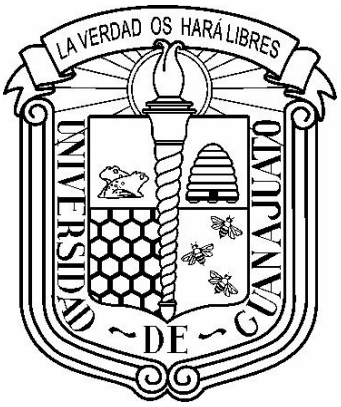

University of Guanajuato

Bachelor's Thesis

Study of "Domain Wall Dynamics under Nonlocal Spin-Transfer Torque" using heterogeneous computing

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A thesis to obtain the degree of Bachelor of Computacional Systems Engineering

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Abstract

Campus Irapuato Salamanca
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Study of "Domain Wall Dynamics under Nonlocal Spin-Transfer Torque" using heterogeneous computing

by Thomas Sanchez Lengeling

This is an exploration analysis on the role the GPUs can play in the acceleration on applied physics software and simulations, specifically on the GPU implementation from Dr. Cludio's "Domain Wall Dynamics under NonLocal Spin-Transfer Torque" research. This is a quantitatively test the effects of spin-diffusion, on real Domain Wall (DW) structures, by numerically implementing the Zhang-LI model[Phys. Rev. Lett. 93, 127204 (2004)] into a NiFe soft nanostrip. Using the massive parallel capabilities of a GPU we can accomplish a 60x speed-up increase with a NVIDIA Tesla K20M over the eight core Intel Xeon optimized CPU version, this done with a double precession arithmetic and with GPU accelerated kernel 4th Runge Kutta implementation.

Acknowledgements

The acknowledgements ...

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Introduction

Commodity graphics processing units (GPUs) are becoming increasingly popular to accelerate scientific applications due to their low cost and potential for high performance when compared with central processing units (CPUs). A large number of contemporary problems and scientific research are being benefit from this new technology .There has been considerable progress in implementing the hardware and the supporting infrastructure for GPUs programming and streaming architectures. This thesis is a exploration and study of the role of accelerator hardware like the use of the GPUs on physical computing, more specific in the area of spin-diffusion effects within a continuously variable magnetization distribution.

The work begins with a overview of the current trends in computing, focusing our attention specifically on GPUs, on how they differ from the CPUs and common programming practices that uses heterogeneous computing. The second chapter focus on the use of techniques of heterogeneous computing to gain more performance out the GPUs when applying to a specific task. Also the necessary means how to test the speed-up against the CPU. The next chapter is overview of the GPU implementation by Dr. Claudio base on his work "Domain Wall Dynamics under Non-local Spin-Transfer Torque". The forth chapter is the results obtained from benchmarking the GPU implementation on various GPUs nodes, also the optimization results after applying several GPUs memories techniques to Dr. Cluadio's GPU implementation. The last chapter of the thesis is a conclusion of the work and future research.

Chapter 1

Heterogeneous Computing

Heterogeneous computing refers a system that combines several processor types to gain more performance. Typically using a single or multi-core computer processing units (CPUs) and a graphics processing units (GPUs). Typically GPUs are know for 3D graphics rendering and video games, but GPUs are becoming increasingly popular for accelerating computing applications and scientific research due to their low price, high performance and relatively low energy consumption per FLOPS (floating point operations per second) when compared with the CPUs. This chapter provides an overview of GPUs within the High Performance Computing (HPC) context, their advantages and disadvantages and how they can be integrated in to a scientific software and research.

1.1 Motivation

The GPU has been essential part of personal computer since the early use of them. Over the course of 30 years the graphics architecture has evolve form drawing a simple 3d scene to be able to program each part of the GPU graphics pipeline. Their role became more important in the 90s with the first-person shooting video game DOOM by id Software. The demanding video game industry has brought year by year more realistic 3D graphics. . Concurrently many new innovated hardware capabilities has became in creating a more sophisticated user programming environment. This is leading the GPU to massive computational power. In till resent years the GPU has been used as general-purpose computing on graphics processing units (GPGPU)[6].

GPUs are attractive for certain type of scientific computation as they offer potential seed-up of multi-processors devices with the added advantages of being low cost, low maintenance, energy efficient, and relative simple to program. Many algorithms in

applied physics are using GPUs to improve there performance over the CPU. Some examples are Euler Solver 16x seepd-up (add Reference seed-up).

In any case, for a given simulation a compromise between speed and accuracy is always made. The current tendency of the CPU relies on increases the clock seeped and adding more cores per unit and be able to work and a parallel manner, because of the there are some limitations[13]

Power Wall

The CPUs single core has not gone beyond the 4GHz barrier, a paradigm shift from a single core to a multi-core CPUs, also the power use of CPUs is very high per Watt. The figure 1.1 shows the comparison of performance between the GPU and CPU.

