessor.
SP	Streaming Processor.
STL	Standard Template Library.
TLP	Thread/Task Level Parallelism.
VAO	Vertex Array Object.
VBO	Vertex Buffer Object.

Chapter 1

Introduction

1.1 Overview

The work described in this document aims to implement a deformed model simulation algorithm in parallel on the GPU (Graphics Processing Unit) using modal warping, based on physics techniques to approximate the behavior of an object when its subject totally or partially to a force applied. Using the architectural advantages of GPUs, this GPGPU (General Purpose Computing on the GPU) algorithm can be implemented efficiently even with a small device, obtaining a considerable speed improvement over conventional algorithms and also providing accurate results.
In the following sections an explanation of why certain tools such as computer languages were chosen and how they were used to implement the algorithm can be found.

1.2 Computer Simulation

1.2.1 History

Computer simulation has become one of the most important areas of research in the last couple of decades, its history dates back to the World War II era, when 2 mathematicians: John Von Neumann and Stanislaw Ulam, faced the complicated problem of neutrons behavior.
Stan made the following remarks about his ideas in the 1980's:

" 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 solitaires. 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 combinational 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, 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 the actual calculations".[1]

Von Neumann was intrigued, doing statistical sampling using newly developed electronic computing techniques seemed a great idea, in March of 1947 Von Neumann wrote a letter to Robert Richtmyer, who was the Theoretical Division Leader at

Los Alamos National Laboratory, where he concluded: *"the statistical approach is very well suited to a digital treatment"*, he outlined in some detail how this method could be used to solve neutron diffusion and multiplication problems in fission devices,further details about this method lay beyond the scope of this document.
Finally at the end of the letter, Von Neumann attached a tentative "computing sheet", that he felt would serve as a basis for setting up this calculation on the ENIAC, the ENIAC was the first general purpose computer built in secret at the University of Philadelphia's Moore's School of Electrical Engineering [2].
The outline was the first formulation of a Monte Carlo computation for an electronic machine.
From that moment on, hardware always predominated the simulation field, it wasn't until the 1950's when programming languages began to emerge and computer simulation started to be developed in several different areas. Computer simulations main applications vary in different areas nowadays, such as:

- Medical
- Science
- Physics
- Engineering
- Military

One of the specific areas of research in computer simulation is deformable model simulation, which is also applied in all the areas stated before.
This area has specifically been subject of research in the past three decades, the reason being that, until the 1980's computer based modelling techniques only allowed modelling of rigid bodies. In 1984 a series of geometric operators for deforming a

solid object by transforming the coordinate space were introduced [3]. These were the starting point for the development of better and improved techniques for deformed object modelling.

Computer based deformed modelling techniques are classified in non-physical, physical and approximate physical techniques:

- Non-Physical Techniques: Purely geometric techniques used to deform virtual objects, accuracy is sacrificed for more computational efficiency.
  - Splines and Patches.
  - Free Form Deformation.

- Physical Techniques: Based on principles of continuum mechanics applied to a geometric structure of a model, these techniques sacrifice computational complexity but provide a more accurate, and realistic result.
  - Discrete Models: Mass Spring Damper Methods.
  - Continuum Models: Finite Element Methods (FEM).

- Approximate Physical Techniques: These techniques are not derived directly from continuum mechanics equations, although they are physically motivated.
  - Active Contour Models

While non-physical techniques are the most efficient and more simply implemented computationally speaking, accuracy is also greatly sacrificed, the most widely used techniques are physical based techniques [4], where FEM are state of the art in physically based modelling becoming more used in the last few years as computational power increases.

Physics based techniques are more complex computationally speaking due to the fact that they handle nonlinearities, this has the main advantage of providing a more accurate and realistic result, but it becomes complex, for this specific case, handling nonlinearities would not easily allow for a parallel algorithm to be created, but omitting the nonlinear term would create unrealistic results, increasing the volume of the model inaccurately.

The modal warping technique used in this work omits the nonlinear term initially when precomputing, although once the simulation is being run, the rotation information is kept, even when the object is deformed, the precomputed modal basis is warped according to the rotational information obtained [5], giving a realistic result but also providing the opportunity of approaching the problem in a parallelizable way.
A more profound classification survey and explanation of these techniques and their advantages and disadvantages can be found on [6] and [4].

1.2.2 OpenGL

OpenGL is merely an API; a software library for accessing features in graphics hardware, as of today it contains more than 500 different commands, used to specify objects, images and operations needed to produce interactive 3-dimensional com-

puter graphics applications[7].
OpenGL is designed to be implemented on many different types of graphics hardware, or it could even be implemented entirely in software, it is also independent of the operating system the computer is running on, due to this type of implementation, some limitations may be considered, it does not provide functions to process user input or creating windows, which means it needs to be used along with some other library that performs this functions and complement it, OpenGL also has the limitation if it may be called that, that lacks a functionality for describing models or 3D objects in any way, neither to read files of any sort. Instead the programmer must read these files or construct the 3D objects from a small set of *geometric primitives* (points, lines, triangles, etc.) these primitives will be explained in further detail on section 2.1 of this document.

1.3 Parallel Computing

1.3.1 History

Computer technology made incredible progress in over 60 years since the first general purpose computer was created, if we analyze the progress over time, we see that during the first 25 years, progress was made in both creating new architectures and developing new technologies, delivering a raise of approximately 25% per year on performance.
By 1970 when the microprocessor emerged, it led to a higher rate of performance improvement, around 35% per year.
In the early 1980's a set of changes made possible the development of RISC (Reduced Instruction Set Computer), which used new performance techniques such as instruction level parallelism and the use of caches, this started what some people

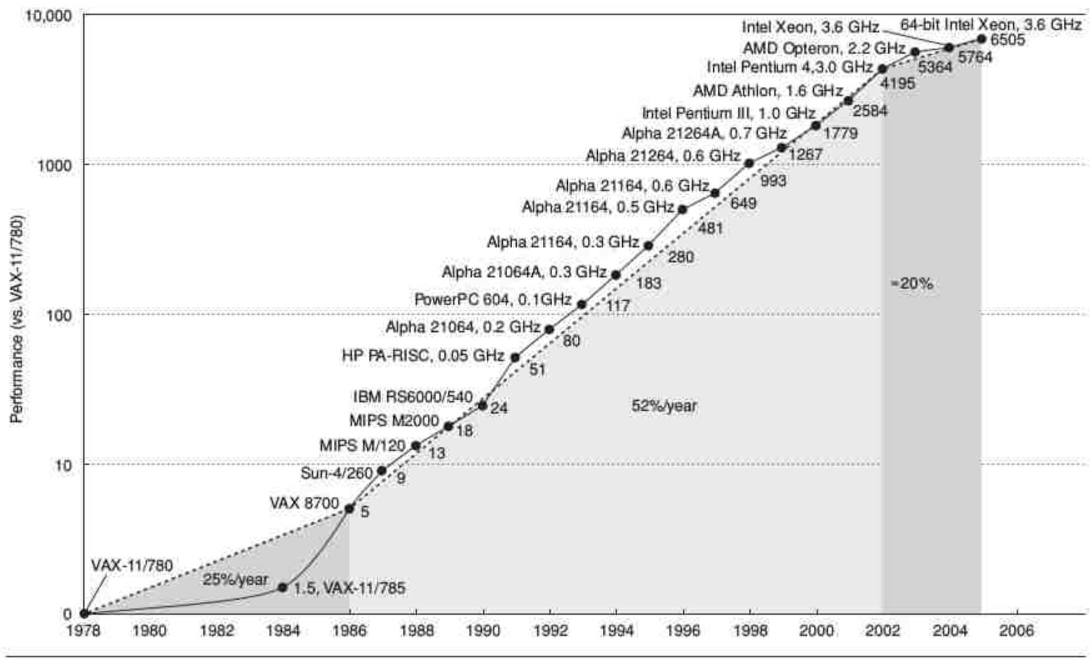


Figure 1.1: Processor Performance Over Time[8]

call the hardware renaissance of computers, where a 52% of improvement per year was achieved. As figure 1.1 shows, the renaissance ended on the year of 2003, this happened because as time passed transistors got smaller, faster and used less power, so processor makers not only added more and more transistors on the same chip, but they also increased the clock frequency of processors.

The question is: Why did they stop?. The simplest answer to that power, both power and heat are the main issue when developing a microprocessor, due to the fact that a billion of transistors generate a lot of heat , and when running at that speed it is impossible to keep the chip from melting. The CPU's or main processors may have been hurt by this parameter, but GPUs have not, or at least not in the same way, due to the fact that GPUs are different in architecture, they have a lot more of compute units or ALU's (Arithmetic Logic Units), but each of those is a lot simpler too, they have small caches, memory accesses are extremely coherent, and memory modules are usually a lot faster than the ones used for CPU's (also known as system memory), this means that when we have a problem which can be organized in a way that there are a wide amount simple computations to do, instead of small amount of complex ones, GPUs are a good option to solve this type of problem [9].

1.3.2 Classification

There are several types of different parallelization techniques, they are mainly classified according to how the calculations are organized to be computed in parallel.

1.3.2.1 Levels of Parallelism

Parallelism can be characterized in levels or forms of where the parallelism is applied to, which could be exploited differently depending on the parallel architecture. Levels of parallelism may be classified as follows:

- Bit Level Parallelism (BLP): BLP is a form of parallelism achieved by increasing the processor word size, doing so reduces the number of instructions the processor has to execute in order to perform an operation on variables whose sizes are greater than the length of the processor word size, an addition between two 32-bit integers using a 16-bit processor, requires the processor to first add the 16 lower order bits from each of the integers and then add the 16 higher order bits, requiring two instructions to complete a single operation [10].
- Instruction Level Parallelism (ILP): ILP is a form of parallelism achieved by applying different techniques to the instructions sent to the processor, tech-

niques such as pipelining, which overlaps the execution of instructions and improves performance, or loop unrolling, performing several loop operations in just one cycle instead of one operation per cycle, limitations for this type of parallelism include data dependencies and control hazards, when exploiting this type of parallelism one must be sure that the data is independent from one cycle to another, otherwise those 2 or more instructions cannot be executed simultaneously or be completely overlapped, and also that the instructions are not control dependent, meaning that the order in which the instructions are executed does not matter, since it cannot be known for sure which operation will be executed first when executed in parallel.

There are 2 main approaches for exploiting ILP, an approach that relies on hardware to help discover and exploit the parallelism dynamically, and an approach relying on software technology to find parallelism statically at compile time [8].

- Data Level Parallelism (DLP): DLP is a form of parallelism where parallelism is focused on the data itself, in a multiprocessor system when executing a single set of instructions (SIMD) 1.3.2.2, data parallelism is achieved when each processor performs the same computations on different pieces of distributed data.

- Thread/Task Level Parallelism (TLP): TLP is a form of parallelism, focused on distributing execution processes or threads across different computer nodes, or processors, this is achieved when a thread or process is executed on each different processor, where this threads may execute the same or different code and on the same or different data, this form of parallelization requires inter-communication amongst threads, in general TLP is more flexible than DLP and thus more generally applicable[8].

1.3.2.2 Parallel Architectures

The most popular characterization of different types of parallel architectures was defined by Flynn in 1966 [11] and is specified as follows:

- SISD: Simple Instruction Simple Data - Conventional single processors computers are classified as SISD systems, each arithmetic instruction initiates an operation on a data item taken from a single stream of data elements.

- SIMD: Simple Instruction Multiple Data - The same instruction is executed by multiple processors using different data streams, these type of systems exploit DLP (Data Level Parallelism), by applying the same operations to multiple items of data in parallel. In these type of systems each processor has its own data memory, but there is only one instruction memory and control processor, whose function is to fetch and dispatch instructions. There are three main variants of SIMD: Vector Architectures, Multimedia SIMD Set extensions and GPUs.
  Given the fact that in this work I use a variant of SIMD's I will explain a little further each of these:

  – Vector Architectures:
    Vector architectures grab sets of data elements scattered in memory, place them into large, sequential register files, operate on the data in those register files and then disperse the results back into memory.
    A single instruction operates on vectors of data, which in turn, results in dozens of register-register operations on independent data elements. These register files act as compiler-controlled buffers, both hide memory latency and leverage memory bandwidth, vector loads/stores are also

deeply pipelined, so the program pays the long memory latency only once per load/store instruction instead of doing it on every element.

  - Instruction Set Extensions For Multimedia:

    These extensions as the name implies are often used for multimedia purposes or applications, since many of these applications operate on narrower data types, than what conventional processors are optimized for, they can be used for audio, graphics, etc. An instruction specifies the same operation on vectors of data, but unlike vector architectures, which have register files, these instructions tend to specify fewer operands and use much smaller registers.

  - Graphic Processing Units:

    This variation of the SIMD taxonomy, offers high potential performance, GPUs share some features with vector architectures, but they also have their own distinguishing characteristics, these systems have a conventional system processor and a system memory in addition to their own processing units and graphics memory, that is why these systems are often called heterogeneous [8]. Although GPUs do fall inside this category, this explains their functionality mainly for what they were initially developed for: computer graphics; when these are utilized to perform GPGPU or in other words, for applications traditionally handled by the CPU, they fall into a new category (not part of Flynn's taxonomy) SIMT (Simple Instruction Multiple Thread) [12] which will be explained in further detail later in this document 1.3.3.2.1 .

- MISD: Multiple Instruction Simple Data - Multiple instruction streams and a single data stream, no commercial multiprocessor of this type has been built to this date.

- MIMD: Multiple Instruction Multiple Data - Multiple instruction streams and also multiple data streams, where each processor fetches its own instructions and operates on its own data, these type of systems exploit TLP (Thread Level Parallelism) 1.3.2.1.

Although Flynn's taxonomy characterizes very well the majority of commercial parallel architectures, it is a coarse model, and some multiprocessors are hybrids of these categories.

1.3.3 GPU Computing Languages

GPU languages first appeared in 2003, it is shown how they have evolved over the years in figure 1.2.

1.3.3.1 Brook

Back in the year 2003: Brook, or BrookGPU appeared [14], developed at Stanford University, researchers realized GPUs could also be used to perform general computing calculations, due to their underlying architecture, but at the time, the only way to access GPUs resources was to use one of the graphics API's (Application Programming Interfaces): OpenGL or Direct3D, so researchers had to use them if they wanted to perform calculations on the GPU, the problem was that one had to become an expert in graphics programming to do this, which seriously complicated things, since graphics programmers think in terms of shaders and textures, while parallel programmers think in terms of kernels or streams. Brook was presented as

a set of extensions to the C language; ”C with streams” is how they called it, brook proposed to encapsulate all the management part of the 3D API and expose the GPU as a coprocessor to perform parallel calculations, brook included a compiler, which took a *.br file containing C++ code and extensions and generated standard C++ code to be linked to a run-time library (DirectX, OpenGL, etc).
Brook's collaboration to the GPGPU technology was primarily to popularize the use of GPUs for high performance computing, it simplified access to GPU resources but had some issues too, it generated excess of workload by using the 3D API, and it had no compatibility, every time the GPU manufacturers updated their drivers, brook compatibility could break. Figure 1.4 shows the performance improvement on the first generation of programmable GPUs using Brook.

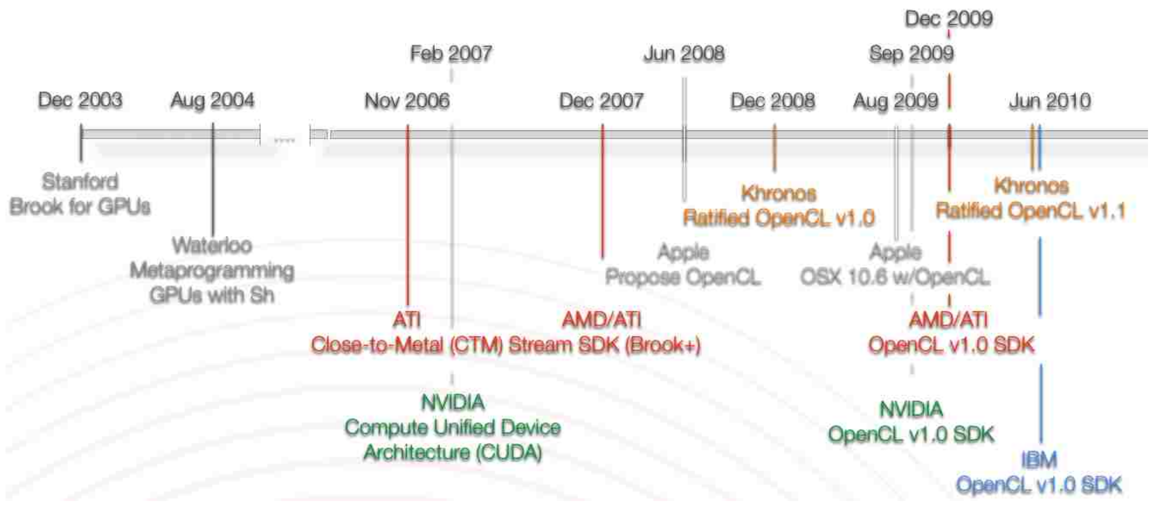


Figure 1.2: GPU Computing Language Timeline [13]

1.3.3.2 NVIDIA CUDA

Brook's success was enough to attract the attention of both major GPU manufacturing companies: ATI and specially of NVIDIA, so Brook's researchers got into development teams at NVIDIA's headquarters with the idea of offering hardware/-software suited for this type of calculations. But, since NVIDIA architects and developers knew all about their own design there was no need to rely on graphics API's anymore, and they were able to design a set of software layers to communicate with the GPU: CUDA (Compute Unified Device Architecture) [15].

