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Le choix des architectures hybrides, une stratégie réaliste pour atteindre l'échelle exaflopique

The choose of hybrids architectures, a realistic strategy to reach the Exascale

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Introduction

The world of High Performance Computing (HPC) will reach another milestone in the power of machines with Exascale. The United States of America and Europe will reach Exascale capability by 2020 or 2021, but China may have the power by 2019.

These supercomputers will be 100 times faster than the estimated overall operations performed by the human brain and its 10^{16} **FLoating point Operations Per Second** (FLOPS) [Kur10] and achieve a computational power of a quintillion (10^{18}) of FLOPS. This odyssey began with the first vacuum tubes computers and the need of ballistic computation for war. Nowadays, supercomputers extended their fields of application and the power of a nation is represented not only by its army and money, but also by the computational power of its supercomputers. HPC's applications has now spread into all the areas of science and technology.

Since 1962, considering the Cray CDC 6600 as the first supercomputer, the power of these machines has increased following an observation of the co-founder of the Intel company, Gordon Moore. Better known under the name of "Moore's Law", it speculated in 1965 that, considering the constant evolution of technology, the number of transistors on a dense integrated circuit will double approximately every two years. Thus, the computational power, that intrinsically depends on the number of transistors on the chip, will increase. More importantly, as "*money is the sinews of war*", the cost of the die for the same performances will decrease. This observation can be compared to the supercomputers results throughout the years in the TOP500 list. As presented on figure 1 the Moore's law appears to be accurate and sustainable even though it was estimated in early 1965.

The shrink in the semiconductor with smaller transistors was not the only driver of the linear evolution. The first one-core Central Processing Units (CPUs) were made using more transistors and had a faster frequency. They later faced limitations to reach high frequencies because of the power consumption and the inherent cooling of the heat generated by the chip. This is why IBM proposed the first multi-core processor on the same die, the Power4, in early twentieth century. The constructors started to create chips with more than one core to increase the computational power in conjunction with the shrink of semiconductors, answering the constant demand of more powerful devices and allowing the Moore's law to thrive. This increase of the overall power of the chip comes with some downside, such as costs in synchronization steps between the cores for memory access, work sharing and complexity. Currently, the general-purpose CPU features from two to less than a hundred of cores on a single chip.

In order to reach even more computational power some researchers started to use many-core approaches. By using hundreds of cores, these devices take advantage of very "simple" computing units, with slow frequency and low power consumption but add more complexity and requirement for their efficient programming with even more synchronizations needed between the cores. Typically, those many-core architectures are used coupled with a CPU that sends the data and drives them. Some accelerators like the Intel Xeon Phi can be driven or driver depending on their configuration. Usually called accelerators, those devices are used in addition to the host processor to provide their efficient computational power in the key parts of execution. The most famous accelerators are the Xeon Phi, the General-Purpose Graphics Processing Unit (GPGPU) initially used for graphic processing, Field Programmable Gates Array



Figure 1: Computational power evolution in the TOP500 list

(FPGA) or dedicated Application-Specific Integrated Circuit (ASIC). The model using a host with additional device(s) appears and we will be referred to as "Hybrid Architecture". In fact, a cluster can be composed of CPUs, CPUs with accelerator(s) of the same kind, CPUs with heterogeneous accelerators or even accelerators like Xeon Phi driving different kinds of accelerators.

Since either 2013 or 2014 many companies, like the Gordon Moore's company *Intel* itself, stated that the Moore's law is over. This can be seen on figure 1: on the right part of the graph, the evolution is no longer linear and tends to decrease slowly in time. This can be contributed to two main factors. First, we slowly reach the maximal shrink size of the transistors implying hard to handle side effects. Second, the power wall implied by the power consumption required by so many transistors and frequency speed on the chip.

Even with all these devices, current supercomputers face several problems in their conception and utilization. The three main walls bounding the overall computational power of the machines are: the power consumption wall, the communication wall and the memory wall. Sub-problems like the interconnect wall, resilience wall or even the complexity wall also arise and make the task even more difficult.

In this context of doubts and questions about the future of HPC, this study proposes several points of view. We believe the future of HPC is made with these hybrid architectures or acceleration devices adapted to the need, using well suited API, framework and code. We consider that the classical benchmarks, like the TOP500, are not enough to target the main walls of those architectures, especially accelerators. Domain scientists' applications like physics/astrophysics/chemist/biologist require benchmarks based on more irregular cases with heavy computation, communications and memory accesses.

In this document, we propose a metric that extracts the three main issues of HPC and apply them to accelerated architectures to determine how to take advantage of these architectures and what are the limitations for them. The first step of this metrics is obtained when merging two characteristic problems and then a third problem, combining all our knowledge. The first two are targeting computation and communication wall over very irregular cases with high memory accesses, using an academic combinatorial problem and the Graph500 benchmark. The last is a computational scientific problem that will cover both difficulties of the previous problems and appears to be hard to implement on supercomputers and even more on accelerated ones. The results obtain supports our thesis and show hybrid architectures as the best solution to reach Exascale.

This thesis is composed of three parts.

The first part explores the state of the art in HPC from the main laws to the hardware. We go through the basic laws from Amdahl's to Gustafson's laws and the specification of speedup and efficiency. Classical CPUs, GPGPUs and other accelerators are described and discussed regarding the state of the art. The main methods of ranking and the issues regarding them are presented.

In the second part we propose our metric based on characteristic problems to target classical and hybrid architectures. The Langford problem is described as an irregular and computationally heavy problem. This demonstrates how the accelerators, in this case GPUs, are able to support the memory and computation wall. This work leads to the publication of one journal paper [KLAJ16b] and many conferences, presentations and posters [DJK⁺14, LJAK16, JDK⁺14]. Our implementation of the Langford problem allowed us to beat a world record with the last instances of this academic problem.

The Graph500 problem is then proposed as an irregular and communications heavy problem. We present our implementation, and moreover, the logic to take advantage of the GPUs computational power for characteristic applications. This work leaded to the publication of a

conference paper [KLAJ16a] and many presentations and posters [LAJK15, LJAK15].

In the third part, we consider a problem that is substantial and irregular in regard to computation and communications. We analyze this problem and show that it combines all the previous limitations. Then we apply our methodology and show how modern supercomputers can overcome these issues. This computational science problem is based on the Smoothed Particle Hydrodynamics method. The former application began with the development of the FleCSI framework from the Los Alamos National Laboratory which allowed us to exchange directly with the LANL domain scientists on their needs. We intent to provide an efficient tool for physicists and astrophysicists, called FleCSPH, based on our global work to efficiently parallelize these types of production applications. This work leaded to several conference papers [LLB⁺18, LAJK18] and posters [DBGH⁺16, LLMB17].

The last part summarizes on this work and results to show some of the main prospects of this study and my future researches.

Part I

HPC and Exascale

Introduction

This part of this thesis contains a state of the art presentation for theory and applications of High Performance Computing. It describes the tools we need for our study. High Performance Computing, HPC, does not have a strict definition. Its history starts with domain scientists in need of more complex and more reliable computation for models checking or simulations. They developed their own tools beginning with vacuum tubes computers which can be consider as a milestone in HPC history. Since this first machine the technology became more and more complex at every layer: the hardware conception, the software to handle it and even the models and topologies. HPC is now a scientific field on its own but always dedicated to the end purpose, domain scientist computations. HPC experts are interested in supercomputer construction, architecture and code optimization, interconnection behaviors and creating more software, framework or tools to facilitate access to these very complex machines.

In this part we give a non-exhaustive definition of HPC focusing on models, hardware and tools required for our study in three chapters.

We first focus on what are the theoretic models for the machines and the memory we base our work on. This first chapter also presents what is defined as performance for HPC and the main laws that define it.

The second chapter details the architecture base on these models. We present nowadays platforms with dominant constructors and architectures from multi-core to specific many-core machines. Representative members of today's supercomputers are described. We show that hybrid architectures seem to be the only plausible way to reach the exascale: they offer the best performance per watt ratio and nowadays API/tools allow to target them more easily and efficiently than ever.

In the third chapter we detail the main software to target those complex architectures. We present tools, frameworks and API for shared and distributed memory. We also introduce the main benchmarks used in the HPC world in order to rank the most powerful supercomputers. This chapter also shows that those benchmarks are not the best to give an accurate score or scale for "realistic" domain scientists' applications.

Chapter 1

Models for HPC

1.1 Introduction

High Performance Computing (HPC) takes its roots from the beginning of computer odyssey in the middle of 20th century. From this emerged rules, observations, theories and most computer science fields. Knowledge of the theory is required to understand and characterize HPC and supercomputers. This part describes the Von Neumann model, the generic model of sequential computer on which every modern machine is built. The Von Neumann model, along with the Flynn taxonomy which is the classification of the different execution models, will be presented. We also review the different memory models based on those elements.

Parallelism will be discussed in detail and we present how it can be used to reach performances, and thus examine what performance implies in HPC. The Amdahl's and Gustafson's laws are presented in detail, along with the strong and weak scaling used in our study.

1.2 Von Neumann Model

The first early 20th century computers were built using vacuum tubes making them high power consuming, and therefore were hard to maintain and expensive to build. The most famous of first vacuum tubes supercomputers, the ENIAC, was based on a decimal system. As well-known as this supercomputer may be, the real revolution came from its successor. The first binary system based computer was created in 1944 and was called the Electric Discrete Variable Automatic Computer (EDVAC). A physicist from the EDVAC team a described the logical model of this computer and provided a model on which every modern computing device is based.

John Von Neumann published the *First Draft of a Report on the EDVAC* [VN93] in 1945. The model known as the Von Neumann model, more commonly referred as the Von Neumann Machine, came from this work. The model is presented on figure 1.1. The figure has three identified parts: the input and output devices and, in the middle, the computational device itself in the middle.

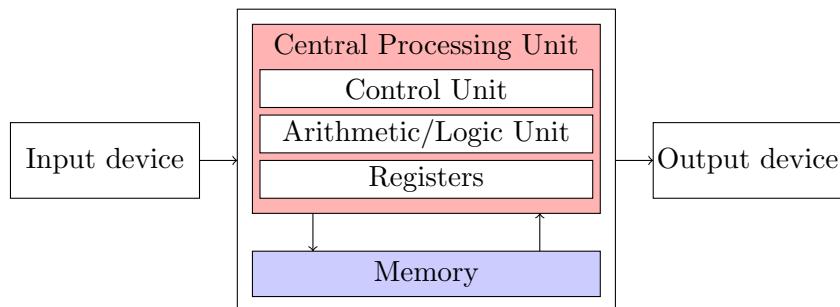


Figure 1.1: Von Neumann model

Input/Output devices The input and output devices are used to store data in a read/write way. They can be represented as hard drives, solid state drives, monitors, printers or even mouse and keyboard. The input and output devices can also be the same, reading and writing in the same area.

Memory Inside the computational unit we find the general memory to store program and data. The most common architectures it can be considered as a Random Access Memory (RAM). There are several types of memory and will be discussed later in this thesis.

Central Processing Unit The Central Processing Unit (CPU) is composed of several elements in this model.

- On one hand, the *Arithmetic and Logic Unit* (ALU) takes as input one or two values, the data and applies an operation on them. The operation can be either logic with operators such as AND, OR, XOR, etc. or arithmetic with operators such as ADD, MUL, SUB, etc. These operators may be more complex on modern CPUs.
- Conversely, we find the *Control Unit* (CU) which controls the data carriage to the ALU from the memory and the operation to be performed on data. It is also involved in the Program Counter (PC), which is the address of the next instruction in the program.
- We can identify the *Registers* section which represents data location used for both ALU and CU to store temporary results, the current instruction address, etc. Some representations may vary since the *Registers* can be represented directly inside the ALU or the CU.

Buses The links between those elements are called buses and can be separated in data buses, control buses and addresses buses. These will have a huge importance for the first machines optimizations, growing the size of the buses from 2, 8, 16, 32, 64 and even more for vector machines with 128 and 256 bits.

The usual processing flow on such architectures can be summarized as a loop:

- Fetch instruction at current PC from memory;
- Decode instruction using the Instruction Set Architecture (ISA). The main ISA are Reduce Instruction Set Computer architecture (RISC) and Complex Instruction Set Computer architecture (CISC);
- Evaluate operand(s) address(es);
- Fetch operand(s) from memory;
- Execute operation(s).
- Store results, increase PC.

With the instruction sets and new architectures, several similar operations can be processed in the same clock time. Every device or machine we describe in the next chapter has this architecture as a basis. One will consider execution models and architecture models to characterize HPC architectures.

1.3 Flynn taxonomy and execution models

The Von Neumann model gives us a general idea of how a computational unit is fashioned. The constant demand for more powerful computers required scientists to find different ways to provide this computational power. In 2001, IBM proposed the first multi-core processor on the same die: the Power4 with its 2 cores. This evolution required new paradigms. A right characterization become essential to be able to target the right architecture for the right purpose. The Flynn taxonomy presents a hierarchical organization of computation machines and executions models.

	Data Stream(s) →	
Instruction Stream(s) ↓	Single Data (SD)	Multiple Data (MD)
Single Instruction (SI)	SISD	SIMD <i>SIMT</i>
Multiple Instruction (MI)	MISD	MIMD <i>SPMD/MPMD</i>

Table 1.1: Flynn taxonomy for execution models completed with SPMD and SIMT models

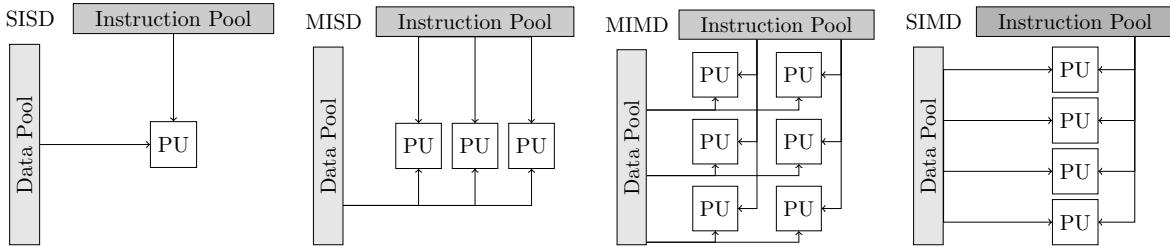


Figure 1.2: Flynn taxonomy schematic representation of execution models

In this classification [Fly72] from 1972, Michael J. Flynn presents the SISD, MISD, MIMD, and SIMD models. Each of those execution models, presented on table 1.1 and figure 1.2, corresponds to a specific machine and function.

1.3.1 Single Instruction, Single Data: SISD

The model corresponding to a single core CPU is similar to the Von Neumann model. This sequential model takes one instruction, operates on one data and the result is then stored before the process continues over. SISD is important to consider for a reference computational time and will be taken into account in the next part for Amdahl's and Gustafson's laws.

1.3.2 Multiple Instructions, Single Data: MISD

This model can correspond to a pipelined computer. Different operation flows are applied to the datum, which is transferred to the next computational unit and so on. This is the least common execution model.

1.3.3 Multiple Instructions, Multiple Data: MIMD

Every element in MIMD executes its own instructions flow on its own data set. This can represent the behavior of a processor using several cores, threads or even the different nodes of a supercomputer cluster. Two subcategories are identified in this model: SPMD and MPMD.

SPMD

The Single Program Multiple Data model (SPMD), where each process executes the same program, is the most famous parallelism way for HPC purpose. All programs are the same, but does not share the same instruction counter. SPMD was proposed for the first time in [DGNP88] in 1988 using Fortran. This is the common approach working with runtime like MPI. The programs are the same and the executions are independent but based on their ID the processes will target different data.

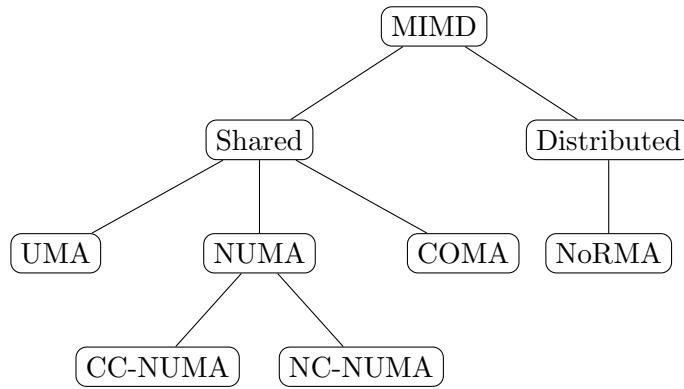


Figure 1.3: MIMD memory models

MPMD

The Multiple Program Multiple Data (MPMD) model is also known for HPC. MPMD involves some of the processes to execute different programs, generally with a separation between a main program generating data for sub-programs. This is the model on which we work in Part II, regarding the Langford problem resolution using a master program generating tasks for the slaves CPUs/GPGPUs programs.

1.3.4 Single Instruction, Multiple Data: SIMD

This execution model corresponds to many-core architectures like a GPU. SIMD can be extended from two to sixteen elements for classical CPUs to hundreds and even thousands of core for GPGPUs. In the same clock cycle, the same operation is executed on every process on different data. A good example is the work on matrices with stencils: the same instruction is executed on every element of the matrix in a synchronous way and the processing elements share one instruction unit and program counter.

1.3.5 SIMT

Another characterization was determined to describe the new GPUs architecture: Single Instruction Multiple Threads. This first appears in one of NVIDIA's company paper [LNOM08]. This model describes a combination of MIMD and SIMD architectures where every block of threads is working with the same control processor on different data and in such a way that every block has its own instruction counter. The model we describe in Part 3.3.3, used for the *warps* model in NVIDIA CUDA.

1.4 Memory

In addition to the execution model and parallelism, the memory access patterns have an important role in performances of SIMD and MIMD. In this classification we identify three categories: UMA, NUMA and NoRMA for shared and distributed cases. This classification has been pointed out in the Johnson's taxonomy[Joh88].

Those different types of memory for SIMD/MIMD model are summarized in figure 1.3, and presented below.

1.4.1 Shared memory

Several kinds of memory models are possible when it comes to multi-threaded and multi-cores execution models like MIMD or SIMD models. We give a description of the most common shared memories architectures. Those shared memory models are the keystone for the next parts of

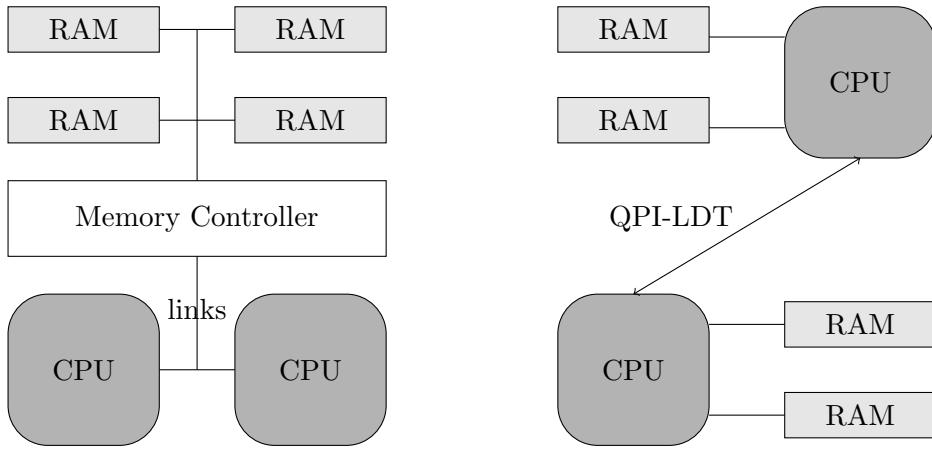


Figure 1.4: UMA vs NUMA memory models

this study. Not only are they found in multi-core but also in many-core architectures with the performances are completely dependent on their usage.

UMA

The Uniform Memory Access architecture have a global memory shared by every threads or cores. Every processor in UMA uses its own cache as local private memory and the accesses consume the same amount of time. The addresses can be accessed directly by each processor which makes the access time ideal. The downside is that more processors require more buses and thus UMA is hardly scalable. Cache consistency problem also appears in this context and will be discussed in next part. Indeed, if a data is loaded in one processor cache and modified, this information has to be spread to the memory and possibly other processes cache.

With the rise of accelerators like GPUs and their own memory, some constructors found ways to create UMA with heterogeneous memory. AMD created the heterogeneous UMA, hUMA [RF13] in 2013, allowed CPU and GPU to target the same memory area, but the performances still needed to be checked in an HPC context.

NUMA

In Non Uniform Memory Access every processor has access to its own private memory but allows other processors to access it though Lightning Data Transport (LDT) or Quick Path Interconnect (QPI) for Intel architectures.

As mentioned for the UMA memory, even if the processors do not directly access to the memory cache, coherency is important. There are two methods possible to aid in coherency. First, the most used is Cache-Coherent NUMA (CC-NUMA) where protocols are used to keep data coherency through the memory. Second, No Cache NUMA (NC-NUMA) forces the processes to avoid cache utilization and write results to main memory, losing all the benefits of caching data.

COMA

In Cache-Only Memory Accesses, the whole memory is seen as a cache shared by all the processes processes. A *Attraction memory* pattern is used to *attract* the data near the process that will use them. This model is less commonly used and, in best cases, leads to same results as NUMA.

1.4.2 Distributed memory

The previous models are dedicated to shared memory, as in the processes can access memory of their neighboring processes. In some cases, like supercomputers, it would be too heavy for

Name	FLOPS	Year	Name	FLOPS	Year
kiloFLOPS	10^3		petaFLOPS	10^{15}	2005
megaFLOPS	10^6		exaFLOPS	10^{18}	2020 ?
gigaFLOPS	10^9	≈ 1980	zettaFLOPS	10^{21}	
teraFLOPS	10^{12}	1996	yottaFLOPS	10^{24}	

Table 1.2: Floating-point Operation per Second and years of reach in HPC.

processors to handle the requests of all the others through the network. Each process or node will then possesses its own local memory that can be shared only between local processes. In order to access to other nodes memory, communications through the network has to be done and copied into local memory. This distributed memory model is called No Remote Memory Access (NoRMA). This requires transfer schemes that have to be added to local read-write accesses.

1.5 Performances characterization in HPC

Previously we described the different execution models and memory models for HPC. We need to be able to emphasize the performances of a computer and a cluster based on those aspects.

There can be several types of performances. First, it can be defined by the speed of the processors themselves with the frequency defined in GHz. We define the notion of *cycle* to be the number that determines the speed of a processor. This is the amount of time between two pulses of the oscillator at the best frequency with higher cycles per seconds being better. This can be used to estimate the highest computational power of a machine. The information is not perfect, however, because the ALU is not constantly busy due to memory accesses, communications or side effects. Therefore, we need to utilize more accurate ways to characterize performance.

1.5.1 FLOPS

The FLoating point Operations Per Second (FLOPS) value considers the number of floating-point operations that the system will execute in a second. Higher FLOPS is better and is the most common scale used to consider supercomputers' computational power. For a cluster we can compute the theoretical FLOPS (peak) based on the processor frequency in GHz with:

$$FLOPS_{cluster} = \#nodes \times \frac{\#sockets}{\#node} \times \frac{\#cores}{\#socket} \times \frac{\#GHz}{\#core} \times \frac{FLOPS}{cycle} \quad (1.1)$$

With $\#nodes$ the number of computational node of the system, $\frac{\#sockets}{\#node}$ the number of sockets (=processors) per node, $\frac{\#cores}{\#socket}$ the number of cores in the processor, $\frac{\#GHz}{\#core}$ the frequency of each core and finally $\frac{FLOPS}{cycle}$ the number of floating-point operations per cycles for this architecture.

Table 1.2 presents the scale of FLOPS and the year that the first world machine reached this step. The next milestone, the exascale, is expected to be reach near 2020.

There still exists many ways to measure computer's performance such as: Instructions Per Seconds (IPS), Instructions per Cycle (IPC) or Operations Per Seconds (OPS). However, it is hard to consider what an operation or instruction can be. Thus, floating point can be considered as a basis, providing a comparison for performance.

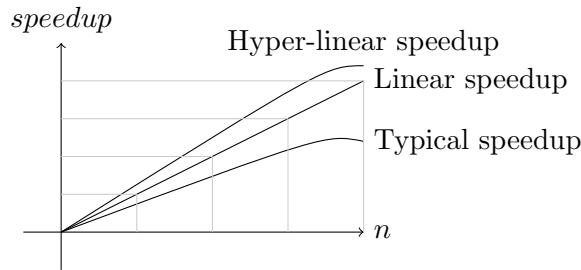


Figure 1.5: Observed speedup: linear, typical and hyper-linear speedups

1.5.2 Power consumption

An additional way to consider machine performance is to estimate the number of operations regarding the power consumption. This considers all the previous metrics like FLOPS, IPS, IPC or OPS. Benchmarks like the Green500 consider the FLOPS delivered over the watts consumed. For current architectures the many-cores accelerated architectures with GPUs seems to deliver the best FLOPS per watt ratio.

This subject is the underlying goal of our study. Without the power consumption limit we would already be able to build exascale or even more powerful machine by combining billions and billions of nodes. This is not doable due to processors power consumption and cooling cost. The question have been studied in our laboratory with the development of tools like *Powmon* (Power Monitor). This power monitor allows to instantaneously query the power consumption with CPU and GPU on a running node of a cluster.

1.5.3 Scalability

After considering architectures evaluation, one have to measure the applications performances. The scalability expresses the way a program reacts to parallelism. When an algorithm is implemented on a serial machine and is ideal to solve a problem, one may consider to use it on more than one core, socket, node or even cluster. Indeed, while using more resources one may expect less computation time or access larger instances, or a combination of both. This is completely dependent of the algorithm's parallelization and is expressed through scalability. A scalable program will scale on as many processors as provided, whereas a poorly scalable one will give the same, or even worst results, than the serial code. Scalability can be approached using speedup and efficiency.

1.5.4 Speedup and efficiency

The latency is the time required to complete a task in a program with lower latency being better.

The speedup compares the latency of both sequential and parallel algorithm. In order to get relevant results, one may consider the given best serial program against the best parallel implementation.

Considering n , the number of processes, and $n = 1$ the sequential case. T_n is the execution time working on n processes and T_1 the sequential execution time. The speedup can be defined using the latency by the formula:

$$\text{speedup} = S_n = \frac{T_1}{T_n} \quad (1.2)$$

In addition to speedup, the efficiency is defined by the speedup divided by the number of workers:

$$\text{efficiency} = E_n = \frac{S_n}{n} = \frac{T_1}{nT_n} \quad (1.3)$$

The efficiency, usually expressed in percent, represents the evolution of the code stability to growing number of processors. As the number of processes grows, a scalable application will keep an efficiency near 100%.

As shown on figure 1.5 several kinds of speedup can be observed.

Linear, reference speedup: The linear speedup usually represents the target for every program in HPC. To have a constant efficiency means that the speedup grows linearly as the number of processors grows is the ideal case. Codes fall typical into two cases: typical and hyper-linear speedup.

Typical speedup: This represents the most common observed speedup. As the number of processors grows, the program faces several of the HPC walls, such as communications wall or memory wall. The increasing number of computational power may be lost in parallel overhead resulting in efficiency being reduced.

Hyper-linear speedup: In some cases, we observe an hyper-linear speedup, meaning the results in parallel are even better than the ideal case. This increasing efficiency can occur if the program fits exactly in memory with less data on each processor or even fit perfectly for the cache utilization. The parallel algorithm can also be more efficient than the sequential one. For example, if the search space in an optimized application is divided over processing units, one can find good solutions more quickly.

1.5.5 Amdahl's and Gustafson's law

The Amdahl's and Gustafson's laws are ways to evaluate the maximal possible speedup for an application taking into account different characteristics.

Amdahl's law

The Amdahl's law[Amd67] is used to find the theoretical speedup in latency of a program. We can separate a program into two parts, the one that can be executed in parallel with optimal speedup and the one that is intrinsically sequential. The law states that even if we reduce the parallel part using an infinity of processes the sequential part will reach 100% of the total computation time.

Extracted from the Amdahl paper the law can be written as:

$$S_n = \frac{1}{Seq + \frac{Par}{n}} \quad (1.4)$$

Where Seq and Par respectively the sequential and parallel ratio of a program ($Seq + Par = 1$). Here if we use up to $n = \inf$ processes, $S_n \leq \frac{1}{Seq}$ the sequential part of the code become the most time consuming.

And the efficiency become:

$$E_n = \frac{1}{n \times Seq + Par} \quad (1.5)$$

A representation of Amdahl's speedup is presented on Fig. 1.6 with varying percentage of serial part.