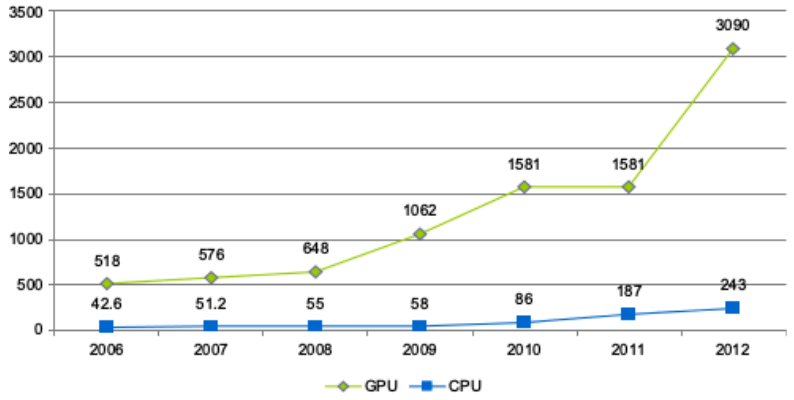

FIGURE 1.1: GPU and CPU peak performance in gigaflops

Memory Wall

This refers to the growing disparity of speed between CPU and the memory outside the CPU chip. Some applications have become memory bound, that is to say computing time is bounded by the transfer memory between the CPU and all the hardware devices connected to the CPU, commonly to the PCIe chip. In conclusion the computing time is bounded by the memory not by the time calculations done on the CPU.

Parallelism Wall

This indicates a law that indicates the number of parallel processes. The number N parallel processes is never ideal and always depends on the problem. The seed-up can be described by Amdahl's Law in terms of the fraction of parallelized work (f). [13].

$$speedup \leq \frac{N}{f + N(1-f)}$$

The current paradigm of using CPUs for computing growth is unsustainable. the largest supercomputers use around 10 megawatts (MWs) of power, this is enough to power a small town of 10,000 homes. If the current thread of power use continues, the next supercomputer would require 200 MWs of power, this would require a nuclear power reactor to run it! [17]

1.2 GPUs as computing units

A insight of the architecture of GPU can give a idea of why it outperforms the CPU on various benchmarking.

The GPU, unlike its CPU cousin, has thousands for registers per SM (streaming multi-processor), this are arithmetic processing units.An SM can thought of like a multi-thread CPU core. On a typical CPU has two, four, six or eight cores. On a GPU as many as N SM core. We can see this in the figure 1.2. For a particular calculation, all the stream processors within a group execute exactly the same instruction on a particular data stream, then the data is sent to the upper level, the host (CPU). [4]

FIGURE 1.2: Architecture of a NVIDIA GeForce GTX 580

Being able to efficiently use a GPU for an application requires to expose the inherent data-parallelism Optimized for low-latency, serial computation. This can be seen in contrast with a CPU, which is optimized for sequential code performance, fast switching registers and sophisticated control logic allowing to run single complex programs as fast as possible, which is not possible on the GPU. Memory management is very important for GPUs. this refers how to allocate memory space and transfer data between host (CPU) and device (GPU). While the CPU memory hierarchy is almost non-existent, on the GPU inherent data is important. In figure 1.3 different levels of memory can be observer between the host and the device, which differs form the CPU [7].

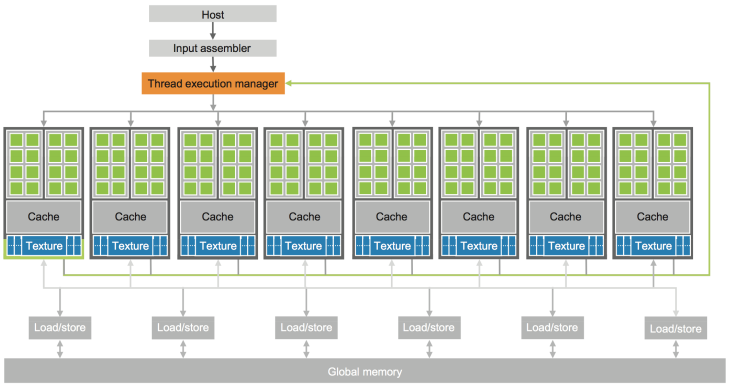

FIGURE 1.3: Memory transfer between the host and device

On the GPU precision and optimization are very important but there is a penalty for choosing performance or precession. All the GPUs are optimized for single precision floating operations, 24 bit size, Also provides double precision point, size of 53 bits. This is using the standard notation IEEE 754. Normally the GPU uses single precession(SP) by default, if choosed double precision (DP), normally there is a penalty of 2x - 4x seed-up. [19] Libraries such as CUBLAS and CUFFT provides useful information how NVIDIA handles floating point operations under the hood.

talk about different types of NVIDIA architecture, Fermin, Kepler.