CUDA provides 2 API's:

- CUDA Runtime API (High-Level)
- CUDA Driver API (Low-Level)

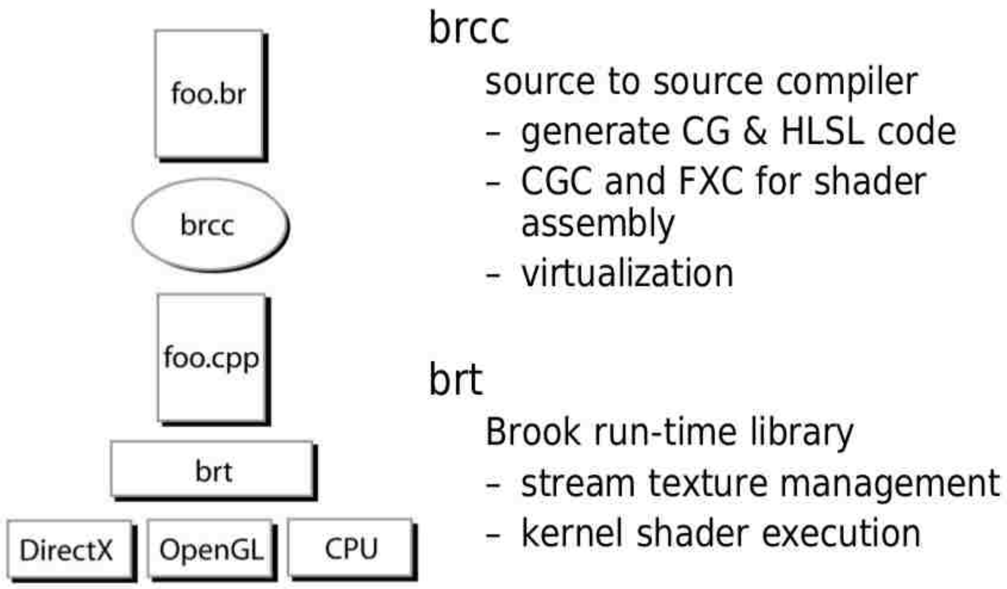

foo.br
brcc
foo.cpp
brt
DirectX
OpenGL
CPU
brcc
source to source compiler
- generate CG & HLSL code
- CGC and FXC for shader assembly
- virtualization
brt
Brook run-time library
- stream texture management
- kernel shader execution

Figure 1.3: BrookGPU System Outline[14]

Although, each call to a function of the high level API is broken down into more basic instructions managed by the low level API.
The CUDA Runtime API can be considered as very low level too, since it requires knowledge of the hardware that is being used, but it still offers functions that are highly practical in terms of initialization and context management.
Both API's are able to communicate with graphics libraries such as Direct3D and OpenGL, this is useful since one can generate resources using CUDA and these can be passed to the graphics API, the advantage here being that the resources remain stored in GPUs RAM without having to transit through the bottleneck of the PCI-Express bus.

1.3.3.2.1 CUDA Hierarchy: SIMT Architecture

CUDA extends the C programming language by allowing the programmer to define C parallel functions called kernels, when called, these functions are executed N times

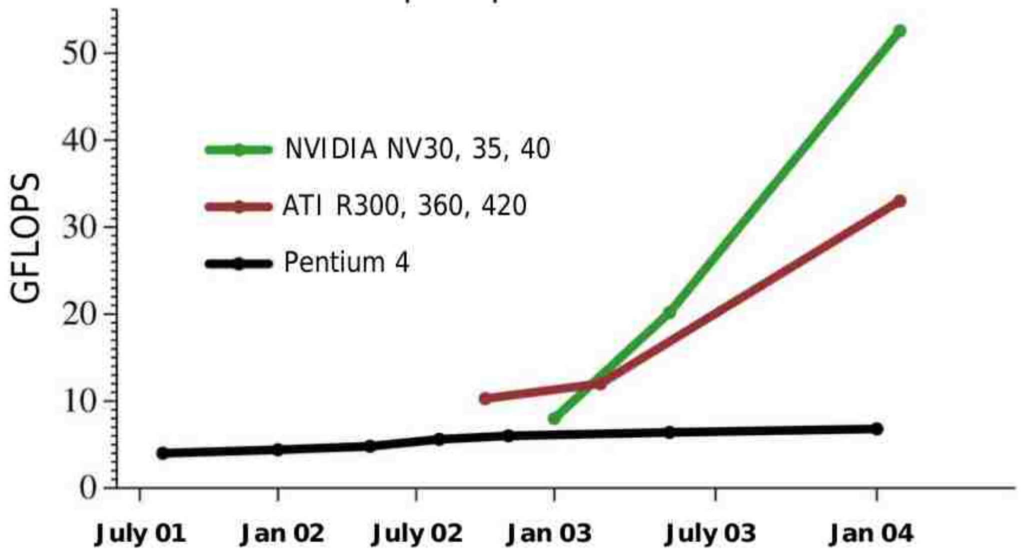


Figure 1.4: Brook's performance on 1st generation of programmable GPUs[14]

in parallel by N different CUDA threads as opposed to regular C functions. Note that originally the kernels could only be "launched" from using the CPU, although has NVIDIA introduced the Kepler architecture featuring the ability to launch kernels from the GPU without CPU involvement.

Each thread that executes the kernel has its own local memory, and its given a unique thread ID, which is accessible within the kernel. This unique ID variable is a 3 component vector or 3 dimensional vector.

These threads are organized in warps, warps are groups of 32 threads, which is the minimum size of the data processed in SIMD by a CUDA SM (Streaming Multiprocessor). Due to granularity issues in CUDA; instead of manipulating warps directly, threads are organized into blocks that can contain from 64 to 1024 threads on current GPUs, and they all share a memory called "shared memory".

CUDA capable devices use this new execution model or architecture called SIMT to manage and execute thousands of threads efficiently, which were both first introduced by NVIDIA in 2006 with the G80 (Tesla Family) of GPUs [12].

Finally these blocks are organized into a one-dimensional, two-dimensional or three-dimensional grid, where the number of thread blocks in a grid is usually dictated by the size of the data being processed or the number of processors in the system, this is where a the global memory is used, it is the slowest of them all but it can be accessed from any threads on the device [16]. The advantage of grouping them in this sort of hierarchy is that the number of blocks processed simultaneously by the GPU are closely linked to the architecture of the GPU (hardware resources), the number of blocks in a grid make it possible to totally abstract that constraint and apply a kernel to a large quantity of threads in a single call, without worrying about fixed resources. The CUDA Runtime library takes care of that, making this model extremely extensible, if the GPU has only a few resources it executes the blocks sequentially, but if it has a large number of processing units instead, it can process them all in

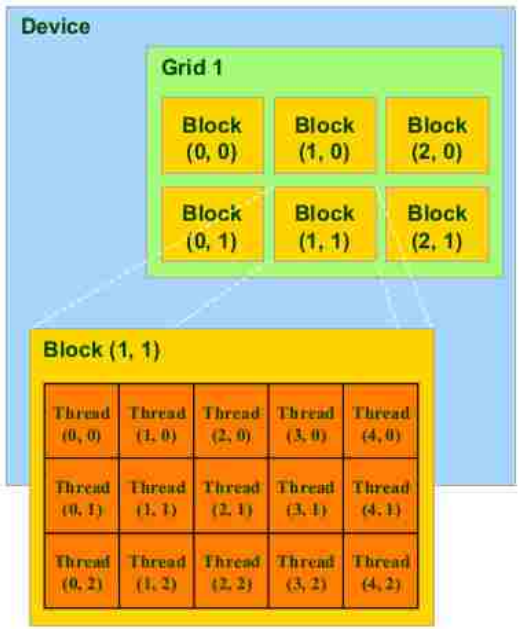


Figure 1.5: CUDA Hierarchy [17]

parallel, this is why the same code can be run on different GPUs. NVIDIA's GPU architectures have evolved over the years, figure 1.7 shows the basic processing unit utilized by NVIDIA for the Fermi Architecture, called SP (Streaming Processor) or

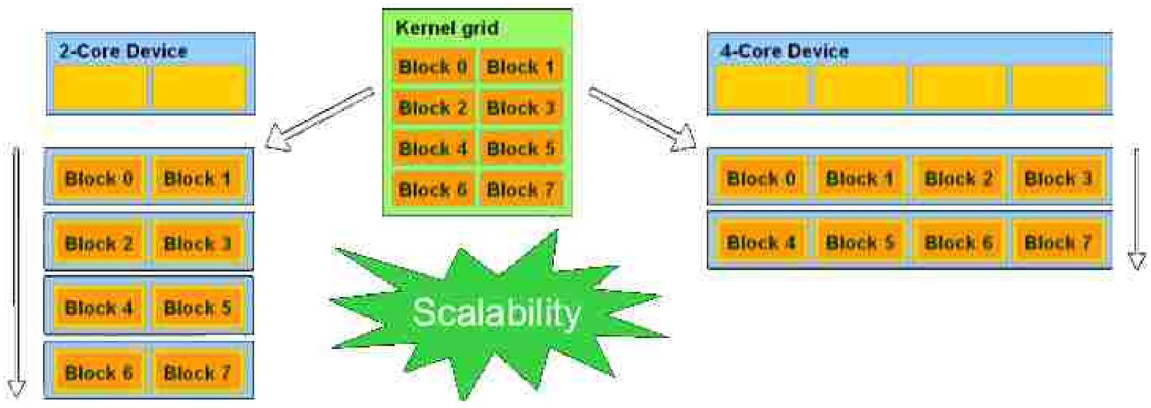


Figure 1.6: CUDA Scalability [17]

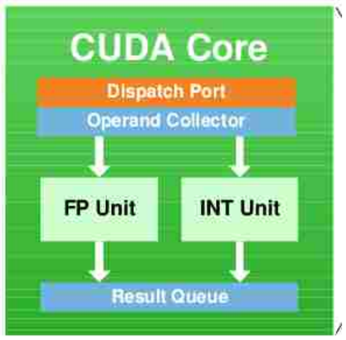


Figure 1.7: Fermi Streaming Processor (CUDA Core) [18]

also called CUDA core, which is in charge of actually performing the calculations, and figures 1.8 and 1.9 show the Streaming Multiprocessor units from the Tesla Architecture (G80) (1st Generation) and the Fermi Architecture (3rd Generation), and lastly figure 1.10 shows a new type of Streaming Multiprocessor introduced with

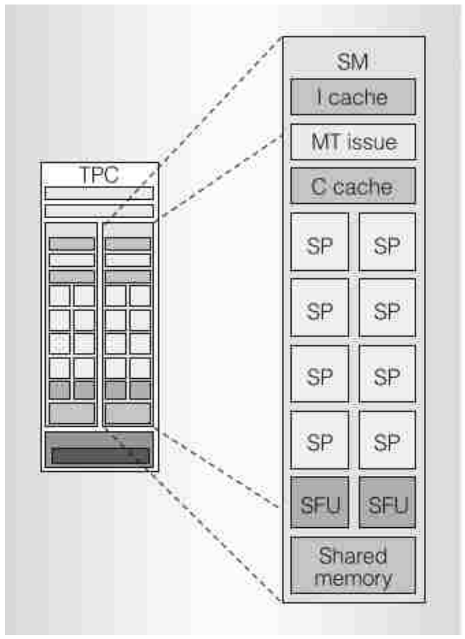


Figure 1.8: Tesla Streaming Multiprocessor [12]

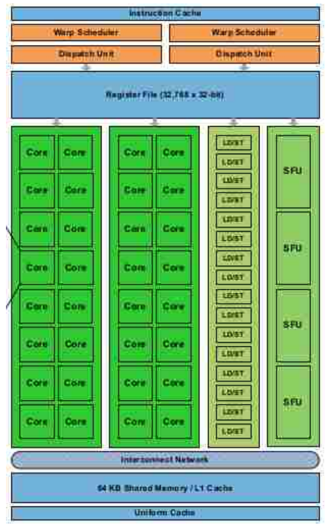


Figure 1.9: Fermi Streaming Multiprocessor [18]

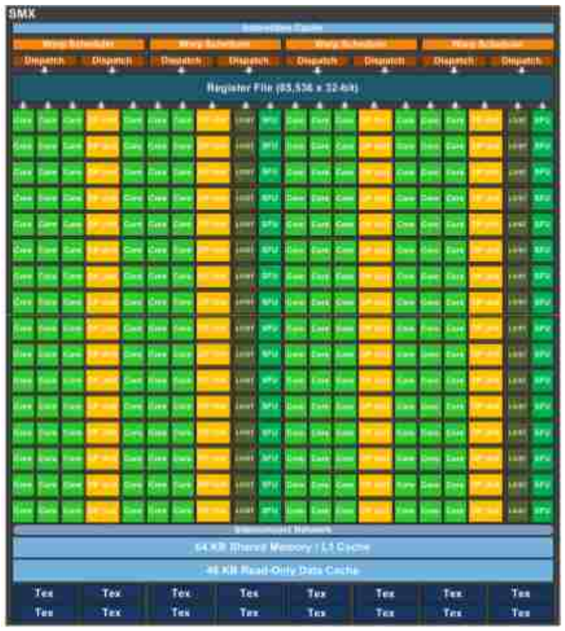

SMX
Instruction Cache
Warp Scheduler
Dispatch
Register File (65,536 x 32-bit)
Core
DP Unit
LD/ST
SFU
Interconnect Network
64 KB Shared Memory / L1 Cache
48 KB Read-Only Data Cache
Tex

Figure 1.10: Kepler Streaming Multiprocessor (SMX) [19]

the Kepler Architecture called SMX, the first one capable of launching kernels from the GPU. We can definitely see how the architectures have evolved in just a couple of years.

1.3.3.3 OpenCL

The OpenCL (Open Computing Language) initiative was first introduced by Apple, but the final proposal included support from several companies like AMD, NVIDIA, IBM and Qualcomm, this proposal was submitted to the Khronos Group, a non-profit organization that focuses on creation of open standards; on June 2008 the Khronos Compute Working Group was formed, with representatives from these and other companies, they released the specification for OpenCL 1.0 on November of the same year [20].
Their design goals were as follows:

- Use all computational resources in the system (CPU's, GPU, and/or other processors).
- Consistent results on all platforms.
- Create an efficient parallel programming model.
  - Provide data and task parallelism.
  - Avoid the specifics of the underlying hardware.
  - Specify the accuracy of floating-point operations.
  - Based on ANSI C99 standard.
- Interoperability with graphics API's
  - Enable advanced visual computing applications.

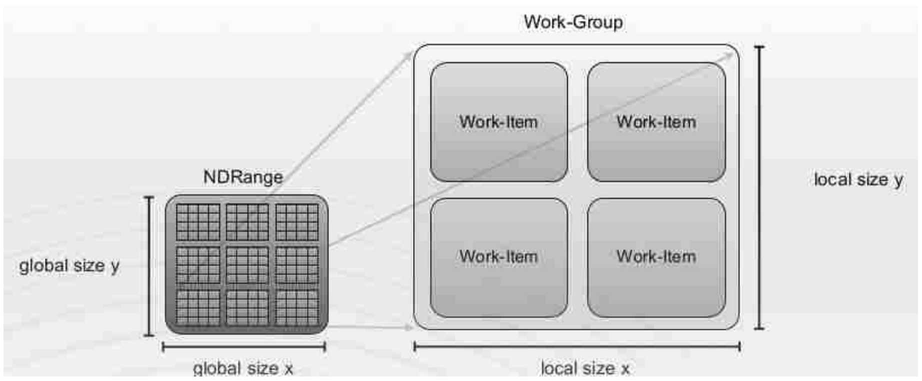


Figure 1.11: OpenCL Hierarchy [13]

- Efficient resource sharing for graphics data.
- Support graphics oriented built-in methods.

Then OpenCL is defined as: ”The open standard for developing cross-platform, vendor agnostic, parallel programs that run on current and future multi-core processors within workstations, desktops, notebooks and mobile devices”. OpenCL 2.0 specification was released on November 14th, 2013 , and it supports the following vendors: NVIDIA, AMD, Apple, Samsung, Qualcomm, ARM, Intel, IBM and others [21].