Gustafson's law

The Amdahl's law focuses on time with problem of the same size. John L. Gustafson's idea is that using more computational units and the same amount of time, the problem size can grow accordingly. He considered a constant computation time with evolving problem, growing the

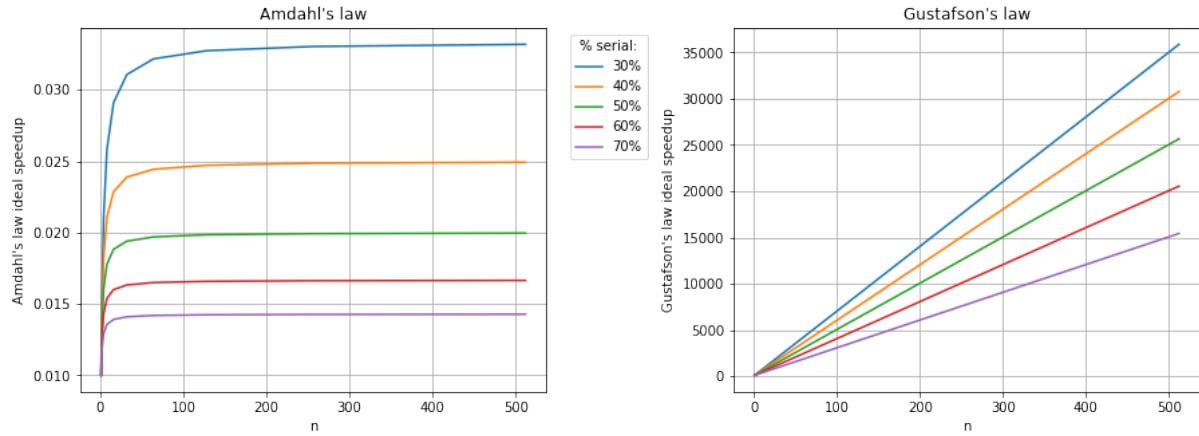


Figure 1.6: Theoretical speedup for Amdahl's (left) and Gustafson's (right) law

size accordingly to the number of processes. Indeed the parallel part grows as the problem size does, reducing the percentage of the serial part for the overall resolution.

The speedup can now be estimated by:

$$S_n = Seq + Par \times n \quad (1.6)$$

And the efficiency:

$$E_n = \frac{Seq}{n} + Par \quad (1.7)$$

Both Amdahl's and Gustafson's law are applicable and they represent two solutions to check the speedup of our applications. **The strong scaling**, looking at how the computation time vary evolving only the number of processes, not the problem size. **The weak scaling**, at the opposite to strong scaling, regards to how the computation time changes with the varying of the problem size, but keeping the same amount of work per processes.

1.6 Conclusions

In this chapter, we presented the different basic considerations to be able to understand HPC: the Von Neumann model that is implemented in every current architecture and the Flynn taxonomy that is in constantly in evolution with new paradigms like recent SIMT from NVIDIA. We discussed the memory types that will be used with the different layers in our clusters, from node memory, CPU-GPGPU shared memory space to global fast shared memory. We finished by presenting the most important laws with Amdahl's and Gustafson's laws. The concept of strong and weak scaling was introduced and will lead our tests through all the examples in Part II and Part III.

Those models have now to be confronted to the reality with hardware implementation and market reality, the vendors. The next chapter introduces chronologically hardware enhancements and their optimization, always keeping a link with the models presented in this part.

We will have to find ways to rank and characterize those architectures as there is always a gap between models and implementation. This will be discussed in the last chapter.

Chapter 2

Hardware in HPC

2.1 Introduction

Parallel models address most of the key points for application performance, but it may also depend on architectures hardware, which may influence how to consider the problems' resolution. Thus, the knowledge of hardware architecture is essential to reach performances through optimizations. Even if the current software, API, framework or runtime already handle most of the optimizations, the last percents of performance gain are architecture dependent. In this chapter, we describe the most important devices architectures from classical processors, General Purpose Graphics Processing Units (GPGPUs), Field Programmable Gate Arrays (FPGAs) and Application-Specific Integrated Circuits (ASICs). This study focuses on multi-core processors and GPUs as we based our tests on these devices.

This chapter describes the architecture of some remarkable supercomputers. This comes with the description of interconnection network for the most used interconnection topologies.

We choose to present the architectures in a chronological order following the models presented in the previous chapter - SISD, MIMD and SIMD/SIMT - and presenting the most recently released technologies. We also present the optimizations of current technologies with the rise of parallelism and new types of memories.

2.2 Early improvements of Von Neumann machine

In this section, we present the different hardware evolution from the 1970s single core processors to modern multi-core and many-core architectures that are the milestones, and the basic units, for building supercomputers. We can observe the most important optimizations that are always implemented in the most recent machines: in/out of order processors, pre-fetching strategies, vectorization and the memory technologies breakthroughs.

2.2.1 Single core processors

The first processors were developed in the 1970s and were built using a single computation core as described in the Von Neumann model. The single core processors were improved with many optimizations from the memory, the order of the instructions and the frequency to increase.

Transistor shrink and frequency

Many new approaches to produce smaller transistors have been discovered. Transistor sizes were about $10\mu m$ in 1971 and reach $10nm$ in current machines. This allowed the constructors to add more transistors on the same die and build more complex ISA and features for the CPUs.

In parallel of the shrink of transistors, the main feature for better performances with the single core architectures came from the frequency augmentation, the clock rate. As the clock rate increases, more operations can be performed on the core in the same amount of time. In the

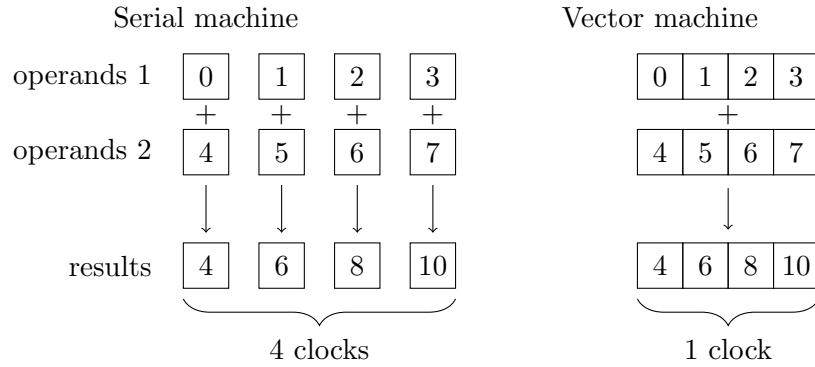


Figure 2.1: Vectorized processor example on 4 integer addition: 128 bits wide bus

1970s, the frequency was about 4 MHz allowing a maximum of 4 million of cycles per seconds. Nowadays, single cores can work at a frequency of 4GHz and even 5GHz performing billions of operations per cycles, but the following sections will demonstrate that due to power consumption and coding considerations, frequency is no longer used to improve performances.

In/Out-Of-Order execution

In-order-process is described in the previous chapter. This control unit fetches instructions and the operands from memory. The ALU then computes the operation before the final result is stored to the memory.

In this model, the time to perform an instruction is the accumulation of: instruction fetching + operand(s) fetching + *computation* + result storage. This time may be high regarding the use of the ALU for *computation*, technically just one clock cycle. The idea of *out-of-order* execution is to compute the instructions without following the Program Counter order. Indeed, for independent tasks, (indicated by dependency graphs) while the process fetches the next instruction data, the ALU can perform another operation with already available operands. This leads to better usage of computational resources in the CPU, and thus better overall performances.

Vectorization

Vector processors allow the instructions to be executed at the same time in a SIMD manner. If the same instruction is executed on coalescent data they can be executed in the same clock cycle. For an example, we can execute operations simultaneously on four to eight floats with a bus size of 128 or 256 bits. This requires specific care for coding with *unrolling* and *loop tiling* to avoid bad behavior leading to poor performances and will be addressed later in this study. The latest architectures vectorization imposes to slightly lower the frequency of processors.

The Cray-1 supercomputer[Rus78], installed in 1975 in the Los Alamos National Laboratory, is a perfect example of vector processor supercomputer. This supercomputer was designed by Seymour Cray, the founder of Cray Research, and was able to deliver up to 160 MFLOPS based on vector processor. It was the fastest supercomputer in 1978 and due to its shape and price it was humorously called *the world's most expansive love-seat*.

The behavior of vector machine is presented on figure 2.1 for a 16 bytes vector machine (4 integer of 4 bytes = 128 bits bus). We see on the left that performing the 4 operations requests in 4 cycle and, at the opposite, 1 cycle on the right with the vectorized machine.

Linked with the CPU optimizations, the memory optimizations also needs to be considered. Even if the ALU can perform billions of operations per second, it needs to be fed with data by fast transfers.

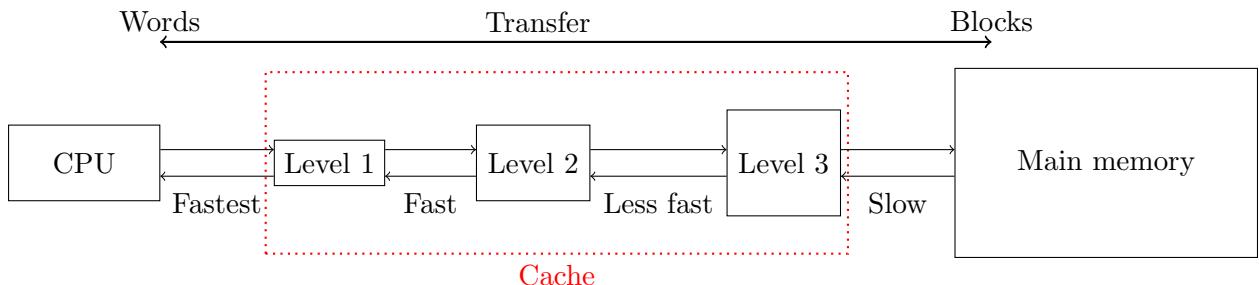


Figure 2.2: Cache memory technology on three levels L1, L2 and L3

Memory technology evolution

The memories technologies optimizations address several aspects. The early 1980s saw the augmentation of bus size from 4 bits to presently 32 bits for single precision and 64 bits for double precision. Buses with 128 bits or 256 bits can also be used to allow vectorization presented just before.

Different kind of technologies are considered in this study: the SRAM and DRAM.

SRAM: The Static Random Access Memory (SRAM) is built using so called "flip-flop" circuits that can store data at any time with no time lost in "refresh operations". This kind of memory is very expensive to produce due to the number of transistors by memory cell, therefore, it is usually limited for small amounts of storage. The SRAM is mainly used for cache memory.

DRAM: The Dynamic Random Access Memory (DRAM) is based on transistors and capacitors to store binary information. This memory is less expensive to produce but needs to be refreshed at a determined frequency, otherwise the data are lost. This refresh step is a read-write operation on the whole memory at a specific frequency. There are several sub-categories of DRAM used in different device depending on the way the bus are used with Single Data Rate (SDR), Double Data Rate (DDR) and Quad Data Rates (QDR). The number of data carried can vary from one times to four times, but the limitation of those products is the price and are constantly rising.

The latest more efficient memory is the 3D memory. This is a stack of the different components instead of usual 2D distribution. This memory, 3D XPoint, was created by Intel and Micron Technology and announced in July 2015. It can now be found in the NVIDIA GPUs, named 3D-stacked in P100 and V100.

Cache memory:

Cache is a memory mechanism that is useful to consider when targeting performance. The main idea of cache technology is presented on figure 2.2. This memory is built hierarchically over several levels. L1 is the closest to the CPU followed by L2 with generally no levels past L3 except on specific architectures. When looking for data, the CPU first checks if the data is present in the L1 cache, otherwise it will look in L2 and L3 to get the data to higher level. From the main memory to the L3 cache *blocks* are exchanged, by chunks. With levels L1 and L2, lines of information are exchanged, usually referred to as *words*. This is based on the idea that if a data is used, it shall be used again in the near future. Many cache architectures exist: direct, associative, fully associative, etc. Cache-hits occur when the data required is present in cache versus a cache-miss occurs when it has to be retrieved from lower levels or main memory. The ratio of cache-miss has to be kept low in a program in order to reach performance, and the impact may be very high.

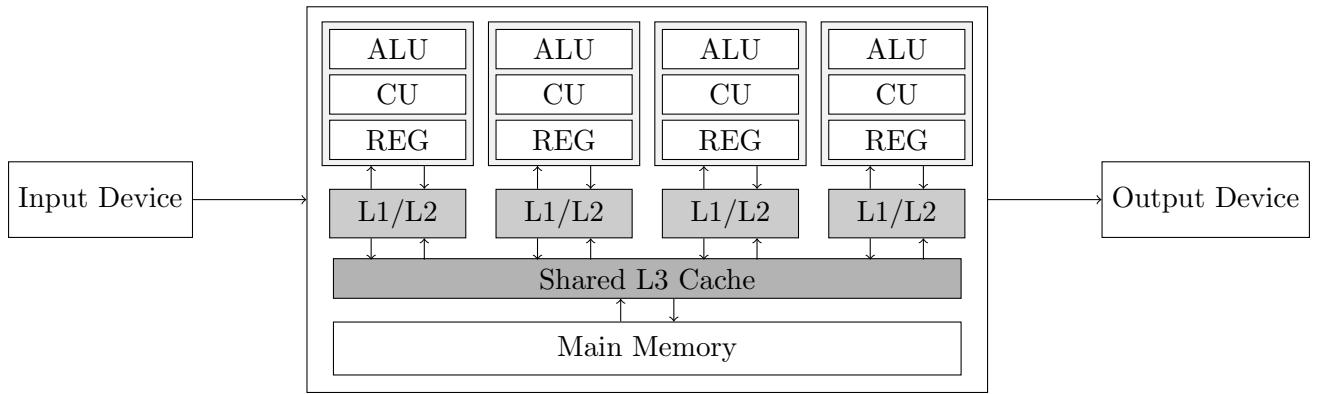


Figure 2.3: Multi-core CPU with 4 cores based on Von Neumann Model

Pre-fetching

Pre-fectching was developed based on memory optimization and especially for the cache. When data are not available in L1 cache, it has to be moved from either L2 to L1 or L3 to L2 to L1 or in the worst case from RAM to L3 to L2 to L1. Pre-fectching technology is a way to, knowing the next instructions operands, pre-fetch the data in closer cache before the instruction is decoded. The pre-fetch can either be hardware or software implemented and can concern data and even instructions.

2.2.2 Multi-CPU servers and multi-core processors

Around the beginning of the 2000s, the limitations of single core processors were very important. The frequency was already high and requested more power consumption causing more heat dissipation. The first solution to this problem was to provide multi-CPU devices, embedding several CPU on the same motherboard and allowing them to share memory. The evolution of the mono-core is the multi-core having several processing units on the same die allowed more optimization inside the die and combining all the advantages of single core processors. But by embedding each CPU, the function and units required consume n times more energy with cumulate heat effects. Thus, unable to answer the constant augmentation of computational power needed for research and HPC, IBM was the first company to create a multi-core CPU in 2001, the Power4.

Compared to the core inside multi-CPU, multi-core CPU shared one of the material (L3 caches, buses, etc.) and are implemented on the same die; this allows to reach the same CPU performances with less transistors and less power consumption, avoiding most of the heating issues.

This architecture is presented on figure 2.3. The main memory is now shared between the cores. The registers and L1/L2 cache are the same but a L3 layer is added to the cache, and consistency has to be maintained over all the cores. If a process modifies a data in the memory this information has to be spread over all the other users of this data, even in their local cache.

We note here that in current language the CPU, as describe in the Von Neumann model, is also the name of the die containing several cores. This is the architecture of most of current processors and these multi-cores provide two to 32 cores in most cases. Thus, the multi-core CPU are called "Host" and the attached accelerators are called "Devices".

2.3 21th century architectures

After years of development and research on hardware for Computer Science and specifically HPC, we present here the latest and best technologies to produce efficient and general-purpose

The Tick-Tock model through the years

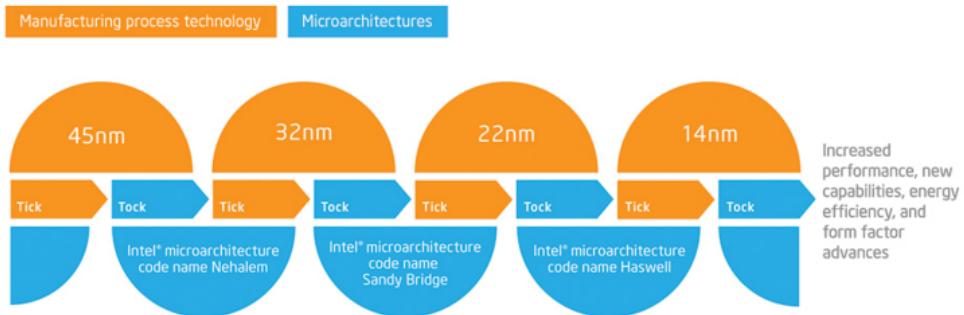


Figure 2.4: Intel Tick-Tock model

supercomputers.

We present the latest architectures with multi-core, many-core and specific processors, and the most famous manufacturers.

2.3.1 Multi-core implementations

The most world spread architecture in public and high performance computing is the multi-core processors. Most present-day accelerators require a classical processor to offload tasks and data on it.

We start this presentation from the most popular processors in HPC world from the Intel company ones. We also present ARM which is a different multi-core architecture based on RISC instructions set.

Intel

Intel was created in 1968 by a chemist and a physicist, Gordon E. Moore and Robert Noyce, in Mountain View, California. Processors today are typically from Intel, the world leader which equips around 90% of the supercomputers (November 2017 TOP500 list).

In 2007, Intel adopted a production model called the "Tick-Tock", presented on figure 2.4. Since the creation of the Tick-Tock model, it always followed the same fashion: a new manufacturing technology, such as shrinking the chip with better engraving, on a "Tick" followed by a "Tock" which delivers a new micro-architecture. The Intel processors for HPC are called Xeon and feature ECC memory, higher number of cores, large RAM support, large cache-memory, Hyper-threading, etc. Compared to desktop processors, their performances are of a different magnitude. Intel has given every new processor a code name. The last generations are chronologically called Westemere (2011), Sandy Bridge (2012), Ivy Bridge(2013), Haswell (2014), Broadwell (2015), Skylake (2015) and Kaby lake (2016).

Kaby Lake, the last architecture provided, does not exactly fit the typical "Tick-Tock" process because it is just based on optimizations of the Skylake architecture. The Kaby Lake is produced like Skylake with an engraving of 14 nm. The Tick-Tock model appears to be hard to maintain due to the difficulties to engrave in less than 10 nm with quantum tunneling. This leads to using larger many-cores architecture and the bases of the next supercomputer evolutions, the road-map to hybrid models.

Hyper-threading Another specificity of Intel Xeon processors is Hyper-threading (HT). This technology makes a single physical processing unit (core) appearing as two logical ones for the user's level. In fact, a processor embedding 8 cores appears as a 16 cores for user. Adding more computation per node can technically allow the cores to switch context when data are fetched from the memory using the processor 100% during all the computation. Multiple studies have been published on HT from Intel itself [Mar02] to independent researchers [BBDD06, LAH⁺02]. This optimization does not fit to all the cases of applications and can be disabled for normal use of the processors in the context of general purpose HPC architectures.

ARM

Back in the 1980s, ARM stood for Acorn RISC Machine in reference to the first company to implement this kind of architecture, Acorn Computers. This company later changed the name to Advanced RISC Machine (ARM). ARM is a specific kind of processors based on RISC architecture as its ISA, despite usual processors using CISC. The downside of CISC machines are they are difficult to create and they require way more transistor and thus more energy to work. The ISA from the RISC is simpler and requires multiple many transistors to operate and thus a smaller silicon area on the die. Therefore, the energy required and the heat dissipated is less important. It becomes easier to create massively parallel processors based on ARM. On the other hand, simple ISA imposes more work on the source code compilation to fit the simple architecture. This makes the instructions sources longer, and therefore, more single instructions to execute.

The ARM company provides several versions of ARM processors named Cortex-A7X (2015), Cortex-A5X (2014) and Cortex-A3X (2015) featured for highest-performances, for balancing performances and efficiency or for less power consumption, respectively.

The new ARMv8 architecture starts to provide the tools to target HPC context [RJAJVH17]. The European approach towards energy efficient HPC, Mont-Blanc project¹, already constructs ARM based supercomputers. The exascale project in Horizon 2020 this project focuses on using ARM-based systems for HPC with many famous contributors, such as Atos/Bull as a project coordinator, ARM, French Alternative Energies and Atomic Energy Commission (CEA), Barcelona Supercomputing Center (BSC), etc. The project is separated into several steps to finally reach Exascale near 2020. The last step, Mont-Blanc 3, is about to work on a pre-Exascale prototype powered by Cavium's ThunderX2 ARM chip based on 64-bits ARMv8.

2.3.2 Intel Xeon Phi

Another specific HPC product from Intel is the Xeon Phi. This device can be considered as a Host or Device/Accelerator machine. Intel describes it as "a bootable host processor that delivers massive parallelism and vectorization". This architecture embed multiple multi-cores processors interconnected and is called Intel's Many Integrated Core (MIC). We placed this architecture here because it provides hundreds of conventional computation core but the program counter is not shared between them. It does not fit in the many-core architecture but is a step in the multi-core one. This is the technology on which Intel bases its Exascale machines.

The architectures names are Knights Ferry, Knights Corner and Knight Landing [SGC⁺16]. The last architecture, Knight Hill, was recently canceled by Intel due to low performances and to focus the Xeon Phi for Exascale. The main advantage of this architecture compared to GPGPUs is the x86 compatibility of the embedded cores and the fact this device can boot and use to drive other accelerators. They also feature more complex operations and handle double precision natively.

¹<http://montblanc-project.eu/>

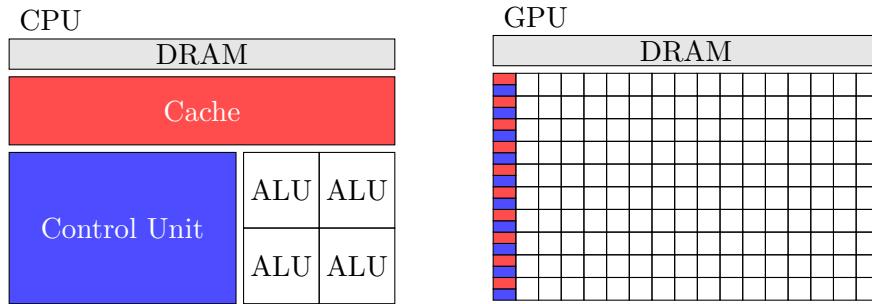


Figure 2.5: Multi-core versus Many-core architecture, case of GPUs

2.3.3 Many-core architecture, SIMT execution model

Several architectures can be defined as many-cores and follow the SIMD model from Flynn taxonomy. These devices integrate thousands of cores that are usually controlled by fewer control units. We can consider these cores as "simpler" since they have to work synchronously and under the coordination of a control unit. Some devices are specific like the Xeon Phi of Intel, integrating a hundred of regular processor cores which can work independently.

GPU

A CPU can usually have two to 32 computation cores that can operate on different instruction streams, but the SIMT architecture of the GPU is slightly different. The cores are grouped and must share the same instruction at the same clock time, but different groups can have their own instructions.

Figure 2.5 present the vision between CPU and GPU processors. We note in this figure that the usual topology with the ALU lined up in front of their control unit and shared cache memory. Every ALU has its own memory and registers to operate local computations.

These devices are called General Purpose Graphics Processing Units (GPGPUs). They are derivative from classical GPUs used for graphical purpose. Pioneers show that GPGPUs can be used efficiently for classical scientific computations. The vendor provides then specific GPU for general purpose computing. We present here the two main companies providing GPGPUs for HPC world: NVIDIA and AMD.

NVIDIA GPU architecture The NVIDIA company was founded in April 1993 in Santa Clara, California by three persons, one being the current CEO, Jensen Huang. The company name originated from *invidia* the Latin word for Envy and vision for graphical rendering.

NVIDIA is known as the pioneer in graphics, cryptocurrency, portable devices, and now Artificial Intelligence (IA) and appears to be even the creator of the name "GPU". NVIDIA's GPUs, inspired from visualization and gaming at a first glance, are available as a dedicated device for HPC purpose since the company released the brand named *Tesla*. The public GPUs can also be used for dedicated computation, but does not feature ECC memory, double precision or special functions/FFT cores. The different versions of the architecture are named following famous physicists, chronologically: Tesla, Fermi, Kepler, Maxwell, Pascal and Volta.

We describe here the Kepler brand GPU and more specifically the K20Xm GPU on which we based our study. This NVIDIA Tesla Kepler GPU is based on the GK110 graphics processor described in the white-paper[Nvi12] on 28nm process. The figure 2.6 is a representation of the physical elements of this graphics processor. The K20X comes in active and passive cooling mode with K20Xc and K20Xm, respectively. This GPU embeds 2688 CUDA cores distributed in 14 SMX (we note that GK110 normally provides 15 SMX but only 14 are present on the K20X). In this model each SMX contains 192 single precision cores, 64 double precision cores, 32 special function units and 32 load/store units. In a SMX the memory provides 65536 32-bits



Figure 2.6: NVIDIA Tesla Kepler architecture. Single-precision in green and double-precision in yellow

registers, 64 KB of shared memory L1 cache, 48 KB of read-only cache. The L2 cache is 1546 KB shared by the SMX for a total of 6 GB of memory adding the DRAM. The whole memory is protected using Single-Error Correct Double-Error Detect (SECDED) ECC code. The power consumption is estimated to 225 W. This GPGPU is expected to produce 1.31 TFLOPS for double-precision and 3.95 TFLOPS of single-precision.

AMD Another company is providing GPUs for HPC, Advanced Micro Devices (AMD). In front of the huge success of NVIDIA GPU that leads from far the HPC market, it is hard for AMD to find a place for its GPGPUs, the FirePro, in HPC. The FirePro is targeted using a language near CUDA, not held by a single company by NVIDIA like CUDA, called OpenCL. An interesting creation of AMD is the Accelerated Processing Units (APUs) which embedded the processor and the GPU on the same die since 2011. This solution allows them to target the same memory.

In the race to market and performances, AMD found an accord with Intel to provide dies featuring Intel processor, AMD GPU and common HBM memory. The project is call Kaby Lake-G and announced it would be available in the first semester of 2018 for public, not HPC itself.

PEZY

Another many-core architecture only appeared in the last benchmarks. The PEZY Super Computer 2, PEZY-SC2, is the third many-core microprocessor developed by the company PEZY. The three first machines ranked in the GREEN500 list are accelerator using this many-core die. We also note that in the November 2017 list, the fourth supercomputer, Gyokou, is also powered by PEZY-SC2 cards.

2.3.4 Other architectures

Numerous architectures have not been presented here because they are out of scope of this study. We present here two technologies we have encountered in our researches and that may be tomorrow solution for Exascale in HPC.

FPGA

Field Programmable Gates Array (FPGA) are devices that can be reprogram to fit the needs of the user after their construction. The leader were historically Altera with the Stratix, Arria and Cyclone FPGAs, which is now part of Intel. With the FPGAs, the users have access to the hardware and can design their own circuits. Currently, FPGA can be targeted with OpenCL programming language. The arrival of Intel in this market assures the best hopes for HPC version of FPGAs. The main gap for users is the circuit building that can be designed for specific needs but may be hard to setup.

ASIC

Application Specified Integrated Circuits are dedicated device construct for on purpose. An example of ASIC is the Gravity Pipe (GRAPE) which is dedicated to compute gravitation given mass and positions. Google leads the way for ASIC and recently created its dedicated devices to boost AI bots. ASIC may be found in some optimized communication devices, such as fast interconnection network in HPC.

2.4 Distributed architectures

The technologies presented in previous part is the milestone of supercomputers. They are used together in a whole system to create machine delivering incredible computational power.

2.4.1 Architecture of a supercomputer

From the hardware described before, we can create the architecture of a cluster from the smallest unit, cores, nodes, to the whole system.

Core: A core is the smallest unit in our devices. It refers to the Von Neumann model in case of core with ALU and CU. We can separate cores from CPU to GPU, the first one able to be independent whereas the second ones working together and share the same program counter.

Socket/Host: A socket is mistakenly called a CPU in current language. It is, for multi-cores sockets, composed of several cores. The name Host comes from the Host-Device architecture using accelerators.

Accelerators/Devices: Accelerators are devices that, when attached to the Host, provide additional computational power. We can identify them as GPUs, FPGAs, ASICs, etc. A socket can have access to one or more accelerators and can also share the accelerator usage.

Computation node: The next layer of our HPC system is the computation node, which is a group of several sockets and accelerators sharing memory;

Rack: A rack is a set of computation nodes, generally in vertical stack. It may also include specific nodes dedicated to the network or the Input/Output.

Interconnection: The nodes are grouped together with hard wire connection following a specific interconnection topology with very high bandwidth.

System/Cluster/Supercomputer The cluster group several racks though an interconnection network.