1.3 Programming on GPUs

There exist, among many, two main computing platforms, NVIDIA's Compute Unified Device Architecture (CUDA), and Khronos's Open Computing Language (OpenCL). CUDA provides the necessary tools, frameworks and library to programs parallel computing using there GPUs. While OpenCL is a open standard framework meaning is not locked like CUDA. This two frameworks are develop in C language this is because C is close to the hardware layer. CUDA provides both a low level API and a higher level API. [7]

The CUDA programming model views the GPU as an accelerator processor which calls parallel programs throughout all the SMI. This programs are only executed on the device and are called kernels. The basic idea of programming on a GPU is simple. We can observer this in the figure 1.4

- Create memory(data) for the host and device

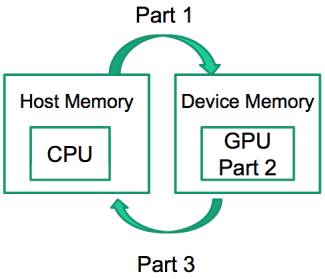

FIGURE 1.4: Programming Cycle between the CPU and GPU

- Send the data created from the host to the highly parallel device.
- Do something with data on the device, e.g. matrix multiplication,calculation, parallel algorithm.
- Return the data from the device to the host.

A kernel is organized as a one, two or three dimensional grid of thread blocks, This is a thread is the simple executing process. Many threads form a block, and many blocks form a grid. This can be observer in figure 1.5. All the threads in a kernel can access the global memory, figure 1.3. Each of the threads can be access by implicit variable that identifies its position within the thread block and its grid. In a case of 1-D block. [16]

$$blockIdx.x \times blockDim.x + threadId.x$$

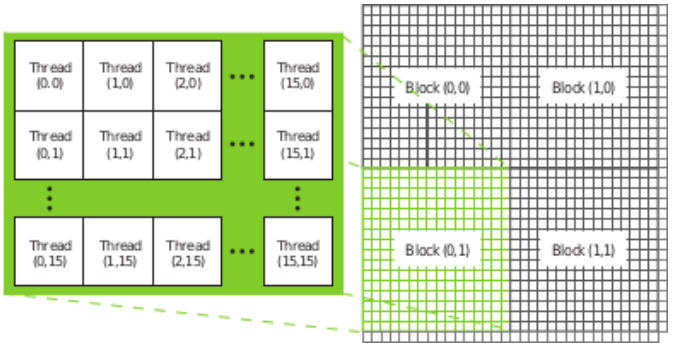

FIGURE 1.5: Part of a 2D CUDA's thread grid, divided in blocks, each block with its own respective threads.

Chapter 2

Heterogeneous Performance Analysis

In the conventional CPU model we have what is called linear or flat memory model. This appears to the programmer as a single contiguous address space. The CPU can directly address all the available memory, in other words there is almost no efficiency penalty in creating global data, local data, or even access data that is located on the opposite memory location, all of this can be access in the contiguous block. [4] Meanwhile on the GPU there are expectations, there exist are different levels in how to access the memory. Using the right type of memory allocations can dramatically accelerate applications and increase the throughput. To ensure that seed-up, benchmarking are actually being useful when optimizing GPU kernels, some analysis should be made, like comparing time and bandwidth, between kernels.

2.1 Performance Metrics

[11]

2.1.1 Timing

2.1.2 Bandwidth

The bandwidth refers to the rate at which data can be transferred, this one of the most important factors for testing performance o the GPUs . Choosing the right type of memory could dramatically increase performance and bandwidth of each kernel that is

executing on the device. There are two main memory to indicate performance, theoretical bandwidth and effective bandwidth. The theoretical bandwidth is base on the hardware specifications that is available by NVIDIA. This is calculated using the following formula:

$$theoreticalbandwidth = (clockrate * (bit - wide - memory - interface/8) * 2)/10^9$$

For example the NVIDIA GeForce GTX 280 uses DDR RAM with a memory clock rate of 1,105 MhZ and a 512-bit-wide memory interface

$$(1107 * 10^6 * (512/8.0) * 2)/10^9 = 141.6Gb/sec$$

The GTX 280 has a theoretical bandwidth of $141.6Gb/sec$

The effective bandwidth is calculated by timing specific program activities and by knowing how data is accessed by the application. [11]

$$effective - bandwidth = ((Br - Bw)/109)/time$$

Where Br is the number of bytes read per kernel, Bw is the number of bytes written per kernel and t is the elapsed time given in seconds. [15]

In practice the difference between theoretical bandwidth and effective bandwidth indicated how much bandwidth is wasted on accessing memory and calculations.