1.3.3.3.1 OpenCL Hierarchy :

In OpenCL programs are divided in 2 parts: One that executes on the device (GPU) and the other that executes on the host (CPU); code that is to be executed on the device must be inside a kernel and is where all the parallelism must happen, these kernels can only be called from the host. Much like NVIDIA's CUDA, OpenCL kernels are executed N times in parallel by N different work-items, which are the smallest execution entity, each work-item has its own ID, accessible from the kernel and distinguishes it from the other ones, making it possible to process different data, every work-item also has its own memory, referred to as private memory. Work-

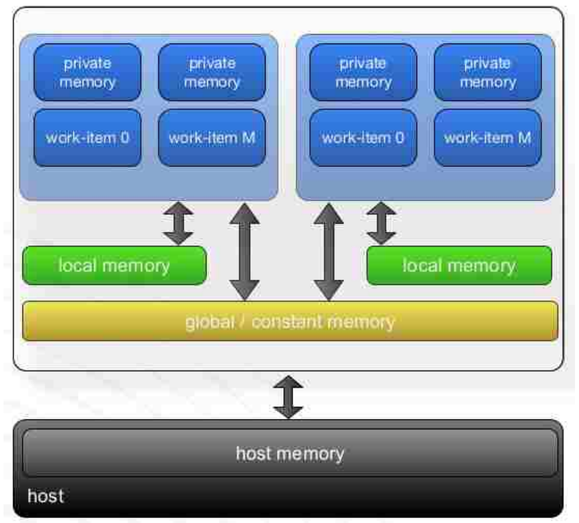


Figure 1.12: OpenCL Hierarchy [20]

items are grouped into work-groups, where they can share a memory called local memory, these work groups also have their unique ID. Finally the work groups are organized into an N-Dimensional grid called ND-Range, where N=1,2 or 3, and a global memory is shared between the whole grid.

1.4 Conclusions

The work explained in section 3.1 was initially thought to be developed using MATLAB, it was, and it provided advantages over the previous related work, being able to accurately simulate rotations on large objects, but MATLAB libraries still provided a slower and slower rendering and computations as the object became larger and larger, performance started to become an issue, that motivated the work explained in this document, to be able to provide not only a better and more efficient renderer engine; using OpenGL, but also to be able to perform the computations faster, doing this in a compiled language such as C or C++, if programmed correctly, would have provided better results than the ones obtained using MATLAB, although a better option was to use parallel programming on the GPU (GPGPU), since the modal warping method efficiently decouples the physics equations on which the simulation is based, making calculations independent from each other, it requires a vast amount of operations on matrices, which also may be computed on an element by element basis on independent data, meaning that an operation to compute element i is independent on the one used to compute element j, these type of operations are a perfect example to use parallel programming and more specifically on the GPU.

The parallel version was programmed using C++ as its main language, OpenGL was used to program the renderer for the 3 dimensional object simulation, and CUDA as its parallel programming platform, it must be noted that as explained in section 1.3.3.3 OpenCL and CUDA programming models are very similar, meaning that in the future would allow for an OpenCL version to be developed "easily" based on the already existing version programmed in CUDA.

Chapter 2

Rendering on OpenGL

This part of the document will aim to explain in some basic level of detail what was used in this work to render the 3-dimensional object or model onto the display, including OpenGL functionality, functions, and external libraries.

2.1 OpenGL Primitives

The primary objective of using OpenGL is to render graphics into a framebuffer, which will be displayed on a screen, complex objects are broken up into OpenGL primitives, that when drawn at high enough density, give the appearance of a 3-dimensional object.
OpenGL includes a vast amount of functions to describe the layout of primitives in computer memory, these are arguably the most important functions in OpenGL, since without them, the programmer would not be able to display anything on the screen.
The are 3 primary types of primitives in OpenGL, even though OpenGL supports

many primitives, in the end they all get rendered as one of the main primitives:Points, Lines and Triangles, these may also be called native primitives, hence they are supported on most graphics hardware. Now a brief explanation of these native primitive types:

- Points : Points are represented on OpenGL by a single vertex, the vertex represents a point in a 4-dimensional homogeneous coordinates, OpenGL uses a set of rules named rasterization rules, to determine which pixels on the screen will be covered by a certain point. These are very simple, if a point falls within a square centered on the point's location, then the respective pixel is covered. Size of the square is determined by the size specified by the programmer for the points, in which one side of the square will equal to the point's size, this is set by an OpenGL state function (*glPointSize()*).
  When points are rendered, each vertex essentially becomes, a single pixel on the screen, if a different size is set, a point may end up being a little more than one pixel.

- Lines: line in OpenGL refers to a line segment, meaning it does not extend to infinity on both directions, lines are represented by pairs of vertices, one for each endpoint of the line, lines may also be joined together to represent a connected series or line segments(line strip), or may even be closed (line loop). The rasterization rule used for lines is called the diamond exit rule: When rasterizing a line running from point A to point B, a pixel should be lit if the line passes through the imaginary edge of a diamond shape drawn inside the pixel's square area on the screen, this is done so if another line going from B to C needs to be drawn, the pixel in which B resides is lit only once.

- Triangles: Triangles are made up of collections of 3 vertices, when separate triangles are rendered, each triangle is independent of all others. A triangle is rendered by projecting each of the 3 vertices into the screen space and forming 3 edges running between the edges. A sample is considered covered if it lies on the positive side of all of the half spaces formed by the lines between the vertices. Rules for triangles are:

- No pixel on a shared edge between 2 triangles that together would cover the pixel should be unlit.
- No pixel on a shared edge between 2 triangles should be lit by more than one of them.

Meaning that there will be no gaps between the triangles and they wont be overdrawn.

Triangles may also be drawn onto strips or fans, which may result in more efficient rendering, reutilizing vertices described on previous triangles, in the case of a triangle strip, the first triangle is drawn using the 3 first vertices, then each subsequent vertex forms another triangle along with the last 2 vertices of the previous triangle, for the triangle fan the first vertex forms a shared point that is included in each subsequent triangle, triangles will be drawn using that shared vertex along with the next two vertices.

2.2 OpenGL Rendering Pipeline

The OpenGL rendering pipeline it's defined as a sequence of processing stages for converting the data the application provides to OpenGL into a final rendered image.

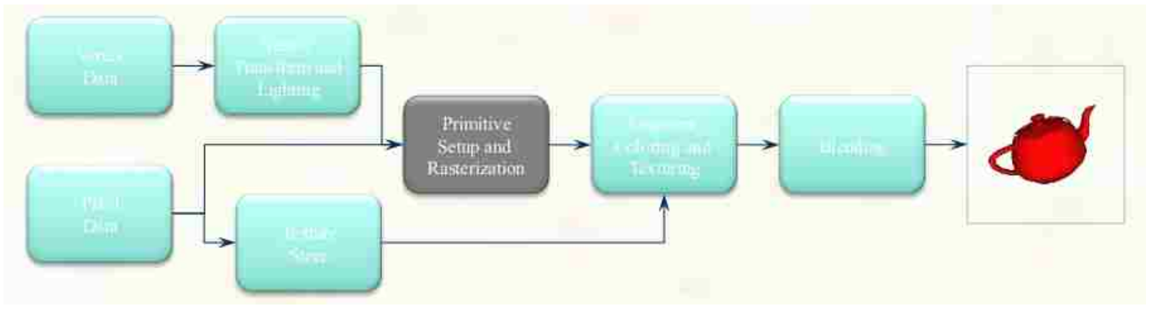


Figure 2.1: OpenGL 1.0 Fixed Pipeline [22]

2.2.1 Fixed Function Pipeline

In the beginning, when OpenGL 1.0 was released in the year of 1994, it's pipeline was entirely *fixed-function*, when an API uses the fixed-function model, it consists of a set of functions entry points that approximately or directly map to a dedicated logic in the GPU specific for its functionality, in other words, the only operations available are fixed by implementation.
Although the pipeline evolved over time, it remained fixed-function until OpenGL 2.0.

2.2.2 Programmable Function Pipeline

As the GPU architecture evolved over time, GPUs were more and more capable of doing different types of computations, more general computations, and not necessarily dedicated to something specific, reason why OpenGL's rendering pipeline evolved too, OpenGL's version 2.0 introduced officially a programmable function pipeline, in the form of *vertex shading* and *fragment shading*.
Figure 2.2 shows a block diagram of OpenGL 4.3 (newest to this day) rendering pipeline; each stage will be briefly explained next.

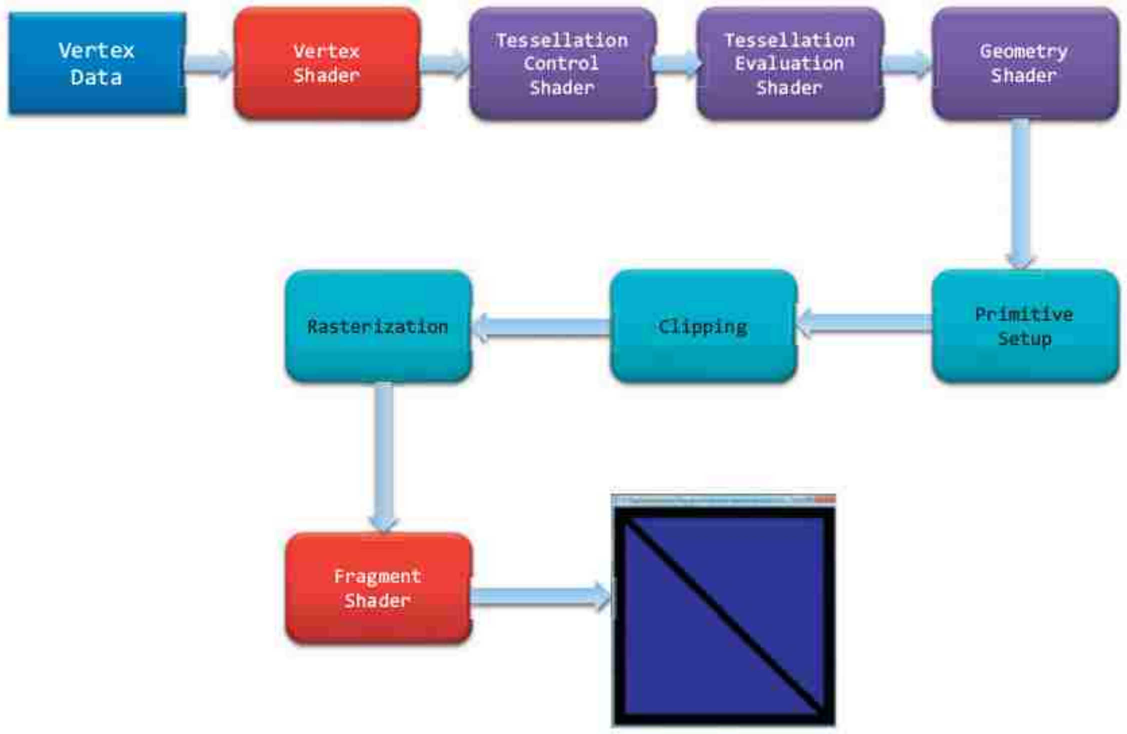


Figure 2.2: OpenGL 4.3 Rendering Pipeline[7]

- Vertex shading: Receives the vertex data, specified in VBOs, processing each vertex separately. This stage is mandatory for all OpenGL programs, and must have a shader bound to it.

- Tessellation shading: This is an optional stage, that generates additional geometry within the OpenGL pipeline, as compared to having the application specify each geometric primitive explicitly. This stage receives the output of the vertex shading stage, and does further processing of the received vertices.

- Geometry shading: This is another optional stage, that can modify the entire geometric primitives within the OpenGL pipeline, this stage operates on individual geometric primitives allowing each to be modified, additionally more geometry may be generated from the input primitive,change the type of geometric primitive or discarding geometry altogether. It receives its input after vertex shading has completed processing the vertices of a geometric primitive or from the primitives generated from the tessellation shading stage.

- Fragment shading: This stage processes the individual fragments generated by the OpenGL's rasterizer, it must have a shader bound to it, here a fragment's color and depth values are computed and then sent for further processing in the fragment-testing and blending parts of the pipeline.
- Compute shading: Although it is not part of the graphics pipeline as all the other stages. A computer shader processes generic work items, driven by an application-chosen range, rather than by graphical inputs like vertices and fragments. Compute shaders can process buffers created and consumed by other shader programs in the application.

2.2.2.1 GLSL

It is important to understand what shaders are, they work like a function call, where data is passed in, some process is applied to the data and then its returned, these functions are written in the OpenGL Shading Language (GLSL), which is a special language very similar to C++ used specifically for constructing shaders. Here I will give a very brief explanation on how to load GLSL shaders.
A GLSL shader is provided in a string of characters, it can either be loaded from a file of declared as a string of characters on code, most times the first method being more effective since, those files may be changed after compiling without a problem. The first line on a shader file must specify the version of GLSL to be used, if it is not specified GLSL 110 will be assumed and may be incompatible with the current OpenGL version, just as in C or C++ variables are declared before the declaration

of the *main()* function, these variables are the connection to the outside world, the shader does not know where its data is coming from but it only sees its input variables populated with data every time it executes, hence the importance of these shader variables, if they are not specified correctly the shader won't be able to do much.

In the *main()* function is where the shader actually performs calculations using the variables populated with the input, a good and simple example is passing the position of a node as the input to the vertex shader, using the vertex shader as a pass-through shader copying the input to the output, which will; eventually be the input of the fragment shader, in which in its *main()* function will perform some calculation and based on the node's position a different color may be obtained. The shaders utilized for this work are located in the appendix of this document.
To associate data going into the vertex shader we need to connect the shader variables declared as "in" to a vertex attribute array, which will be explained in section 2.3. Shaders also need to be compiled before they are used, they work in a similar way as C programs, the compiler analyses the program, checking for errors, translates it into object code, which is then linked to generate an executable program, the main difference is that the compiler and linker are also part of the OpenGL API. This process is shown on figure 2.3. To create a shader object, the function *glCreateShader()* is used as follows:

```
GLuint glCreateShader(GLenum type);
/* Allocates a shader object, type must be one of
GL_VERTEX_SHADER, GL_FRAGMENT_SHADER, GL_TESS_CONTROL_SHADER,
 GL_TESS_EVALUATION_SHADER, or GL_GEOMETRY_SHADER */
```

Once the shader object is created it needs to be associated with the source code of the shader, that is done with the function *glShaderSource()*.

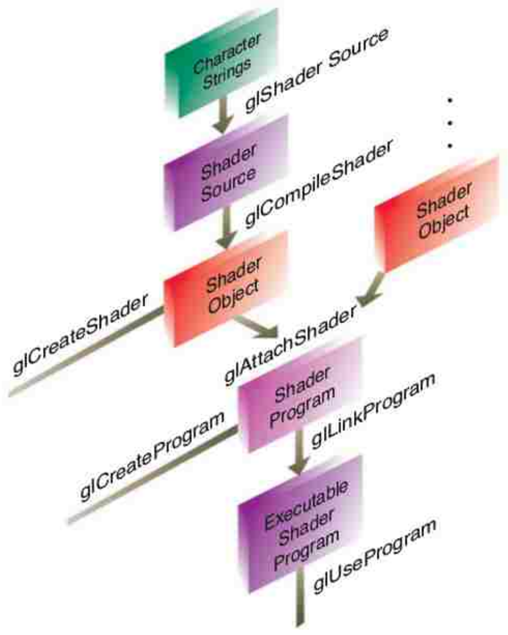


Figure 2.3: Shader compilation process[7]

```
void glShaderSource(GLuint shader, GLsizei count,
const GLchar **string, const GLint *length);
/* Associates the source of a shader with a shader object shader.
string is an array of count GLchar strings that compose the
```

As explained in the figure the next step is to compile the shader object:

```
void glCompileShader(GLuint shader);
/* Compiles the source code for shader. The results of the
 compilation can be queried by calling glGetShaderiv() with
 an argument of GL_COMPILE_STATUS. */
```

After the shader object was compiled, they need to be linked to create an executable shader program, this is a similar process as the one explained before for creating shader objects, first a shader program needs to be created, to be able to attach those shader objects to it.

```
GLuint glCreateProgram(void);
/* Creates an empty shader program. The return value is either
a nonzero integer, or zero if an error occurred. */
```

and to attach shader objects to it:

```
void glAttachShader(GLuint program, GLuint shader);
/* Associates the shader object, "shader" , with the shader
program, "program". A shader object can be attached to a shader
program at any time, although its functionality will only be
available after a successful link of the shader program.
A shader object can be attached to multiple shader programs
simultaneously. */
```

A shader object may be removed from a program with:

```
void glDetachShader(GLuint program, GLuint shader);
/* Removes the association of a shader object, "shader", from
the shader program, "program". If shader is detached from program
 and had been previously marked for deletion (by calling
glDeleteShader()), it is deleted at that time. */
```

Now with all the shader objects attached to the program, they need to be linked in order to become an executable program:

```
void glLinkProgram(GLuint program);
/* Processes all shader objects attached to "program" to generate
a completed shader program. The result of the linking operation
can be queried by calling glGetProgramiv() with GL_LINK_STATUS.
```

```
GL_TRUE is returned for a successful link; GL_FALSE otherwise. */
```

After a program has been successfully linked it can be used like this:

```
void glUseProgram(GLuint program);
/* Use the linked shader program "program". */
```

Shader objects and shader programs may be deleted as follows respectively:

```
void glDeleteShader(GLuint shader);
/* Deletes shader. If shader is currently linked to one or more
active shader programs, the object is tagged for deletion and
deleted once the shader program is no longer being used by any
shader program. */
```

```
void glDeleteProgram(GLuint program);
/* Deletes program immediately if not currently in use in any
context, or schedules program for deletion when the program is
no longer in use by any contexts. */
```

2.3 Buffer Objects

Buffers objects are general purpose memory storage blocks allocated by OpenGL, they give OpenGL implementations flexibility and improve performance, although they are generic by definition, the programmer is required to specify or describe the usage for them during the implementation, they can be used to store many types of data, but in this work buffers are used for storing vertex information, hence they are called Vertex Buffer Objects (VBOs).