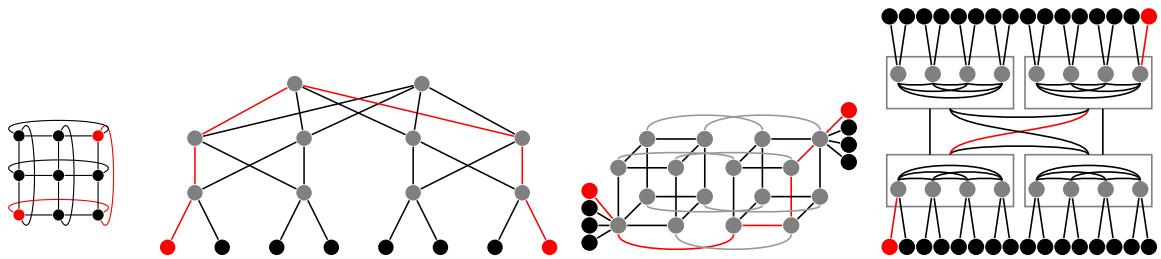


Figure 2.7: Torus, Fat-Tree, HyperX, DragonFly

Name	Gbs	Year	Name	Gbs	Year
Single DR	2.5	2003	Enhanced DR	25	2014
Double DR	5	2005	Highg DR	50	2017
Quad DR	10	2007	Next DR	100	2020
Fourth DR	14	2011			

Table 2.1: InfiniBand technologies name, year and bandwidth

An interconnect technology is required in order to connect nodes together and allow distributed programming. Interconnection networks are the way the nodes of a cluster are connected together.

2.4.2 Interconnection topologies

Several topologies exist from point to point to multi-dimensional torus. The figure 2.7 is a representation of famous topologies. Each interconnect technology has its own specificity. These networks take in account the number of nodes to interconnect and the targeted bandwidth/budget. Several declination of each network are not detailed here. The Mesh and the Torus are used as a basis in lower layers of others more complex interconnection networks. A perfect example is the supercomputer called K-Computer describe in the next section. The Fat Tree presented here is a k-ary Fat Tree, the higher the position in the tree, the more connections are found and with a bandwidth being important. The nodes are available as the leaves, on the middle level we find the switches and on top the routers. This is the topology of the ROMEO supercomputer we used for our tests. Another topology, HyperX[ABD⁺09], is based on Hyper-Cube. The DragonFly[KDSA08] interconnect is recent, 2008, and is used in modern day supercomputers.

InfiniBand (IB) is the most widespread technology used for interconnection with different kind of bandwidth presented in figure 2.1. It provides high bandwidth and small latency and companies such as Intel, Mellanox, etc. provide directly adapters and switches specifically for IB.

Unfortunately, this augmentation of clock rate is not sustainable due to the energy required and the heat generated by the running component. Another idea originated in the 19th century with the first multi-core processors.

2.4.3 Remarkable supercomputers

The TOP500² is the reference benchmarks for the world rank supercomputers. This benchmark is based on the LINPACK and aim to solve a dense system of linear equations. Most of the TOP10 machines have specific architectures and, of course, the most efficient ones. In this

²<https://www.top500.org>

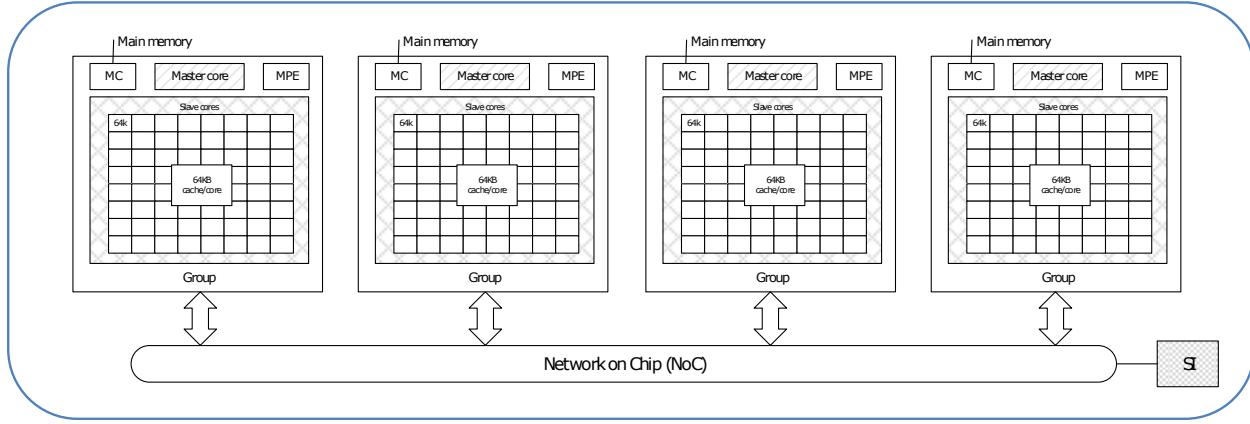


Figure 2.8: Sunway Taihulight node architecture from *Report on the Sunway TaihuLight System*, Jack Dongarra, June 24, 2016.

section, we describe several supercomputers about their interconnect, processors and specific accelerators.

Sunway Taihulight

Sunway Taihulight is the third Chinese supercomputer to be ranked in the first position of the TOP500 list, in November 2017. A recent report from Jack J. Dongarra, a figure in HPC, decrypted the architecture of this supercomputer[Don16]. The most interesting point is the conception of this machine, completely done in China. The Sunway CPUs were designed and built in China by the Shanghai High Performance IC Design Center.

The SW26010, a many core architecture processor, features 260 cores based on RISC architecture and a specific conception, depicted on figure 2.8. The processor is composed of the master core, a Memory Controller (MC) and a Management Processing Element (MPE) that manages the Computing Processing Elements (CPE), which are the slaves' cores.

The interconnect network is called Sunway Network and is connected using Mellanox Host Channel Adapter (HCA) and switches. This is a five-level interconnect going through computing nodes, computing board, super-nodes and cabinets to the complete system. For the latest TOP500 list, from November 2017, the total memory is 1.31 PB and the number of cores available is 10,649,600. The peak performance is 125.4 PFLOPS but the Linpack is only 93 PFLOPS which is 74.16% of theoretic efficiency.

Piz Daint

The supercomputer of the CSCS, Swiss National Supercomputing Center, is currently ranked second on the November 2017 TOP500 list. This GPUs accelerated supercomputer is a most powerful representative of GPU hybrid acceleration and is the most powerful European supercomputer. This supercomputer is composed of 4761 hybrids and 1210 multi-core nodes. There are hybrids nodes embedding an Intel Xeon E5-2690v3 and an NVIDIA Tesla Pascal P100 GPGPU. The interconnect is based on a Dragonfly network topology and Cray Aries routing and communications ASICs. The peak performance is 25.326 TFLOPS using only the hybrid nodes with Linpack generating 19.590 TFLOPS. The low power consumption ranks Piz Daint as tenth in the November 2017 GREEN500.

K-Computer

The K-Computer was the top 1 supercomputer of the 2011 TOP500. The TOFU interconnect network makes the K-Computer unique [ASS09] and stands for TOrus FUision. This interconnect presented in figure 2.9 mixes a 6D Mesh/Torus interconnect. The basic units are based on

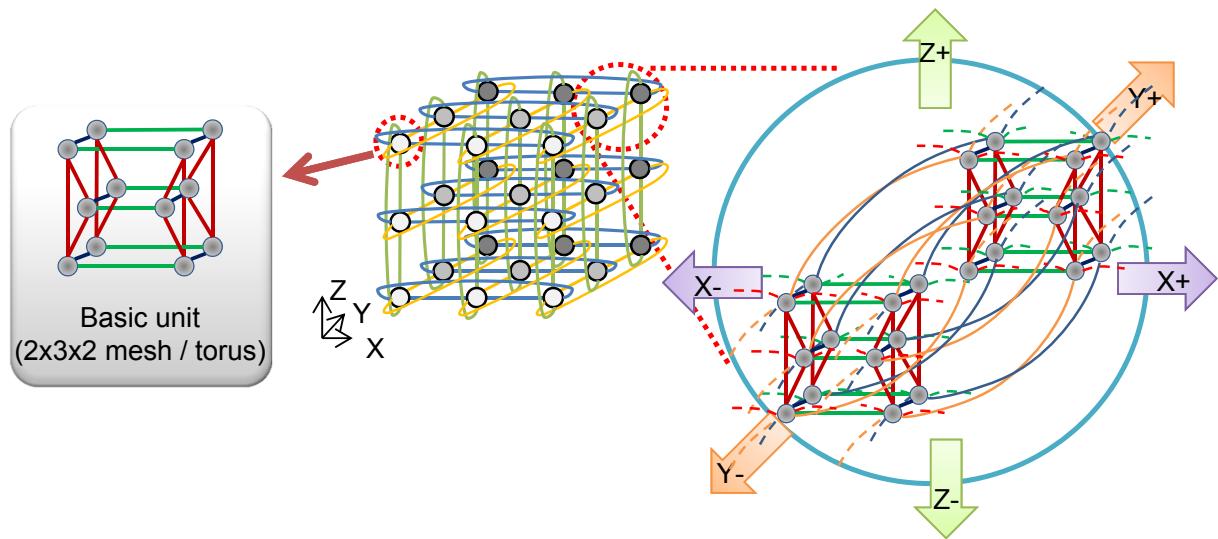


Figure 2.9: TOFU Interconnect schematic from *The K-Computer: System Overview*, Atsuya Uno, SC11

a mesh and are interconnected together in a three-dimensional torus. In this configuration, each node can access to its 12 neighbors directly. It also provide a fault tolerant network with many routes to reach distant node.

Sequoia/Mira

The Sequoia supercomputer was ranked first on the 2012 TOP500 list. It is based on BlueGene from IBM. The BlueGene project made up to three main architectures with BlueGene/L, BlueGene/P and BlueGene/Q. It is very interesting to note the BlueGene architecture because 15 machine utilizing this architecture were in the top 200 in the last GRAPH500 list in November 2017. The algorithm used on these supercomputers will be our basis in the Part II regarding our implementation of the GRAPH500 benchmark.

2.5 ROMEO Supercomputer

The ROMEO supercomputer center is the computation center of the Champagne-Ardenne region in France. Hosted since 2002 by the University of Reims Champagne-Ardenne, this so called meso-center (Medium size HPC center) is used for HPC in theoretic research and domain science like applied mathematics, physics, biophysics and chemistry.

This project is supported by Europe, National Fundings, Grand-Est region and Reims Metropole. It aims to host research and production codes of the region for industrial, research and academics purposes.

We are currently working on the fourth version of ROMEO, last updated in 2013. As many of our tests in this study have been done on this machine, we will carefully describe its architecture.

This supercomputer was ranked 151st in the TOP500 and fifth in the GREEN500 list. It was ranked with a RPeak of 384.1 TFlops and a RMax of 254.9 TFlops.

2.5.1 ROMEO hardware architecture

ROMEO is a Bull/Atos supercomputer composed of 130 BullX R421 computing nodes.

Each node is composed of two processors Intel Ivy Bridge 8 cores @ 2,6 GHz. Each processor has access to 16 GB of memory for a total of 32 GB per node, the total memory of 4.160 TB. Each processor is linked, using PCIe-v3, to an NVIDIA Tesla K20Xm GPGPU. This cluster

provides then 260 processors for a total of 2080 CPU cores and 260 GPGPU providing 698880 GPU cores. The computation nodes are interconnected with an Infiniband QDR non-blocking network structured as a FatTree. The Infiniband is a QDR providing 10 GB/s.

The storage for users is 57 TB and the cluster also provide 195 GB of Lustre and 88TB of parallel scratch file-system.

In addition to the 130 computations nodes, the cluster provides a visualization node NVIDIA GRID with two K2 cards and 250GB of DDR3 RAM. The old machine, renamed Clovis, is also available but does not features GPUs.

The supercomputer supports MPI with GPU Aware and GPUDirect.

ROMEO is based on the Slurm³ workload manager for node distribution among the users. This manager allows different usage of the cluster with classical reservation-submission or more asynchronous computation with best-effort. We developed advantages of both submissions systems in Part II.

2.5.2 New ROMEO supercomputer, June 2018

In June 2018 a new version of the supercomputer ROMEO will be installed at the University of Reims Champagne Ardenne. This project intents to feature a supercomputer ranked around 250th in TOP500. It is a renewed partnership between ATOS/BULL and NVIDIA.

The new ROMEO will feature 115 computation nodes with a total of 3220 CPU cores. The technology selected is the BULL *Sequana* with its high energy saving, BXI network technology, NVLink support for GPUs and the density of the cluster. Each node will provide a Skylake 6132 CPU with 14 cores with a maximum frequency of 2.6GHz.

Two different types of node are present:

- 70 of the with 4 GPUs and 96GB of RAM featuring a total of 280 Pascal P100 SMX2 GPUs.
- 45 last generation Intel CPUs with 192GB of memory per CPU.

The machine will feature up to 15.3TB of global memory.

The aim is to provide a performance of 964.6 TFLOPS in LINPACK and to be present in several TOP500 lists with a starting position around 232th or 297th.

2.6 Conclusion

In this chapter, we reviewed the most important modern day hardware architectures and technologies. In order to use the driver or API in the most efficient way, we need to keep in mind the way the data and instructions are proceed by the machine.

Efficiency is based on computation power, but also communications, we showed different interconnection topologies and their specificities. We present perfect use cases of the technologies in the current top ranked systems. We show that every architecture is unique in its construction and justify the optimization work dedicated to reach performance.

We determine from the new technologies presented here that supercomputers are moving toward hybrids architectures featuring multi-core processors accelerated by one or more devices such as many-core architectures. The Exascale supercomputer of 2020 will be shaped using hybrid architectures and they represent the best of nowadays technology for purpose of HPC this day and age. Combining CPU and GPUs or FPGA on the same die and sharing the same memory space may also be another solution.

³<https://slurm.schedmd.com/>

Chapter 3

Software in HPC

3.1 Introduction

After presenting the rules of HPC and the hardware that compose the cluster, we introduce the most famous ways to target those architectures and supercomputers with programming models. Then, fitting those models, we present the possible options in the language, the API, the distribution and the accelerators code.

This chapter details the most important programming models and the software options for HPC programming and include the choices we made for our applications. Then it presents the software used to benchmark the supercomputers. We present here the most famous, the TOP500, GRAPH500, HPGC and GREEN500 to give their advantages and weaknesses.

3.2 Parallel and distributed programming Models

The Flynn taxonomy developed in chapter 1 was a characterization of the executions models. This model can be extended to programming models which are an extension of MIMD. We consider here a *Random Access Machine* (RAM). The memory of this machine consists of an unbounded sequence of registers each of which may hold an integer value. In this model the applications can access to every memory words directly in write or read manner. There are three main operations: load from memory to register; compute operation between data; store from register to memory. This model is used to estimate the complexity of sequential algorithms. If we consider the unit of time of each operation (like in cycle) we can have an idea of the overall time of the application. We identify two types of RAM, the Parallel-RAM using shared memory and the Distributed-RAM using distributed memory.

3.2.1 Parallel Random Access Machine

The Parallel Random Access Machine [FW78], PRAM, is a model in which the global memory is shared between the processes and each process has its own local memory/registers. The execution is synchronous, processes execute the same instructions at the same time. In this model each process is identified with its own index enabling to target different data. The problem in this model will be the concurrency in reading (R) and writing (W) data as the memory is shared between the processes. Indeed, mutual exclusion have to be set with exclusive (E) or concurrent (C) behaviors and we find 4 combinations: EREW, ERCW, CREW and CRCW. As the reading is not critical for data concurrency the standard model will be Concurrent Reading and Exclusive Writing: CREW.

An example of PRAM model applied on a reduction is given on figure 3.1. In this example the computation of minimum, maximum or a reduction can be performed on an array of n values in $\log(n)$ steps and $n - 1$ operations. This kind of reduction or scan are used to reach performances

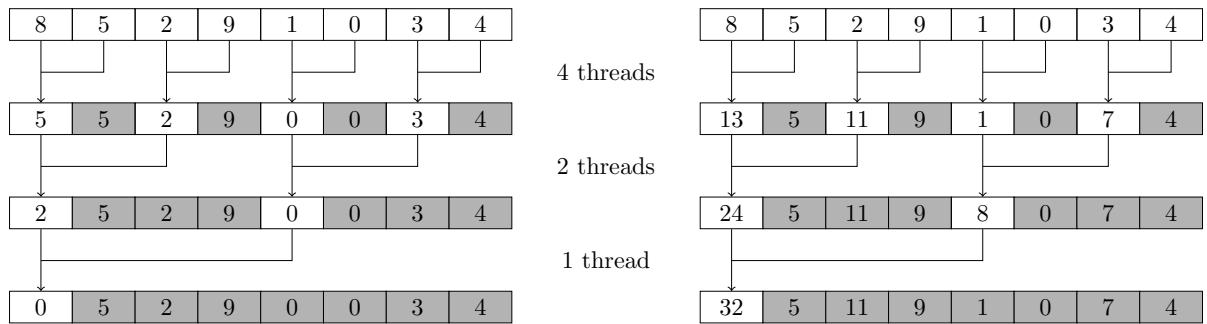


Figure 3.1: PRAM model example on minimum and reduction computation

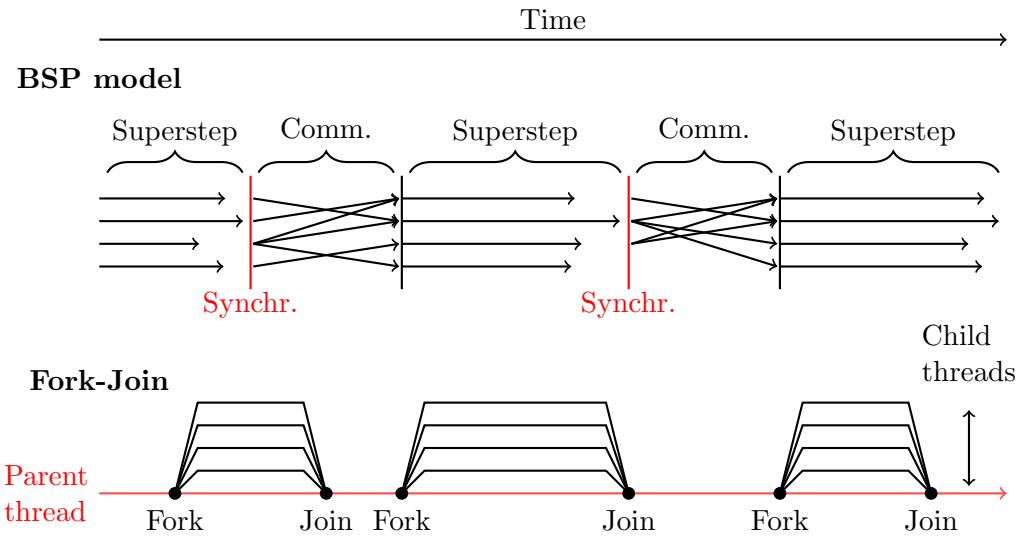


Figure 3.2: Bulk Synchronous Parallel model and Fork-Join model

on multi-core and many-core code in this study. We will give example of those reductions in different languages and API.

3.2.2 Distributed Random Access Machine

For machine that base their memory model on NoRMA the execution model can be qualify of Distributed Random Access Machine, DRAM. It is based on NoRMA memories detailed in part 1.4. This model is in opposition to PRAM because the synchronization between processes is made by communications and messages. Those communications can be of several kind and depend of physical architecture, interconnection network and software used.

3.2.3 H-PRAM

A DRAM can be composed of an ensemble of PRAM system interconnected. Each of them working on their own data and instructions. This is an intermediate model between PRAM and DRAM having a set of shared memory and synchronous execution, the overall execution being asynchronous and having distributed memory.

3.2.4 Bulk Synchronous Parallelism

This model was presented in 1990 in [Val90]. Being the link of HRAM and PRAM, the Bulk Synchronous Parallelism model is based on three elements:

- a set of processor and their local memory;

- a network for point-to-point communications between processors;
- a unit allowing global synchronization and barriers.

This model is the most common on HPC clusters. It can be present even on node themselves: a process can be assigned on a core or set of cores and the shared memory is separated between the processes. The synchronization can be hardware but in most cases it is handled by the runtime used. A perfect example of runtime, presented later, is MPI.

In this model the applications apply a succession of *supersteps* separated by *synchronizations* steps and data exchanges.

At opposite to H-PRAM which represent the execution as a succession of independent blocks working synchronously, BSP propose independent blocks of asynchronous applications synchronized by synchronization steps.

In a communication/synchronization step we can consider the number of received messages h_r and the number of send ones h_s .

The time lost in communication in one synchronization step is:

$$T_{comm} = hg + I \quad (3.1)$$

With $h = \max(h_s, h_r)$, g the time to transfer data and I the start-up latency of the algorithm. Indeed, the entry points and exit points of communications super-step can be a bottleneck considered in I .

The time for computing a super-step is:

$$T_{comp} = \frac{w}{r} + I \quad (3.2)$$

With w the maximum number of flops in the computation of this super-step, r the speed of the CPU expressed in FLOPS and I the start-up latency of the algorithm. Indeed, the entry points and exit points of communications super-step can be a bottleneck considered in I .

The BSP model estimates the cost of one super-step with:

$$T_{comm} + T_{comp} = w + gh + 2l \quad (3.3)$$

With T a measure of time, a wall clock that measures elapsed time. We also note that usually g and I are function of the number of processes involved.

It can then be used to compute the overall cost in BSP model summing all super-steps s :

$$T = \sum_s \frac{\max(w_s)}{r} + h_s g + I \quad (3.4)$$

The problem of performances in this model can come from unequal repartitions of work, the load balancing. The processes with less than w of work will be idle.

3.2.5 Fork-Join model

The Fork-Join model or pattern is presented in figure 3.2. A main thread pilot the overall execution. When requested by the application, typically following the idea of *divide-and-conquer* approach, the main thread will fork and then join other threads. The *Fork* operation, called by a logical thread parent, creates new logical threads children working in concurrency. There is no limitations in the model and we find nested fork-join where a child can also call fork to generate sub-child and so on. The *Join* can be called by both parents and child. Children call join when done and the parent join by wait until children completion. The Fork operation increase concurrency and join decrease concurrency.

3.3 Software/API

In this section we present the main runtime, API and frameworks used in HPC and in this study in particular. The considered language will be C/C++, the most present in HPC world along with Fortran.

```

...
int min_val = MAX;
#pragma omp parallel for reduction(min:min_val)
for(int i = 0 ; i < X ; ++i){
    min_val = arr[i] < min_val ? arr[i] : min_val;
}
...

```

Figure 3.3: OpenMP reduction code for minimum

3.3.1 Shared memory programming

On the supercomputers nodes we find one or several processors that access to UMA or NUMA memory. Several API and language provide tools to target and handle concurrency and data sharing in this context. The two main ones are PThreads and OpenMP for multi-core processors. We can also cite Cilk++ or TBB from Intel.

PThreads

The Portable Operating System Interface (POSIX) threads API is an execution model based on threading interfaces. It is developed by the IEEE Computer Society. It allows the user to define threads that will execute concurrently on the processor resources using shared/private memory. PThreads is the low level handling of threads and the user need to handle concurrency with semaphores, conditions variables and synchronization "by hand". This makes the PThreads hard to use in complex applications and used only for very fine-grained control over the threads management.

OpenMP

Open Multi-Processing, OpenMP¹ [Cha08, Sup17, CDK⁺⁰⁰], is an API for multi-processing shared memory like UMA and CC-NUMA. It is available in C/C++ and Fortran. The user is provided with pragmas and functions to declare parallel loop and regions in the code. In this model the main thread, the first one before forks, command the fork-join operations.

The last versions of OpenMP 4.0 also allow the user to target accelerators. During compilation the user specify on which processor or accelerator the code will be executed in parallel.

We use OpenMP as a basis for the implementation of our CPU algorithms. Perfect for loop parallelization and parallel sections, we show that we can have the best results for CPU algorithms in most of the case. In our case, OpenMP is always use on the node to target all the processors cores in the shared memory.

We note that the new versions of OpenMP also allows to target directly accelerators like NVIDIA ones.

The code corresponding to a reduction using OpenMP API is presented on figure 3.3. This is linked with the PRAM model reduction presented at the beginning of this part.

3.3.2 Distributed programming

In the cluster once the code have been developed locally and using the multiple cores available, the new step is to distribute it all over the nodes of the cluster. This step requires the processes to access NoRMA memory from a node to another. Several runtime are possible for this purpose and concerning our study. We should also cite HPX, the C++ standard distribution library, or AMPI for Adaptive MPI, Multi-Processor Computing (MPC) from CEA, etc.

¹<http://www.openmp.org>

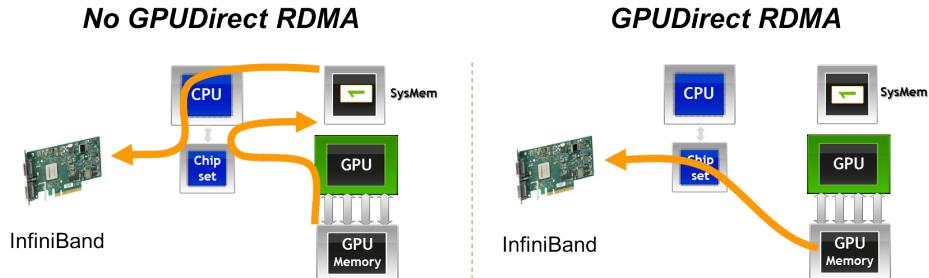


Figure 3.4: GPUDirect RDMA from NVIDIA Developer Blog, *An Introduction to CUDA-Aware MPI*

MPI

The Message Passing Interface, MPI, is the most famous runtime for distributed computing [Gro14, Gro15]. Several implementations exists from Intel MPI² (IMPI), MVAPICH³ by the Ohio State University and OpenMPI⁴ combining several MPI work like Los Alamos MPI (LA-MPI). Those implementation follow the MPI standards 1.0, 2.0 or the latest, 3.0.

This runtime provides directs, collectives and asynchronous functions for process(es) to process(es) communication. A process can be a whole node or one or several cores on a processor.

Some MPI implementations offer a support for accelerators targeting directly their memory through the network without multiple copies on host memory. The data go through one GPU to the other through network and PCIe. This feature is used in our code in part 2 and 3.

Most of our code presented here are based on MPI for the distribution on the cluster. The advantage is its presence on all the cluster and the control over the data transfers.

For NVIDIA this technology is called GPUDirect RDMA and presented on figure 3.4.

In term of development MPI can be very efficient if use carefully. Indeed, the collectives communications such as *MPI_Alltoall*, *MPI_Allgather*, etc. can be a bottleneck when scaling up to thousands of processes. A specific care have to be taken in those implementation with privilege to asynchronous communications to hide computation than synchronous idle CPU time.

Charm++

Charm++⁵ is an API for distributed programming developed by the University of Illinois Urbana-Champaign. It is asynchronous messages paradigm driven. In contrary of runtime like MPI that are synchronous but can handle asynchronous, Charm++ is natively asynchronous. It is based on *chare object* that can be activated in response to messages from other *chare objects* with triggered actions and callbacks. The repartition of data to processors is completely done by the API, the user just have to define correctly the partition and functions of the program. Charm++ also provides a GPU manager implementing data movement, asynchronous kernel launch, callbacks, etc.

A perfect example can be the hydrodynamics N-body simulation code Charm++ N-body Gravity Solver, ChaNGa [JWG⁺10], implemented with Charm++ and GPU support.

Legion

Legion⁶ is a distributed runtime support by Stanford University, Los Alamos National Laboratory (LANL) and NVIDIA. This runtime is data-centered targeting distributed heterogeneous

²<https://software.intel.com/en-us/intel-mpi-library>

³<http://mvapich.cse.ohio-state.edu/>

⁴<http://www.open-mpi.org>

⁵<http://charmplusplus.org/>

⁶<http://legion.stanford.edu/>

```
--inline__ __device__ void warpReduceMin(int& val, int& idx)
{
    for (int offset = warpSize / 2; offset > 0; offset /= 2) {
        int tmpVal = __shfl_down(val, offset);
        int tmpIdx = __shfl_down(idx, offset);
        if (tmpVal < val) {
            val = tmpVal;
            idx = tmpIdx;
        }
    }
}
```

Figure 3.5: CUDA kernel for reduction of minimum

architectures. Data-centered runtime focuses to keep the data dependency and locality moving the tasks to the data and moving data only if requested. In this runtime the user defines data organization, partitions, privileges and coherency. Many aspect of the distribution and parallelization are then handle by the runtime itself.

The FleCSI runtime develops at LANL provide a template framework for multi-physics applications and is built on top of Legion. We give more details on this project and Legion on part 3.