Throughput is how many operations completed per cycle.

2.2 Visual Profiler

Visual Profiler is a tool provider by NVIDIA that allows to collect several information about different memory throughput measures. Is possible to analyze memory request inside the applications with the profiler.

GPUs. From each kernel is possible to obtain various memory throughput measures, like global load Throughput

The requested Global Load Throughput and request global store Throughput values indicate the global memory throughput requested by the kernel and therefore corresponding to the effective bandwidth mentioned in the last section. The Visual profiler is very useful to indicate how much load and work is being done on the GPU, it also information about the memory throughput that can be helpful to indicate if the kernel is being actually optimized. [11]

2.2.1 Kernel Analysis

Trough the Profiler the kernels are invoked several times to calculate all the necessary information about how to optimze each kernel depending on several results. Also the profilers

Memory Bandwidth Bound
: This refers when the code/application is limited by memory access. Most GPUs card have 1GB- 6GB of memory, this is used to process the data on the GPU, while the CPU has massively amount of memory available for use. A solution to this is to reuse the data, change the type of memory used in the GPU. A multi-GPU approach, where is possible to handle more amount of memory in the device.

Compute Bound
: Is one which computations dominates the kernel time, under the assumption that theres no problem with the memory on the kernel. This is actually the analysis time operations on the kernels. Theoretical bandwidth vs effective Bandwidth can measure performance for a compute-bound Kernel. This a good way to measure if its possible to increase the FLOPS per device.

Latency Bound
: Is one whose predominate stall reason is due to memory fetches. This actually say if not saturating the global memory, or any type, but still have to wait to get the data into the kernel. Physically can be the data being sent from one part of the Device to the other. Also depends the time required to perform an operation, and are counted in cycles of operations. A way to reduce the latency is to increase the number of parallel instructions (more calls per thread), in other words more work per thread and fewer threads.

The performance of relatively simple kernels, which perform computations across a large number of data elements, is more a function of the GPU's memory system performance than the processing performance. It can be beneficial for such memory-bound kernels

to decrease the amount of memory access required by increasing the complexity of the computation. [4]

2.3 Memory Handling with CUDA

In this section four types of memory handling are going to be explained, shared memory, global memory (device memory) and finally host memory. In figure 2.1 each memory type has it's bandwidth penalty of used and latency in cycles. Each one can be used in different applications to maximize the memory used. The shared Memory is very limited so it cannot be handler for all the kernels, when performed wrong on the device there is a huge latency and bandwidth penalty, instead having a gain in performance [4].

Storage Type	Registers	Shared Memory	Texture Memory	Constant Memory	Global Memory
Bandwidth	~8 TB/s	~1.5 TB/s	~200 MB/s	~200 MB/s	~200 MB/s
Latency	1 cycle	1 to 32 cycles	~400 to 600	~400 to 600	~400 to 600

FIGURE 2.1: Different memory type and penalties usage

2.3.1 Global Memory

Understanding how to efficiently use global memory is essential in CUDA memory management. Focusing on data reuse within the SM and caches avoids memory bandwidth limitations. Global memory on the GPU is designed to quickly stream memory blocks of data into the SM.

- Get the data on to the Device, keep it there.
- Give the GPU enough workload, this using all the resources available from the GPU.
- Focus on data reuse within the GPGPU to avoid memory bandwidth limitations.

In other words the global memory resides on the device, and it can be anything from 0GB to 8GB. Also the memory is visible to all the threads of the grid. Any thread can read and write to any location of the global memory, The memory is always allocated with *cadaMalloc*. And only global memory can be passed to the kernels and are called with _global _.

[5]

2.3.2 Shared Memory

CUDA C compiler treats variables differently than typical variable, it creates a copy of the variable for each block that is launched on the GPU, now every thread in that block can access the memory, this is why is called shared memory. This memory reside physically on the GPU, because the memory is very close the cache, the latency is typical very low.[16]. One thing comes to mind, if the threads can communicate with others threads, so there should be way to synchronize all the threads. A simple case should be if thread A writes a value into the shared memory, and Thread B wants to access we need to synchronize, when thread A finish writing then Thread B can access it. This is typical case when shared memory with synchronize thread is needed. [4] Shared memory is magnitudes faster to access than global memory, essentially is like a local cache for each threads of a block. While the shared memory is limited to 48K a block, the global memory is the amount of DRAM on the device. The duration of the shared memory on the device is the lifetime of the thread block. Using _shared _to the kernel call invocate shared memory.