To allocate data on a buffer object, a buffer object first need to be created, this is done using the *glGenBuffers()* command, and it has the following prototype:

```
void glGenBuffers(GLsizei n, GLuint *buffers);
/* Returns n currently unused names for buffer
objects in the array buffers. */
```

This will create an array of buffer objects names located at &*buffers*, although they are not object buffers yet, they are only placeholders. The buffer objects are not created until the name is bound to one of the buffer binding points on the context. There are several types of buffer binding points or also called targets, such as: *GL_ARRAY_BUFFER* for VBOs and *GL_ELEMENT_ARRAY_BUFFER* for Element Buffer Objects, which is where the vertex indices are contained.
Buffer objects will be actually created after the binding is done, using the *glBindBuffer()* command, with the following prototype:

```
void glBindBuffer(GLenum target, GLuint buffer);
/* Binds the buffer object "buffer" to the specified
buffer binding point as specified by "target". */
```

After creating the buffer, the next step to make something useful out of it, is to put data on it. This is done via the *glBufferData()* function:

```
void glBufferData(GLenum target, GLsizeiptr size,
  const GLvoid *data, GLenum usage);
/* Allocate size bytes of storage for the object bound
to the target, data must be non-null, usage describes
the intended usage for that buffer */
```

The function *glBufferData()* allocates storage, if *size* is larger than the space allocated for that buffer, the buffer will be resized, it is important to note the *usage* parameter, since it may have big influence on the performance of the program, it should be specified as one of the OpenGL usage tokens.

These usage tokens are composed of 2 parts: The first one can be either *STATIC, DYNAMIC, STREAM*, while the second one can be *DRAW, READ or COPY*, these are explained in further detail in table 2.3. OpenGL will make decisions based on

STATIC	Contents will be modified once and used many times.
DYNAMIC	Contents will be modified repeatedly, and used many times.
STREAM	Contents will be modified once and used at most a few times.
_DRAW	Contents are modified by the application and used as the source for OpenGL drawing and image specification commands.
_READ	Contents are modified by reading data from OpenGL and used to return that data when queried by the application.
_COPY	Contents are modified by reading data from OpenGL and used as the source for OpenGL drawing and image specification commands.

Table 2.1: Buffer Usage Tokens [7]

this parameter, such as placing the data on fast memory or avoiding to do so, if considers it not convenient.

To modify a buffer, completely or partially, the function *glBufferSubData()* is used like this:

```
void glBufferSubData(GLenum target, GLintptr offset,
GLsizeiptr size, const GLvoid *data);
/* Replaces a subset of a buffer object's data store
with new data. The section of the buffer object bound
to "target" starting at "offset" bytes is updated with
```

```
"size" bytes of data addressed by "data". */
```

When the buffers are correctly populated with the required data, this data needs to be hooked up to the shader. Vertex Array Objects (VAOs) are OpenGL objects that describe how the vertex attributes are stored in a Vertex Buffer Object (VBO), the VAO is not the object storing the vertex data but it is only the descriptor of this data. To associate the data going into the vertex shader, the shader "in" variables need to be connected to a Vertex Attribute Array, doing so with the function *glVertexAttribPointer()*:

```
void glVertexAttribPointer(GLuint index, GLint size, GLenum type,
GLboolean normalized, GLsizei stride, const GLvoid *pointer);
/* Specifies where the data values for the vertex attribute with
location "index" can be accessed. "pointer" is the offset in
bytes from the start of the buffer object currently bound to the
GL_ARRAY_BUFFER target for the first set of values in the array.
"size" represents the number of components to be updated per
vertex. "type" specifies the data type of each element in the
array. "normalized" indicates that the vertex data should be
normalized before being presented to the vertex shader. "stride"
is the byte offset between consecutive elements in the array. */
```

The state set by this function is stored in the currently bound VAO, there is only one thing left to do to be able to use this data, the VAO needs to be enabled, and this is done by the function *glEnableVertexAttribArray()*:

```
void glEnableVertexAttribArray(GLuint index);
void glDisableVertexAttribArray(GLuint index);
/* Specifies that the vertex array associated with variable index
be enabled or disabled. index must be a value between zero and
```

```
GL_MAX_VERTEX_ATTRIBS      1. */
```

Once the data is ready to be used by OpenGL, all that needs to be done is draw it on the screen, for this the function *glDrawElements()* will be used.

```
void glDrawElements(GLenum mode, GLsizei count,
GLenum type, const GLvoid *indices);
/* Defines a sequence of geometric primitives using "count"
number of elements, whose indices are stored in the buffer bound
to the Element Array Buffer (EAB). "indices" represents an offset
,in bytes, into the EAB where the indices begin. "type" must be
one of GL_UNSIGNED_BYTE, GL_UNSIGNED_SHORT, or GL_UNSIGNED_INT,
indicating the data type of the indices the EAB. "mode" specifies
what kind of primitives are constructed. */
```

2.4 External Libraries

2.4.1 GLUT

As explained before, OpenGL is designed to be implemented on different hardware and it is independent of the operating system running on the computer, for this very reason, OpenGL does not contain any functions or commands to manage windows, this needs to be done manually depending on the operating system the software is intended to run on, in this work the GLUT (OpenGL Utility Toolkit) library was used to overcome this, facilitating the OpenGL initialization and window managing. The version of GLUT used is called *freeglut*, it is based on the original version, but it's more updated and more compatible in many cases, a more in depth explanation

of how GLUT works can be found at [23].
GLUT makes making OpenGL applications a simpler process, this is done in its most basic form in the following way:

- Initialization: In the initialization part several functions are called, such as *glutInit()*, and *glutCreateWindow()*, their names are very obvious of what they do, but also in this phase other functions may be called, to specify the window size, position or OpenGL display mode for example.

- Registering Callbacks: In this phase, the programmer must specify the functions that will be called when a specific event happens, this functions could be for example, what function to call when a key was pressed or released on the keyboard (*glutKeyboardFunc()*), when the user uses a mouse button or even moves the mouse(*glutMouseFunc()* and *glutMotionFunc()*), and some of them more needed than others, such like what function to call when it's time to display or render something on the screen (*glutDisplayFunc()*), when OpenGL is idle (*glutIdleFunc()*), or when the window is resized(*glutReshapeFunc()*).

- Main Loop: Lastly what needs to be done is to call the *glutMainLoop()* function which basically loops between the functions previously specified and has an event handler to perform the correct callback for a specific event.

2.4.2 GLEW

GLEW is the OpenGL Extension Wrangler, which is another external library used in this work, it is a cross platform open source C/C++ extension loading library, GLEW provides efficient runtime mechanisms for determining which OpenGL extensions are supported on the target platform, OpenGL core and extension functionality is exposed in a single header file *glew.h*, all that needs to be done is to initialize it calling the function *glewInit()* after creating the window using GLUT[].

2.4.3 GLM

OpenGL Mathematics or GLM is a header only c++ mathematics library for graphics software based on the OpenGL Shading Language (GLSL), this library intends to provide classes and functions designed and implemented following as strictly as possible the GLSL conventions and functionalities so that when a programmer knows GLSL, GLM will also look familiar, although it is not limited to GLSL, it provides extended capabilities including matrix transformations, quaternions, random number generation, among others, it also ensures interoperability with third party libraries , SDKs and OpenGL, it replaces deprecated functions, and as a general purpose library it can be used in many applications. In this work the GLM library is used primarily to perform the object manipulations using matrices for transformations and rotations, and camera manipulation.

Chapter 3

Parallelization

When using parallel computing to develop parallel algorithms it is a good idea to follow some software engineering discipline or programming model, one good example is the APOD (Analyze Parallelize Optimize and Deploy) model, which is defined as a systematic automation process, that the programmer must follow to break down the optimization process and succeeding not only at developing fast algorithms, but also be efficient and organized about it.
First an explanation of the theory behind the algorithm will be explained

3.1 Modal Warping

This work is based primarily on the paper presented at the IEEE transactions on visualization and computer graphics by Min Gyu Choi and Hyeong-Seok Ko [5].
In their work they present a technique to perform real time simulation of objects, their work is based on implementing a special type modal analysis called modal warping to FEM to improve simulation speed when using large objects, however what

modal warping fails to achieve is being accurate for large deformations, extending their modal analysis work to identify a rotational component of an infinitesimal deformation and being able to keep track of it, achieving accurate results.
Reason why modal analysis is a good choice of algorithm to be implemented on a GPU; it provides accurate results and applying modal analysis to FEM, as its explained further in the next section makes it easy to decouple the calculation of the modal amplitudes making every calculation independent from each other fitting for the most part the threads organization used in GPGPU computing.

3.1.1 Rotational Part in a Small Deformation

The non-linear term in a strain sensor is the one responsible for the appearance and disappearance of rotational deformations, since it is generally known that every infinitesimal deformation can be decomposed into a rotation followed by a strain this serves as a basis for this technique, basically: at every timestep of the simulation, small rotations are identified on every point of the material, then the effect of them is integrated to obtain the deformed shape.
A brief explanation of this calculation goes as follows:

3.1.1.1 Kinematics of Infinitesimal Deformation

Given an elastic solid object; $x \in \mathbb{R}^3$ denotes the position of a material node/point in an undeformed state, which will in turn move to a new position given by $a(x)$ due to a subsequent deformation.

$$a(x) = x + u(x), x \in \Omega$$

where Ω is the domain of the solid.
Differentiating both sides with respect to x gives us:

$$da = (I + \nabla u)dx \tag{3.1}$$

The *infinitesimal strain tensor* ε which measures the change in the squared length of dx during an infinitesimal deformation is defined as:

$$\varepsilon = \frac{1}{2}(\nabla u + \nabla u^T)$$

if we note that $\frac{1}{2}(\nabla u + \nabla u^T)$ is a meaningful quantity, ∇u can be decomposed as:

$$\nabla u = \frac{1}{2}(\nabla u + \nabla u^T) + \frac{1}{2}(\nabla u - \nabla u^T) = \varepsilon + \omega \tag{3.2}$$

The skew-symmetric tensor ω, is closely related to the curl of the displacement field ∇u and it may rewritten as:

$$\omega = \frac{1}{2}(\nabla u - \nabla u^T) = \frac{1}{2}(\nabla \times u)\times = w\times \tag{3.3}$$

Where $w\times$ denotes the standard skew symmetric matrix of vector w. Therefore $\frac{1}{2}(\nabla \times u)\times$ can be viewed as a rotation vector that causes rotation of the material points at and near x, by an angle given by $\theta = \|w\|$ about the unit axis $\hat{w} = \frac{w}{\|w\|}$
ω is called the *infinitesimal rotation tensor*
Finally if we substitute equations 3.3 and 3.2 into 3.1 we obtain:

$$da = dx + \underbrace{\varepsilon dx} + \underbrace{\theta \hat{w} \times dx} \tag{3.4}$$

Showing that an infinitesimal deformation can be decomposed correctly into *strain* and *rotation*.

3.1.1.2 Extended Modal Analysis

The purpose of extending the modal analysis is to keep track of the rotation experienced by each material point during deformation.

The governing equation for a finite element model is given by:

$$M\ddot{u} + C\dot{u} + Ku = F \tag{3.5}$$

Where $u(t)$ is a 3n-dimensional vector representing the displacements of the n nodes, from their original positions and $F(t)$ is a vector that represents the external forces acting on the nodes. The mass, damping and stiffness matrices M, C and K respectively are independent of time and are completely characterized at the rest state under the commonly adopted assumption that $C = \xi M + \zeta K$ where ξ and ζ are scalar weighting factors (Rayleigh Damping) [5].

In general M and K are not diagonal, thus equation 3.5 is a coupled system of ordinary differential equations (ODEs). Let Φ and a diagonal matrix Λ be the solution matrices to the generalized eigenvalue problem: $K\Phi = M\Phi\Lambda$, such that $\Phi^T M\Phi = I$ and $\Phi^T K\Phi = \Lambda$.

Since the columns of matrix Φ form a basis of the 3n-dimensional space, u can be expressed as a linear combination of the columns:

$$u(t) = \Phi q(t) \tag{3.6}$$

Where Φ is the *modal displacement matrix*; every column represents a different mode, and $q(t)$ is a vector containing the corresponding modal amplitudes.

Examining the *eigenvalues*, allows to only take dominant columns (modes) of Φ, reducing significantly the amount of computation to be performed.

Substituting equation 3.6 in equation 3.5 followed by a premultiplication of Φ^T decouples 3.5 as:

$$M_q\ddot{q} + C_q\dot{q} + K_q q = \Phi^T F \tag{3.7}$$

where $M_q = I$, $C_q = \xi I + \zeta\Lambda$, and $K_q = \Lambda$ are now all diagonal matrices and $\Phi^T F$ is defined as the modal force.

Manipulating the previous equation the following equations can be obtained:

$$\dot{q}^k = \frac{(\alpha - I) * q^{k-1} + \beta * \dot{q}^{k-1} + \gamma * \Phi^T * F^{k-1}}{h} \tag{3.8}$$

$$q^k = \alpha * q^{k-1} + \beta * \dot{q}^{k-1} + \gamma * \Phi^T * F^{k-1} \tag{3.9}$$

Where h is the time step size and the coefficient matrices can be obtained by:

$$\alpha_i = 1 - \frac{h^2 * k_i}{d_i}$$

$$\beta_i = h * (1 - \frac{h * C_i + h^2 * k_i}{d_i})$$

$$\gamma_i = \frac{h^2}{d_i}$$

$$d_i = M_i + h * C_i + h^2 * k_i$$

Where: M_i, C_i and K_i represent the diagonal entries of M_q,C_q and K_q

3.1.1.3 Modal Rotation

While the conventional way of accurately calculating strain and deformation is defined as:

$$\varepsilon = \nabla u * \nabla u^T \tag{3.10}$$

The previous equation provides accurate results but it is computationally complex, reason why it is chosen to use the infinitesimal strain sensor from equation 3.3, trading off accuracy for complexity, to overcome this problem the calculation of displacement for every node needs to be independent of rotation, and the rotation must be included afterwards.

The rotation matrix is defined as follows:

$$R = \int_0^t \omega(t) * dt \tag{3.11}$$

Where $\omega(t)$ is the angular velocity of a certain node for in a specific timestep.

It can be assumed that the rotation linearly varies from 0 to t starting at 0 and ending in w, for a certain time $\frac{w*\tau}{t} \rightarrow R$, given this we can include define the composite vector $w(t)$ as follows:

$$w(t) = W * \Phi * q(t) = \Psi(q(t) \tag{3.12}$$

To make the calculation time independent Ψ can be defined as and be precomputed as:

$$\Psi = W * \Phi \tag{3.13}$$

Equation 3.12, will later be used to calculate the rotation using Rodrigues formula [24]

$$R_i = [I + (\hat{w}_i \times) \frac{1 - cos\|w_i\|}{\|w_i\|} (\hat{w}_i \times)^2 (1 - \frac{sin\|w_i\|}{\|w_i\|})] \tag{3.14}$$

Where: i indicates this calculation is for a specific node , $\hat{w}_i \times$ is defined as the *skew symmetric matrix* for that specific node and $\|w_i\|$ is the magnitude of the *skew symmetric matrix* and I is the identity matrix with a size of $n * n$, given that it is a 3 dimensional node $n = 3$, and finally R_i will also be a $n * n$ matrix.

Lastly what needs to be done is to include the rotational part in the displacement calculation doing so by applying R_i on equation 3.6 for a specific node:

$$u_i(t) = R_i * u_i(t) \tag{3.15}$$

After doing so $u(t)$ will contain not only displacement information for all nodes but also rotation information, which will only need to be applied to the nodes original location to get the new location for a specific timestep.

3.1.2 Implementation

The implementation of the modal warping technique will be explained in this section. The displacement is given by equation 3.6, it is obtained by the multiplication of the *modal displacement matrix* by the vector containing the corresponding *modal amplitudes*, to get these two elements, we need to solve the eigen problem first to get Φ; which in this case its precomputed and use equations 3.8 and 3.9 to obtain q. Lastly using equation 3.14 we can also include the rotational information, providing an accurate result.
A brief analysis of the equations previously will give the chronological order in which the elements need to be obtained: The final goal is to obtain a displacement per 3-dimensonal node, which is given by:

$$u(t) = \Phi q(t)$$

To obtain u first Φ and q need to be obtained, in the case of Φ it is assumed it was previously computed, and q will be given by the following equation:

$$q^k = \alpha * q^{k-1} + \beta * \dot{q}^{k-1} + \gamma * \Phi^T * F^{k-1}$$

Asit can be seen to get q we not only need to get $\dot{q}$ first using equation:

$$\dot{q}^k = \frac{(\alpha - I) * q^{k-1} + \beta * \dot{q}^{k-1} + \gamma * \Phi^T * F^{k-1}}{h}$$

But also the coefficients matrices which are given by:

$$\alpha_i = 1 - \frac{h^2 * k_i}{d_i}$$

$$\beta_i = h * (1 - \frac{h * C_i + h^2 * k_i}{d_i})$$

$$\gamma_i = \frac{h^2}{d_i}$$

$$d_i = M_i + h * C_i + h^2 * k_i$$

Where: M_i, C_i and K_i represent the diagonal entries of M_q,C_q and K_q, and as explained in section 3.1 we can assume that K contains the eigenvalues, M is the Identity matrix and C is a linear combination of both. In chronological order of execution, calculations need to be performed as follows:

1. Solve the Eigenproblem: From this: Φ and K will be obtained, being the eigenvectors and the eigenvalues respectively.

2. Compute C : After getting K and knowing that M is the Identity matrix, C can be computed as a linear combination of both.