3.3.3 Accelerators

In order to target accelerators like GPU, several specific API have been developed. At first they were targeted for matrix computation with OpenGL or DirectX through specific devices languages to change the first purpose of the graphic pipeline. The GPGPUs arriving forced an evolution and new dedicated language to appear.

CUDA

The Compute Device Unified Architecture is the API develop in C/C++ Fortran by NVIDIA to target its GPGPUs. The API provide high and low level functions. The driver API allows a fine grain control over the executions.

The CUDA compiler is called NVidia C Compiler, NVCC. It converts the device code into Parallel Thread eXecution, PTX, and rely to the C++ host compiler for host code. PTX is a pseudo assembly language translated by the GPU in binary code that is then execute. As the ISA is simpler than CPU ones and able the user to work directly in assembly for very fine grain optimizations.

As presented in figure 3.6, NVIDIA GPUs include many *Streaming Multiprocessors* (SM), each of which is composed of many *Streaming Processors* (SP). In the Kepler architecture, the SM new generation is called SMX. Grouped into *blocks*, *threads* execute *kernels* functions synchronously. Threads within a block can cooperate by sharing data on an SMX and synchronizing their execution to coordinate memory accesses; inside a block, the scheduler organizes *warps* of 32 threads which execute the instructions simultaneously. The blocks are distributed over the GPU SMXs to be executed independently.

In order to use data in a device kernel, it has to be first created on the CPU, allocated on the GPU and then transferred from the CPU to the GPU; after the kernel execution, the results have to be transferred back from the GPU to the CPU. GPUs consist of several memory categories, organized hierarchically and differing by size, bandwidth and latency. On the one hand, the device's main memory is relatively large but has a slow access time due to a huge latency. On the other hand, each SMX has a small amount of shared memory and L1 cache, accessible by

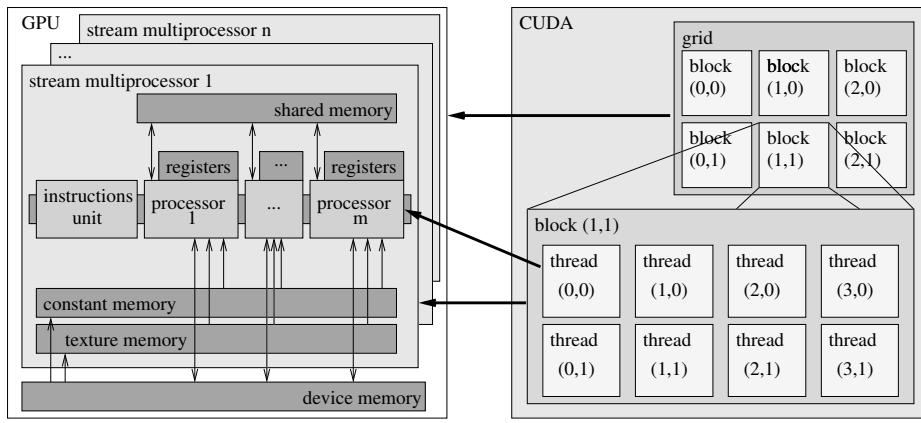


Figure 3.6: NVIDIA GPU and CUDA architecture overview

its SPs, with faster access, and registers organized as an SP-local memory. SMXs also have a constant memory cache and a texture memory cache. Reaching optimal computing efficiency requires considerable effort while programming. Most of the global memory latency can then be hidden by the threads scheduler if there is enough computational effort to be executed while waiting for the global memory access to complete. Another way to hide this latency is to use streams to overlap kernel computation and memory load.

It is also important to note that branching instructions may break the threads synchronous execution inside a warp and thus affect the program efficiency. This is the reason why test-based applications, like combinatorial problems that are inherently irregular, are considered as bad candidates for GPU implementation.

Specific tools have been made for HPC in the NVIDIA GPGPUs.

Dynamic Parallelism This feature allow the GPU kernels to run other kernels themselves.

When more sub-tasks have to be generated this can be done directly on the GPU using dynamic parallelism.

Hyper-Q This technology enable several CPU threads to execute kernels on the same GPU simultaneously. This can help to reduce the synchronization time and idle time of CPU cores for specific applications.

NVIDIA GPU-Direct GPUs' memory and CPU ones are different and the Host much push the data on GPU before allowing it to compute. GPU-Direct allows direct transfers from GPU devices through the network. Usually implemented using MPI.

Indeed, working with a very low level API like CUDA can lead to better performances. This can be very costly in development time. Regarding the time involved in coding compared to the performances gain, one may consider to use higher levels API like OpenACC.

The reduction using the CUDA API is presented on figure 3.5. It shows, compared to OpenMP, the complexity of CUDA code.

OpenCL

OpenCL is a multi-platform framework targeting a large part of nowadays architectures from processors to GPUs, FPGAs, etc. A large group of company already provided conform version of the OpenCL standard: IBM, Intel, NVIDIA, AMD, ARM, etc. This framework allows to produce a single code that can run in all the host or device architectures. It is quite similar to NVIDIA CUDA Driver API and based on kernels that are written and can be used in On-line/Off-line compilation meaning Just In Time (JIT) or not. The idea of OpenCL is great by rely on the vendors wrapper. Indeed, one may wonder, what is the level of work done by NVIDIA on its own CUDA framework compare to the one done to implement OpenCL standards? What is the advantage for NVIDIA GPU to be able to be replace by another component and compare

```

...
int min_val = MAX;
#pragma acc parallel loop copyin(arr[0:n]) reduction(min:min_val)
for (int i=0; i<n; i++) {
    min_val = arr[i]<min_val?arr[i]:min_val;
}
...

```

Figure 3.7: OpenACC code for reduction of minimum

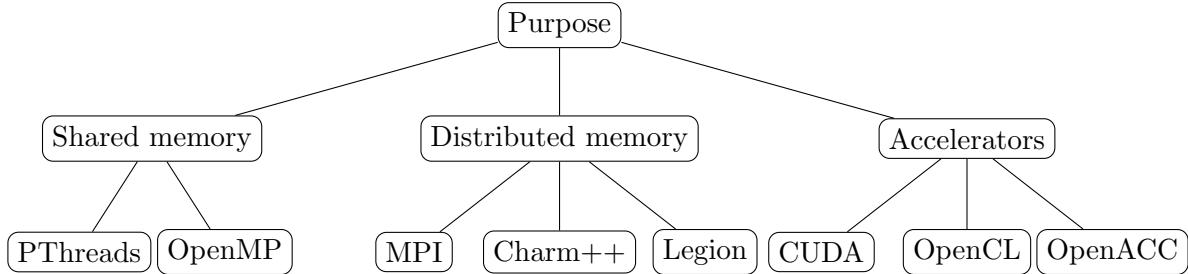


Figure 3.8: Runtimes, libraries, frameworks or APIs

on the same level? Those questions are still empty but many tests prove that OpenCL can be as comparable as CUDA but rarely better[KDH10, FVS11].

In this study most of the code had been developed using CUDA to have the best benefit of the NVIDIA GPUs present in the ROMEO Supercomputer. Also the long time partnership of the University of Reims Champagne-Ardenne and NVIDIA since 2003 allows us to exchange directly with the support and NVIDIA developers.

OpenACC

Open ACCelerators is a "user-driven directive-based performance-portable parallel programming model"⁷ developed with Cray, AMD, NVIDIA, etc. This programming model propose, in a similar way to OpenMP, pragmas to define the loop parallelism and the device behavior. As the device memory is separated specific pragmas are used to define the memory movements. Research works[WStAM12] tend to show that OpenACC performances are good regarding the time spent in the implementation itself compare to fine grain CUDA or OpenCL approaches. The little lack of performances can also be explained by the current contribution to companies in the wrapper for their architectures and devices.

The reduction example is given on figure 3.7. This shows the simplicity of writing accelerator code using high level API like OpenACC compared to the complex CUDA code. Indeed, this approach works in most of the case but for specific ones CUDA might outperform OpenACC.

The runtime, libraries, frameworks and APIs are summarized in figure 3.8. They are used in combination. The usual one is MPI for distribution, OpenMP and CUDA to target processors and GPUs.

3.4 Benchmarks

All those models, theory, hardware and software leads to better understanding and characterization of machines to produce better algorithm and solve bigger and harder problems. The question that arise is: how to know if a machine is better than another? We answer that ques-

⁷<https://www.openacc.org/>

tion with FLOPS, IPC, OPS or just the frequency of the machine. The models like BSP or law's like Amdahl and Gustafson ones propose to find the best/worst case during the execution.

In real application the only way to really know what will be the behavior of a supercomputer is to try, test real code on it. This is call benchmarking. Several kind of benchmarks exists and target a specific application of supercomputers. We present here the most famous benchmarks of HPC and their specificities.

3.4.1 TOP500

The most famous benchmark is certainly the TOP500⁸. It gives the ranking of the 500 most powerful, known, supercomputers of the world as its name indicates. Since 1993 the organization assembles and maintains this list updated twice a year in June and November.

This benchmark is based on the LINPACK[DMS⁺94] a benchmark introduced by Jack J. Dongarra. This benchmark rely on solving dense system of linear equations. As specified in this document this benchmark is just one of the tools to define the performance of a supercomputer. It reflects "the performance of a dedicated system for solving a dense system of linear equations". This kind of benchmark is very regular in computation giving high results for FLOPS.

In 1965 the Intel co-fonder Gordon Moore made an observation[Pre00] on the evolution of devices. He pointed the fact that the number of transistors in a dense integrated circuit doubles approximately every eighteen months. This is know as the Moore's law. Looking at the last TOP500 figure presented on figure 1, in the introduction of this document, we saw that nowadays machines does not fit in the law anymore. This is due to the size of transistor and the energy needed to reach more powerful machines. The Moore's law have been sustains by the arrival of many-cores architectures such as GPU or Xeon Phi. Tomorrow machines architectures will have to be based on hybrid with more paradigms and tools to take part of massive parallelism.

3.4.2 Green500

In conjunction of the TOP500, the Green500⁹ focus on the energy consumption of supercomputers. The scale is based on FLOPS per watts [FC07]. Indeed the energy wall is the main limitation for next generation and exascale supercomputers. In the last list, November 2017, the TOP3 machines are accelerated with PEZY-SC many-core devices. The TOP20 supercomputers are all equipped with many-cores architectures: 5 with PEZY-SC, 14 with NVIDIA P100 and 1 with the Sunway many-core devices. This show clearly that the nowadays energy efficient solutions resides in many-core architecture and more than that, hybrid supercomputers.

3.4.3 GRAPH500

The GRAPH500¹⁰ benchmark[MWBA10] focus on irregular memory accesses, and communications. The authors try to find ways to face the futures large-scale large-data problems and data-driven analysis. This can be see as a complement of the TOP500 for data intensive applications. The aim is to generate a huge graph to fill all the maximum memory on the machine and then operate either:

BFS: A Breadth-First Search which is an algorithm starting from a root and exploring recursively all the neighbors. This requires a lot of irregular communications and memory accesses.

SSSP: A Single Source Shortest Path which is an algorithm searching the shortest path from one node to the others. Like the BFS it has an irregular behavior but also requires to keep more data during the computation.

⁸<http://www.top500.org>

⁹<https://www.top500.org/green500/>

¹⁰<https://www.graph500.org/>

This benchmark will be detailed in Part II Chapter II in our benchmark suite.

3.4.4 HPCG

The High Performance Conjugate Gradient benchmark¹¹ is a new benchmark created in 2015 and presented for the first time at SuperComputing 2015. The last list, November 2017 contains 115 supercomputers ranked. The list also offer to compare the results of Linpack compared to Conjugate Gradient. This benchmark is a first implementation of having both computation and communications aspects of HPC in the same test.

This benchmark is presented and features:

- Sparse matrix-vector multiplication;
- Vector updates;
- Global dot products;
- Local symmetric Gauss-Seidel smoother;
- Sparse triangular solve (as part of the Gauss-Seidel smoother);
- Driven by multigrid preconditioned conjugate gradient algorithm that exercises the key kernels on a nested set of coarse grids;
- Reference implementation is written in C++ with MPI and OpenMP support.

The benchmarks presented in this section are the most famous of HPC world. Indeed, they are not the perfect representative of the nowadays application. The upcoming of big data and artificial intelligence in addition to classical "real life" applications impose HPC to evolute and find new ways to target new architectures. The TOP500 target the computational problem but does not handle a lot of irregularity. Indeed, solving dense linear equation is straight forward and also use the memory in a regular way. The Graph500 is very interesting to focus on communication and does handle irregular behavior for communications and memory. The Green500 does target energy wall but can also be applied to any benchmark. The most interesting one may be the HPCG benchmark. It does create irregularity during computation and communication along to memory traversal.

3.5 Conclusion

In this chapter we presented the most used software tools for HPC. From inside node with shared memory paradigms, accelerators and distributed memory using message passing runtime with asynchronous or synchronous behavior.

The tools to target accelerators architectures tend to be less architecture dependent with API like OpenMP, OpenCL or OpenACC targeting all the machines architectures. Unfortunately the vendor themselves have to be involve to provide the best wrapper for their architecture. In the mean time vendor dependent API like CUDA for NVIDIA seems to deliver the best performances.

We show through the different benchmark that hybrid architecture start to have their place even in computation heavy and communication heavy context. They are the opportunity to reach exascale supercomputers in horizon 2020.

The benchmarks we presented, the most famous ones, does not represent all the types of modern domain scientists problems. This study intents to provide a specific metrics representing computation and communication walls with highly irregular application. These tools will help us to show the real advantage of hybrid architectures over classical clusters.

¹¹<http://www.hpcg-benchmark.org/>

Conclusion

This part detailed the state of the art theory, hardware and software in High Performance Computing and the tools we need to detail our experiences.

In the first chapter we introduced the models for computation and memory. We also detailed the main laws of HPC.

The second chapter was an overview of hardware architectures in HPC. The one that seems to be the most promising regarding computational power and energy consumption seems to be hybrid architectures. Supercomputers equipped with classical processors accelerated by devices like GPGPUs, Xeon Phi or, for tomorrow supercomputers, FPGAs.

In the third section we showed that the tools to target such complex architecture are ready. They provide the developer a two or three layer development model with MPI for distribution over processes, OpenMP/PThreads for tasks between the processor's cores and CUDA/OpenCL/OpenMP/OpenACC to target the accelerator.

We also showed in the last part that the benchmarks proposed to rank those architectures are based on regular computation. They are node facing realistic domain scientists code behavior. The question that arise is: How the hybrid architecture will handle irregularity in term of computation and communication? This question will be developed in the next part through one example for irregular computation and another for irregular communication using accelerators.

Part II

Complex problems metric

Introduction

The tools described in the previous part for comprehension of High Performance Computing from theory, hardware and software give us the basis elements to go toward optimizations and benchmarking. We showed through examples that hybrid architectures seem to be the way to reach exascale in few years. In the same time many optimizations need to be done. On one hand, the exascale supercomputer will need to fit the energy envelope imposed, to be able to sustain the computational power and the price of the hardware itself for economical reasons. This is made by vendors and is a specific area of optimization. On the other hand, we focus on the performances we obtained using a specific architecture/accelerator to fit the targeted application with the best resources usage. The need of regular memory accesses, synchronization and the host-device memory separation put some constraint on their usage. As many-core architectures presented nowadays come with several downsides we need to confront them to classical processors on a specific set of problems, a metric, a dedicated benchmark suite.

In benchmarks like the TOP500 the target is to solve a problem with regular computation and communication behavior. We think that this behavior does not fit realistic and production applications. In many domains like meteorology, oceanography, astrophysics, big data, ... the underlying issue are the irregular input and behavior. The irregularity in an application can have several definitions. This is defined by [JTB] as a problem which: can not be characterize a priori, is input data dependent and evolves with the computation itself. In [SL06] the author specifies that the work involves subcomputations which cannot be determined before and implies work distribution during runtime. The irregularity can then spread on all the layers of the resolution: the communications, the computation and the memory searches.

In order to target more representative applications of nowadays realistic problems, we identify several bottlenecks and limitations in HPC. Those limitations are called *walls* against which nowadays architectures are confronted to reach exascale.

Memory Wall: This problem was targeted for the first time in [WM95]. The authors explain that:

We all know that the rate of improvement in microprocessor speed exceeds the rate of improvement in DRAM memory speed, each is improving exponentially, but the exponent for microprocessors is substantially larger than that for DRAMs.

In the case of accelerators another layer of memory is added. The memory of the host processors and device accelerators cannot be accessed directly and copies from one to the other are requested. The problems of coalescent accesses are also addressed in this study. Some companies try to find ways using shared memory between host and device but this technology is always under development and test for HPC purpose.

The two problems we propose for our metric implement heavy memory utilization. The first one dynamically uses the memory in an irregular way. The tree traversal of the first method generates temporary data and binary tests. The algebraic method uses a dedicated big integers library and carries propagation is applied just when necessary. In the second benchmark the memory is saturated and prepared at the startup. It is then accessed in an irregular way during all the computation.

Communication wall: We showed that the supercomputers' architecture is based on a set of racks, composed of nodes composed of computation units. The network topology can never be perfect for all the kinds of problems and even the fastest technologies are limited to the software handling. Limiting the big synchronization steps, like in the BSP model, allows the system to be asynchronous and hide computation by communications. Unfortunately this is not applicable to all the applications and a huge care have to be taken to approach perfect scaling.

We decided to target this problem in two main ways. In the first benchmark the model corresponds to FIIT: Finite number of Independent and Irregular Tasks, introduced in [FKF03]. The tasks can be solved independently and then merged at the end. We show that the accelerators can also take advantage of specific distribution methods like Best-Effort. In the second problem communications are central because the data are too big to be represented on a single machine and cannot be computed independently. The irregularity in communication is very high. In this benchmark the amount of data shared is never known before reaching the end of a superstep.

Power wall: The energy consumption of nowadays and future supercomputers is the main wall in HPC. Indeed, an exascale supercomputer could be built using several petascale supercomputers but, with todays architectures, will require a full nuclear plant to operate. In this objective low energy consumption and innovative architectures need to be found. The energy considered is required to power the machine itself but also handle the heat generated.

This wall is the underlying goal of this study. The hybrid architectures seem to deliver better performances for less watts. This thesis shows through different benchmarks what the real benefit of accelerators is on realistic problems and that the performances can be even better for less watts of power consumption.

Computational wall: The computational wall is a combination of the wall presented before. By increasing the memory wall, the energy consumption and the communications we can increase the overall computation power of the supercomputer. The limitation in computational power also comes from the fact that the Moore's law seems to be over. Vendors have more difficulties to shrink transistors due to physical side effects. The frequency itself seems to reach its highest values due to the energy required to operate, the heat dissipated and synchronization issues.

This is targeted in the first benchmark we propose. The algebraic method is heavy in computation with irregular memory accesses. The second one does focus on irregular communication and memory usage with test based operations.

This is the reason why we propose in this part a new metric for the main HPC walls to confront many-core architectures to multi-core architectures. The two applications we targeted cover all the walls we specify.

The first academic problem is a perfect candidate for our benchmark since it characterizes the behavior of accelerators and more specifically GPUs focusing on irregular computations and memory accesses. It is the problem of Langford and it shows how we can take advantage of accelerators for this kind of problem. Several paper were published on this problem [KLAJ16b, DJK⁺14, LJAK16, JDK⁺14]

The second problem focuses on irregular memory accesses and communications. It is based on a benchmark we presented in the previous part, the Graph500 benchmark. This problem was presented to the community with [KLAJ16a, LAJK15, LJAK15].

The combination of those two problems creates a metric covering all the walls and limitations we are facing in HPC. This allows us to emphasize on the behavior of hybrid architecture on several type of problems.

Chapter 4

Computational Wall: Langford Problem

4.1 Introduction

Our goal is to determine the behavior of accelerators compared to classical processor in case of heavy irregular-computationally problems. For this purpose we choose the Langford problem which is an academic problem of combinatorial counting.

We present the problem and expose the two possible methods to solve it:

- The tree traversal, called Miller's method, providing us benchmark targeting irregular memory and computation.
- The algebraic version, called Godfrey's method, showing the performances of many-core versus multi-core architectures in respect to computationally heavy and memory irregular behaviors.

We show the optimizations made to the regular processor algorithm to efficiently implement this application on GPU. We compare the two approaches for classical processor and GPU implementation. The results are then presented to show the acceleration using the whole ROMEO supercomputer.

4.1.1 The Langford problem

C. Dudley Langford gave his name to a classic permutation problem [Gar56, Sim83]. While observing his son manipulating blocks of different colors, he noticed that it was possible to arrange three pairs of different colored blocks (yellow, red and blue) in such a way that only one block separates the red pair - noted as pair 1 -, two blocks separate the blue pair - noted as pair 2 - and finally three blocks separate the yellow one - noted as pair 3 -, see figure 4.1.

This problem has been generalized to any number n of colors and any number s of blocks having the same color. $L(s, n)$ consists in searching for the number of solutions to the Langford problem, up to a symmetry. In November 1967, Martin Gardner presented $L(2, 4)$ (two cubes and four colors) as being part of a collection of small mathematical games and he stated that

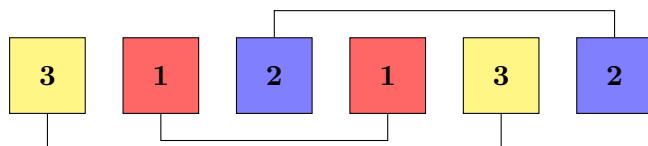


Figure 4.1: $L(2,3)$ arrangement

Instance	Solutions	Method	Computation time
L(2,3)	1	Miller algorithm	-
L(2,4)	1		-
...
L(2,16)	326,721,800		120 hours
L(2,19)	256,814,891,280		2.5 years (1999) DEC Alpha
L(2,20)	2,636,337,861,200	Godfrey algorithm	1 week
L(2,23)	3,799,455,942,515,488		4 days with CONFIIT
L(2,24)	46,845,158,056,515,936		3 months with CONFIIT
L(2,27)	111,683,611,098,764,903,232		2 days on ROMEO
L(2,28)	1,607,383,260,609,382,393,152		23 days on ROMEO

Table 4.1: Solutions and time for Langford problem using different methods

$L(2, n)$ has solutions for all n such that:

$$\text{solutions for: } \begin{cases} n = 4k \\ n = 4k - 1 \end{cases} \quad k \in \mathbb{N}^+ \quad (4.1)$$

The central resolution method consists in placing the pairs of cubes, one after the other, on the free places and backtracking if no place is available (see figure 4.3 for detailed algorithm).

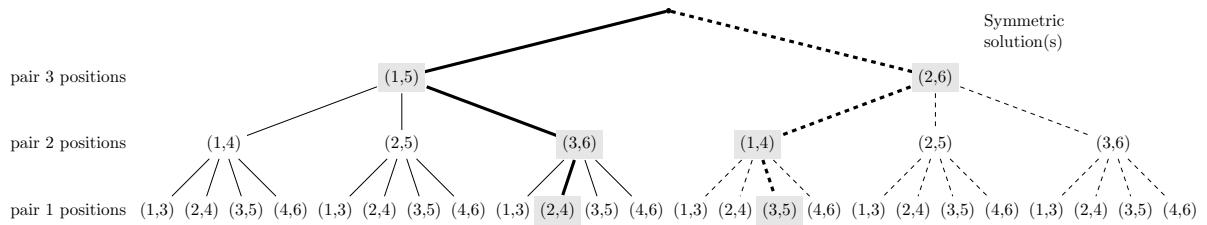
The Langford problem has been approached in different ways: discrete mathematics results, specific algorithms, specific encoding, constraint satisfaction problem (CSP), inclusion-exclusion ... [Mil99, Wal01, Smi00, Lar09]. In 2004, the last solved instance, $L(2, 24)$, was computed by our team [JK04] using a specific algorithm. Table 4.1 presents the latest results and number of solutions. $L(2, 27)$ and $L(2, 28)$ have just been computed but no details were given.

The most efficient known algorithms are: the Miller backtrack method, the Godfrey algebraic method and the Larsen inclusion-exclusion method. The Miller one is based on backtracking and can be modeled as a CSP[HKS00, HKS05]; it allowed us to move the limit of explicits solutions building up to $L(2, 21)$ but combinatorial explosion did not allow us to go further. Then, we use the Godfrey method to achieve $L(2, 24)$ more quickly and then recompute $L(2, 27)$ and $L(2, 28)$, presently known as the last instances. The Larsen method is based on inclusion-exclusion [Lar09]; although this method is effective, practically the Godfrey one is better. The latest known work on the Langford Problem is a GPU implementation proposed in [ABL15] in 2015. Unfortunately this study does not provide any performance considerations but just gives the number of solution of $L(2, 27)$ and $L(2, 28)$.

4.2 Miller algorithm

The Miller's method is based on a tree traversal to be able to check all the cubes positions. This method finds its limits because even using branch cutting algorithm to traverse the tree, the number of branches to explore stay very high. We implemented a multi-core and many-core version of it for the purpose of our benchmark. Indeed, this huge tree traversal requires irregular computation and memory accesses: two elements fitting the wall we want to confront to our architectures.

In this section we present our multi-GPU cluster implementation of the Miller's algorithm. First, we introduce the backtrack method itself and the elements allowing us to consider it as a good candidate for our metric. Then we present our implementation in order to fit the GPUs architecture. The last section presents our results.

Figure 4.2: Search tree for $L(2, 3)$

4.2.1 CSP

Combinatorial problems are NP-complete [GJ79] and can be described as satisfiability problems (SAT) using a polynomial transformation. They can be transformed into CSP formalism. A *Constraint Satisfaction Problem* (CSP), first introduced by Montanari [Mon74], is defined as a triple $\langle X, D, C \rangle$ where:

$$\begin{cases} X = \{X_1, \dots, X_n\}: \text{a finite set of variables} \\ D = \{D_1, \dots, D_n\}: \text{their finite domains of values} \\ C = \{C_1, \dots, C_p\}: \text{a finite set of constraints} \end{cases} \quad (4.2)$$

The goal in this formalism is to assign values in D to n -uple X respecting all the C p -uple constraints. This approach is a large field of research. [AC14] developed *local search* and compares GPU to CPU. This first work brings to light that GPU is a real contributor to the global computation speed. [CDPD⁺14] proposes a solver using *propagator* on a GPU architecture to solve CSP problems. [JAO⁺11] cares about GPU weak points, loading bandwidth and global memory latency.

Considering a basic approach, combinatorial problems formed into CSP can be represented as a tree search. Each level corresponds to a given variable, with values in its domain. Leaves of the tree correspond to a complete assignment (all variables are set). If it meets all the constraints this assignment is called an acceptor state. Depending on the constraints set, the satisfiability evaluation can be made either on complete or partial assignment.

4.2.2 Backtrack resolution

As presented above the Langford problem is known to be a highly irregular combinatorial problem. We first present here the general tree representation and the ways we regularize the computation for GPUs. Then we show how to parallelize the resolution over a multi-GPU cluster.

Langford's problem tree representation

As explained, CSP formalized problems can be transformed into tree evaluations. In order to solve $L(2, n)$, we consider a tree of height n : see example of $L(2, 3)$ in figure 7.6.

- Every level of the tree corresponds to a cube color.
- Each node of the tree corresponds to the placement of a pair of cubes without worrying about the other colors. Color p is represented at depth $n - p + 1$, where the first node corresponds to the first possible placement (positions 1 and $p+2$) and i^{th} node corresponds to the placement of the first cube of color p in position i , $i \in [1, 2n - 1 - p]$.
- Solutions are leaves generated without any placement conflict.

```

while not done do
  test pair           <- test
  if successful then
    if max depth then
      count solution
      higher pair
    else
      lower pair       <- remove
    else
      higher pair     <- add
  for pair 1 positions
    assignment
    for pair 2 positions
      assignment
      for ...
    for pair n positions
      assignment
      if final test ok then
        count solution
      <- add
    <- add
  <- add

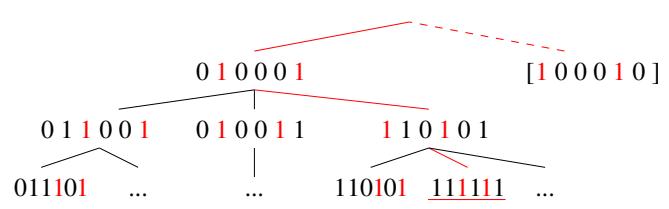
```

Figure 4.3: Backtrack algorithm

	pair 1	pair 2	pair 3
1	0 0 0 1 0 1	0 0 1 0 0 1	0 1 0 0 0 1
2	0 0 1 0 1 0	0 1 0 0 1 0	1 0 0 0 1 0
3	0 1 0 1 0 0	1 0 0 1 0 0	
4	1 0 1 0 0 0		

Figure 4.5: Bitwise representation of pairs positions in $L(2, 3)$

Figure 4.4: Regularized algorithm

Figure 4.6: Bitwise representation of the Langford $L(2, 3)$ placement tree

- As we consider the solution up to a symmetry, the left part is represented dashed and is in fact not traversed.