2.3.3 Constant Memory

Is an excellent way to store and broadcast read-only data to all the threads on the GPU. One thing to keep in mind is that the constant memory is limited to 64KB. [5]. A simple analogue is the *#define* or *const* attribute in the c++ programming language, the variable performed like a variable that cannot be modified. On CUDA is excitability the same, the value can only be read and not written, the value will not change over the course of a kernel execution and only the host can write the constant memory.[16]

2.3.4 Texture Memory

Like constant memory, texture memory is another variety of read-only memory that can improve performance and reduce memory traffic when reads have certain access patterns. . Traditionally Texture memory id used for computer graphics applications, but it can also be use for HPC. The main idea of this read-only memory is that threads are likely to read from address "near' the address they nearby threads.[16]

This can be summarized in the following table:

The texture Memory in a form works like the GPU graphics Texture, when you want to use the texture bind with some sort of data is necessary and when you finish using it unbind the texture from the data. The usage can be summarized in the following table.

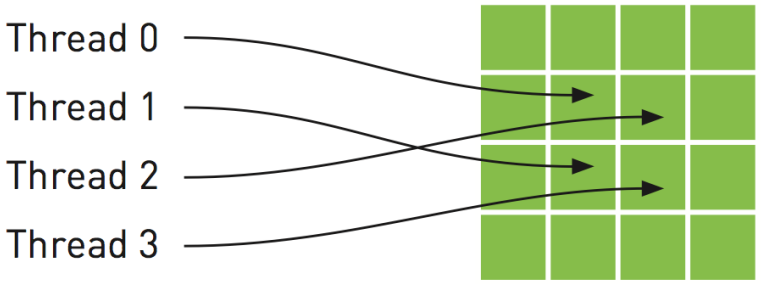

FIGURE 2.2: Mapping of threads into a two dimensional array of texture memory

- Allocate global memory in the Host.
- Create Texture reference and bind it to memory object.
- On the device obtain the reference from the texture.
- Use Texture memory operations on the device
- When the work is done on the Texture, unbind the texture reference on the host.

2.3.5 Thread Synchronization

This refers to synchronizing threads operations,

Will wait for all threads to finish there job.

2.4 Performance Issue

2.4.1 Hardware constraints

This refers to the limit how many threads pero block a kernel lacuh can have. If exceed this values they kernel will never run. The threads per block really depends of the hardware capabilities. In a roughy summarized as:

- Each block cannot have more than 512/1024 threads in total, with compute Capability 1.x or 2.x-3.x
- The Maximum dimensions of each block are limited to [512,512, 64]/[1024, 1024, 64](compute 1,1.2,
- Each block cannot consume more than to 8k, 16k, 32K registers total

- Each block cannot consume more than 16kb/48kb of shared memory

SM Resources, improve performance of an application by trading one resource usage for another. [11]

Another inefficiency that can cause low performance to the applications is the number transfers memory calls between the CPU and GPU. The GPU communicates with the CPU via a *ePCI*, by this all the massive FLOPS per second that can be achieve cannot actually be sent to CPU. The GPU should be filled with the enough workload at the beginning of the application and at the end only return it to the CPU.

2.4.2 Thread Division

The hardware has its limits in how much thread per block a kernel can handle. Launching a kernel with the hardware constrains for above can only ensure that the kernel will actually be executed in the device, not a optimize set of threads per block. For this is necessary launch kernel with the amount of threads per block base on the hardware constains that will optimize the performance of the GPU. The impact of the block size that is choosed impacts on how much faster the code will run. By Benchmarking, is possible to find what configuration is the best for the problem. One thing to notice is that thread blocks should be a multiple number of SMs, with this idead is possible to obtain optimal thread block configuration.

Chapter 3

Introduction to Domain Wall Dynamics and a Implementation with CUDA

In this chapter a overview of the theory and experiments behind the work of Dr. Cluadio "Domain Wall Dynamics under Nonlocal Spin-Transfer Torque". This is a quantitatively test the effects of spin-diffusion, on real Domain Wall (DW) structures, by numerically implementing the Zhang-LI model into a NiFe soft nanostrip [3]. Also the implementation of the theory in to CUDA code.

3.1 Theory

We study spin-diffuse effect within a continuously variable magnetization distribution, integrating with micromagenectis with diffuse model of Zhang and LI [3]

Spin-transfer torque is a torque that exerts on a magnetization by conduction electron spins, in other words the angular momentum transferred from spins to magnetic moment [21].