3. Compute Coefficient Matrices: All the coefficient matrices will be diagonal matrices obtained from the equations previously explained.

The elements previously mentioned are time independent and can be computed at the beginning of the program, while the following need to be computed at every timestep or iteration of the program:

1. Compute $\dot{q}$

2. Compute q

3. Compute u

4. Compute rotation: rotational information needs to be calculated, and it can be obtained using the Rodrigues's formula

5. Include rotation: Including the rotational information obtained in the last element is vital since it will give an accurate result

3.2 Analyze Stage

The first step of the model is to analyze the problem, or in this case analyze the current algorithm, which was developed using conventional computing, executing CPU code exclusively, the original algorithm was developed using MATLAB as stated before, so the first step was to create or translate the original algorithm from MATLAB to C/C++, doing so to not only to get a better performance already, but also to be able to reuse parts of this code on the parallel version programmed in CUDA.

3.2.1 GNU Profiler

A good way of analyzing a program is using a technique called profile based analysis, profiling an application will output some vital information of where the program spends its time, and this in turn will facilitate developing algorithms that will improve performance on the parts of the code where its most important, GNU profiler (gprof) was the tool selected to do this task [25]. Below is the filtered output of the GNU profiler:

```
$ gprof -p mwgpu

%    cumulative  self           self     total
time   seconds  seconds  calls  ms/call  ms/call   name
83.01   1.71    1.71    135378  0.01  0.01   matrixByVec(...)
8.25    1.88    0.17       414  0.41  0.41   matrixTranspose(...)
3.88    1.96    0.08    132480  0.00  0.00   matrixMult(...)
3.40    2.03    0.07       414  0.17  0.17   insertZeros(...)
0.49    2.05    0.01      1656  0.01  0.01   vectorAdd(...)
```

Listing 3.1: GNU Profiler Filtered Output

From this output we can see easily in what functions the program spends more time, it is important to also note the amount of times a certain function was called, since noticing that a programs spends a lot of time on a certain function might not necessarily mean its inefficient, it might be that it just needs to call that function a lot of times.
As noted before the functions where the program spends more time are, in order of time spent:

- *matrixByVec()*
- *matrixTranspose()*
- *matrixMult()*
- *insertZeros()*
- *vectorAdd()*
- *computeR()*

This is valuable information, since it gives a good start point on where the parallelization would improve more the original algorithm, after getting this information, singling out every one of this functions to analyze is the next step.
After analyzing all the functions, it can be stated that the functions *matrixByVec()*, *matrixTranspose()* and *matrixMult()* can be parallelized in most of their computations, while *insertZeros()* and *computeR()* not so much, but since most of the time spent is on the first three functions mentioned, it can be presumed that a good optimization will be achieved.

3.2.2 Amdahl's Law

To be able to approximate the performance gain that can be obtained by improving some portion of an algorithm may be improved, Amdahl's Law is used. Amdahl's law states that the performance improvement to be gained from using some faster mode of execution is limited by the fraction of time the faster mode can be used. Amdahl's law defines the speedup that can be gained by using a particular feature[8]. Where speedup is defined as:

$$Speedup = \frac{Performance\,using\,the\,enhancement\,when\,possible}{Performance\,without\,using\,the\,enhancement} \tag{3.16}$$

Amdahl's law gives a quick way to find the speedup from some enhancement, depending on two factors: The fraction of the computation time in the original algorithms that can be converted to take advantage of the enhancement, and the improvement gained by the enhanced execution mode (how much faster the task would run if the enhanced mode where to be used for the entire algorithm. The execution time is defined as follows:

$$ExecTime_{new} = ExecTime_{old} * ((1 - Fraction_{enhanced}) + \frac{Fraction_{enhanced}}{Speedup_{enhanced}}) \tag{3.17}$$

and the overall speedup is the ration of the execution times:

$$Speedup_{overall} = \frac{ExecTime_{old}}{ExecTime_{new}} \tag{3.18}$$

or:

$$Speedup_{overall} = \frac{1}{((1 - Fraction_{enhanced}) + \frac{Fraction_{enhanced}}{Speedup_{enhanced}})} \tag{3.19}$$

Amdahl's law expresses the law of diminishing returns: The incremental improvement is the speedup gained by an improvement of just a portion of the computation, it diminishes as improvements are added. Analyzing the specific case of this algorithm we can note that the fraction of the code that can be improved is a constant, where this fraction was approximated using the profiler in section 3.2.1, although the time spent on executing it's a variable, depending on how large the object used on the simulation is, the number of nodes the object has and the number of eigenvalues used in the calculation, will define the time spent on calculating the modal displacement. It can be presumed then that as the object gets larger and larger, the gain on algorithm performance will also increase.

3.2.3 Computer and device specs

It is also important to specify the specifications of the devices and software used to measure performance improvement, these will be described in the following listings:

```
OS: Arch Linux x86_64 GNU/Linux
Kernel: 3.14.0-5-ARCH

GCC: gcc (GCC) 4.8.2 20140206 (prerelease)

Make: GNU Make 4.0

NVCC: NVIDIA (R) Cuda compiler driver
Cuda compilation tools, release 6.0, V6.0.1
```

Listing 3.2: Operating System & Software Specifications

The CPU and system memory specifications are a filtered version of the information taken from the files */proc/cpuinfo* and */proc/meminfo*, gotten using the Linux kernel, and some information using other commands.

```
Processor: Genuine Intel (R) Core 2 Duo CPU U7300 @ 1.30 Ghz
CPU MHz: 1733.00
Cache Size: 3072 KB

Memory:
Size: 4096 MB
Form Factor: SODIMM
Type: DDR3
Speed: 800 MHz
```

Listing 3.3: CPU and System Memory Specifications

GPU or device specifications listed below are a filtered version of the output obtained by the deviceQuery utility given by NVIDIA with the CUDA release, and also the information obtained using the NVIDIA Visual Profiler [26], whose functionality will be explained in section 3.4.

```
GPU: GeForce GT 335M
CUDA Driver Version / Runtime Version           6.0 / 5.5
CUDA Capability Major/Minor version number:     1.2
Total amount of global memory:                  1023 MBytes
( 9) Multiprocessors, (  8) CUDA Cores/MP:      72 CUDA Cores
GPU Clock rate:                                 1080 MHz
Memory Clock rate:                              790 Mhz
Memory Bus Width:                               128-bit
Warp size:                                      32
Maximum number of threads per multiprocessor:   1024
Maximum number of threads per block:            512
Max dimension size of a thread block (x,y,z): (512, 512, 64)
Max dimension size of a grid size    (x,y,z): (65535, 65535, 1)
```

```
Integrated GPU sharing Host Memory:             No
Support host page—locked memory mapping:        Yes
Device supports Unified Addressing (UVA):       No
```

Listing 3.4: GPU Specifications

The above is perhaps the most valuable information of all, since as specified before in section 1.3.3.2, when using parallel computing on the GPU; the programmer must develop algorithms somewhat based on the underlying architecture of the device, for example the amount of maximum threads possible to execute per block is a very important parameter, which was thought of when developing the algorithm, or another important parameter would be the amount of CUDA cores available for a specific device.

3.3 Parallelize Stage

With all the information previously obtained, CUDA can be integrated to an existing C/C++ application, the CUDA entry point being a host only function, containing the kernel or kernels, called from C/C++ code.
The compiler needed for CUDA code is called *nvcc*, and it only needs to compile the file that contains the function previously specified, while any other file can be compiled with a conventional compiler such as *gcc*. First, a host only function was created called *displacement()*, parameters such as the force vector, number of nodes, eigenvalues, among others were passed to it, the purpose of this function as mentioned before was to be a entry point to CUDA, in this function the *environment* to use CUDA is created, allocating GPU memory, copying memory from host to device or vice-versa, calculating the amount of threads needed to be run per block (there is a

maximum amount of threads depending on the device), etc. Although once all that is done this function is also in charge of one of the most important things, which is launching the kernels.
To implement the parallel algorithm the same ”sequence” found on the conventional algorithm was followed, creating a parallel version of the functions needed, as it was shown before the most important ones were *matrixByVec()*, *matrixTranspose()*, etc. These functions were ”replicated” in the form or kernels.
In this first version the *displacement()* function would be called from inside the OpenGL loop created by GLUT [23], it would allocate and copy all the memory needed on the GPU, launch the kernels to perform different calculations, and after a result for that node displacement was obtained it would return that result in the form of an array which would then be used in the main code to modify the OpenGL buffer previously created, to render the object on the screen.

3.3.1 Kernel Development

In this section a basic explanation of the kernels developed will be given.
The major kernels used in this work as it was shown in figure 3.3 are:

- kMatVector
- kInsertZeros
- kVectorAdd
- kModBuffer
- kComputeR

These kernels are used to implement the equations found on section 3.1.2, the purpose of these equations is to be able to get the location displacement from every node contained on the object, while keeping the rotation information too.
The calculations that need to be parallelized are the ones to be computed on every iteration of the program, hence obtaining a better improvement in performance.
Analyzing the following equation the $\dot{q}$ vector can be obtained:

$$\dot{q}^k = \frac{(\alpha - I) * q^{k-1} + \beta * \dot{q}^{k-1} + \gamma * \Phi^T * F^{k-1}}{h}$$

It can be separated in 5 main operations:

$$result_1 = (\alpha - I) * q^{k-1}$$

$$result_2 = \beta * \dot{q}^{k-1}$$

$$result_3 = \gamma * \Phi^T * F^{k-1}$$

$$result = \Sigma_i^n result_i$$

$$\dot{q} = \frac{result}{h} = result * \frac{1}{h}$$

- The first part ($result_1$) can also be separated in an addition between matrices ($\alpha + (-Identity)$) multiplied by q^{k-1} which is a vector.

- The second part ($result_2$) is merely a matrix (β) multiplication by a vector ($\dot{q}^{k-1}$).

- The third part ($result_3$) performs two sequential multiplications, the first one a matrix by a vector $\Phi^T * F^{k-1}$ assuming that the transpose of Φ was previously calculated, and the second one, multiplying the result obtained by the coefficient matrix γ.

- The next operation is to perform an addition of the result obtained from all the previous ones.
- And the last one is to multiply that result which is a vector by a scalar ($\frac{1}{h}$).

With the next equation q can be obtained:

$$q^k = \alpha * q^{k-1} + \beta * \dot{q}^{k-1} + \gamma * \Phi^T * F^{k-1}$$

Looking at the previous equation, it can be seen that it could be separated in the following operations:

$$result_1 = (\alpha) * q^{k-1}$$

$$result_2 = \beta * \dot{q}^{k-1}$$

$$result_3 = \gamma * \Phi^T * F^{k-1}$$

$$q = \Sigma_i^n result_i$$

But looking closely, two of these operations were already calculated previously to get $\dot{q}$ ($\beta * \dot{q}^{k-1}$ and $\gamma * \Phi^T * F^{k-1}$), so the only one different is $(\alpha) * q^{k-1}$ and then adding them all together. This will take more space in memory but save time not performing unnecessary calculations. With these results now the following calculation can be computed:

$$u(t) = \Phi q(t)$$

This is again a matrix (Φ) multiplication by a vector ($q(t)$)
After this the only computation needed is to include the rotational information in vector $u(t)$ although it is not that simple, to do this we need to implement equation 3.15:

$$u_i(t) = R_i * u_i(t)$$

This will include the rotation information in the $u(t)$ but it will do it for every node, the R_i matrix can be obtained using Rodrigues's formula like this:

$$R_i = [I + (\hat{w}_i \times)\frac{1 - cos\|w_i\|}{\|w_i\|}(\hat{w}_i \times)^2(1 - \frac{sin\|w_i\|}{\|w_i\|})]$$

To implement this the following calculations need to be performed first:

1. Compute w vector
2. Compute $\hat{w}_i$ skew symmetric matrix
3. Calculate w_i vector's norm
4. Calculate the skew symmetric matrix squared: $\hat{w}_i \times^2$

Vector $w(t)$ can be obtained by multiplying the Ψ matrix by vector $q(t)$, where it is assumed that this matrix was previously precomputed.
And the skew symmetric matrix of vector w_i is given by:

$$\begin{bmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{bmatrix}$$

.

Generic kernels were created to perform matrix and vector operations, it was decided this way instead of creating one major kernel to perform calculations per element because the device available was not powerful computationally speaking.
After several tests and performance measurements it was proven that using generic kernels was more efficient for this device while the same code could still work on better devices.
A good example of this is the *kmatrixByVec* kernel which performs the multiplication of a matrix by a vector, the original code developed was this:

```
__global__ void kMatVector(float *mat, float *vec, float *res,
 unsigned int RowsMat, unsigned int ColsMat) {
  float c = 0;
  const unsigned int TID = threadIdx.x;
  const unsigned int BID = blockIdx.x;
  const unsigned int BDIM = blockDim.x;

  unsigned int i=BDIM*BID+TID;

  if(i > RowsMat) return;

  extern __shared__ float vecsh[];
  for(int j=0;j<ColsMat;j++){
    vecsh[j]=vec[j];
  }

  __syncthreads();

  for(int j=0;j<ColsMat;j++){
    c += mat[i*ColsMat+j]*vec[j];
  }
  res[i]=c;
}
```

This used some interesting features of CUDA, first it used the *__shared__* variable declaration to specify that memory will be contained in shared memory, which as explained in section 1.3.3.2.1: shared memory is faster than global memory, after that it copied values from global memory to shared memory, using *__syncthreads()* to make sure all threads were synchronized and the vector in shared memory contained all the information needed, after that the actual matrix by vector multiplication was calculated, nonetheless performance was slow and the code had to be modified to:

```
__global__ void kMatVector(float *mat, float *vec, float *res,
  unsigned int RowsMat, unsigned int ColsMat) {
   float c = 0;
   const unsigned int TID = threadIdx.x;
   const unsigned int BID = blockIdx.x;
   const unsigned int BDIM = blockDim.x;

   unsigned int i=BDIM*BID+TID;

   for(int j=0;j<ColsMat;j++){
     c += mat[i*ColsMat+j]*vec[j];
   }
   res[i]=c;
}
```

Getting rid of all shared memory operations.

The architecture on this device was not able to hold enough shared memory for the vector in some of the models, and while a workaround could have been found for this, the processors were still too slow and sacrificing the use of another *for* loop to use shared memory, creating another branch in the thread code was simply not feasible.

Two other important kernels used were the *kModBuffer* and *kVectorAdd*, which as the name suggests, the first one modifies the OpenGL graphics buffer and the second one adds two vectors, these two kernels basically perform the same operation since the graphics buffer is nothing more than a vector in memory. Again shared memory operations had to be avoided:

```
__global__ void kModBuffer(float *buffer, float *d_nodes,  float
 *u, unsigned int totalThreads)
{
  const unsigned int TID = threadIdx.x;
  const unsigned int BID = blockIdx.x;
  const unsigned int BDIM = blockDim.x;

  unsigned int index=BDIM*BID+TID;



  if(index>totalThreads)
    return;
  // Add displacement to original nodes
  buffer[index]=d_nodes[index]+u[index];

}
```

The first part of the kernel is to know which thread is actually being executed, this is how the index for the memory location to be modified is obtained. The *if* branch is to make sure the that none of the threads will try to modify memory locations not part of the buffer, as explained before this was part of the warp optimizations. While these two kernels seem very simple, they are executed many times hence their importance on performance.

Lastly another important kernel to mention is the *kInsertZeros* kernel, this is particularly important because along with the *kComputeR* kernel its one of the less parallelizable parts of the program, in fact to be able to do this in parallel it has to be executed several times, unlike the serial version which is able to do it in only one execution.

```
__global__ void kInsertZeros(float *Input, float *Output,
  unsigned int position, unsigned int number, unsigned int
  numElements) {
  //Get element to work on
  const unsigned int TID = threadIdx.x;
  const unsigned int BID = blockIdx.x;
  const unsigned int BDIM = blockDim.x;

  unsigned int i=BDIM*BID+TID;
  //Array wil be increasin its size per execution
  if(i<numElements){
    // Do it 3 times
    // i for insert 0's
    if(i>position-1 && i<=position+number-1)
      Output[i]=0;
    // i After 0's
    else if(i>=position+number)
      Output[i]=Input[i-number];
    // i before 0's
    else if(i<position)
      Output[i]=Input[i];
  }
}
```

This kernel inserts three 0's on the array containing the displacement, each zero corresponds to a dimension (x,y,z), this is because some of the nodes of the object are fixed to analyze the object's behavior, meaning that these nodes should not have a displacement, and since they are not used for the calculation, these locations in memory need to be 0. The complex part here is that since it is being done in parallel, there is no communication between the threads, the programmer cannot know the order in which threads will be executed, and for this specific operation order does matter, this is why this kernel needs to be executed several times. It is important to note that a workaround for this is to use sparse structures which is one of the items on future work to improve performance of this program.