There are many ways to browse the tree and find the solutions: *backtracking*, *forward-checking*, *backjumping*, etc [Pro93]. We limit our study to the naive *backtrack* resolution and choose to evaluate the variables and their values in a static order; in a depth-first manner, the solutions are built incrementally and if a partial assignment can be aborted, the branch is cut. A solution is found each time a leaf is reached.

The recommendation for performance on GPU accelerators is to use non test-based programs. Due to its irregularity, the basic *backtracking* algorithm, presented on figure 4.3, is not supposed to suit the GPU architecture. Thus a vectorized version is given when evaluating the assignments at the leaves' level, with one of the two following ways: assignments can be prepared on each tree node or totally set on final leaves before testing the satisfiability of the built solution (figure 4.4).

Data representation

In order to count every Langford problem solution, we first identify all possible combinations for one color without worrying about the other ones. Each possible combination is coded within an integer, a bit to 1 corresponding to a cube presence, a 0 to its absence. This is what we called a *mask*. This way figure 4.5 presents the possible combinations to place the one, two and three weight cubes for the $L(2, 3)$ Langford instance.

Furthermore the masks can be used to evaluate the partial placements of a chosen set of colors: all the 1 correspond to occupied positions; the assignment is consistent *iff* there are as many 1 as the number of cubes set for the assignment.

With the aim to find solutions, we just have to go all over the tree and *sum* one combination of each of the colors: a solution is found *iff* all the bits of the sum are set to 1.

Each route on the tree can be evaluated individually and independently; then it can be evaluated as a thread on the GPU. This way the problem is massively parallel and can be, indeed, computed on GPU. figure 4.6 represents the tree masks' representation.

a) adding a pair

mask	or	$\begin{array}{r} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{array}$	or	$\begin{array}{r} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{array}$
pair		$\underline{\begin{array}{r} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{array}}$		$\underline{\begin{array}{r} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{array}}$
		$\begin{array}{r} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{array}$		$\begin{array}{r} 1 \\ 0 \\ 1 \\ 1 \\ 1 \\ 1 \end{array}$

b) testing a pair

mask	and	$\begin{array}{r} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{array}$	and	$\begin{array}{r} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{array}$
pair		$\underline{\begin{array}{r} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{array}}$		$\underline{\begin{array}{r} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{array}}$
		$= 0$		$= 1$

Figure 4.7: Testing and adding position

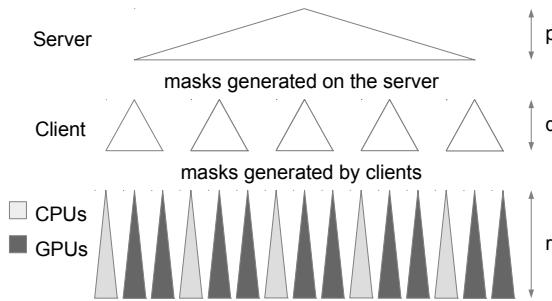


Figure 4.8: Server client distribution

Specific operations and algorithms

Three main operations are required in order to perform the tree search. The first one, used for both backtrack and regularized methods, aims to add a pair to a given assignment. The second one, allowing to check if a pair can be added to a given partial assignment, is only necessary for the original backtrack scheme. The last one is used for testing if a global assignment is an available solution: it is involved in the regularized version of the Miller algorithm.

Add a pair: Top of figure 4.7 presents the way to add a pair to a given assignment. With a *binary OR*, the new mask contains the combination of the original mask and of the added pair. This operation can be performed even if the position is not available for the pair (however the resulting mask is inconsistent).

Test a pair position: On the bottom part of the same figure, we test the positioning of a pair on a given mask. For this, it is necessary to perform a *binary AND* between the mask and the pair.

$= 0$: *success*, the pair can be placed here

$\neq 0$: *error*, try another position

Final validity test: The last operation is for *a posteriori* checking. For example the mask 101111, corresponding to a leaf of the tree, is inconsistent and should not be counted among the solutions. The final placement mask corresponds to a solution *iff* all the places are occupied, which can be tested as $\neg \text{mask} = 0$.

Using this data representation, we implemented both *backtrack* and *regularized* versions of the Miller algorithm, as presented in figure 4.3 and 4.4.

The next section presents the way we hybridize these two schemes in order to get an efficient parallel implementation of the Miller algorithm.

4.2.3 Hybrid parallel implementation

Section 4.2.2 presents the Miller algorithm and the tools needed for the resolution. The irregularity is present in the tree traversal and specific data representation has been chosen for efficient use of the memory. This section presents our methodology to implement Miller's method on a multi-GPU cluster.

Tasks generation: In order to parallelize the resolution we have to generate tasks. Considering the tree representation, we construct tasks by fixing the different values of a first set of variables [pairs] up to a given level. Choosing the development level allows to generate as many tasks as necessary. This leads to a *Finite number of Irregular and Independent Tasks*, *FIIT* applications [Kra99, KFM04, SKF10].

Cluster parallelization: The generated tasks are independent and we spread them in a client-server manner: a server generates them and makes them available for clients. As we consider the cluster as a set of CPU-GPU(s) machines, the clients are these machines. At the machines level, the role of the CPU is, first, to generate work for the GPU(s): it has to generate sub-tasks, by continuing the tree development as if it were a second-level server, and the GPU(s) can be considered as second-level client(s).

The sub-tasks generation, at the CPU level, can be made in parallel by the CPU cores. Depending on the GPUs number and their computation power the sub-tasks generation rhythm may be adapted, to maintain a regular workload both for the CPU cores and GPU threads: some CPU cores, not involved in the sub-tasks generation, could be made available for sub-tasks computing.

This leads to the 3-level parallelism scheme presented in figure 4.8, where p , q and r respectively correspond to: (p) the server-level tasks generation depth, (q) the client-level sub-tasks generation one, (r) the remaining depth in the tree evaluation, *i.e.* the number of remaining variables to be set before reaching the leaves.

Backtrack and regularized methods hybridization: The Backtrack version of the Miller algorithm suits CPU execution and allows to cut branches during the tree evaluation, reducing the search space and limiting the combinatorial explosion effects. A regularized version had to be developed, since GPUs execution requires synchronous execution of the threads, with as few branching divergence as possible; however this method imposes to browse the entire search space and is too time-consuming.

We propose to hybridize the two methods in order to take advantage of both of them for the multiGPU parallel execution: for tasks and sub-tasks generated at sever and client levels, the tree development by the CPU cores is made using the backtrack method, cutting branches as soon as possible [and generating only possible tasks]; when computing the sub-tasks generated at client-level, the CPU cores involved in the sub-tasks resolution use the backtrack method and the GPU threads the regularized one.

4.2.4 Experiments tuning

In order to take advantage of all the computing power of the GPU we have to refine the way we use them: this section presents the experimental study required to choose optimal settings. This tuning allowed us to prove our proposal on significant instances of the Langford problem.

Registers, blocks and grid: In order to use all GPUs capabilities, the first way was to fill the blocks and grid. To maximize occupancy (ratio between active warps and the total number of warps) NVIDIA suggests to use 1024 threads per block to improve GPU performances and proposes a CUDA occupancy calculator¹. But, confirmed by the Volkov's results[Vol10], we experimented that better performances may be obtained using lower occupancy. Indeed, another critical criterion is the inner GPU registers occupation. The optimal number of registers (57 registers) is obtained by setting 9 pairs placed on the client for $L(2, 15)$, thus 6 pairs are remaining for GPU computation.

In order to tune the blocks and grid sizes, we performed tests on the ROMEO architecture. Figure 4.9 represents the time in relation with the number of blocks per grid and the number of threads per block. The most relevant result, observed as a local minimum on the 3D surface, is obtained near 64 or 96 threads per block; for the grid size, the limitation is relative to the GPU global memory size. It can be noted that we do not need shared memory because their are no data exchanges between threads. This allows us to use the total available memory for the L1 cache for each thread.

¹http://developer.download.nvidia.com/compute/cuda/CUDA_Occupancy_calculator.xls

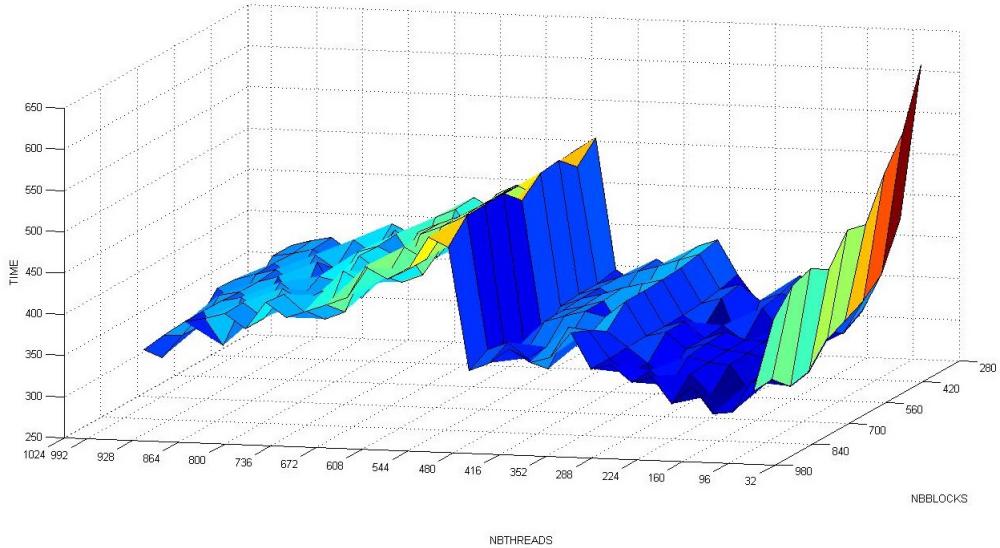
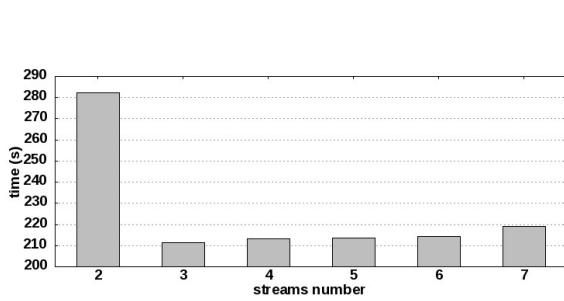
Figure 4.9: Time depending on grid and block size on $n = 15$ 

Figure 4.10: Computing time depending on streams number

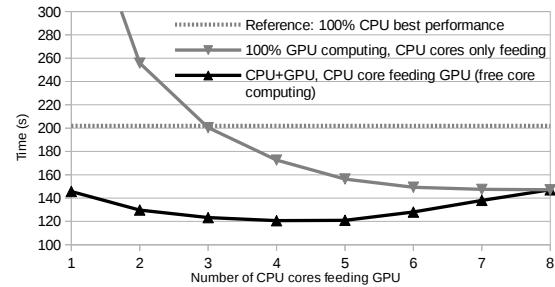


Figure 4.11: CPU cores optimal distribution for GPU feeding

Streams: A client has to prepare work for GPU. There are four main steps: generate the tasks, load them into the device memory, process the task on the GPU and then get the results.

CPU-GPU memory transfers cause huge time penalties (about 400 cycles latency for transfers between CPU memory and GPU *device memory*). At first, we had no overlapping between memory transfer and kernel computation because the tasks generation on CPU was too long compared to the kernel computation. To reduce the tasks generation time we used OpenMP in order to use the eight available CPU cores. Thus CPU computation was totally hidden by memory transfers and GPU kernel computation. We tried using up to 7 streams; as shown by figure 4.10, using only two simultaneous streams did not improve efficiency because the four steps did not overlap completely; the best performances were obtained with three streams; the slow increase in the next values is caused by synchronization overhead and CUDA streams management.

Setting up the server, client and GPU depths: We now have to set the depths of each actor, server (p), client (q) and GPU (r) (see figure 4.8).

First we set the $r = 5$ for large instances because of the GPU limitation in terms of registers by threads, exacerbated by the use of numerous 64bits integers. For $r \geq 6$, we get too many registers (64) and for $r \leq 4$ the GPU computation is too fast compared to the memory load overhead.

Clients are the buffers between the server and the GPUs: $q = n - p - r$. So we have conducted tests by varying the server depth, p . The best result is obtained for $p = 3$ and

n	CPU (8c)	GPU (4c) + CPU (4c)	n	CPU (8c)	GPU (4c) + CPU (4c)
15	2.5	1.5	17	29.8	7.3
16	21.2	14.3	18	290.0	73.6
17	200.3	120.5	19	3197.5	803.5
18	1971.0	1178.2	20	—	9436.9
19	22594.2	13960.8	21	—	118512.4

(a) Regularized method (seconds)

(b) Backtrack (seconds)

Table 4.2: Comparison between multi-core processors and GPUs for regularized and backtrack method

performance decreases quickly for higher values. This can be explained since more levels on the server generates smaller tasks; thus GPU use is not long enough to overlap memory exchanges.

CPU: Feed the GPUs and compute The first work of CPU cores is to prepare tasks for GPU so that we can generate overlapping between memory load and kernel computation. In this configuration using eight cores to generate GPU tasks under-uses CPU computation power. It is the reason why we propose to use some of the CPU cores to take part of the sub-problems treatment. Figure 4.11 represents computation time in relation with different task distributions between CPU and GPU. We experimentally demonstrated that only 4 or 5 CPU cores are enough to feed GPU, the other ones can be used to perform backtrack resolution in competition with GPUs.

4.2.5 Results

Regularized method results We now show the results obtained for our massively parallel scheme using the previous optimizations, comparing the computation times of successive instances of the Langford problem. These tests were performed on 20 nodes of the ROMEO supercomputer, hence 40 CPU/GPU machines.

The previous limit with Miller’s algorithm was $L(2, 19)$, obtained in 1999 after 2.5 years of sequential effort and at the same time after 2 months with a distributed approach[Mil99]. Our computation scheme allowed us to obtain it in less than 4 hours (Table 4.2a), this being not only due to Moore law progress.

Note that the computation is 1.6 faster with CPU+GPU together than using 8 CPU cores. In addition, the GPUs compute $200,000\times$ more nodes of the search tree than the CPUs, with a faster time.

The computation time between two different consecutive instances being multiplied by 10 approximately, this could allow us to obtain $L(2, 20)$ in a reasonable time.

Backtracking on GPUs It appears at first sight that using backtracking on GPUs without any regularization is a bad idea due to threads synchronization issues. But in order to compare CPU and GPU computation power in the same conditions we decided to implement the original backtrack method on GPU (see figure 4.3) with only minor modifications. In these conditions we observe very efficient work of the NVIDIA scheduler, which perfectly handles threads desynchronization. Thus we use the same server-client distribution as in 4.2.3, each client generates masks for both CPU and GPU cores. The workload is then statically distributed on GPU and CPU cores. Executing the backtrack algorithm on a randomly chosen set of sub-problems allowed us to set the GPU/CPU distribution ratio experimentally to 80/20%.

The experiments were performed on 129 nodes of the ROMEO supercomputer, hence 258 CPU/GPU machines and one node for the server. Table 4.2b shows the results with this configuration. This method first allowed us to perform the computation of $L(2, 19)$ in less than 15 minutes, $15\times$ faster than with the regularized method; then, we pushed the limitations of the

Miller algorithm up to $L(2, 20)$ in less than 3 hours and even $L(2, 21)$ in about 33 hours².

This first benchmark application provides a perfect example for the behavior of many-core accelerators confronted to irregular application. Even if the application does not seem to fit with the direct tree traversal, the results prove that if used in the right way performance can be achieved in this case.

4.3 Godfrey's algebraic method

The previous part presents the Miller algorithm for the Langford problem, this method cannot achieve bigger instances than the $L(2, 21)$. It allows us the target specific walls with memory and computation irregularities.

An algebraic representation of the Langford problem has been proposed by M. Godfrey in 2002. This example is perfect in our study to target computationally heavy context with irregular memory behavior. In this part we describe this algorithm and optimizations, and then our implementation on multiGPU clusters. As a side note, this implementation also allowed us to break a new world record on the computation time needed to solve the last instances, $L(2, 27)$ and $L(2, 28)$.

4.3.1 Method description

Consider $L(2, 3)$ and $X = (X_1, X_2, X_3, X_4, X_5, X_6)$. It proposes to modelize $L(2, 3)$ by:

$$\begin{aligned} F(X, 3) = & (X_1 X_3 + X_2 X_4 + X_3 X_5 + X_4 X_6) \times \\ & (X_1 X_4 + X_2 X_5 + X_3 X_6) \times \\ & (X_1 X_5 + X_2 X_6) \end{aligned} \tag{4.3}$$

In this approach each term represents a position of both cubes of a given color and a solution to the problem corresponds to a term developed as $(X_1 X_2 X_3 X_4 X_5 X_6)$; thus the number of solutions is equal to the coefficient of this monomial in the development. More generally, the solutions to $L(2, n)$ can be deduced from $(X_1 X_2 X_3 X_4 X_5 \dots X_{2n})$ terms in the development of $F(X, n)$.

If $G(X, n) = X_1 \dots X_{2n} F(X, n)$ then it has been shown that:

$$\sum_{(x_1, \dots, x_{2n}) \in \{-1, 1\}^{2n}} G(X, n)_{(x_1, \dots, x_{2n})} = 2^{2n+1} L(2, n) \tag{4.4}$$

So

$$\sum_{(x_1, \dots, x_{2n}) \in \{-1, 1\}^{2n}} \left(\prod_{i=1}^{2n} x_i \right) \prod_{i=1}^n \sum_{k=1}^{2n-i-1} x_k x_{k+i+1} = 2^{2n+1} L(2, n) \tag{4.5}$$

That allows to get $L(2, n)$ from polynomial evaluations. The computational complexity of $L(2, n)$ is of $O(4^n \times n^2)$ and an efficient big integer arithmetic is necessary. This principle can be optimized by taking into account the symmetries of the problem and using the Gray code: these optimizations are described below.

4.3.2 Method optimizations

Some works focused on finding optimizations for this arithmetic method[Jai05]. Here we explain the symmetric and computation optimizations used in our algorithm.

²Even if this instance has no interest since it is known to have no solution

Evaluation parity:

As $[F(-X, n) = F(X, n)]$, G is not affected by a global sign change. In the same way the global sign does not change if we change the sign of each pair or impair variable.

Using these optimizations we can set the value of two variables and accordingly divide the computation time and result size by four.

Symmetry summing:

In this problem we have to count each solution up to a symmetry; thus for the first pair of cubes we can stop the computation at half of the available positions considering

$$S'_1(x) = \sum_{k=1}^{n-1} x_k x_{k+2} \text{ instead of } S_1(x) = \sum_{k=1}^{2n-2} x_k x_{k+2}. \text{ The result is divided by 2.}$$

Sums order:

Each evaluation of $S_i(x) = \sum_{k=1}^{2n-i-1} x_k x_{k+i+1}$, before multiplying might be very important regarding to the computation time for this sum. Changing only one value of x_i at a time, we can recompute the sum using the previous one without global re-computation. Indeed, we order the evaluations of the outer sum using Gray code sequence. Then the computation time is considerably reduced.

Based on all these improvements and optimizations we can use the Godfrey method in order to solve huge instances of the Langford problem. The next section develops the main issues of our multiGPU architecture implementation.

4.3.3 Implementation details

In this part we present the specific adaptations required to implement the Godfrey method on a multiGPU architecture.

Optimized big integer arithmetic:

In each step of computation, the value of each S_i can reach $2n - i - 1$ in absolute value, and their product can reach $\frac{(2n-2)!}{(n-2)!}$. As we have to sum the S_i product on 2^{2n} values, in the worst case we have to store a value up to $2^{2n} \frac{(2n-2)!}{(n-2)!}$, which corresponds to 10^{61} for $n = 28$, with about 200 bits.

So we need few big integer arithmetic functions. After testing existing libraries like GMP for CPU or CUMP for GPU, we came to the conclusion that they implement a huge number of functionalities and are not really optimized for our specific problem implementation: product of "small" values and sum of "huge" values.

Finally, we developed a light CPU and GPU library adapted to our needs. In the summation, for example, as maintaining carries has an important time penalty, we have chosen to delay the spread of carries by using buffers: carries are accumulated and spread only when useful (for example when the buffer is full). Figure 4.12 represents this big integer handling.

This big integer library imposes many constraint on the accelerator memory. We conduct tests using simple and double precision for the basic unit. The carries propagation is also triggered when necessary only. This strategy implies random memory accesses to the words and irregular behavior between the threads.

Gray sequence in memory:

The Gray sequence cannot be stored in an array because it would be too large (it would contain 2^{2n} byte values). This is the reason why only one part of the Gray code sequence is stored in memory and the missing terms are directly computed from the known ones using arithmetic

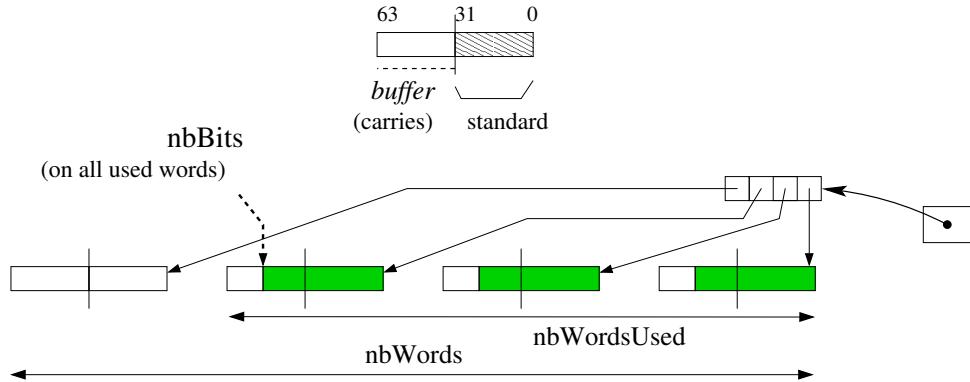


Figure 4.12: Big integer representation, 64 bits words

considerations. The size of the stored part of the Gray code sequence is chosen to be as large as possible to be contained in the processor's cache memory, the L1 cache for the GPUs threads: so the accesses are fastened and the computation of the Gray code is optimized. For an efficient use of the E5-2650 v2 ROMEO's CPUs, which disposes of 20 MB of level-3 cache, the CPU Gray code sequence is developed recursively up to depth 25. For the K20Xm ROMEO's GPUs, which dispose of 8 KB of constant memory, the sequence is developed up to depth 15. The rest of the memory is used for the computation itself.

Tasks generation and computation:

In order to perform the computation of the polynomial, two variables can be set among the $2n$ available. For the tasks generation we choose a number p of variables to generate 2^p tasks by developing the evaluation tree to depth p .

The tasks are spread over the cluster, either synchronously or asynchronously.

Synchronous computation: A first experiment was carried out with an MPI distribution of the tasks of the previous model. Each MPI process finds its tasks list based on its process *id*; then converting each task number into binary gives the task's initialization. The processes work independently; finally the root process (*id* = 0) gathers all the computed numbers of solutions and sums them.

Asynchronous computation: In this case the tasks can be computed independently. As with the synchronous computation, the tasks' initializations are retrieved from their number. Each machine can get a task, compute it, and then store its result; then when all the tasks have been computed, the partial sums are added together and the total result is provided.

4.3.4 Experimental settings

This part presents the experimental context and methodology, and the way the experiments were carried out. This study has similar goals as for the Miller's resolution experiments.

Methodology:

We present here the way the experimental settings were chosen. Firstly we define the tasks distribution, secondly we set the number of threads per GPU block; finally, we set the CPU/GPU distribution.

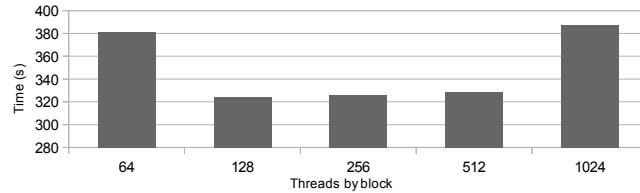
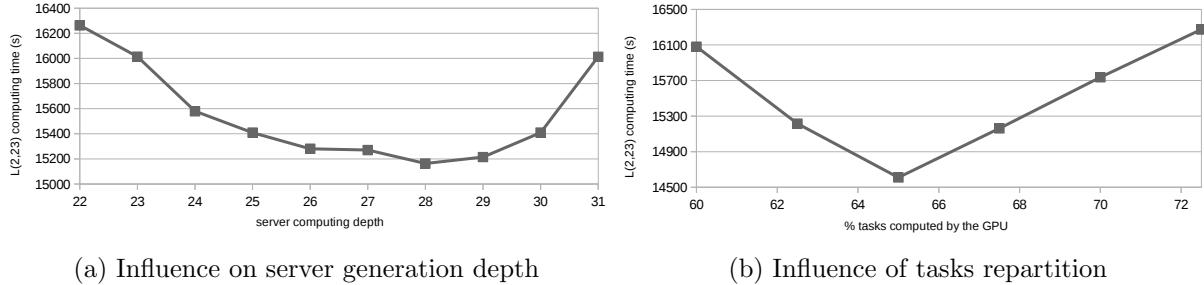
Figure 4.13: $L(2, 20)$, number of threads per block

Figure 4.14: Influences of repartitions of depths and CPU-GPU tasks

Tasks distribution depth: This value being set it is important to get a high number of blocks to maintain sufficient GPU load. Thus we have to determine the best number of tasks for the distribution. As presented in part 4.3.3 the number p of bits determines 2^p tasks. On the one hand, too many tasks are a limitation for the GPU that cannot store all the tasks in its 6GB memory. On the other hand, not enough tasks means longer tasks and too few blocks to fill the GPU grid. figure 4.14a shows that for the $L(2, 23)$ instance the best task number is with generation depth 28.

Number of threads per block: In order to take advantage of the GPU computation power, we have to determine the threads/block distribution. Inspired by our experiments with Miller's algorithm we know that the best value may appear at lower occupancy. We perform tests on a given tasks set varying the threads/block number and grid size associated. Figure 4.13 presents the tests performed on the $n = 20$ problem: the best distribution is around 128 threads per block.

CPU vs GPU distribution:

The GPU and CPU computation algorithm will approximately be the same. In order to take advantage of all the computational power of both components we have to balance tasks between CPU and GPU. We performed tests by changing the CPU/GPU distribution based on simulations on a chosen set of tasks. Figure 4.14b shows that the best distribution is obtained when the GPU handles 65% of the tasks. This optimal load repartition directly results from the intrinsics computational power of each component; this repartition should be adapted if using a more powerful GPU like Tesla K40 or K80.

Computing context:

As presented in part 2.5.1, we used the ROMEO supercomputer to perform our tests and computations. On this supercomputer SLURM[JG03] is used as a reservation and job queue manager. This software allows two reservation modes: a static one-job limited reservation or the opportunity to dynamically submit several jobs in a Best-Effort manner.

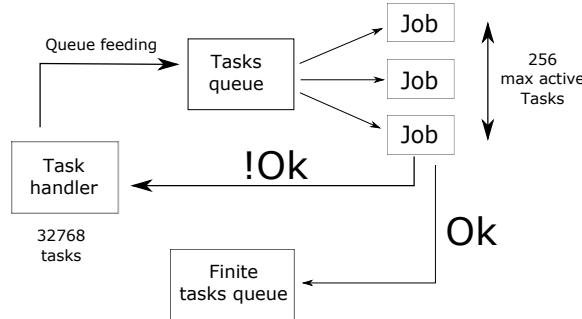


Figure 4.15: Best-effort distribution

Static distribution: In this case we used the synchronous distribution presented in 4.3.3. We submitted a reservation with the number of MPI processes and the number of cores per process. This method is useful to get the results quickly if we can get at once a large amount of computation resources. It was used to perform the computation of small problems, and even for $L(2, 23)$ and $L(2, 24)$.

As an issue, it has to be noted that it is difficult to quickly obtain a very large reservation on such a shared cluster, since many projects are currently running.

Best effort: SLURM allows to submit tasks in the specific Best-Effort queue, which does not count in the user *fair-share*. In this queue, if a node is free and nobody is using it, the reservation is set for a job in the best effort queue for a minimum time reservation. If another user asks for a reservation and requests this node, the best effort job is killed (with, for example, a SIGTERM signal). This method, based on asynchronous computation, enables a maximal use of the computational resources without blocking for a long time the entire cluster.