This has simulated reaserch into domain wall (DW) dynamics, particularly those resulting from interactions with current passing through the DW via the phenomenon of spin momemntum transfer (SMT) [18]

Some application include racetrack technology by fellow IBM scientific Parkin [12]

Contrarily to charge, spin accumulate in metals, The associated diffusion curretn flows in all directions, giving rise to nonlocal effects, Beyond transport properties, conduction

electrons spin resonance and spin pumping provide further testimonies for nonlocality in spin transport. These works all refer to samples consisting in piecewise uniform layers or blocks, magnetic or not. Of special significance to the present work in the noncolinear geometry where a spin current with polarization transverse to the magnetization exists, whose absorpton in the vicinty of the surface of a magnetic layer creates a torque on the magnetization, known as spin transfer torque (SFF),

We Quantitatively test the effects of spin diffusion, on real Domain walls structures, this is done by numerically solve the Zhang-Li model [21] into micromagnetics. The Zhang Li model refers to:

which is the following equation.

Base on the work of Dr. Claudio [3]

At first we investigate the steady-sate velocity regime of DWs in NiFe soft nanostrips. applying current desities similar to those reported in experiments. The results that we are going to obtain

Experimentally measured spin-diffusion parametres are used, we want to the solution of.

$$\frac{\partial \delta\vec{m}}{\partial t} = D \triangle \delta\vec{m} + \frac{1}{\tau_{sd}}\vec{m} \times \delta\vec{m} - \frac{1}{\tau_{sf}}\delta\vec{m} - u\partial_x\vec{m} \tag{3.1}$$

The sample that is considerate is a 300 nm wide and 5 nm tick NiFe soft nanostrip. This dimentions are widely used for experimental use.

Advances in spintronics recognized by 2007 Nobel Prize in Physics have ennable over the last decade advaces in computer memory, in hard drives, this is a metal based structures which utilize magnetoresisite effects to save and read data from a magnetic disk. [18]

Base on this study numeris applications have been unfold. A interesting applicaion using spintronics is new design for a new memory disk drive called racetrack memory by Parkin in 2008[12]

Therefore, a simulatenous solution of the diffusive Zhang and Li model togethr with the magnetization dynamics equation has uncovered a qualitativiely new feature of the spin-trasnfer torque effec in the presence of spin diffusion.

3.2 Domain Wall Dynamics on the GPU

The implementation of the GPU of Dr. Claudio is based on launching several kernels.

3.2.1 Rungge and Kutta

The basic structure is computational solve rungge and kutta of for other.

There exist several computational numeric methods to solver such equations, methods like euler, Midpoint Method and Runge-Kutta integrator method. The RG4 this method is used for the simulation because its numerically more accurate when compared to the others.

This method differs widely from the Euler method and the Midpoint method. The euler method is the simplest, the derivative at the starting point of each interval is extrapolated to find the next function value, see figure 3.1. The method is only has first order accuracy while RG4 its fourth order integrator.

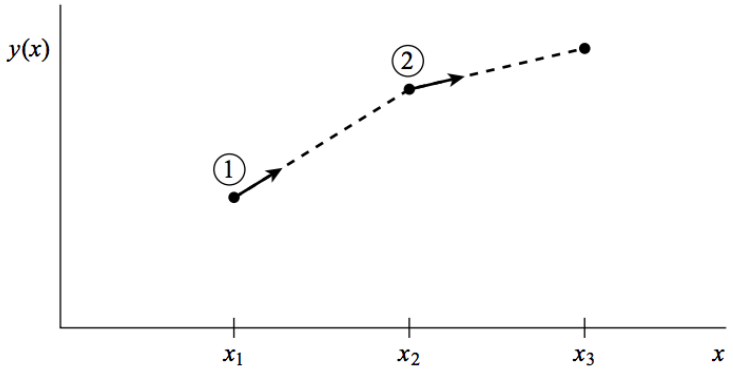

FIGURE 3.1: Euler Method, Is the simplest approximate to solver differential equation or numerically solve equations.

RK4 goes as follows:

$$y_{n+1} = y_n + 1/6K_1 + 1/3K_2 + 1/3K_3 + 1/6K_4 \tag{3.2}$$

where

$$K_1 = h\dot{f}(x_n, y_n)$$
$$K_2 = h\dot{f}(x_n + h/2, y_n + k_1/2)$$
$$K_3 = h\dot{f}(x_n + h/2, y_n + k_2/2)$$
$$K_4 = h\dot{f}(x_n + h, y_n + k_3)$$

As the equations shows, each step the derivative is evaluated four times, once at the initial point, twice at trial midpoints, and once at a trial endpoint. From these four values, the final value is calculated, just like the equation is shown 3.2

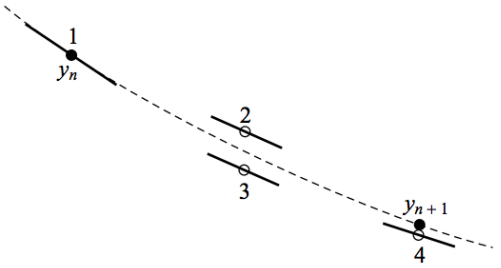

FIGURE 3.2: Fourth-order Runge and Kutta method, Each step the derivative is evaluated four times.