The *kComputeR* kernel is very long but some important parts will be explained here, this kernel implements the Rodrigues's formula shown in equation 3.14, and it then includes this information on vector $u(t)$ it is not very parallelizable with the CUDA version compatible with this device.

```
float sum=0;
// Compute Norm
for(j=0;j<size;j++){
  sum+=d_w[rI+j]*d_w[rI+j];
}
if(sum<0.00001)
  norm=1;
else
  norm=sqrtf(sum);
```

This part is used to obtain the norm of the vector w, avoiding a future division by zero, although it is a simple operation, but the usage of *sqrt* which is unavoidable makes it slow.

This kernel has to work per node, meaning that unlike most other kernels that perform operations per location in memory, this one perform operations on three locations of memory, since every node contains information about its three dimensions. Using CUDA 6 a kernel is able to launch more kernels, which could avoid this and make every kernel to work on only one location per memory.

```
// Get skew matrix ^2
for (j=0;j<size;j++){
  for (k=0;k<size;k++){
    sum=0;
    for(l=0;l<size;l++){
      sum+=skew_w[j*size+l]*skew_w[l*size+k];
    }
    skew_w2[j*size+k]=sum;
  }
}

// Get R Matrix
for(j=0;j<size*size;j++){
  R[j]=Identity[j]+skew_w[j]*b+skew_w2[j]*c;
}

// Multiply R by uc and modify u
for (j=0;j<size;j++){
  sum=0;
  for(k=0;k<size;k++)
    sum+=R[j*size+k]*d_uc[rI+k];
  d_u[rI+j]=sum;
}
```

It is clearly seen that inside this kernel many operations for which another kernel was already developed (such as matrix multiplication, or multiplying a matrix by a vector) are executed, again the usage of CUDA 6 could greatly improve performance, by launching kernels from the GPU.
It is important to note that this kernel uses functions such as *sine* and *cosine*, the implementation of this kernel uses a special library made available by NVIDIA which contain intrinsics functions developed specifically to be executed on the GPU and work a lot faster than their equivalent implementations of the *Math.h* library on C.

There were some other kernels developed to perform operations like matrix by matrix multiplication, using shared memory which is not used at the moment but in a future version it can be very well implemented, and a matrix transpose kernel which is not as important since after the optimizations it is only executed once.

Another important fact is that, after analyzing the code it might seem serialized in some way due to the fact that when launching kernels, one launch needs to wait until the previous kernel finishes, but to overcome this problem *CUDA Streams* were used, a CUDA stream is defined as a single operation sequence that will be executed on a GPU device.

CUDA kernels by default are executed in the default stream, if all the kernels are on the same stream, they do have to wait for the previous one to finish to be launched, although if they are put on different CUDA streams, multiple kernels can run concurrently, performance can be improved by increasing the number of concurrent kernels setting a higher degree of parallelism.

A stream can be declared as follows:

```
//Declare the stream
cudaStream_t stream_1;
//Create the actual stream on CUDA
cudaStreamCreate(&stream_1)
```

After being declared the stream can be used when launching a kernel, by specifying on the kernel launch parameters on which stream it should run.

```
//Launch kMatVector Kernel on stream 1
kMatVector<<< blocksPerGrid, threadsPerBlock,stream_1>>>
```

And lastly when the program will not use the stream for any other calculations it should be destroyed:

```
//Destroy the stream
cudaStreamDestroy(stream_1);
```

An array of streams can also be created:

```
//Create array of streams
int nstreams= 3;
// Allocate and Initialize Array
cudaStream_t *streams = (cudaStream_t *)
  malloc(nstreams * sizeof(cudaStream_t));
for (int i = 0; i < nstreams; i++){
  cudaStreamCreate(&(streams[i]));
}
```

This way many kernels can be launched on the several streams contained in the array. The programmer needs to be aware that in some cases a synchronization between steams needs to be performed, this to make sure that the data needed has already been calculated correctly avoiding unwanted results.

```
//Synchronize streams
cudaStreamSynchronize()
```

So as an example: in the calculation of vector $\dot{q}(t)$, the first and second operations are independent from each other so they can and should be executed on different streams as it is shown in the following code snippet.

```
//Create array of streams
int nstreams= 2;
// Allocate and Initialize Array
cudaStream_t *streams = (cudaStream_t *)
  malloc(nstreams * sizeof(cudaStream_t));
for (int i = 0; i < nstreams; i++){
  cudaStreamCreate(&(streams[i]));
}

//Arguments: Matrix , Vector, Result Array Location,
// Size of Matrix (m,n)
kMatVector<<< blocksPerGrid, threadsPerBlock,streams[0]>>>(
  d_alphaI, d_qo, d_u1, eigencount, eigencount);
//Make sure no error was returned from CUDA
error = cudaGetLastError();
if (error != cudaSuccess)
{
  //Print Error Code and Line
  fprintf(stderr, "Failed to launch MatByVec kernel
    (result_1) (error code %s)!\n", cudaGetErrorString(error));
  exit(EXIT_FAILURE);
}

//Arguments: Matrix , Vector, Result Array Location,
// Size of Matrix (m,n)
kMatVector<<< blocksPerGrid, threadsPerBlock,streams[1]>>>(d_beta
  , d_qdo, d_u2, eigencount, eigencount);
//Make sure no error was returned from CUDA
error = cudaGetLastError();
if (error != cudaSuccess)
{
  //Print Error Code and Line
  fprintf(stderr, "Failed to launch MatByVec kernel
    (result_2) (error code %s)!\n", cudaGetErrorString(error));
  exit(EXIT_FAILURE);
}

//Synchronize streams
cudaStreamSynchronize()
```

Basic chronologic diagrams of execution are shown in figures 3.1 and 3.2; the first one shows how kernels are executed one after another when they are all in the default stream, while the second one shows how kernels can be executed concurrently if they are on different streams.

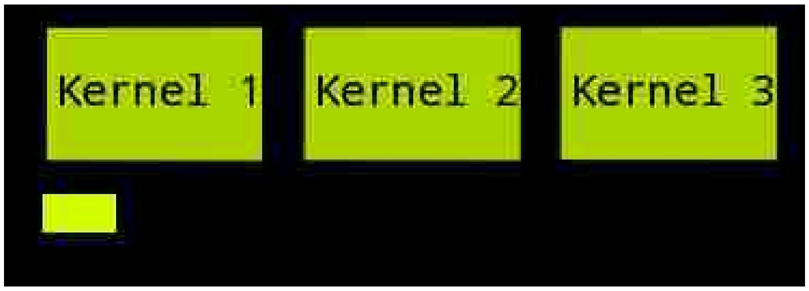


Figure 3.1: CUDA's Default Stream Behavior

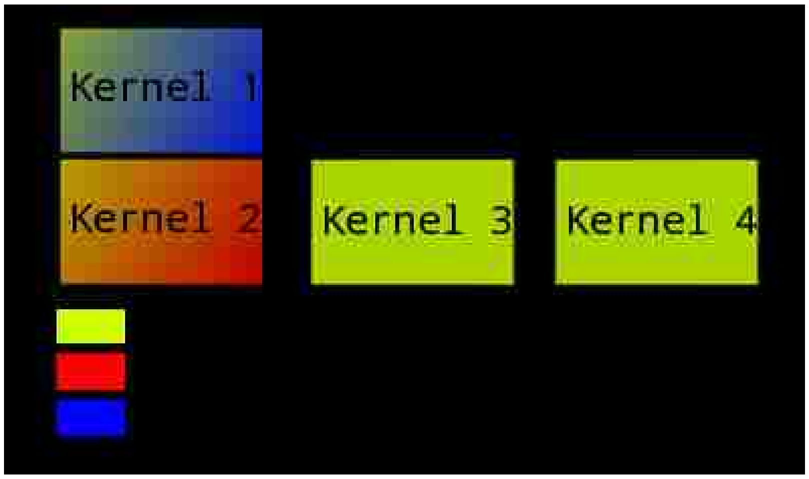


Figure 3.2: CUDA's Streams Behavior

3.4 Experimentation Results - Deploy Stage

In this first occasion the optimize stage was skipped since the initial parallelization may be considered as part of the optimize stage.

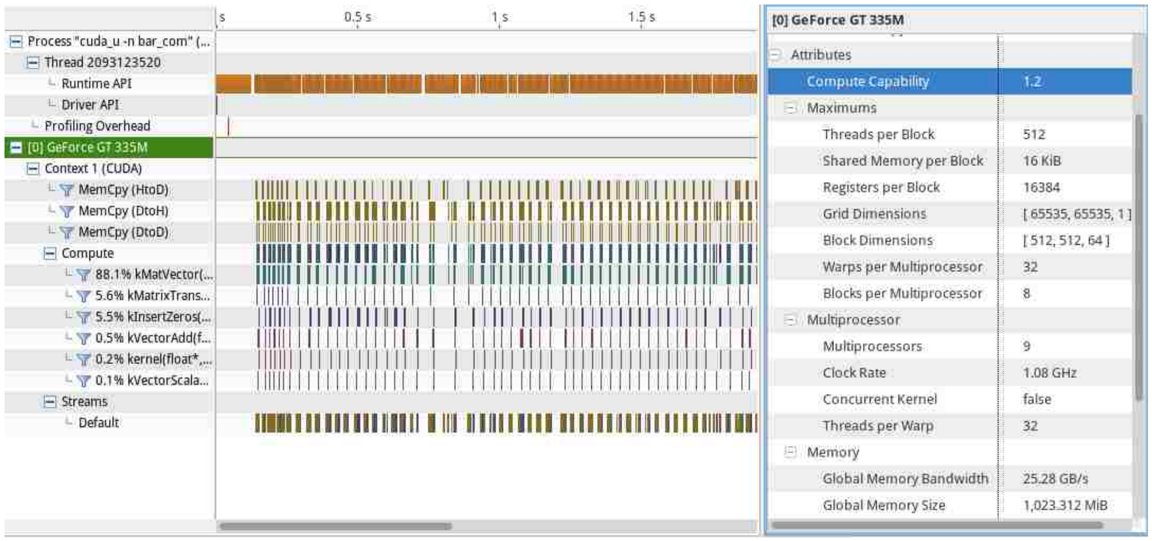
Here are the results in terms of simulation time when comparing the conventional algorithm vs the parallel algorithm Although this work is to be tested only on much

# of Nodes	# of Eigenvalues	SimTime (ms)	SimTime CUDA (ms)
336	100	7.2	13.3
336	500	31.97	30.3
336	900	95.33	70.32
48	100	2.1	4.12

Table 3.1: Initial Experimentation Results

larger objects, this table shows that even for small objects the parallel version does not work as initially expected, it is even slower than the serial version in some cases, it also shows that as the number of eigenvalues used increases, the parallel version performance improves over the serial version, confirming what was explained in section 3.2.2. To debug and check what is happening NVIDIA released a vital tool called NVIDIA Visual Profiler [26], which does basically the same thing as the GNU Profiler explained before in section 3.2.1, but working on CUDA programs.

The NVIDIA Visual Profiler not only gives information about the profiled program such as the time spent on different kernels, allocating GPU memory, or performing memory copy operations, but it also shows important information about the device the program is being run on, similar information as the one obtained using the *deviceQuery()* tool from NVIDIA.



[0] GeForce GT 335M

Attributes	
Compute Capability	1.2
Maximums	
Threads per Block	512
Shared Memory per Block	16 KiB
Registers per Block	16384
Grid Dimensions	[65535, 65535, 1]
Block Dimensions	[512, 512, 64]
Warps per Multiprocessor	32
Blocks per Multiprocessor	8
Multiprocessor	
Multiprocessors	9
Clock Rate	1.08 GHz
Concurrent Kernel	false
Threads per Warp	32
Memory	
Global Memory Bandwidth	25.28 GB/s
Global Memory Size	1,023.312 MiB

Figure 3.3: NVIDIA Visual Profiler Analysis

Figure 3.3 shows the result of profiling the parallel application just developed.

After the initial analysis, it can clearly be seen that the program spends a lot of time doing memory operations; either allocating GPU memory or copying memory, mostly copying it from host to device, to perform operations on the data. Figure 3.4 shows the current flow diagram of the program in its most basic form. The OpenGL Loop is where the calculations are performed, along with its main OpenGL functions, the flow diagram of the the process followed to perform calculations on the GPU is shown in figure 3.5.

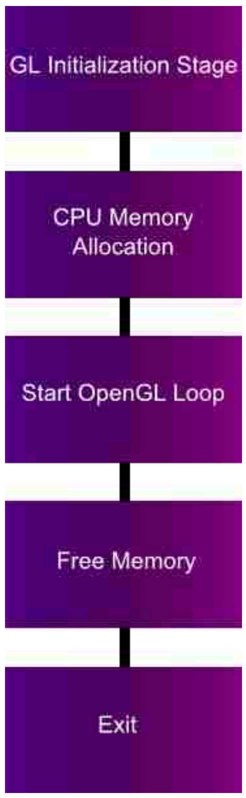


Figure 3.4: Basic Flow Diagram

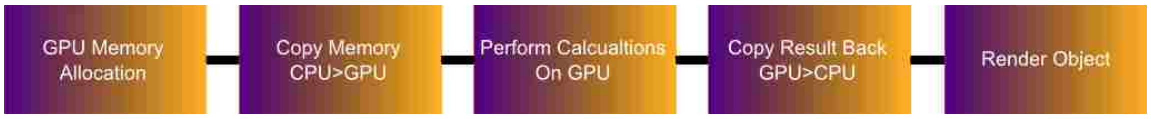


Figure 3.5: CUDA Program Basic Flow Diagram

3.5 Potential Improvements - Optimize Stage

After deploying the first application a loop can be created between the stages Optimize and Deploy, performing optimizations on the algorithm, as minimal as they might be, deploying the application and testing it to see improvements, then going back to the optimize stage to perform optimizations on different areas of the code and so on.
After further analysis of the profile application, focusing on time spent on specific operations, some stages of the diagrams shown in figures 3.4 and 3.5 may be improved:

- GPU memory allocation:
  Although it is technically better to work on Local memory than to work on Global memory when performing calculations using the GPU, in this case it was better to work on global memory, this avoid transferring vast amounts of memory from host to device in every loop iteration. For this, the function *allocate_GPUmem()* was created; it does more than then name indicates, it allocates global memory on the GPU, transfers data from host to device, amongst other small functionalities.

- Memory transfers:
  Using the previous optimization, allows the GPU to keep in memory data that will be used on the next iteration, again avoiding unnecessary data transfers in in every iteration.

- Initial Transpose:
  One of the operations needed to be calculates is a matrix transpose, it is unnecessary to calculate this inside the loop since it can be calculated at the

beginning of the program, and saved to global memory for it to be used later during the execution of the loop.

- CUDA Streams:
  Using CUDA streams can improve a program's performance greatly, since several operations can be executing at the same time.

- OpenGL Buffer modification:
  Another way to avoid unnecessary usage of the PCI-Express bus is to take advantage of the CUDA and OpenGL interoperability, basically rendering the object directly from the result obtained; this is further explained in section 3.5.1

These were the main or more important optimizations that should be done, the basic flow diagram of the whole program after these optimizations have been introduced is shown in figure 3.6.

Some other optimizations that might seem minimal are very important, such as optimizing kernel launches per warp, as explained in section 1.3.3.2.1 warps are groups of 32 threads, these groups are the ones actually executed at the same time, and it has been discovered that there is a small but noticeable lag, that happens when launching a number of threads different than a multiple of 32, this can be corrected by launching more threads than needed, rounding up the number of threads launched to the next multiple of 32, this would represent a problem since when executing the kernel code for a certain thread, it might try to operate on an undesired memory location, causing in many cases a segmentation fault or other errors, this is corrected by using a simple *if()* branch to make sure the thread to be executed will only operate up to a desired index.