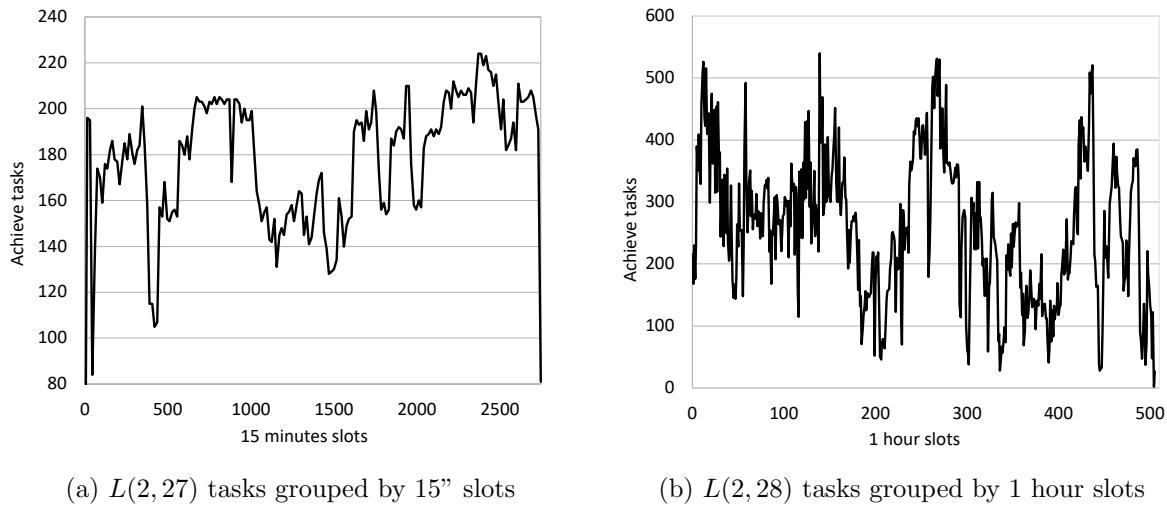
For $L(2, 27)$ and even more for $L(2, 28)$ the total time required is too important to use the whole machine off a challenge period, thus we chose to compute in a Best-Effort manner. In order to fit with this submission method we chose a reasonable time-per-task, sufficient to optimize the treatments with low loading overhead, but not too long so that killed tasks are not too penalizing for the global computation time. We empirically chose to run 15-20 minute tasks and thus we considered $p = 15$ for $n = 27$ and $p = 17$ for $n = 28$.

The best effort based algorithm is presented on figure 4.15. The task handler maintains a maximum of 256 tasks in the queue; in addition the entire process is designed to be fault-tolerant since killed tasks have to be launched again. When finished, the tasks generate an output containing the number of solutions and computation time, that is stored as a file or database entry. At the end the outputs of the different tasks are merged and the global result can be provided.

4.3.5 Results

After these optimizations and implementation tuning steps, we conducted tests on the ROMEO supercomputer using best-effort queue to solve $L(2, 27)$ and $L(2, 28)$. We started the experiment after an update of the supercomputer, that implied a cluster shutdown. Then the machine was restarted and was about 50% idle for the duration of our challenge. The computation lasted less than 2 days for $L(2, 27)$ and 23 days for $L(2, 28)$. The following describes performances considerations.

Computing effort - For $L(2, 27)$, the effective computation time of the 32,768 tasks was about 30 million seconds (345.4 days), and 165,000" elapsed time (1.9 days); the average time of the tasks was 911", with a standard deviation of 20%. For the $L(2, 28)$ 131,072 tasks the total computation time was about 1365 days (117 million seconds), as 23 day elapsed time; the tasks lasted 1321" on average with a 12% standard deviation.

Figure 4.16: Task repartition for $L(2, 27)$ and $L(2, 28)$

Best-effort overhead - With $L(2, 27)$ we used a specific database to maintain information concerning the tasks: 617 tasks were aborted [by regular user jobs] before finishing (1.9%), with an average computing time of 766" (43% of the maximum requested time for a task). This consumed 472873", which overhead represents 1.6% of the effective computing effort.

Cluster occupancy - Figure 4.16a presents the tasks resolution over the two computation days for $L(2, 27)$. The experiment elapse time was 164700" (1.9 days). Compared to the effective computation time, we used an average of 181.2 machines (CPU-GPU couples): this represents 69.7% of the entire cluster.

Figure 4.16b presents the tasks resolution flow during the 23 days computation for $L(2, 28)$. We used about 99 machines, which represents 38% of the 230 available nodes.

For $L(2, 27)$, these results confirm that the computation took great advantage of the low occupancy of the cluster during the experiment. This allowed us to obtain a weak best-effort overhead, and an important cluster occupancy. Unfortunately for $L(2, 28)$ on such a long period we got a lower part of the supercomputer dedicated to our computational project. Thus we are confident in good perspectives for the $L(2, 31)$ instance if computed on an even larger cluster or several distributed clusters.

4.4 Conclusion

We propose as a benchmark the two methods to solve the Langford pairing problem on multi-GPU clusters, presented as the Miller's and Godfrey's algorithms.

4.4.1 Miller's method: irregular memory + computation

In this first implementation we showed that the accelerators can target irregularity in memory and computation. The tree traversal, even with branch cutting, gives us excellent results on many-core architectures. They GPUs handle 80% of the computation effort. Also as any combinatorial problem can be represented as a CSP, the Miller algorithm can be seen as general resolution scheme based on the backtrack tree browsing. A three-level tasks generation allows to fit the multiGPU architecture. MPI or Best-Effort are used to spread tasks over the cluster, OpenMP for the CPU cores distribution and then CUDA to take advantage of the GPU computation power. We were able to compute $L(2, 20)$ with this regularized method and to get an even better computation time with the basic backtrack. The proposed approach exhibits that the GPU scheduler is very efficient at managing highly divergent threads.

4.4.2 Godfrey's method: irregular memory + heavy computation

We also presented the Godfrey's method which targets irregular memory accesses but also heavy computational behavior. The results show that the many-core version completely exceed the classical processor best performances. The GPU handle 65% of the computation effort. In addition we beat the Langford limits using multi-GPUs. In order to use the ROMEO supercomputer, which is shared by a large scientific community, we have implemented a work distribution that does not affect the machine load, using a best-effort queue. The computation is fault-tolerant and totally asynchronous. The utilization of this technology also shows the reliability of nowadays accelerators technologies. Indeed, they can be used at demand for specific tasks without specific warm-up.

Langford problem results: This work also enabled us to compute $L(2, 27)$ and $L(2, 28)$ in respectively less than 2 days and 23 days on the University of Reims ROMEO supercomputer. This is nowadays the fastest time for those problems. The total number of solutions is:

$$\begin{aligned} L(2,27) &= 111,683,611,098,764,903,232 \\ L(2,28) &= 1,607,383,260,609,382,393,152 \end{aligned}$$

This first benchmark implementation is clearly in favor of hybrid architecture. The many-core architectures show a perfect handling of irregularity and heavy computations.

Chapter 5

Communication Wall: Graph500

5.1 Introduction

In order to face the communication wall in our metric for multi-accelerator's architectures, we choose the Graph500 problem. This benchmark is based on huge tree traversal through a randomly generated graph. We already work on this kind of memory intensive problem with the first implementation of the Langford algorithm. The Graph500 pushes this example to its limits using terabytes to petabytes of data to represent the graph on which the traversal is executed. In this case the computation is absent or just reduce to tests on datum. This metric directly targets the memory and communication wall in an irregular case.

In this part we present the benchmark itself, from the graph generation to its traversal. We focus on the BFS part, we do not work on the latest Graph500 using SSSP. We explain why this benchmark is perfect to target communication wall and memory wall. We present our implementation on multi-GPUs architectures and the results are compared to the multi-core processor version.

5.1.1 Breadth First Search

The most commonly used search algorithms for graphs are Breadth First Search (BFS) and Depth First Search (DFS). Many graph analysis methods, such as the finding of shortest path for unweighted graphs and centrality, are based on BFS.

As it is a standard approach method in graph theory, its implementation and optimization require extensive work. This algorithm can be seen as frontier expansion and exploration. At each step the frontier is expanded with the unvisited neighbors.

The sequential and basic algorithm is well known and is presented on Algorithm 1.

This algorithm is presented on figure 5.1. At each step from the current queue we search

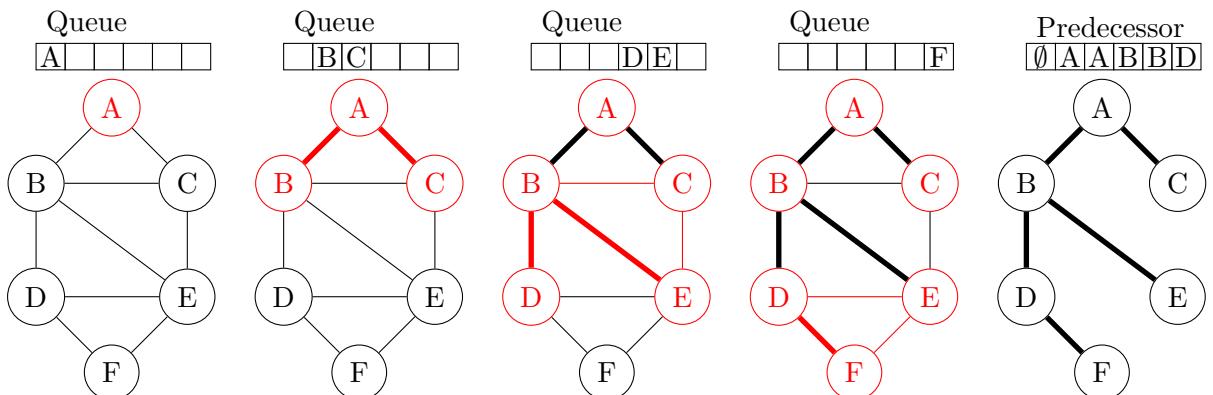


Figure 5.1: Example of Breadth First Search in an undirected graph

Algorithm 1 Sequential Breadth First Search algorithm

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1: function COMPUTE_BFS( $G = (V, E)$ : graph representation,  $v_s$ : source vertex,  $In$ : current
   level input,  $Out$ : current level output,  $Vis$ : already visited vertices)
2:    $In \leftarrow \{v_s\}$ ;
3:    $Vis \leftarrow \{v_s\}$ ;
4:    $P(v) \leftarrow \perp \forall v \in V$ ;
5:   while  $In \neq \emptyset$  do
6:      $Out \leftarrow \emptyset$ 
7:     for  $u \in In$  do
8:       for  $v|(u, v) \in E$  do
9:         if  $v \notin Vis$  then
10:           $Out \leftarrow Out \cup \{v\}$ ;
11:           $Vis \leftarrow Vis \cup \{v\}$ ;
12:           $P(v) \leftarrow u$ ;
13:        end if
14:      end for
15:    end for
16:     $In \leftarrow Out$ 
17:  end while
18: end function

```

through the neighbors of nodes. All the new nodes, not yet traversed, are added in the queue for the next step. We keep the information of neighbors' exploration in order to recreate the predecessor array.

This algorithm is very famous thanks to its use in many applications but also thanks to the world supercomputer ranking called Graph500¹. This benchmark is designed to measure the performance on very irregular problems like BFS on a large scale randomized generated graph. The first Graph500 list was released in November 2010. The last list, issued in November 2017, is composed of 235 machines ranked using a specific metric: Traversed Edges Per Second, denoted as TEPS. The aim is to perform a succession of 64 BFS on a large-scale graph in the fastest possible way. Then the ratio of edges traversed per the time of computation is used to rank the machines.

This benchmark is more representative of communication and memory accesses than computation itself. Other benchmarks can be used to rank computational power such as LINPACK for the TOP500 list. Indeed, the best supercomputers (K-Computer, Sequoia, Mira, ...) on the ladder have a very specific communication topology and sufficient memory, and are large enough to quickly visit all the nodes of the graph.

This benchmark is conduct using GPUs as accelerators. There are many CPU algorithms available, which are listed on the Graph500 website. In order to rank the ROMEO supercomputer, we had to create a dedicated version of the Graph500 benchmark in order to fit the supercomputer architecture. As this supercomputer is accelerated by GPUs, three successive approaches had to be applied: first create an optimized CPU algorithm; second provide a GPU specific version and third take advantage of both CPU and GPU computation power.

The first section performs a survey of graph representation and analysis; it also describes some specific implementations. The second section describes the Graph500 protocol and focuses on the Kronecker graph generation method and the BFS validation. The third section presents the chosen methods to implement graph representation and work distribution over the supercomputer nodes. It particularly focuses on the interest of a hybrid CSR and CSC representation. We compare the results for different graph scales and load distributions.

¹<http://www.graph500.org>

This work also leads us to work on similar algorithms like the evaluation of centrality[BM06, BP07, Bra01, GSS08, JHC⁺10, SZ11, SKS⁺13] and SSSP/APSP[DBG014, DTC⁺14] on large graphs. This similar application gave us hint for the best BFS implementation. The betweenness centrality computation in particular was interesting and we will apply it in the case of power grid analysis or nowadays problems like network mapping[Kre02, SN11].

5.2 Existing methods

The most efficient algorithm to compute BFS traversal is used and detailed in [CPW⁺12]. It uses a 2D partition of the graph which will be detailed later. This algorithm is used on the BlueGene/P and BlueGene/Q architectures but can be easily adapted to any parallel cluster. Several other work[GLG⁺12] propose a distributed graph traversal but are very similar to the BlueGene version.

We use another key study in order to build our Graph500 CPU/GPU implementation. [MGG15] proposes various effective methods on GPU for BFS. Merrill & al. explain and test a few efficient methods to optimize memory access and work sharing between threads on a large set of graphs. It focuses on Kronecker graphs in particular. First, they propose several methods for neighbor-gathering with a serial code versus a warp-based and a CTA-based approach. They also use hybridization of these methods to reach the performance level. In a second part they describe the way to perform label-lookup, to check if a vertex is already visited or not. They propose to use a bitmap representation of the graph with texture memory on the GPU for fast random accesses. In the last phase, they propose methods to suppress duplicated vertices generated during the neighbor exploration phase. Then based on these operations they propose *expand-contract*, *contract-expand*, *two-phase* and finally *hybrid* algorithms to adapt the method with all the studied graph classes. The last part they propose a multi-GPU implementation. They use a 1D partition of the graph and each GPU works on its subset of vertices and edges.

In [FDB⁺14], a first work is proposed to implement a multi-GPU cluster version of the Graph500 benchmark. The scheme used in their approach is quite similar to the one in our study but with a more powerful communication network, namely FDR InfiniBand.

In our work we focus on the GPUDirect usage on the ROMEO supercomputer.

5.3 Environment

As previously mentioned, a CPU implementation is available on the official Graph500 website. A large range of software technology is covered with MPI, OpenMP, etc. All these versions use the same generator and the same validation pattern which is described in this part below.

The Graph500 benchmark is based on the following stages:

- *Graph generation.* The first step is to generate the Kronecker graph and mix the edges and vertices. The graph size is chosen by the user (represented as a base-2 number of vertices). The *EDGEFACTOR*, average ratio of edges by vertex, is always 16. Self-loop and multiple edges are possible with Kronecker graphs. Then 64 vertices for the BFS are randomly chosen. The only rule is that a chosen vertex must have at least one link with another vertex in the graph. *This stage is not timed*;
- *Structure generation.* The specific code part begins here. Based on the edge list and its structure the user is free to distribute the graph over the machines. In a following section we describe our choices for the graph representation. *This stage is timed*;
- *BFS iterations.* This is the key part of the ranking. Based on the graph representation, the user implements a specific optimized BFS. Starting with a root vertex the aim is to build the correct BFS tree (up to a race condition at every level), storing the result in a predecessor list for each vertex;

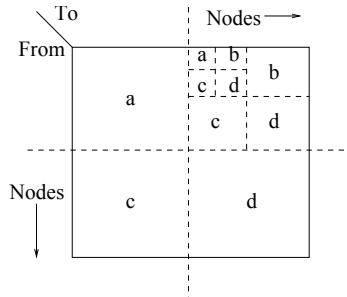


Figure 5.2: Kronecker generation scheme based on edge probability

- *BFS verification.* The user-computed BFS is validated. The number of traversed edges is determined during this stage.

The process is fairly simple, and sources can be found at <http://www.graph500.org>. The real problem is to find an optimized way to use parallelism at several levels: node distribution, CPU and GPU distribution and then massive parallelism on accelerators.

5.3.1 Generator

The *Kronecker graphs*, based on Kronecker products, represent a specific graph class imposed by the Graph500 benchmark. These graphs represent realistic networks and are very useful in our case due to their irregular aspect [LCK⁺10]. The main generation method uses the Kronecker matrix product. Based on an initiator adjacency matrix K_1 , we can generate a Kronecker graph of order $K_1^{[k]}$ by multiplying K_1 by itself k times. The Graph500 generator uses Stochastic Kronecker graphs, avoiding large scale matrix multiplying, to generate an edge list which is utterly mixed (vertex number and edge position) to avoid locality.

As presented on figure 5.2, the generation is based on edge presence probability on a part of the adjacency matrix. For the Graph500 the probabilities are $a = 0.57$, $b = c = 0.19$ and $d = 0.05$. The generator handle can be stored in a file or directly split in the RAM memory of each process. The first option is not very efficient and imposes a lot of I/O for the generation and verification stage but can be very useful for large scale problems. The second option is faster but uses a part of the RAM thus less resources are available for the current BFS execution.

5.3.2 Validation

The validation stage is completed after the end of each BFS. The aim is to check if the tree is valid and if the edges are in the original graph. This is why we must keep a copy of the original graph in memory, file or RAM. This validation is based on the following stages, presented on the official Graph500 website. First, the BFS tree is a tree and does not contain cycles. Second, each tree edge connects vertices whose BFS levels differ by exactly one. Third, every edge in the input list has vertices with levels that differ by at most one or that both are not in the BFS tree. Finally, the BFS tree spans an entire connected component's vertices, and a node and its parent are joined by an edge of the original graph.

In order to meet the Graph500 requirements we use the proposed verification function provided in the official code.

5.4 BFS traversal

In this section we present the actual algorithm we used to perform the BFS on a multi-GPU cluster. In a first part we introduce the data structure; then we present the algorithm and the optimizations used.

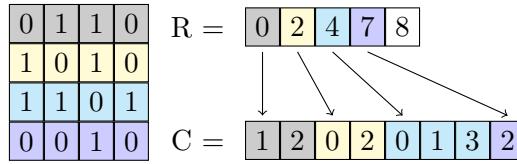


Figure 5.3: Compressed Sparse Row example

5.4.1 Data structure

We performed tests of several data structures. In a first work we tried to work with bitmap. Indeed, the regularity of computation can fit very well with the GPU architecture. But this representation imposes a significant limitation on the graph size. This representation is used on the BlueGene/Q architecture. Indeed, they have some specific hardware bit-wise operations implemented in their processors and have a large amount of memory, allowing them to perform very large scale graph analysis.

In a second time we used common graph representations, Compressed Sparse Row (CSR) and Compressed Sparse Column (CSC) representation, which fit very well with sparse graphs such as the Graph500 ones.

Figure 5.3 is an example illustrating the CSR compression. The M adjacency matrix represents the graph. R vector contains the cumulative number of neighbors for each vertex, of size ($\#vertices + 1$). C , of size ($\#edges$), is, for each index of R , the edges of a vertex. This representation is very compact and very efficient to work with sparse graphs.

5.4.2 General algorithm

When looking at the latest Graph500 list we see that the best machines are the BlueGene ones. We count about 26 BlueGene/Q and BlueGene/P machines in the first 50 machines. This is due to a quite specific version of the BFS algorithm proposed in [CPW⁺12]. It proposes a very specific 2D distribution for parallelism and massive use of the 5D torus interconnect.

In the BFS algorithm, like other graph algorithms, parallelism can take several shapes. We can split the vertices into partitions using 1D partition. Each thread/machine can then work on a subset of vertices. The main issue with this method is that the partitions are not equal since the number of edges per vertex can be very different; moreover, in graphs like Kronecker ones where some vertices have a very high degree compared to other ones. Thus, we are confronted with a major load balancing problem.

In [CPW⁺12] they propose a new vision of graph traversal, here BFS, on distributed-memory machines. Instead of using standard 1D distribution their BFS is based on a 2D distribution. The adjacency matrix is split into blocks of same number of vertices. If we consider $l \times l$ blocks $A_{i,j}$ we can split the matrix as follows:

$$M = \begin{bmatrix} A_{0,0} & A_{0,1} & \cdots & A_{0,l-1} \\ A_{1,0} & A_{1,1} & \cdots & A_{1,l-1} \\ \vdots & \vdots & \ddots & \vdots \\ A_{l-1,0} & A_{l-1,1} & \cdots & A_{l-1,l-1} \end{bmatrix}$$

Each bloc $A_{x,y}$ is a subset of edges. We notice that blocks $A_{0,l-1}$ and $A_{l-1,0}$ have the same edges but in a reverse direction for undirected graphs. Based on this distribution they use *virtual processors*, which are either machines or nodes, each associated with a block. This has several advantages. First, we reduce the load balancing overhead and a communication pattern can be set up. Indeed, each column shares the same *in-queue* and each row will generate an *out-queue* in the same range. Thus, for all the exploration stages, communications are only on line and

we just need a column communication phase to exchange the queues for the next BFS iteration. Algorithm 2 presents the BlueGene/Q and BlueGene/P parallel BFS.

Algorithm 3 Algorithm for tree traversal presented for BlueGene

```

1:  $Vis_{i,j} \leftarrow In_{i,j}$ 
2:  $P(N_{i,j}, v) \leftarrow \perp$  for all  $v \in R_{i,j}^{1D}$ 
3: if  $v_s \in R_{i,j}^{1D}$  then
4:    $P(N_{i,j}, v_s) \leftarrow v_s$ 
5: end if
6: while true do
7:    $(Out_{i,j}, Marks_{i,j}) \leftarrow ExploreFrontier();$ 
8:    $done \leftarrow \bigwedge_{0 \leq k, l \leq n} (Out_{k,l} = \emptyset)$ 
9:   if  $done$  then
10:    exit loop
11:   end if
12:   if  $j = 0$  then
13:      $prefix_{i,j} = \emptyset$ 
14:   else
15:     receive  $prefix_{i,j}$  from  $N_{i,j-1}$ 
16:   end if
17:    $assigned_{i,j} \leftarrow Out_{i,j} \setminus prefix_{i,j}$ 
18:   if  $j \neq n - 1$  then
19:     send  $prefix_{i,j} \cup Out_{i,j}$  to  $N_{i,j+1}$ 
20:   end if
21:    $Out_{i,j} \leftarrow \bigcup_{0 \leq k \leq n} Out_{i,k}$ 
22:   WritePred()
23:    $Vis_{i,j} \leftarrow Vis_{i,j} \cup Out_{i,j}$ 
24:    $In_{i,j} \leftarrow Out_{j,i}$ 
25: end while

```

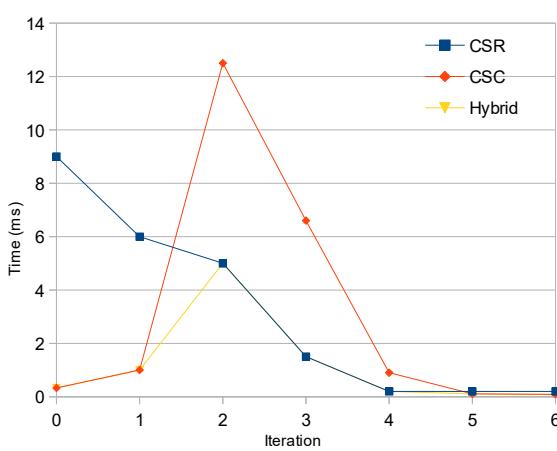
This algorithm is presented in algorithm 3 and is based on the exploration phase, denoted by *ExploreFrontier()*. It performs the exploration phase independently on all the machines. Then several communication phases follow. The first two phases are performed on the same processes line. The last one is performed on a processes column.

- On line 15, an exclusive scan is performed for each process on the same line, all the $A_{i,x}$ with $i \in [0, l - 1]$. This operation allows us to know which vertices have been discovered in this iteration.
- On line 19, a broadcast of the current *out_queue* is sent to the processes on the same line. With this information they would be able to update the predecessor list only if they are the first parent of a vertex.
- On line 24, a global communication on each column is needed to prepare the next iteration. The aim is to replace the previous *in_queue* by the newly computed *out_queue*.

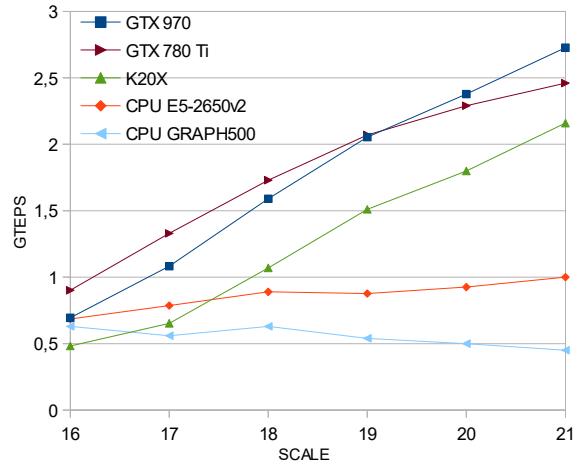
Two functions are not specified: *ExploreFrontier()* converts the *in_queue* into *out_queue* taking account of the previously visited vertices; *WritePred()* aims to generate the BFS tree and therefore store the predecessor list. In this algorithm the predecessor distribution is still in 1D to avoid vertex duplication. This part can be done using RDMA communication to update predecessor value or with traditional MPI all-to-all exchanges. It can be done during each iteration stage or at the end of the BFS but this requires using a part of the memory to store this data.

Iteration	Top-down	Bottom-up	Hybridization
0	27	22 090 111	27
1	8 156	1 568 798	8 156
2	3 695 684	587 893	587 893
3	19 565 465	12 586	12 586
4	214 578	8 256	8 256
5	5 865	1 201	1 201
6	12	156	12
Total	23,489,787	24,269,001	618,131

Table 5.1: BFS directions change from top-down to bottom-up



(a) CSR and CSC approach comparison. On a 6 iterations BFS, the time with the two method is compared. The hybridization just takes the best time of each method



(b) Single CPU and accelerators comparison. CPU Graph500 represent the best implementation proposed by the Graph500 website.

This algorithm, which is the basis of many implementations, is the main structure of our distribution.

5.4.3 Direction optimization

In order to get an optimized computation in terms of TEPS we decided to sacrifice a small part of the memory for storing both the CSC and CSR representations. Indeed, during the different BFS iterations the *in_queue* size varies a lot and, taking this into account, it is wiser to perform exploration from *top-down* or *bottom-up*. So, as proposed in [BAP13], we perform a direction-optimized BFS.

In the first case, *top-down*, we start from the vertices in the *in_queue* and check all the neighbors verifying each time if this neighbor has ever been visited. Then if not, it is added to the *out_queue*. When the *in_queue* is sparse, like for the first and latest iterations, this method is very efficient. In the second case, *bottom-up*, we start the exploration by the not-yet-visited vertices and verify if there is a link between those vertices and the *in_queue* ones. If yes, the not-yet-visited vertex is added to the *out_queue*. Table 5.1 shows the advantages of switching from top-down to bottom-up regarding the number of edges traversed. Figure 5.4a presents the two approaches, with the time visiting all the edges, and the benefits of their hybridization.

5.4.4 GPU optimization

In algorithm 2, two parts are not developed. namely *ExploreFrontier()* and *WritePred()*. Indeed, these phases are optimized using the GPU. Based on the Merill et al. implementation, the

algorithm is optimized to use the shared memory and the texture memory of the GPU. For our version we decided to keep the bitmap implementation for the communications and the queues. So, we have to fit the CSR and CSC implementations. On algorithm 4 we present the CSR algorithm; CSC is based on the same approach but starting from the *visited* queue.

In the CSR version each warp is attached to a 32-bits word of the *in_queue* bitmap. Then if this word is empty the whole warp is released; if it contains some vertices, the threads collaborate to load the entire neighbor list. Then they access the coalescent area in the main memory to load the neighbor list. A texture memory is used to accelerate the verification concerning this vertex. Indeed, this memory is optimized to be randomly accessed. Then the vertex is added in the bitmap *out_queue*.

5.4.5 Communications

Based on the algorithm 2 communications pattern, we first used MPI with the CPU transferring the data. But the host-device transfer time between the CPU and the GPU was too time-consuming. In order to accelerate the transfers between the GPUs, we used a specific GPU MPI-aware library. This library allows direct MPI operations from the memory of one GPU to another and also implements direct GPU collective operations. GPUDirect can be used coupled with this library. In the last version we used this optimization with GDRCopy.

5.5 Results

5.5.1 CPU and GPU comparison

On figure 5.4b we present the single node implementation. Here we compare the best CPU implementation proposed by the Graph500 benchmark with our GPU implementation. On our cluster we worked with K20Xm GPUs. The GPU result is twice times better than the CPU one. We also carried out tests on some "general public" GPUs like GTX980 and GTX780Ti. The result is better on these GPUs because they do not implement the ECC memory and do not provide double precision CUDA cores. Indeed all the cores can be used for the Exploration phase.

5.5.2 Strong and weak scaling

Figure 5.5b and figure 5.5a present the results of strong and weak scaling, respectively. In the strong scaling we used a *SCALE* of 21 for different numbers of GPUs. The application scales up to 16 GPUs but then the data exchanges are too penalizing; performance for 64 GPUs is lower. Indeed as the problem scale does not change, the computational part is reduced compared to the communication one. Using 16 GPUs we were able to perform up to 4.80 GTEPS.

For the weak scaling, the *SCALE* evolves with the number of GPUs. So the computation part grows and the limitation of communications is reduced. On figure 5.5a, the problem *SCALE* is presented on each point. With our method we were able to reach up to 12 GTEPS using this scaling.

5.5.3 Communications and GPUDirect

Each node of the ROMEO supercomputer is composed of two CPU sockets and two GPUs, named GPU 0 and GPU 1. Yet the node just has one HCA (Host Channel Adapters), linked with CPU 0 and GPU 0. In order to use this link GPU 1 has to pass through a Quick Path Interconnect link (QPI) between the two CPU sockets. This link considerably reduces the bandwidth available for node-to-node communication. Another problem is that the two GPUs have to share the same HCA for their communication.

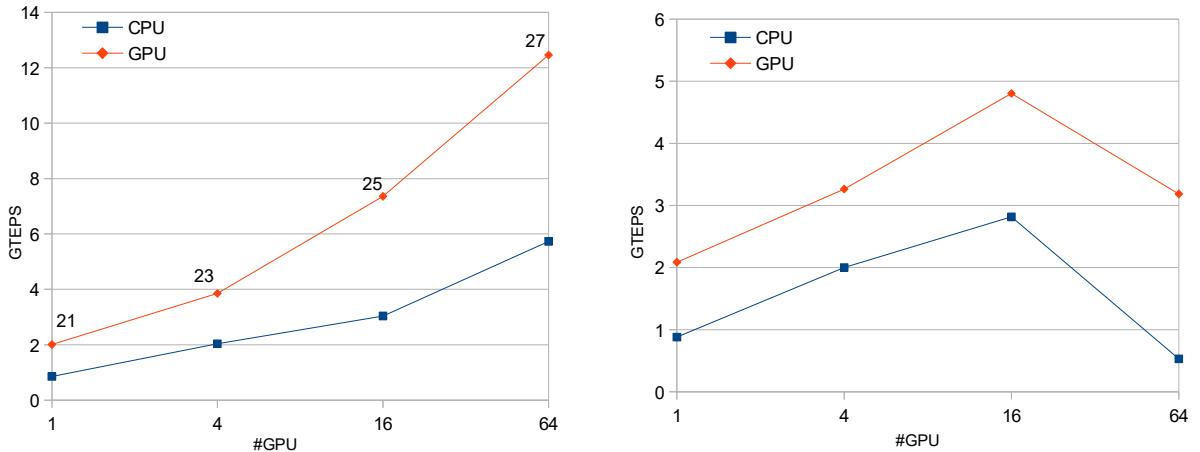
On figure 5.6, the tests are based on the GPU-only implementation. First we worked with the two GPUs of the nodes. We were able to perform up to to *SCALE* 29 with 12 GTEPS. The

Algorithm 4 Exploration kernel based on CSR