[14]

3.2.2 Kernels

The GPU implementation. the application reads

At inicialize the applications first it allocates all the CUDA arraries, and C arries.

The CUDA Array is done with:

```
1 cudaMalloc
```

And C with

```
1 calloc
```

In the initialization function it also reads the magenetizacion data from a especific file in this specific case from “upVW-magn-2.5nm.data”

The initial values for the simulation are

```
#define NX  480
//Number of cells along direction y
#define NY  120
//Number of cells along direction z
#define NZ  1

//Size of calculation box
#define TX  1200.0
#define TY  300.0
#define TZ  5.0

//Diffusion parameters
#define u_const 1     //nm/ns
#define D   1.0e3   //nm^2/ns
#define tau_sd_const  1.0e-3    //ns
#define tau_sf_const  25.0e-3   //ns
#define unitsfactor 1e-3  //needed to scale integer arguments to real value

//Threads and array sizes parameteres
#define XTHREADS_PERBLOCK 32
#define YTHREADS_PERBLOCK 32
```

The calculations are divided into two parts, the CPU code and GPU code. Most of the code is on the GPU. On the CPU only minor process are taken place, like I/O to a .data. On GPU is were all the computation is happening and simulation.

3.2.3 CPU

In the $initial_calculations$ functions it calculates the terms on magnetization components

the read magnetization data. This function basically reads data from a .dat file and allocates the memory for each blocks, it reads

The file is divide into two blocks of data, the first block of 57600 rows are the coordinate X and the coordinate Y. Then the next 57600 rows by 3 columns are the magnetization data. Base on the information read the matrices of data is created.

here two data sets are created. The coordinates point data (x, y) and the magnetization data (x, y, z).

Afther this initilization data, the next step is to send this data, that is actually read on the CPU (host) to de GPU(device).

First we print the Initial and final coordinates that read, this is to ensure that the values ared sucuefully.

3.2.4 GPU

Array are created on the on the Host and sento the Device using

In the type it can be either cudaMemcpyHostToDevice or cudaMemcpyDeviceToHost, depeding, if the memory thats is beeing copied is sent to the host or to the device.

```
1 cudaMemcpy(dst, src, size_in_bytes, type);
```

after initilizacion the coordinates points an the manetization data in the device are done, does values are sent to the GPU, with the function cudaMemcpy() and value set to cudaMemcpyHostToDevice.

In the Initialization of the calculations most of the arrays are filled up with values base on the data read from the .dat magenetization.

```
1 __global__ void gsource(double *sm_out, double *matrix_in, double u, int
      grid_width);
2
3 __global__ void gm_x_source(double *tempx, double *tempy, double *tempz,
4                 double *mx, double *my, double *mz,
5                 double *sm_x, double *sm_y, double *sm_z,
6                 int grid_width);
```

The function gsource

Makes the following calculation of the $double * matrix\_in$ or m

$$out[i] = (m[i-2] - 8.0 * m[i-1] + 8.0 * m[i+1] - m[i+2]) * \frac{u}{12 * deltaX} \tag{3.3}$$

where

$$deltaX = \frac{TX}{NX}$$

This calculation is done for the arrays read from the .dat file, for dev_mx, dev_my and dev_mz and are saved in a temporary arrays dev_sm_x, dev_sm_y, and dev_sm_z.

The method.

gm_x_source calculates the coss producto of the array m_{xyx} and sm_{xyz}, this is done twice.

THis data is saved on the arrays $dev_s m_{xyz}$,

Afther launching this two kernels the initial setup is done, the next step is the actual simulation using runge and kutta integrator.

3.2.5 KG4

As seed in Runge and Kutta section, this method is implementation to numerically solve the differential equation. Intuitivelly the implementation on CUDA code is done with 4 kernls, where each kernel calculates respectivelly the order of the integrator. In the last term calculation is where all the magic occurr, the sum of the previous 3 calculated terms.

```
1 __global__ void gterm1_RK1( . . .);
2 __global__ void gterm2_RK2( . . .);
3 __global__ void gterm3_RK3( . . .);
4 __global__ void gterm4_RK4( . . .);
```

Between each term calculation of RG4 laplacian calculation kernels are launched.

```
1 __global__ void glaplacianx( . . . );
2 __global__ void glaplacianyboundaries( . . . );
3 __global__ void glaplaciany( . . . );
```

The final kernel is launched $voidgterm4_R K4()$ obtain the array $deltam_{xyz}$, which is the final result of the RK4 integrator. This array is sent to the last step.