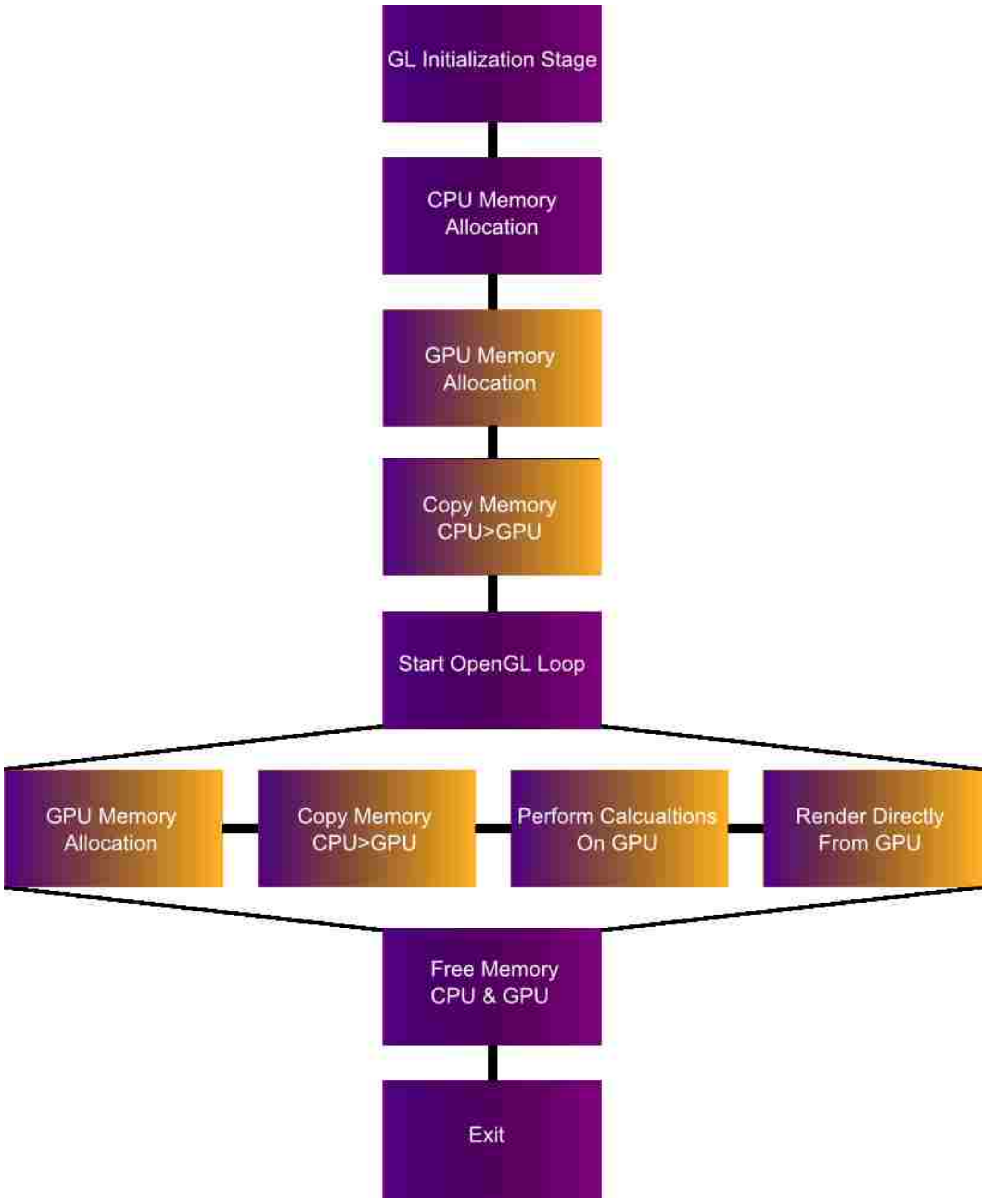


Figure 3.6: Basic Flow Diagram After Optimizations

3.5.1 OpenGL CUDA Interoperability

Benchmarks dedicated to measure performance of parallel algorithms on heterogeneous architectures, such as Parboil [27] and Rodinia [28], based on statistical methods such as Principal Component Analysis and Clustering Analysis provide metrics independent of the underlying GPU architecture [29]. As an example; the Rodinia benchmark suite was tested, comparing CPU vs GPU performance, where the GPU showed a speedup of 5.5 to 80.8 CPU implementation and from 1.6 to 26.3 of the CPU implementation [29].

Performing general purpose computing on the GPU, has some drawbacks, nevertheless all benchmark suites correlate on one point, amongst all of them, the most important drawback is the time spent on memory transfers between CPU memory and GPU memory this due to the fact that the GPU is located on a different chip than the CPU and they communicate through the PCI-Express bus, which as of this date has a bandwidth on the order of 6GB/s and creates a bottleneck [30].
This means that when developing parallel algorithms the programmer must try to avoid memory transfers between system and device as much as possible, in this case, the program is performing some type of computer simulation which is being rendered on the screen using OpenGL, the object is described using nodes, and the simulation calculates the nodes new location after some force has been applied to it, after this; in memory the nodes location is updated so it can be rendered once again, this is located on GPU or device memory, although to change it, it is first changed on system memory, involving memory transfer between the CPU and GPU every single time the new location for the nodes is calculated, to avoid this CUDA API provides some interoperability with the graphics API, in this case OpenGL.
Vertex Buffer Objects are relatively easy to handle in CUDA, since the programmer

needs not to be concerned about texture element fetching or texture filtering, VBOs work much like C arrays that reside in device memory instead of system memory. After declaring the VBO as previously referenced, the buffer object needs to be registered so it can be used in CUDA, this is done using the *cudaGraphicsGLRegisterBuffer()* method as follows:

```
cudaError_t cudaGraphicsGLRegisterBuffer(struct
cudaGraphicsResource ** resource,GLuint buffer,
unsigned int flags);
/* Registers the "buffer" object specified by buffer for access
by CUDA. A handle to the registered object is returned as
"resource". The register flags flags specify the intended
usage.*/
```

Before the registered resource can be accessed in CUDA, the resource must be mapped , this will lock the resource to the CUDA resource object, if the VBO was accessed while it was mapped in CUDA, an error will be thrown, after using the resource in CUDA it must be unmapped when it is no longer needed.

```
cudaError_t cudaGraphicsMapResources(int count,
cudaGraphicsResource_t * resources, cudaStream_t stream = 0);
/* Maps the "count" graphics resources in "resources" for access
by CUDA. The resources in resources may be accessed by CUDA until
they are unmapped. The graphics API from which resources were
registered should not access any resources while they are mapped
by CUDA. If an application does so, the results are undefined. */
```

So far the resource is mapped in memory so it can be guaranteed that it is safe to use inside a CUDA kernel, but still have no access to the contents of that resource, the last step needed to use the buffer object on CUDA is to get a pointer to the device memory, which will be used to access the contents of the resource inside a CUDA kernel, this is done via the function *cudaGraphicsResourceGetMappedPointer()*:

```
cudaError_t cudaGraphicsSubResourceGetMappedArray(struct
cudaArray** array, cudaGraphicsResource_t resource,
unsigned int arrayIndex, unsigned int mipLevel);
/* Returns in *devPtr a pointer through which the mapped graphics
resource resource may be accessed. Returns in *size the size of
the memory in bytes which may be accessed from that pointer.
The value set in devPtr may change every time that resource
is mapped. */
```

After getting the pointer to device memory this can be accessed inside any CUDA kernel, in this case, computing the nodes new location is done purely on device memory, avoiding unneeded memory transfers. These avoided memory transfers vary depending on the model used on the simulation, since models are of different sizes, being all 3 dimensional, but containing a different amount of nodes.

3.6 Results

The models used to test performance of the first parallel version from section 3.4, are considered small meshes, table 3.6 describe the models used to test performance on the optimized version and their characteristics, another reason why these were not tested at first was that at the time it was simply not feasible mostly due to memory limitations; the only model considered in both the first and optimized version was the *Bar* model, which can be used as a point of comparison between both, table 3.6 shows the results obtained when testing this specific model, and the tables that follow, show the speedup obtained on all the other different models.

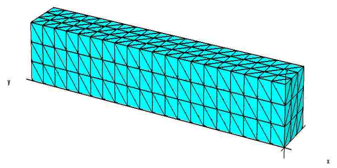
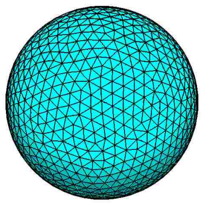
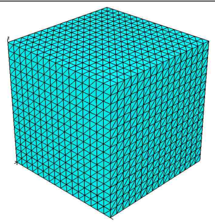
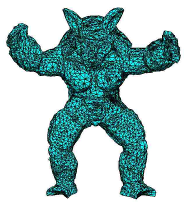
Figure	Object	# of Nodes	# of Elements
	Bar	336	1080
	Sphere	1130	3341
	Cube	4913	24576
	Armadillo	13144	49736

Table 3.2: Objects Tested

# of Eigenvalues	SimTime (ms)	SimTime CUDA (ms)	Speedup (x)
10	1.65	3.21	0.51
100	6.45	5.07	1.27
500	65.37	17.82	3.66
900	147.18	28.22	5.21

Table 3.3: Bar Performance Results

# of Eigenvalues	SimTime (ms)	SimTime CUDA (ms)	Speedup (x)
10	42.01	15.94	2.63
100	54.63	17.95	3.04
500	103.93	32.11	3.23
700	155.09	39.80	3.89
1000	233.56	47.73	4.89
1500	411.03	66.31	6.19

Table 3.4: Sphere Performance Results

# of Eigenvalues	SimTime (ms)	SimTime CUDA (ms)	Speedup (x)
10	108.94	53.33	2.04
100	167.23	60.04	2.78
200	356.77	66.69	5.34
300	422.09	77.08	5.47
500	577.55	108.5	5.77
1000	1039.41	172.37	6.03
2000	2570.36	331.27	7.75

Table 3.5: Cube Performance Results

# of Eigenvalues	SimTime (ms)	SimTime CUDA (ms)	Speedup (x)
5	170.02	128.69	1.32
50	336.43	142.21	2.36
100	546.71	150.03	3.64
200	917.85	174.41	5.26
300	1590.38	192.96	8.24
500	2667.89	297.61	8.96
700	3691.06	343.01	10.76

Table 3.6: Armadillo Performance Results

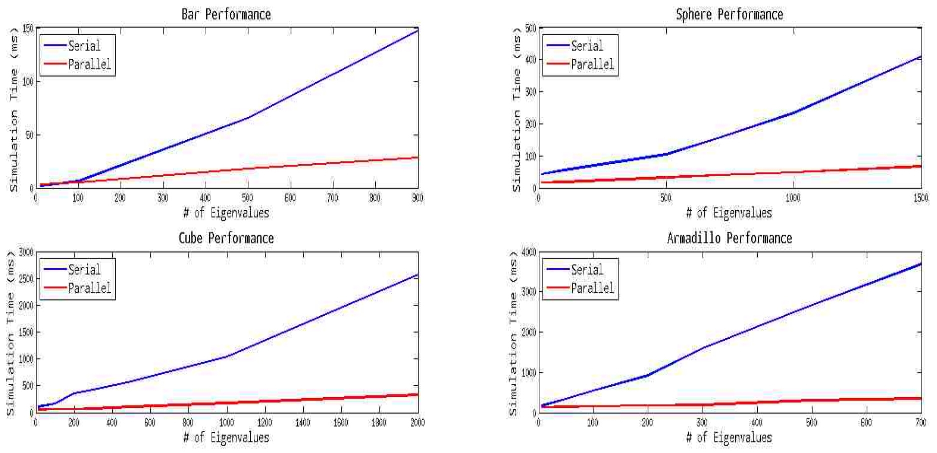


Figure 3.7: Performance by # Eigenvalues on Different Objects

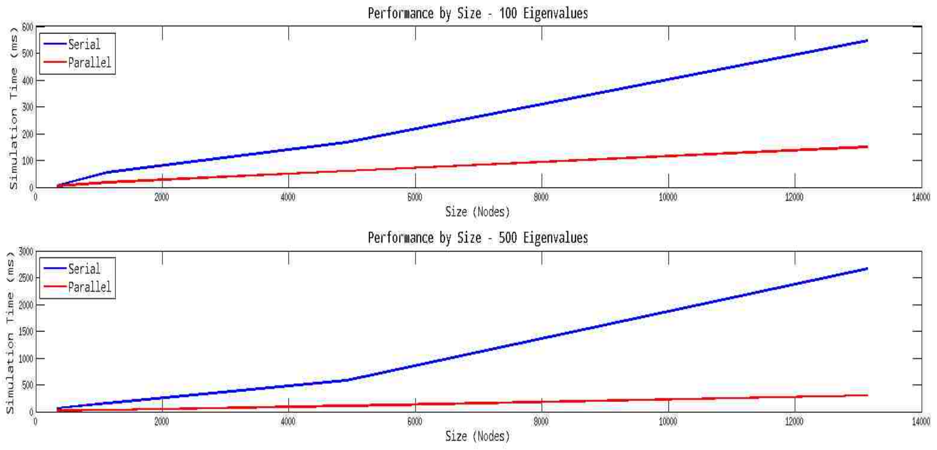


Figure 3.8: Performance by Object's Size

Analyzing figure 3.7 we can see the behavior of the algorithm according to each different object, varying the amount of eigenvalues used, and on figure 3.8, we can analyze its behavior as the number of nodes contained within the object is increased. All the optimizations applied represented a large performance improvement, it was proven what was only presumed before, the parallel program performance improves over the conventional program's performance as the object becomes larger and the number of eigenvalues increases, this is not surprising given the fact that GPUs in general perform better when used on large datasets.
While the time taken to perform calculations on the serial version behaves somewhat exponentially as the number of eigenvalues is increased, the parallel version's behavior is rather linear.
Profiling the optimized application to examine the memory transfers shows us that in case of the armadillo for example the memory transfers between system and device memory is now 40.54 KB per displacement calculation, we can then see that according to table 3.6 the armadillo has 13144 3-dimensional nodes, stored in floating point numbers (4 $bytes$):

$$ArmadilloKB = \frac{13144 * (3) * (4)}{1024} = 154.03$$

So by using the CUDA and OpenGL interoperability copying back the result to system memory and then copying it back to GPU to render it is avoided, a total of $154.06 * 2 = 308.06KB$ of memory transfers are avoided per displacement call, which would account for:

$$\frac{308.06}{308.06 + 40.54} * 100 = 88.36\%$$

of transfers per call.

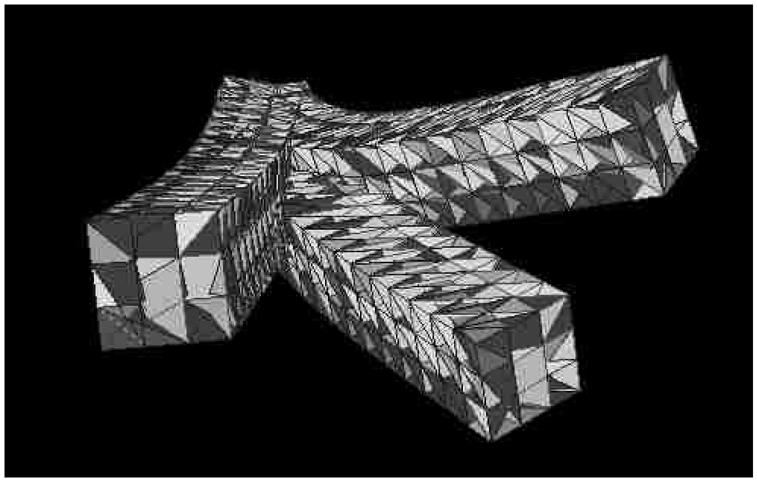


Figure 3.9: Bar Analysis

The program also has the capability to save the object's nodes location at a certain time, giving the opportunity to the user perform a post simulation analysis of the object's behavior, figures 3.9 and 3.10 show an example of how an object may be analyzed afterwards.

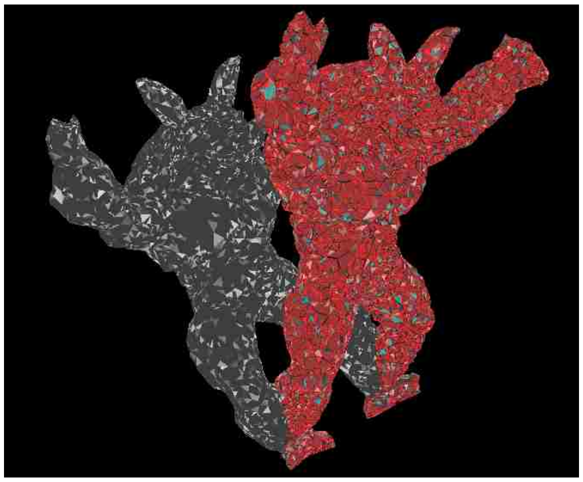


Figure 3.10: Armadillo Analysis

Chapter 4

Conclusion and Future Work

4.1 Limitations and Future Work

During the development of this project, possible new features and limitations were encountered.
The limitations found are mostly related to the hardware available, the graphics card used (NVIDIA GeForce GT 335M) is not only old but it is also only found on personal computers, it is considered a small device, table 4.1 shows the comparison of the hardware specifications of this card, against a newer one.

4.1.1 APU's

Although using CUDA and OpenGL Interoperability minimizes memory transfers between device and system memory, somewhat overcoming the PCI-Express bottleneck in some cases, there are other alternatives, this bottleneck is a known issue for

	GeForce GT 335M	GeForce GTX Titan Z
CUDA Compute capability	1.2 (Legacy)	3.5
Architecture	Tesla G80	Kepler
# of Transistors	727 Million	14.2 Billion
Interface	PCI-E 2.0	PCI-E 3.0
Memory	1GB GDDR3 (800MHz)	12GB GDDR5 (7 GHz)
Memory Interface Width	128 bit	768 bit
Streaming Processors	72	5760
L1 cache	16K	48K
L2 cache		1536
Warp Scheduler	1	4
Precision	32 bit	64 bit

Table 4.1: GPU Comparison

a vast number of applications in many different areas, and for this same reason it has been tried to be fixed also on an architectural level.