```

1: Constants:
2:  $NWARP$ : number of WARPS per block
3:
4: Variables:
5:  $pos\_word$ : position of the word in  $in\_queue$ 
6:  $word$ : value of the word in  $in\_queue$ 
7:  $lane\_id$ : thread ID in the WARP
8:  $warp\_id$ : WARP number if this block
9:  $comm[NWARP][3]$ : shared memory array
10:  $shared\_vertex[NWARP]$ : vertex in shared memory
11:
12: Begin
13: if  $word = 0$  then
14:   free this WARP
15: end if
16: if  $word \& 1 << lane\_id$  then
17:    $id\_sommet \leftarrow pos\_word * 32 + lane\_id$ 
18:    $range[0] \leftarrow C[id\_sommet]$ 
19:    $range[1] \leftarrow C[id\_sommet + 1]$ 
20:    $range[2] \leftarrow range[1] - range[0]$ 
21: end if
22: while  $_any(range[2])$  do
23:   if  $range[2]$  then
24:      $comm[warp\_id][0] \leftarrow lane\_id$ 
25:   end if
26:   if  $comm[warp\_id][0] \leftarrow lane\_id$  then
27:      $comm[warp\_id][0] \leftarrow range[0]$ 
28:      $comm[warp\_id][0] \leftarrow range[1]$ 
29:      $range[2] \leftarrow 0$ 
30:      $share\_vertex[warp\_id] = id\_sommet$ 
31:   end if
32:    $r\_gather \leftarrow comm[warp\_id][0] + lane\_id$ 
33:    $r\_gather\_end \leftarrow comm[warp\_id][2]$ 
34:   while  $r\_gather < r\_gather\_end$  do
35:      $voisin \leftarrow R[r\_gather]$ 
36:     if  $not \in tex\_visited$  then
37:       Adding in  $tex\_visited$ 
38:        $AtomicOr(out\_queue,voisin)$ 
39:     end if
40:      $r\_gather \leftarrow r\_gather + 32$ 
41:   end while
42: end while

```



(a) CPU *vs* GPU weak scaling. The number of CPUs is the same as the number of GPUs.

(b) CPU *vs* GPU strong scaling. The *SCALE* is showed on the GPU line. The number of CPUs is the same as the number of GPUs.

Figure 5.5: Weak and Strong scaling between CPU and GPU

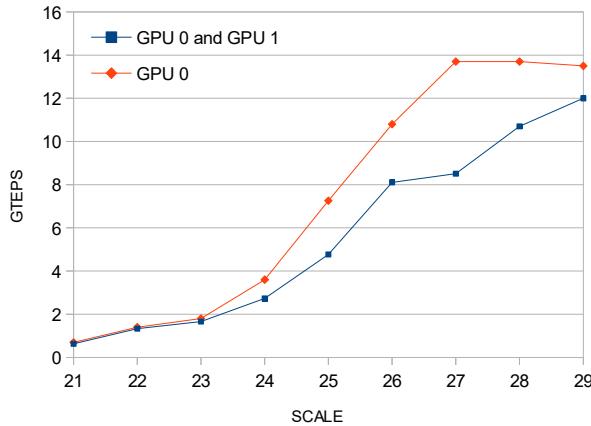


Figure 5.6: Full node GPUs *vs* GPU #0. The GPU #0 implementation not use the QPI link of the two CPU socket.

GPUDirect implementation does not allow the communication with a QPI link. So, in order to compare the results, we only used the GPU #0 of each node of the supercomputer. Based on our algorithm implementation we need to use a number of 2^{2n} GPUs. Then the tests on figure 5.6 are for 256 GPUs (with GPU #0 and GPU #1) and with 64 GPUs (using GPU #0 only). Thus we were able to reach a better GTEPS rate. The major limitation is the communications part, using only GPU #0 allowed us to obtain about 13.70 GTEPS on the ROMEO supercomputer compared to 12.05 GTEPS with GPU #0 and GPU #1 and the QPI link communications reducing the GPUDirect interest.

5.6 Conclusions

The Graph500 is already a benchmark that focuses on memory and communication wall in an irregular behavior. We presented an optimized implementation of the Graph500 benchmark for the ROMEO multi-GPU cluster for the purpose of our metric to emphasize behavior of hybrid architectures. It is based on the BlueGene/Q algorithm and GPU optimization for BFS traversal introduced by Merrill et al. This work highlights different key points. First, we have chosen a hybrid memory representation of the graphs using both CSR and CSC. Although this

double representation requires more memory, it significantly reduces the computation workload and allows us to achieve outstanding performance. Secondly, the inter-node and intra-node communication is a critical bottleneck. Each computation node has two GPUs, however only one shares the PCIe bridge with the Infiniband HCA that allows to take advantage of the GPUDirect technology. Thirdly, due to the low computation power required for BFS traversal, we get better performance by fully loading the GPUs. Otherwise communication time cannot be overlapped with computation time. Thus, to achieve the best performance we had to use only one GPU on each node. Finally, using all these optimizations, we achieved satisfactory results. Indeed, by using GPUDirect on 64 GPUs, we are able to achieve 13.70 GTEPS. In this configuration CPUs are only used to synchronize GPUs kernels. All the communications are directly GPU to GPU using a CUDA-aware MPI library with GPUDirect.

These results have been published in the Graph500 list published in November 2016. The ROMEO supercomputer was ranked 105th.

Another library appears in the same time that our study. The Gunrock library[WDP⁺15] provides a very efficient framework for graph traversal on NVIDIA GPUs. Unfortunately, this work is not implemented in a distributed way. A next part of this work would be to use our distribution strategies on top of Gunrock.

In addition to the previous benchmarks proposed in our thesis, the Graph500 benchmark completes the communication and memory irregular behavior. It shows the benefit of using many-core architectures in this context allowing twice better results using accelerators than CPUs. It shows the advantage of using GPU even up to the scale.

Conclusion

In this part we showed the real advantage of accelerators used in hybrid architectures, toward classical processors in HPC environment. In the two examples presented in this part we confronted both architectures to complex problems representing characteristic walls: irregular applications in computation and communications. In the first one, with the problem of Langford, we worked on an irregular and computationally heavy application that does not require much communication. The second one, the Graph500 BFS, characterized as an irregular communication over irregular memory usage. These two applications are confronted to all the walls that may face realistic applications.

In both cases we showed better results using accelerator, in this case GPU, compared to classical multi-core processors systems.

5.6.1 Computational wall

We studied the Langford problem under two methods of resolution. In the first one, the Miller algorithm, the resolution is based on a tree traversal. We showed that even using the irregular algorithm directly on the GPU gave us better results than on multi-core processors. We showed an acceleration of quad times using the GPUs with the backtrack method.

For the second method, the Godfrey algorithm, we were able to beat a new speed record for the last instances $L(2, 27)$ and $L(2, 28)$. We used the whole ROMEO supercomputer and were able to recompute them in 23 days using best-effort on the cluster, with 38% of the machine on average. Then, this result could be theoretically reduced to a maximum of 10 days using the whole cluster in the same time, with a linear scaling.

5.6.2 Communication wall

Several aspects of the Graph500 BFS make it a good metric candidate in our study. The graph generated is completely random and we cannot know in advance the exact number of edges and thus the perfect behavior for distributing the data. During the search of the BFS algorithm the memory is completely traversed with an irregular behavior due to the random generation of the graph.

In order to get performances, we imposed regularization over our data. The Compressed Sparse Row and Compressed Sparse Column compression methods were used together and the communications were based on bitmap transfers. The communication intensity presents a huge wall for realistic application on large architectures. Proposing an appropriate parallelization scheme can reduce the disadvantage but only well-balanced architectures can fight the problem and allows to reach good performances.

We showed that despite of the irregularity downside and larger memory used we were able to provide an efficient GPU algorithm, faster than the CPU one and the reference code proposed by the Graph500 consortium itself. We provided an acceleration of two times using our CPU algorithm and quad times using our GPU algorithm. This benchmark confirmed that hybrid architectures allow to solve communication-intensive problems with convenient performances.

5.6.3 Reaching performances on accelerators based architectures

From those two metrics we extracted the main factors that allowed us to reach good performances on accelerators like GPUs.

Regularization versus high number of tasks

We showed in both cases that the regularization of the tasks to fit the GPU execution model, based on synchronized execution, is not always the best way to reach performances. Indeed, if the number of tasks to solve on the GPUs is high enough, the SIMD model allows all the computational cores to keep busy while fetching data. The number of blocks in the grid and threads per blocks have to be very high to allow the coordinator to switch from WARPS and cover the data fetching time.

Memory usage

All the kinds of memory have to be considered and have their own interests. We used the constant memory to store the Gray code in the Langford problem. Despite its small size, it was a critical factor avoiding necessary re-computations. The texture memory, perfect for irregular data fetching, was a perfect area to store the neighbors' information for the Graph500 problem. Another very important part of the work is to focus on shared memory usage. Using the same data fetching instruction for all the threads of a WARP and providing shared memory information like for the neighbor search will lead to better performances. Another care has to be taken while considering the bank conflicts during fetching data.

Communication/computation overlapping

For accelerator programming, and especially GPUs, the execution on the device is asynchronous regarding the host. That behavior allows the host to either prepare more data or compute part of the solutions itself. We studied both cases for our benchmarks. This repartition shows interest in the computationally heavy problem like Langford and both CPU and GPU were computing part of the result simultaneously. For the Graph500 benchmark we were able to have an intensive usage of GPUs even if the communications are important and introducing CPUs in the computation did not allow to reach better performances. Empiric tests have to be made for the work distribution regarding the targeted problem. Another critical factor for performance was the utilization of streams since this feature allows to hide communication between the host and device by dividing the communication into smaller chunks and starting the computation while the data are sent.

Distribution on multi-GPU clusters

We showed that hybrid architectures handle multiple distribution strategies. The classical synchronous communications are perfectly handled and lead to good performances. We also used more complex start-stop systems, like best-effort, for the Langford problem. The GPU-Direct technology can also be vital in data driven applications like the Graph500 benchmark. This tool perfectly fits in the HPC environment and allows to reach even better performances.

From this preliminary study, on both applications, we showed that the hybrid architectures give really good results on different representative problems of HPC. The question that arises is now: what will be the behavior of GPUs confronted to both of those aspects together? In order to answer this question, we present in the next part the Smoothed Particle Hydrodynamics problem on which we base the last part of this study. We show that GPUs can also be used in this context, targeting domain scientists codes.

Part III

Application

Introduction

The first part of this thesis presented the tools needed to understand and target performances in HPC. The second part exposed our metric benchmarks provided to test HPC architectures when confronted to the main performances walls, and then showing the benefit of accelerators, in this case GPUs, over classical processors in the two contexts addressed: irregular computation and irregular communication/memory behaviors. We showed that accelerators give a real advantage on these two problems and even allow us to push the limits of performances. We are confident that hybrid architectures will be the way to reach exascale in 2020.

In order to validate our previous results and our metric we decided to target another irregular behavior problem embedding both computation and communication/memory wall over an irregular behavior. This problem can also be considered as a *realistic production* code as it targets current problems of domain scientists. In order to show how accelerators handle real world problems, we searched for an application fulfilling our needs. Our choice fell on the Smoothed Particle Hydrodynamics problem applied to fluid and astrophysics simulation.

We targeted this problem for several reasons. In the first chapter of this part we show the computer science implementation issues and limitations. We present the elements making this application a perfect choice for our metric. This project is also part of an exchange with the Los Alamos National Laboratory in New Mexico, USA. This laboratory is part of the U.S. Department of Energy, DoE, and groups thousands of researchers working on the most advanced nowadays problems. The Los Alamos National Laboratory, LANL, is also one of the three nuclear research facilities of the U.S. National Nuclear Security Administration (NNSA). In the summer of 2016, I had my first internship for a three months period during a program called: *Co-Design Summer School*. This allowed us to discover a particular class of problems, Smoothed Particle Hydrodynamics, and exchange with computer scientists and domain scientists. We extrapolated after the internship and saw what this problem means in a production context and its utility for our study. It represents a perfect example of realistic problem confronting computation and communication walls, with irregular behavior. In order to characterize what physicists requested for this problem, I had a second internship at the LANL in the summer of 2017 for three months.

In this part, we first present the Smoothed Particle Hydrodynamics method from a physical point of view and draw a parallel with the computer science problems involved. Indeed, a huge amount of time has been spent on the understanding of the physics side to be able to do realistic simulations and thus realistic behavior. The second chapter presents a distributed SPH implementation designed for multi-CPU and multi-GPU. The program is called FleCSPH. Starting from FleCSI, the framework which is the base of FleCSPH, we introduce the algorithm and methods needed to efficiently solve this problem on classical processor and the acceleration generated adding GPUs.

Chapter 6

Complex system choice and modelization

6.1 Introduction

In this chapter, we give details on our choice for a generic complex system which encounters several problematics. A complex system is a problem which gathers several layers of complexity. In our case, these complexities are the physics modelization and the computer science implementation with many sub-problems like computation and communication walls with underlying high irregularity.

The problem we choose, the Smoothed Particle Hydrodynamics simulation method, is described on a physical aspect. We point out the difficulties involved in the implementation on supercomputers and especially hybrid architectures. A lot of work was spent on the comprehension of the physical aspects to produce a code that meets the behavior of real astrophysics simulations.

The first section is a presentation of the SPH method and the overall limitations we have to face. Then we describe different types of specific simulations we used as a benchmark of the application, and the application obtained is a good benchmark candidate for testing architectures for computational and communication walls combined with irregular behavior.

6.2 Physical modelization and downsides

We identified two main walls in our metric. The computational, the communication and the memory walls. We conducted tests on all aspects keeping the irregularity behavior as a good representative of production codes. We show how these requirements are met in the same problem with SPH and gravitation. We targeted astrophysical simulations in order to add another complexity layer in term of irregularity for both computation and communication. They require the computation of gravitation in addition to SPH on a very high number of particles. This part describes the SPH method itself and the gravitation computation based on fast multipole methods.

6.2.1 Smoothed Particles Hydrodynamics

Smoothed Particle Hydrodynamics (SPH) is an explicit numerical mesh-free Lagrangian method. It is used to solve hydrodynamical partial differential equations (PDEs) by discretized them into a set of fluid elements called particles. This computational method was invented for the purpose of astrophysics simulations by Monaghan, Gingold and Lucy in 1977 [Luc77, GM77]. This first SPH work conserved mass and they later proposed a method which also conserved linear and angular momenta [GM82]. The method was extended for general fluid simulations and many other fields from ballistics to oceanography. The development of new reliable, parallel and

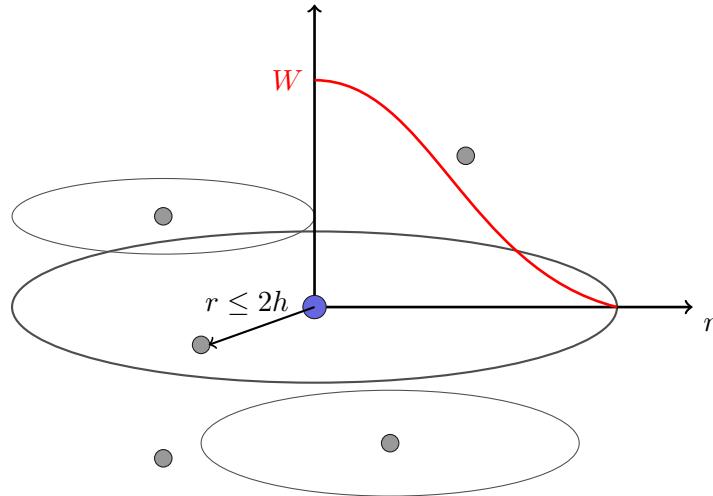


Figure 6.1: SPH kernel W and smoothing length h representation

distributed tools for this method is a challenge for future HPC architectures with the upcoming Exascale systems.

The method, as illustrated in figure 6.1, computes the evolution of a group of particles representing physical quantities. Those physical quantities are either invariant or computed for every particle at each step regarding its neighbors in the radius of its smoothing length h . The particles in this radius are then valued according to their distance using a smoothing function W , also called a kernel. The fundamental SPH formulation computes the physical value of any quantity A of a particle a regarding its neighbors' particles b by:

$$A(\vec{r})_a \simeq \sum_b \frac{m_b}{\rho_b} A(\vec{r}_b) W(|\vec{r} - \vec{r}_b|, h) \quad (6.1)$$

On a physics aspect, this method has several advantages: it can handle deformations, low densities, vacuum and makes particle tracking easier. It also conserves mass, linear and angular momenta and energy by its construction that implies independence of the numerical resolution. Another strong benefit of using SPH is its exact advection of fluid properties. Furthermore, the particle structure of SPH easily combines with tree methods for solving Newtonian gravity through N-body simulations. As a mesh-free method, it avoids the need of grid to calculate the spatial derivatives.

However, there are cons to consider using SPH: it cannot be extended to all PDE formulations; it requires careful setup of initial distribution of particles; further, it can be difficult to resolve turbulence-dominated flows and special care must be taken when handling high gradients such as shocks and surface structure of neutron stars. Many works are exploring how to handle more cases and to push the limitations of this method [DRZR17, LSR16, RDZR16].

In this work, we are solving Lagrangian conservation equations (Euler equations) for density, energy and momentum of an ideal fluid [LL59] such that:

$$\frac{d\rho}{dt} = -\rho(\nabla \cdot \vec{v}), \quad \frac{du}{dt} = -\frac{P}{\rho}(\nabla \cdot \vec{v}), \quad \frac{d\vec{v}}{dt} = -\frac{1}{\rho}(\nabla P) \quad (6.2)$$

with ρ the density, P the pressure, u the internal energy and v the velocity, ∇ the nabla operator and where $d/dt = \partial/\partial_t + \vec{v} \cdot \nabla$ which is convective derivative.

By using the volume element $V_b = m_b/\rho_b$, we can formulate the Newtonian SPH scheme [Ros09] such that:

$$\rho_a = \sum_b m_b W_{ab}(h_a) \quad (6.3)$$

$$\frac{du_a}{dt} = \frac{P_a}{\rho_a^2} \sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab} \quad (6.4)$$

$$\frac{d\vec{v}_a}{dt} = - \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla_a W_{ab} \quad (6.5)$$

where $W_{ab} = W(|\vec{r}_a - \vec{r}_b|, h)$ is the smoothing kernel. The equations we would like to solve allow for emergence of discontinuities from smooth initial data. At discontinuities, the entropy increases in shocks. That dissipation occurs inside the shock-front. The SPH formulation here is inviscid so we need to handle this dissipation near shocks. There are a number of way to handle this problem, but the most widespread approach is to add artificial viscosity (or artificial dissipation) terms in SPH formulation such that:

$$\left(\frac{du_a}{dt} \right)_{art} = \frac{1}{2} \sum_b m_b \Pi_{ab} \vec{v}_{ab} \cdot \nabla_a W_{ab} \quad (6.6)$$

$$\left(\frac{d\vec{v}_a}{dt} \right)_{art} = - \sum_b m_b \Pi_{ab} \nabla_a W_{ab} \quad (6.7)$$

In general, we can express the equations for internal energy and acceleration with artificial viscosity as:

$$\frac{du_a}{dt} = \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{\Pi_{ab}}{2} \right) \vec{v}_{ab} \cdot \nabla_a W_{ab} \quad (6.8)$$

$$\frac{d\vec{v}_a}{dt} = - \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \nabla_a W_{ab} \quad (6.9)$$

Π_{ab} is the artificial viscosity tensor. As long as Π_{ab} is symmetric, the conservation of energy, linear and angular momentum is assured by the form of the equation and antisymmetric of the gradient of kernel with respect to the exchange of indices a and b . Π_{ab} may define in different ways and here we use [MG83] such as:

$$\Pi_{ab} = \begin{cases} \frac{-\alpha \bar{c}_{ab} \mu_{ab} + \beta \mu_{ab}^2}{\bar{\rho}_{ab}} & \text{for } \vec{r}_{ab} \cdot \vec{v}_{ab} < 0 \\ 0 & \text{otherwise} \end{cases} \quad (6.10)$$

$$\mu_{ab} = \frac{\bar{h}_{ab} \vec{r}_{ab} \cdot \vec{v}_{ab}}{r_{ab}^2 + \epsilon \bar{h}_{ab}^2} \quad (6.11)$$

Using the usual form c_s as $c_s = \sqrt{\frac{\partial p}{\partial \rho}}$. The values of ϵ , α and β have to be set regarding the problem targeted. As an example, we used for the Sod shock tube problem: $\epsilon = 0.01h^2$, $\alpha = 1.0$ and $\beta = 2.0$.

There are many possibilities for the smoothing function, called the kernel. For example, the Monaghan's cubic spline kernel is given by:

$$W(\vec{r}_{ij}, h) = \frac{\sigma}{h^D} \begin{cases} 1 - \frac{3}{2}q^2 + \frac{3}{4}q^3 & \text{if } 0 \leq q \leq 1 \\ \frac{1}{4}(2-q)^3 & \text{if } 1 \leq q \leq 2 \\ 0 & \text{otherwise} \end{cases} \quad (6.12)$$

where $q = r/h$, r the distance between the two particles, D is the number of dimensions and σ is a normalization constant with the values:

$$\sigma = \begin{cases} \frac{2}{3} & \text{for 1D} \\ \frac{10}{7\pi} & \text{for 2D} \\ \frac{1}{\pi} & \text{for 3D} \end{cases} \quad (6.13)$$

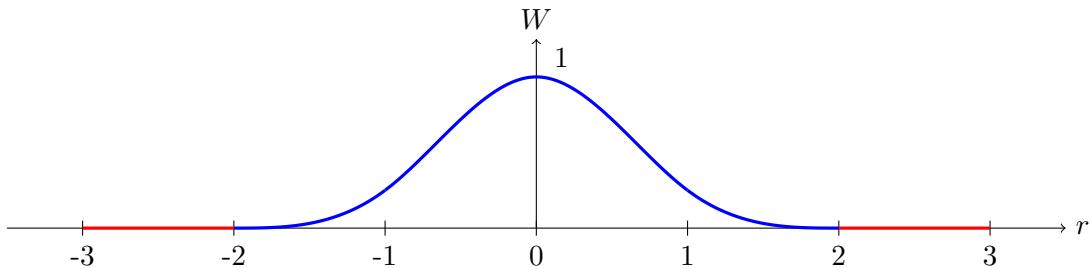


Figure 6.2: Cubic spline kernel example with $\sigma = 1$ and $h = 1$

In the computation of forces, we need to apply the gradient of the smoothing kernel. This is, in our example, for the cubic spline kernel:

$$\vec{\nabla}_i W(r_{ij}, h) = \frac{\sigma}{h^{D+1}} \times \begin{cases} \left(-\frac{3}{h} + \frac{9}{4h}q\right)r_{ij}, & \text{si } 0 \leq \frac{r}{h} < 1 \\ \left(\frac{-3}{r} + \frac{3}{h} - \frac{3}{4h}q\right)r_{ij}, & \text{si } 1 \leq \frac{r}{h} < 2 \\ 0, & \text{si } \frac{r}{h} \geq 2 \end{cases} \quad (6.14)$$

Figure 6.2 is a representation of the cubic spline kernel with $\sigma = 1$ and $h = 1$. The abscissa axis represents r , distance between the particles and the ordinate the value of the smoothing kernel. When the support of the function, 2 is reached the particles are ignored $W = 0$, represented in red on the figure.

To sum up, the SPH resolution scheme and its routines are presented on algorithm 5. The Equation of State (EOS) and the integration are problem dependent and will be define for each test case in section 6.3.

Algorithm 5 SPH loop algorithm

- 1: **while** not last step **do**
 - 2: Compute density for each particle (6.3)
 - 3: Compute pressure using EOS
 - 4: Compute acceleration from pressure forces (6.9)
 - 5: Compute change of internal energy for acceleration (6.8)
 - 6: Advance particles after integration
 - 7: **end while**
-

The main downside for the implementation of this method is the requirement for local computation on every particle. The particles have to be grouped locally to perform the computation of (6.3), (6.8) and (6.9). A communication step is needed before and after (6.3) to get the local physical data to be able to compute (6.8) and (6.9). The tree data structure allows us to perform $O(N \log(N))$ neighbor search, but also add a domain decomposition and distribution layer.

6.2.2 Gravitation

We decided to simulate astrophysical events in order to target hard irregular simulation facing both the communication and computation wall in irregular behavior. This choice is also accurate since our code, FleCSPH, will be used by the LANL astrophysicists in the near future. In order to perform these simulations, the computation of gravitation/self-gravitation is required. This part presents our implementation choice and expose the main problems for HPC implementation.

For classical problems, like fluid flow, the gravitation can directly be applied on the particles with the force:

$$\vec{a}_g = m\vec{g} \quad (6.15)$$

In order to consider astrophysics problems, we need to introduce self-gravitation and gravitation. Each particle implies an action on the others based on its distance and mass. The

equation of gravitation for a particle i with j other particles is:

$$\vec{f}_{ai} = \sum_j -G \frac{m_i m_j}{|\vec{r}_i - \vec{r}_j|^3} \vec{r}_{ij} \quad (6.16)$$

This computation involve an $O(N^2)$ complexity and thus is not applicable directly. We applied the method called Fast Multipole Method (FMM) discussed in [BG97]. This method is perfectly adapted to a tree representation of the domain and particles.