3.2.6 effective values

When the rg4 integretaor is done effective values are calculatated, this values sirve the porpese of calculation the.

```
1 __global__ void gm_x_sm( . . . );
2 __global__ void gu_eff( . . . );
3 __global__ void gu_eff_beta_eff( . . . );
4 __global__ void gbeta_eff( . . . );
5 __global__ void gbeta_diff( . . . );
```

The last kernel $voidgbeta\_diff(...)$; is where the two final arrays are obtain, which then are sent to the CPU for the final calculation.

The final calculation is just the sum of all the elements of $beta_diff_num$ and $beta_diff_den$, there divided. This final single values tells us...

This is the final step of the simulations this is where $beta\_diff$ is obtained.

The final data is saved

3.2.7 time

When the simulation is done, it will repeat the process intil the values converges.

3.3 Validation

The validate the code, that is obtained from the simulation

Once obtain the results from the simulation, the results are saved into two seperated data sets. .eff and .spin. depending of the configuration of the application is possible to obtain the uVW or the. Because CUDA framework is highly parallel system is farly easy to obtain errenois data from the calculations, even setting up the threads per block incorrectly is possible to get data set that a wrong, or results that don't diverge. It is necessary that when finishing making changes to the code validating the results with a valid data set is done.

The validation is done by checking the output the simulation with a valid data set, the output of the validation application tells us the error factor of the current data with the valid set. So for each data set there is a threshold value, that can tell if the that is close enough to the results.

3.4 Help Kernels

3.5 Data Flow

The initial data flow of the kernels goes as follow, Fi

Chapter 4

Optimization Results

This chapter the results obtain by launching the CUDA code on to several GPUs. Also the results after applying several optimizations techniques to the initial implementation from Dr. Claudio. The techniques and optimization scheme are explained in chapter 2 and the theory and code behind the implementation is in chapter 3. The results were obtain using the supercomputer of the University of Guanajuato.

4.1 Supercomputer "piritakua"

The test and analysis are obtain form the cluster piritakua. The supercomputer was design and built by Dr. Claudio from the University of Guanajuato Campus Irapuato-Salamanca. The computer is located in a small town of Mexico called Yuriria. The supercomputer has at the Front-end a 8 core Intel Xeon at 2.4 Ghz with several GPU nodes, one NVIDIA Tesla K20, two Tesla M2070 and GTX 580.

The specifications of the front-end cluster.

Processor	Number	Cores	RAM
Servidor Dell Intel Xeon E5620 2.4 GHz	1	8	12 GB
Servidores HP Proliant SL 350s Gen3 Intel Xeon X5650 2.67 GHz	2	24	32 GB
Servidores HP Proliant SL 250s Gen8 Intel Xeon E5-2670 2.60 GHz	3	48	104 GB
CPU Xeon Phi 5110p	1	8	8 GB
CPU Xeon Phi 7120p	1	8	16 GB

Some test were done one a high-end CPU laptop a eight core intel i7-3630QM, so we obtain results using the Xeon Phi and the Intel i7.When accessing the front-end, it

connects to the Xeon Phi processor, then its possible to access all the GPUs available. The Specifications of the GPU connected to the front-end are as follows.

Model	Cores	RAM	DP	SP	Bandwidth
Tesla K20m	2496	5GB	1.17 Tflops	3.52 Tflops	208 GB/s
Tesla M2070	448	6GB	515 Gflops	1030 Gflops	150 GB/s
Tesla C2050	448	2.5GB	512 Gflops	1030 Gflops	144 GB/s
GeForce GTX 580	512	1.5GB	520 Gflops	1,154 Gflops	192.2 GB/s
GeForce GTX 670MX	960	3GB	520 Gflops	1,154 Gflops	67.2 GB/s

Some test were perform on a laptop with a NVIDIA GPU, the GeForce GTX 670m. This card is design for less power used but with high graphics power, it even has more cores than some Tesla models, but with less Bandwidth.

There two main GPU architectures that NVIDIA developed, the Fermi and Kepler. The Tesla K20m is base on "Kepler" GPU architecture and Tesla M2070, Tesla M2050 and GeForce GTX 580 on the Fermi architecture. The Kepler is a newer architecture than the Fermi. The big difference between the is the number of CUDA cores per SM.

4.1.1 Experiment detail

4.2 Results

The CUDA code was launched in each GPU of the piritakua supercomputer. As we know the supercomputer has different GPU architectures so we can test...

4.2.1 Initial Test

4.2.1.1 Visual profiler

The visual profiler.

The visual profiler was used on Laptop with GeForce GTX 670m with the intel eight core i7-3630QM.

the

4.2.2 Obtimized

4.2.3 Subsection 2

4.3 Main Section 2

Chapter 5

Conclusions and future work

5.1 Main Section 1

Appendix A

Appendix Title Here

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