In 2011 AMD announced the 1st generation of the Fusion project or APUs (Accelerated Processing Units), its first codename was called Llano (high-end) and Brazos (low-power), 2nd generation Trinity and Brazos-2 were announced on June 2012 and 3rd generation Kaveri is expected to be released on 2014, the important thing about the Fusion architecture or APUs is that its the first one to have both the CPU and the GPU on the same chip, as this proposes many challenges its major advantage is that it no longer suffers from the PCI-E bottleneck for memory transfers, although one disadvantage is that they can only be programmed in OpenCL.

The Llano variant combines 4 x86 processor cores, a unified video decoder, a DirectX11 graphics core, it fits on $227mm^2$ of die area in a 32 nm silicon insulator process, it features a node called Northbridge which is where the processor, graphics and multimedia are jointly managed, it connects the processor cores, the I/O interfaces, graphics and video accelerators and 2 64-bit channels of DRAM through a multi-stage memory controller (DDR3-1866). It uses a AMD Turbo Core (ATC)

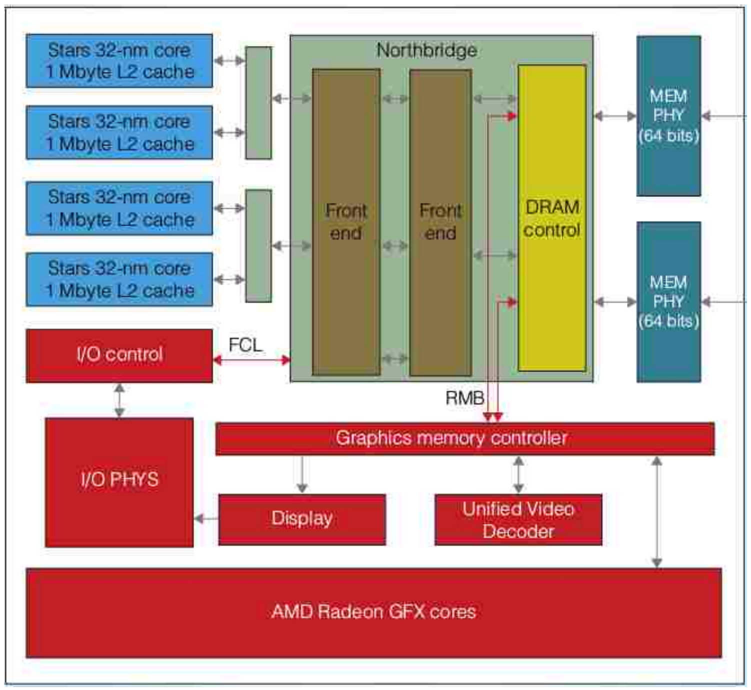


Figure 4.1: Llano APU block diagram [31]

technology to maximize core performance in the systems thermal design power, while balancing power budget between processor and graphics cores using the same cooling solution [31].

A Radeon Memory Bus (RMB) is a 256-bit bus used to access memory with a bandwidth of 29 GB/s, the processor cores use an L2 cache of 1MB, a reordering buffer to accommodate up to 84 micro-ops contributing to better ILP, a load/store buffer handling up to 52 operations and an enhanced instruction-pointer-based prefetcher contributing to better instructions per cycle, the GPU uses a VLIW-5 as a basic building block, includes 4 stream cores, one special function core, a branch unit and some general purpose registers.

16 AMD Radeon VLIW-5 elements combine to form a SIMD processing unit, the graphics core compute unit consists of 5 such SIMDs, forming a structure of 400

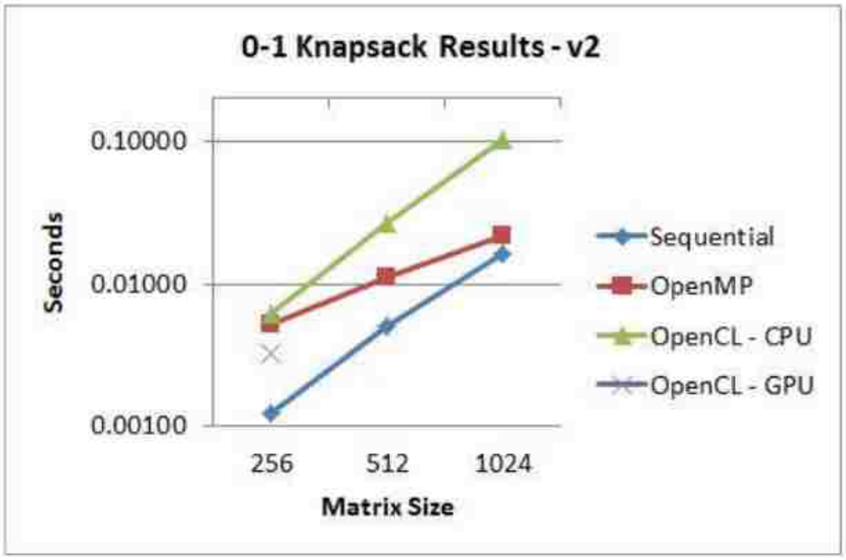


Figure 4.2: Knapsack Algorithm on APU [32]

stream cores, delivering throughput of 480 GFlops [31]. It uses a unified memory architecture (UMA) where GPU and CPU share a common memory and traffic is routed using the GMC (Graphics Memory Controller).
This new technology has already been adopted by the 8th generation of video game consoles, both the Playstation 4 and the Xbox One, use a customized AMD APU.

Only a few researchers have tested/compared algorithm performance on APUs, some examples are shown next: In figure 4.2 the Knapsack algorithm was tested on an APU using a Radeon 5870 as GPU (mid-range) against an Intel i7 at 1.6 GHz.
In figures 4.3 and 4.4 it is shown the implementation of B+ tree searches (heavily used on database management systems) on a high end discrete GPU and a high-end CPU against a (mid-end) APU, where depending on the size of the problem they APU performs better (4.9x best case, 2.5x average) than the discrete GPU implementation, the only case where the discrete GPU implementation is better its when

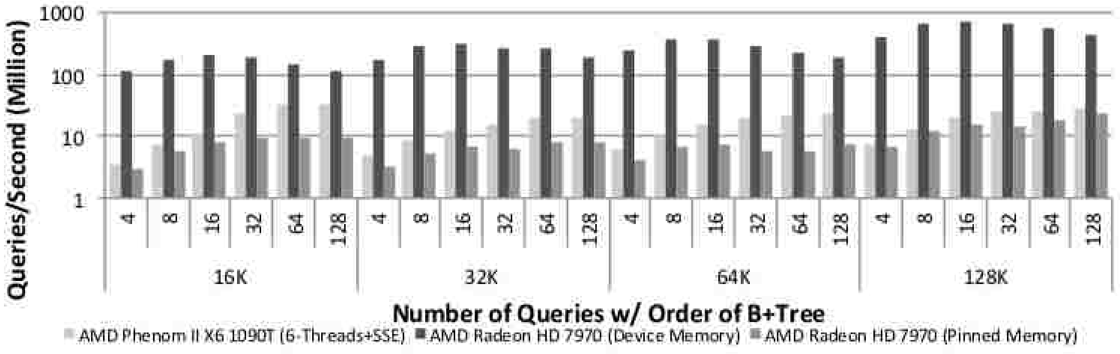


Figure 4.3: Performance measurement on a Discrete GPU [33]

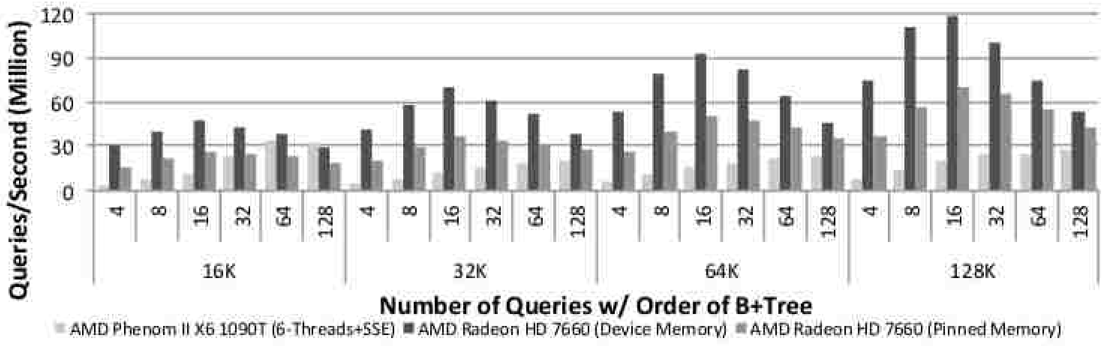
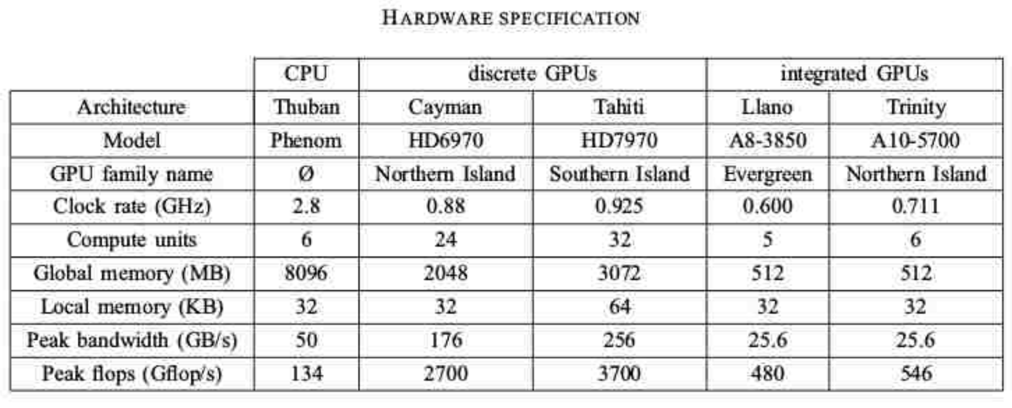


Figure 4.4: Performance measurement on an APU [33]

the tree already resides in the GPU memory (No transfers between the GPU and CPU through the PCI-Express bus).

And finally the implementation of the finite difference stencil using OpenCL on two generations of discrete GPUs and two generations of APUs, hardware specifications are shown in figures 4.5 and performance on figure 4.6.

As it can be seen the best performance (as a function frequency of data snapshotting) is always obtained on the discrete GPU Tahiti, while the 2nd gen trinity APU may match the Tahiti performance and outperform the Cayman performance for a



HARDWARE SPECIFICATION

	CPU	discrete GPUs		integrated GPUs	
Architecture	Thuban	Cayman	Tahiti	Llano	Trinity
Model	Phenom	HD6970	HD7970	A8-3850	A10-5700
GPU family name	Ø	Northern Island	Southern Island	Evergreen	Northern Island
Clock rate (GHz)	2.8	0.88	0.925	0.600	0.711
Compute units	6	24	32	5	6
Global memory (MB)	8096	2048	3072	512	512
Local memory (KB)	32	32	64	32	32
Peak bandwidth (GB/s)	50	176	256	25.6	25.6
Peak flops (Gflop/s)	134	2700	3700	480	546

Figure 4.5: Hardware specs for finite stencil implementation [30]

snapshot retrieval after every stencil computation, also we can note that the APUs always outperform the CPU implementation.

The new AMD APU architecture eliminates the PCI-Express bus which bottlenecks

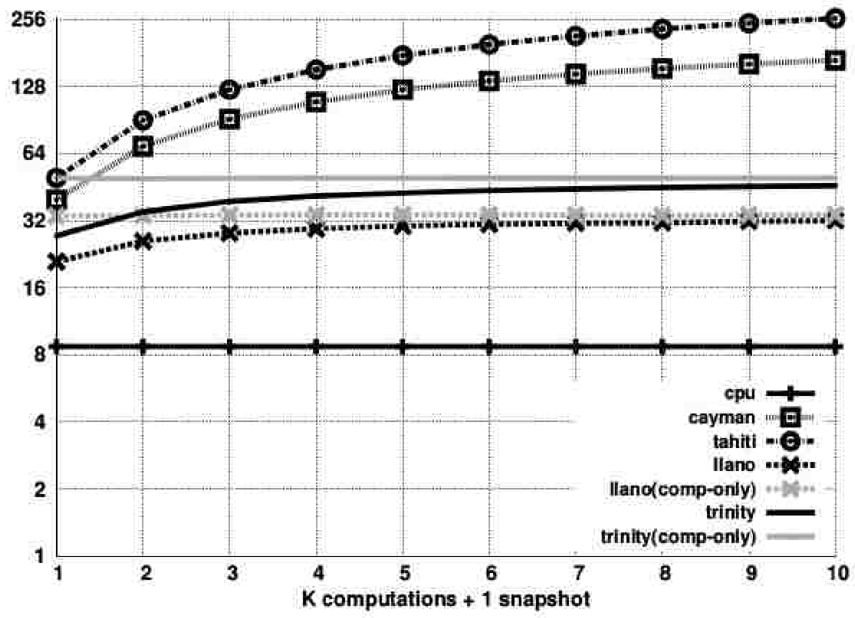


Figure 4.6: Performance Comparison GPU vs GPU vs APU vs APU [30]

many GPU applications, but since it is a new technology the APUs are not powerful computationally speaking, they perform a lot better than what the difference in specifications between the discrete GPUs and APUs show, also the internal memory bandwidth of the APUs its still a lot slower than the one from GPUs, new generations of APUs will rely on unified memory, but 1st and 2nd gen still have a distinct GPU memory partition.Also note that the APUs architecture was designed thinking in performance per watt, these APUs are 100 Watts TDP compared to 250 Watts on the discrete GPUs. Once this technology takes off we can expect a lot of performance improvement.

In contrast NVIDIA released CUDA 6 on November 18th 2013, where they introduce a unified memory programming model, where now the programmer has access to the whole memory address space (both CPU and GPU memory) using a single pointer, and while this provides a simpler programming model, and uses a very complex background process (transparent to the programmer) to migrate memory from the GPU to the CPU and vice-versa, achieving performance improvement, this still does not completely address the problem of having the bottleneck of the PCI-Express bus bandwidth.

After deep analysis, these are some of the possible improvements that can be added to this work in the future:

- C++ Code: At the beginning of this project the C language was selected for many of its features, although it was selected it was not limited to it, during the development of the project I have realized that C++ has some interesting features that may be useful for this work, such as: using STL (Standard Template Library) vectors instead of C arrays; for easier manipulation and in some cases better performance, the use of Object Oriented Programming; for better organization of the code and also better scalability, amongst other features, the goal would be to make the code fully C++ compatible in the future.

- Eigenvectors: For the moment this work assumes the eigenvectors have been precomputed, this is very computationally expensive, although to this date, there is no known accurate algorithm to calculate the eigenvectors in parallel efficiently, it would be an important addition to include this calculation, either serially or in parallel.
- Click-to-Fix Feature: One important addition that is possible if the eigenvectors calculation is included is the click-to-fix feature, using the mouse to interact with the 3D model, to fix certain nodes and not apply a force to them, instead of pre-fixing them.
- Improve Rendering: Rendering may be improved, if the computation is only done for the nodes on the surface, it is unnecessary to perform all the calculations for the nodes that are "inside" the object since they don't affect the behavior of the object as a whole.
- OpenCL: As it was explained before in section 1.3.3.3 OpenCL programming is similar to CUDA programming, and their code organization or hierarchy is also similar, meaning it is potentially possible to create an OpenCL version of the code, which would work on other graphic cards, instead of only NVIDIA cards supported by CUDA.
- OpenMP: With the addition of an OpenCL version it would be also a good addition to use parallel programming on both the CPU and GPU; each used for different calculations that better fit their architecture, this could be done for the CPU using POSIX threads or for more compatibility with OpenCL using OpenMP.
- APUs: Lastly, as explained before, new architectures are arising, including APUs which are still in an initial stage of development, creating an OpenCL

version would also facilitate testing the program on these new architectures, potentially achieving a great improvement in performance.

4.2 Conclusion

The work presented in this document shows how the parallel algorithm developed, improves performance over the one using a conventional approach, with the right conditions it improves performance over 10 times and potentially more, this conditions are mostly met when a sufficiently large object is to be used in the simulation. While performance using the conventional approach decreases in an exponential way as the number of eigenvectors used is increased, this new approach keeps a linear behavior, due to memory limitations of the device used, tests with even larger models were not feasible, but analyzing the behavior shown in plots, it can be presumed a better performance improvement can be achieved.

While the graphics card available was enough to show a good improvement of the usage of this algorithm, it is simply impossible to compare, its hardware capabilities with a newer card, it is also important to note that the newer card used in the comparison table 4.1 is meant for a desktop computer, if a workstation or a server is available, it would potentially have even better hardware specifications.

There is work to be done in the future, such as creating a better and more intuitive user interface and developing different versions of the algorithm capable of running on a wide range of hardware.

The implementation of this new algorithm on new technologies only arising in the last couple of years looks promising, some modifications may have to be done to achieve peak performance, since GPGPU algorithms are indeed closely related to the underlying architecture of the hardware used, but this is not only an important area of research but it also has potential in the coming years.

Appendix A

Appendix A - C++ Code

The updated code can be found at the following location:

`https://github.com/aehs29unm/mwgpu`

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