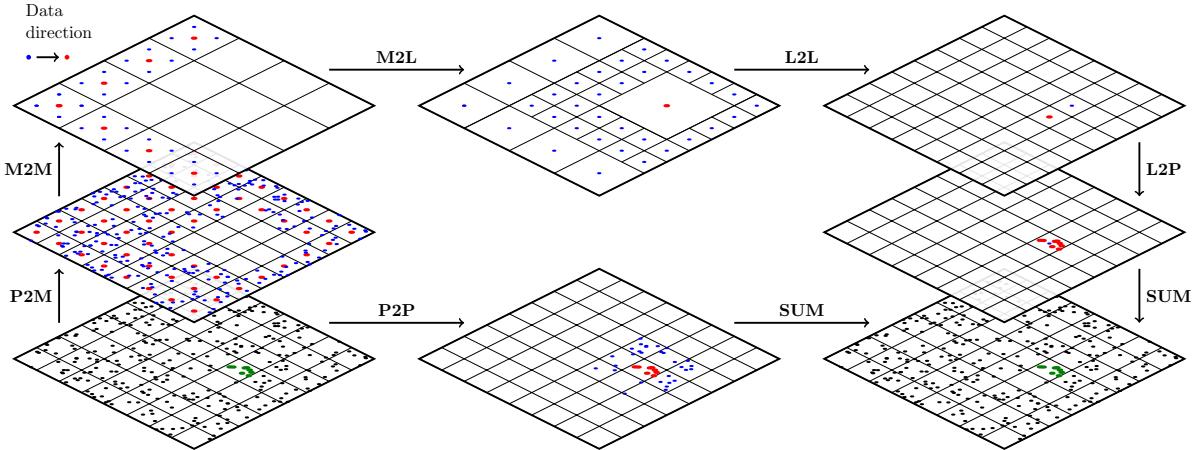


Figure 6.3: Fast Multipole Method schematics. Particles to Multipole (P2M), Multipole to Multipole (M2M), Multipole to Particles (M2P), Multipole to Local (M2L), Local to Local (L2L) and Particles to Particles (P2P). Schematic inspired from [YB11]

This method aims to compute the gravitation up to an approximation determined by the user. Details are given in figure 6.3, from left bottom to right bottom for a group of particles. We identify three main actors in this method:

Particles: the bodies on which we need to compute the gravitation regarding the other particles. In figure 6.3 we separate the green particles, on which we are computing the gravitation, from the other blue particles.

Multipoles: the center of mass for a group of particles. In our example, they regroup the mass and barycenter of the sub-particles. There are several levels of multipoles: particles' multipole and multipoles' multipole.

Locals: the center of mass for the reduction on the particles concerned in this walk. They have the same behavior as the multipoles, but the information goes down to particles instead of up.

In order to compute the gravitation for a group of particles in the domain the steps are:

Particles to Particles (P2P): For the particles that are close, use the direct $O(N^2)$ algorithm. This is the part that grow if the user desires more accurate results.

Particles to Multipoles (P2M): Gathers the data of all the sub-particles to the centers of mass, the multipoles. This is the first layer of the tree, the leaves.

Multipoles to Multipoles (M2M): Gathers the data of multipoles on higher level of the tree from the leaves to the root.

Multipoles to Local (M2L): Computes the gravitation part of all the distant multipole to the local.

Local to Local (L2L): Goes down in the tree and spread the component to sub-locals.

Local to Particles (L2P): When a leaf of the tree is reached, computes the application of the local for all sub-particles.

Summation: At the end of the computation for both P2P and L2P the two interactions can be summed up to compute the gravitation applied to the particles.

This scheme has to be repeat for every group of particles. The P2M-M2M steps are done just once before the FMM method for all the groups of particles. We use a criterion call Multipole Acceptance Criterion (MAC) for the choice between either P2P or M2L. In this study we used an angle between the local center of mass and the edge of distant multipole. If the angle fits the criterion we use the current multipole, otherwise we go lower in the tree to consider smaller multipole. If the criterion never matches, we are too close and consider P2P.

For the P2P step, the classical gravitation computation is used, like presented in equation 6.16. But for the interaction with distant multipoles, we use a Taylor series.

The gravitation function of equation 6.16 can be approximate on a particle at position \vec{r} by the gravitation computed at the centroid at position \vec{r}_c :

$$\vec{f}(\vec{r}) = \vec{f}(\vec{r}_c) + \left\| \frac{\partial \vec{f}}{\partial \vec{r}} \right\| \cdot (\vec{r} - \vec{r}_c) + \frac{1}{2} (\vec{r} - \vec{r}_c)^T \cdot \left\| \frac{\partial^2 \vec{f}}{\partial \vec{r} \partial \vec{r}} \right\| \cdot (\vec{r} - \vec{r}_c) \quad (6.17)$$

From equation 6.16 we compute the term $\left\| \frac{\partial \vec{f}}{\partial \vec{r}} \right\|$:

$$\frac{\partial \vec{f}}{\partial \vec{r}} = - \sum_p \frac{m_p}{|\vec{r}_c - \vec{r}_p|^3} \begin{bmatrix} 1 - \frac{3(x_c - x_p)(x_c - x_p)}{|\vec{r}_c - \vec{r}_p|^2} & -\frac{3(y_c - y_p)(x_c - x_p)}{|\vec{r}_c - \vec{r}_p|^2} & -\frac{3(z_c - z_p)(x_c - x_p)}{|\vec{r}_c - \vec{r}_p|^2} \\ -\frac{3(x_c - x_p)(y_c - y_p)}{|\vec{r}_c - \vec{r}_p|^2} & 1 - \frac{3(y_c - y_p)(y_c - y_p)}{|\vec{r}_c - \vec{r}_p|^2} & -\frac{3(z_c - z_p)(y_c - y_p)}{|\vec{r}_c - \vec{r}_p|^2} \\ -\frac{3(x_c - x_p)(z_c - z_p)}{|\vec{r}_c - \vec{r}_p|^2} & -\frac{3(y_c - y_p)(z_c - z_p)}{|\vec{r}_c - \vec{r}_p|^2} & 1 - \frac{3(z_c - z_p)(z_c - z_p)}{|\vec{r}_c - \vec{r}_p|^2} \end{bmatrix} \quad (6.18)$$

And we propose a compact version of the matrix with:

$$\left\| \frac{\partial f^a}{\partial r^b} \right\| = - \sum_c \frac{m_c}{|\vec{r} - \vec{r}_c|^3} \left[\delta_{ab} - \frac{3 \cdot (r^a - r_c^a)(r^b - r_c^b)}{|\vec{r} - \vec{r}_c|^2} \right] \quad (6.19)$$

With δ_{ab} the Kronecker delta:

$$\delta_{ab} = \begin{cases} 1, & \text{if } a = b. \\ 0, & \text{if } a \neq b. \end{cases} \quad (6.20)$$

We note that a and b variate from 0 to 2 and $r^0 = x$, $r^1 = y$ and $r^2 = z$ as usual sense.

For the term $\left\| \frac{\partial^2 \vec{f}}{\partial \vec{r} \partial \vec{r}} \right\|$ we give the compact version by:

$$\left\| \frac{\partial^2 f^a}{\partial r^b \partial r^c} \right\| = - \sum_c \frac{3m_c}{|\vec{r} - \vec{r}_c|^5} \left[\frac{5(r^a - r_c^a)(r^b - r_c^b)(r^c - r_c^c)}{|\vec{r} - \vec{r}_c|^2} - \left(\delta_{ab}(r^c - r_c^c) + \delta_{bc}(r^a - r_c^a) + \delta_{ac}(r^b - r_c^b) \right) \right] \quad (6.21)$$

The equations 6.19 and 6.21 are use during the M2L step. We use equation 6.17 during the tree traversal and apply the gravitation to locals and then particles in L2L and L2P.

This method imposes a lot of communications and exchanges between the processes. The particles are separate for each process in our distributed version. Indeed, as each of the processes will hold part of the particles, the multipole in M2L computation imposes to share data. The P2P computation will face issues on the edge of each sub-domain. The irregular behavior is also present for the choice of the multipole to consider during the M2L step based on the MAC criterion.

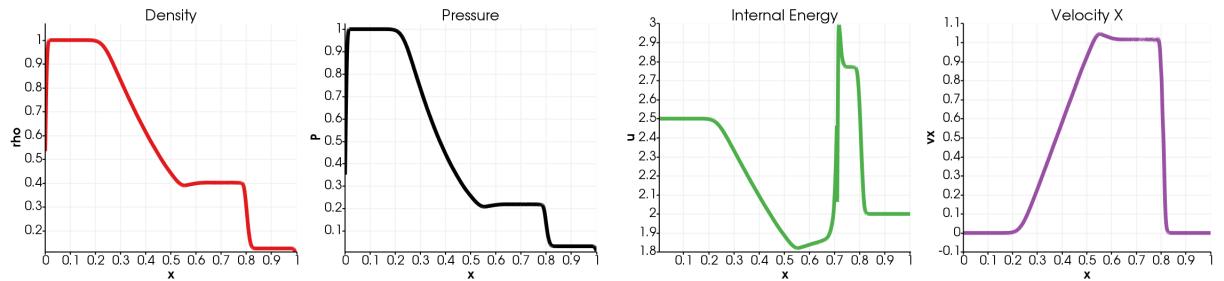


Figure 6.4: Sod shock tube with FleCSPH

6.3 Test cases with SPH

The generic SPH method and the gravitation computation, either simple or with FMM, allow us to run standard example to check the physical accuracy of our code. We choose four mains examples in this purpose: the Sod shock tube, the Sedov blast wave, fluid flow simulation and astrophysical examples like binary neutron stars coalescence. We present those problems in this section and their characteristics regarding the computer science difficulties involved.

6.3.1 Simple tests: tree and communications

Sod shock tube

The Sod shock tube is the test consisting of a one-dimensional Riemann problem with the following initial parameters [Sod78].

$$(\rho, v, p)_{t=0} = \begin{cases} (1.0, 0.0, 1.0) & \text{if } 0 < x \leq 0.5 \\ (0.125, 0.0, 0.1) & \text{if } 0.5 < x < 1.0 \end{cases} \quad (6.22)$$

In our code, we use the same initial data as in section 6.2.1 with ideal gas EOS such as:

$$P(\rho, u) = (\Gamma - 1)\rho u \quad (6.23)$$

where Γ is the adiabatic index of the gas, we set $\Gamma = 5/3$.

This test is used to check the physical accuracy of the code and thus the tree search itself. A simulation of our Sod shock experimentation is presented on figure 6.4 and shows physically correct results. The first difficulty of this problem is the tree repartition, the physics behind is not complicated and does not involve specific optimizations.

Sedov blast wave

A blast wave is the pressure and flow resulting from the deposition of a large amount of energy in a small very localized volume. There are different versions of blast wave test and we consider comparing it with the analytic solution for a point explosion as given by Sedov [Sed46], making the assumption that the atmospheric pressure relative to the pressure inside the explosion negligible. Here, we test 2D blast wave. In this simulation, we use ideal gas EOS with $\Gamma = 5/3$ and we are assuming that the undistributed area is at rest with a pressure $P_0 = 1.0^{-5}$. The density is constant ρ_0 , also in the pressurized region.

An example of our Sedov Blast wave experimentation is presented on figure 6.5 and shows physically correct results. This problem has the same conclusion as the Sod shock tube, his purpose is the test the tree behavior with 2 dimensions.

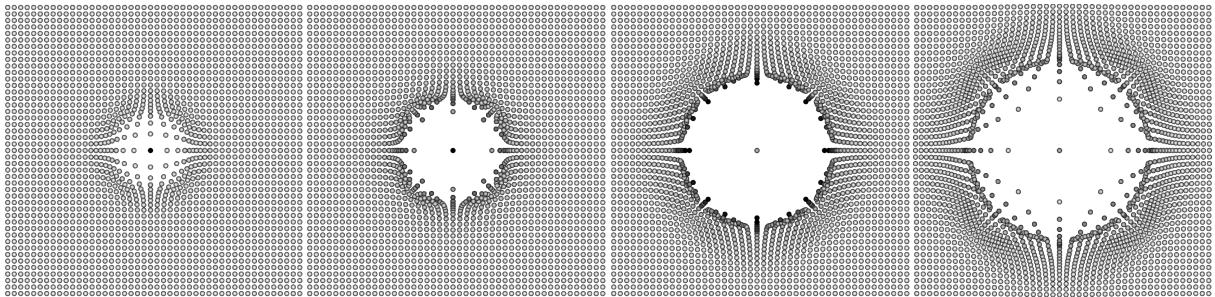


Figure 6.5: Sedov Blast Wave with FleCSPH at respectively $t = 0.01$, $t = 0.03$, $t = 0.06$ and $t = 0.1$

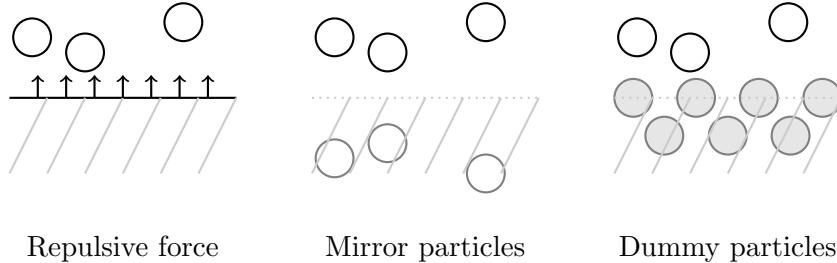


Figure 6.6: Different boundaries condition methods

6.3.2 High number of particles and specific formulation

After performing the tests regarding the physics reliability, we worked on fluid flow problem in 2D and 3D to reach high number of particles. The details can be found in [GGRC⁺12]. This test is based on an ideal EOS given by:

$$P = B \left[\left(\frac{\rho}{\rho_0} \right)^\gamma - 1 \right] \quad (6.24)$$

with $\gamma = 7$ and $B = c_0 \rho_0 / \gamma$ being $\rho_0 = 1000 \text{ kg.m}^{-3}$ the reference density.

Boundary conditions

For this experiment, realistic boundaries conditions were needed. Several methods are possible with SPH and we focused on the main ones: the repulsive wall, the mirror particles [LP91] and the dummies particles implementation [AHA12]. Those boundaries conditions implementation are presented in figure 6.6.

On our first implementation we used repulsive forces, but they imposed a lot of computation during the integration step and does not handle all the shape of boundaries easily.

For the current implementation we used the dummies particles method. This method is accurate and allows us to consider all the shape of boundaries. The wall particles are just considered as normal particles, with specific equations and their quantities are evolved during the run. The main difference is that their position does not evolve at the end of the step. They are identified in the code with a specific type, provided during the data generation.

In this fluid flow example, we were able to go up to a high number of particles with 2 or 3 dimensions. The handling of boundaries conditions added a pressure on the irregularity behavior.

6.3.3 SPH and gravitation

The final aim of our tests is to simulate astrophysical events. We are interested in one of the most important event recently discovered. Last year the Laser Interferometer Gravitational

Wave, LIGO, detected the first gravitational wave generated by binary neutron stars merging [AAA⁺17b] and also more complexes event with Binary Black Holes coalescence in [AAA⁺17a]. We decided to conduct tests on Binary Neutron Star, BNS, coalescence. This problem represents all the aspect needed in our benchmark with the SPH method but also the self-gravitation and gravitation computation. In order to perform realistic simulations, we consider two stars that are stable. We give details on the way to generate those data and the physics of the fusion itself. A lot of work have been involved in this understanding since it is quite out of the field of the primary researches.

The generation of initial data for binary neutron star merging is quite complicated. The first step is to generate the profile of mass regarding the radius of the star. This is made using the Lane-Emden equation. As those data are generated based on a grid with a fixed smoothing length in our case we need to add an extra step for relaxation. We used two relaxation methods with the Roche Lobe and Darwin problems. The last step before the merging is to position the stars and add the rotation velocity.

Solving Lane-Emden Equation

In order to consider BNS we first consider two individual stars. The star is characterized by its radius and mass but also the density repartition inside. Indeed, we have to determine the density function based on the radius. For this purpose, we used the so-called Land-Emden equation.

As we consider the star as a polytropic fluid, we use the equation of Lane-Emden which is a form of the Poisson equation:

$$\frac{d^2\theta}{d\xi^2} + \frac{2}{\xi} \frac{d\theta}{d\xi} + \theta^n = 0 \quad (6.25)$$

With ξ and θ two dimensionless variables. There are only exact solutions for a polytropic index $n = 0.5, 1$ and 2 . In our work we use a polytropic index of 1 which can correspond to a NS simulation.

For $n = 1$ the solution of equation 6.25 is:

$$\theta(\xi) = \frac{\sin(\xi)}{\xi} \quad (6.26)$$

We note $\xi_1 = \pi$, the first value of ξ with $\theta(\xi) = 0$. $\theta(\xi)$ is also defined as:

$$\theta(\xi) = \left(\frac{\rho(\xi)}{\rho_c} \right)^{\frac{1}{n}} = \frac{\rho(\xi)}{\rho_c} \quad (6.27)$$

With ρ_c the internal density of the star and ρ the density at a determined radius. ξ is defined as:

$$\xi = \sqrt{\frac{4\pi G}{K(n+1)}} \rho_c^{(n-1)/n} \times r = \sqrt{\frac{2\pi G}{K}} \times r = Ar \quad (\text{for } n = 1 \text{ and } A = \sqrt{\frac{2\pi G}{K}})$$

With K a proportionality constant, r the radius and G the gravitational constant.

From the previous equations we can write the stellar radius R , the total radius of the star, as:

$$R = \sqrt{\frac{K(n+1)}{4\pi G}} \rho_c^{(1-n)/2} \xi_1 = \sqrt{\frac{K}{2\pi G}} \times \xi_1 \quad (\text{for } n = 1) \quad (6.28)$$

We note that for $n = 1$ the radius does not depend of the central density.

Here as an example, we use dimensionless units as $G = R = M = 1$ (for the other results we use CGS with $G = 6.674 \times 10^{-8} \text{ cm}^3 \text{ g}^{-1} \text{ s}^{-2}$) We can compute K as:

$$K = \frac{R^2 2\pi G}{\xi_1^2} \quad (6.29)$$

	NS ₁	NS ₂	NS ₃	NS ₄
Radius (cm)	$R = G = M = 1$	1500000	1400000	960000
K	0.636619	95598.00	83576.48	39156.94

Table 6.1: Examples of the proportionality constant K regarding the star stellar radius R

Figure 6.1 give example of radius and the proportionality constant K .

Then we deduce the density function of r as:

$$\rho(\xi) = \frac{\sin(A \times r)}{A \times r} \times \rho_c \text{ with } A = \sqrt{\frac{2\pi G}{K}}$$

As we know the total Mass M , the radius R and the gravitational constant G we can compute the central density as:

$$\rho_c = \frac{MA^3}{4\pi(\sin(AR) - AR\cos(AR))}$$

Then we normalize the results to fit $R = M = G = 1$: $K' = K/(R^2G)$, $m'_i = m_i/M$, $h'_i = h_i/R$, $\vec{x}'_i = \vec{x}_i/R$

Generating Binary Neutron Stars initial data

The initial data are based on a cubic lattice within a sphere of radius R . The density function, based on radius, $\rho(\vec{r})$ is known using the result of the Lane-Emden equation (we use polytropic index $n = 1$ here). The mass associate to each particle i of the total N particles:

$$m_i = \frac{\rho(\vec{r}_i)}{n_r} \text{ with } n_r = \frac{3N}{4\pi R^3}$$

The smoothing length is defined constant and the same for all particles for all the simulation:

$$h = \frac{1}{2} \sqrt{\frac{3N_N}{4\pi n}}$$

Here we choose N_N , the average number of neighbors, to be 100.

Relaxation

The last step is to perform a relaxation on the raw data. There are two methods we used: the Roche lobe and Darwin problems. In each of them we apply specific forces during a determined time for the particles to be stabilized.

Roche lobe problem: The Roche Lobe version is used to simulate the halo around the stars which is shaped like a tear-drop. For this Hydrostatic Equilibrium Models, we use a different equation of motion:

$$\frac{d\vec{v}_i}{dt} = \frac{\vec{F}_i^{Grav}}{m_i} + \frac{\vec{F}_i^{Hydro}}{m_i} + \vec{F}_i^{Roche} - \frac{\vec{v}_i}{t_{relax}} \quad (6.30)$$

With $t_{relax} \leq t_{osc} \sim (G\rho)^{-1/2}$ and where \vec{F}_i^{Roche} is:

$$\vec{F}_i^{Roche} = \mu(3+q)x_i\hat{\vec{x}} + \mu q y_i\hat{\vec{y}} - \mu z_i\hat{\vec{z}}$$

With μ to be determined (for us $\mu = 0.069$) and $q = \frac{M'}{M} = 1$ as the two polytropes have the same total mass. This is applied to each star to get the equilibrium and the simulate the tidal effect.

Darwin problem: This is the way we use to generate the final simulation. The equation of motion for the relaxation is now:

$$\frac{d\vec{v}_i}{dt} = \frac{\vec{F}_i^{Grav}}{m_i} + \frac{\vec{F}_i^{Hydro}}{m_i} + \vec{F}_i^{Rot} - \frac{\vec{v}_i}{t_{relax}} \quad (6.31)$$

With t_{relax} same as before and \vec{F}_i^{Rot} defined by:

$$\vec{F}_i^{Rot} = \Omega^2(x_i \vec{\hat{x}} + y_i \vec{\hat{y}}) \quad (6.32)$$

With $\Omega = \sqrt{\frac{G(M+M')}{a^3}}$, $L_z = Q_{zz}\Omega$ and $Q_{zz} = \sum_i(x_i^2 + y_i^2)$. At $t = 0$ we compute the total angular moment L_z which stay constant. Using it during the relaxation we can compute Ω as: $\Omega = \frac{L_z}{Q_{zz}}$ just by recomputing Q_{zz} . Here the scheme is in N^2 but just for the relaxation step.

For this relaxation we use two stars generated as before, applying equation of motion 6.31. Using a as the distance between the two polytropes (Here $a = 2.9$ for $R = 1$) and $\vec{\hat{x}}$ going for the center of the first to the second star and $\vec{\hat{z}}$ is like the rotation vector.

After the generation we are able to perform BNS coalescence. This provides us a code using SPH, self-gravity and gravitation.

This will be the perfect candidate to provide a benchmark for our study. First, a high computation cost with the SPH and FMM computation of hydrodynamics and gravitation. The problem size can grow accordingly to the number of particles but also their physical data like the number of neighbors. Secondly, a lot of communications for both SPH and FMM to share local particles and non-local center of mass. In completion of those two aspect, the irregularity provided by a huge number of particles moving in a 2D or 3D space at every iteration, making impossible the prediction of their position and values.

6.4 Conclusion

The problem we presented in this part fulfills all the objectives for our metric. The computation wall is targeted via the physics and gravitation computation. The communication wall on the other hand is central regarding the exchanges needed for SPH and the fast multipole method. This problem is also very irregular for both cases. Indeed, the particles move at every iteration without any prediction on their new position and data. In the same time the locality imposes a very high level of irregularity to reach efficiently all the neighbors of a specific particle. This implies the usage of a tree data structure and the work of our two metrics can be applied in this context.

As the SPH method is used in a large panel of fields from astrophysics to fluid mechanic, there are numerous related works. We can cite a code developed in the LANL, 2HOT [War13] that introduced the Hashed Oct Tree structure used in our implementation. There is also GADGET-2 [Spr05], GIZMO [Hop14] and the most recent publication is GASOLINE [WKQ17] based on PKDGRAV, a specific tree+gravity implementation. Several implementations already implement GPU code and tree construction and traversal, one can cite GOTHIC [MU17], presenting gravitational tree code accelerated using the latest Fermi, Kepler and Maxwell architectures. But a lot of GPU accelerated work still focused on fluid problems and not on astrophysical problems [HKK07, CDB⁺11]. We also note that these implementations focus on SPH problems and do not provide a general purpose and multi-physics framework as we intend to provide through FleCSI and FleCSPH. Several other works gave us hint for the best implementation of parallel and accelerated SPH [IABT11, IOS⁺14].

Our implementation has not to be considered as a revolution for the SPH method itself, neither the use of accelerators. This study provides a code easy to use by domain scientists moving the complexity of distribution, load balancing and accelerator use to the back-end framework. As it will be shown in next, this tool will allow us to push forward and provide different types

of accelerators in the future keeping a full transparency for the user. The application obtained, ready to be parallelized for HPC CPU architectures and then for hybrid HPC architectures, fulfills both computational and memory/communication walls. Thus, it seems to be a good candidate for testing HPC architectures.

Chapter 7

Complex simulations on hybrid architectures

7.1 Introduction

The previous part described the method we implement to set the last metric of our benchmark for hybrid architectures. It also presented the walls faced with smoothed particle hydrodynamics and gravitation. We showed that this application meets the communication and computation wall in an irregular behavior context.

We intend to target astrophysical simulation using hybrid architectures. This distributed multi-accelerator SPH and gravitation implementation is called FleCSPH. This is a complex application that, beside of being interesting for our purpose, needs to be accurate on the physics aspect to be used by the domain scientists from LANL.

This section gives details about the FleCSPH framework. We first present FleCSI, the base project in the Los Alamos National Laboratory on which FleCSPH is based. Then, we give details on the implementation itself and the tools we implemented to reach a working and efficient code. We give details on the domain decomposition strategy used with Morton Ordering. The tree traversal algorithm choices are then explained.

After this presentation of the native code using multi-CPU clusters we present our strategies for a multi-GPU implementation. The last section exposes the results for both implementation and the simulations.

A lot of code already exists for SPH simulation and some are already designed for hybrid architectures. The contribution of FleCSPH is, like FleCSI, to provide a transparent tool for domain scientists. Those frameworks provide a bunch of topologies and functions and will handle the load balancing and distribution for the domain scientists. This allows the computer scientists to keep track of last hardware evolution and provide efficient algorithms for them while the physicists/astrophysicists/chemists can focus on the simulations themselves. In this context FleCSPH has to take in charge the tree topologies and will be integrated in FleCSI later on.

7.2 FleCSI

FleCSI¹ [BMC16] is a compile-time configurable framework designed to support multi-physics application development. It is developed at the Los Alamos National Laboratory as part of the Los Alamos Ristra project. As such, FleCSI provides a very general set of infrastructure design patterns that can be specialized and extended to suit the needs of a broad variety of solver and data requirements. FleCSI currently supports multi-dimensional mesh topology, geometry, and

¹<http://github.com/laristra/flecsi>

adjacency information, as well as n-dimensional hashed-tree data structures, graph partitioning interfaces, and dependency closures.

FleCSI introduces a functional programming model with control, execution, and data abstractions that are consistent both with MPI and with state-of-the-art, task-based runtimes such as Legion[BTSA12] and Charm++[KK93]. The abstraction layer insulates developers from the underlying runtime, while allowing support for multiple runtime systems including conventional models like asynchronous MPI.

The intent is to provide developers with a concrete set of user-friendly programming tools that can be used now, while allowing flexibility in choosing runtime implementations and optimization that can be applied to future architectures and runtimes.

FleCSI's control and execution models provide formal nomenclature for describing poorly understood concepts such as kernels and tasks. FleCSI's data model provides a low-buy-in approach that makes it an attractive option for many application projects, as developers are not locked into particular layouts or data structure representations.

FleCSI currently provides a parallel but not distributed implementation of Binary, Quad and Oct-tree topology. This implementation is based on space filling curves domain decomposition, the Morton order. The current version allows the user to specify the code main loop and the data distribution requested. The data distribution feature is not available for the tree data structure needed in our SPH code and we provide it in the FleCSPH implementation. The next step will be to incorporate it directly from FleCSPH to FleCSI as we reach a decent level of performance. As FleCSI is an on-development code the structure may change in the future and we keep track of these updates in FleCSPH.

Based on FleCSI the intent is to provide a binary, quad and oct-tree data structure and the methods to create, search and share information for it. In FleCSPH this will be dedicated, apply and tested on the SPH method. In this part we first present the domain decomposition, based on space filling curves, and the tree data structure. We describe the HDF5 files structure used for the I/O. Then we describe the distributed algorithm for the data structure over the MPI processes.

7.3 Distributed SPH on multi-core architectures

Before going further in the SPH implementation and our development, we need to give details on the algorithm and the work involved. The general algorithm is presented on algorithm 6

Algorithm 6 SPH implementation

```

1: Read particles from file
2: while not last step do
3:   Generate keys for particles
4:   Load balance particles
5:   Generate local tree data structure
6:   while Physics not done do
7:     Physics: search and distributed search
8:     Update data
9:   end while
10:  Gravitation = FMM
11:  if Output step then
12:    Output data in H5part format
13:  end if
14: end while
```

and shows the features of SPH exposed in the previous section. In this section we present the main features of our code and the problems involved: the domain decomposition, the tree data

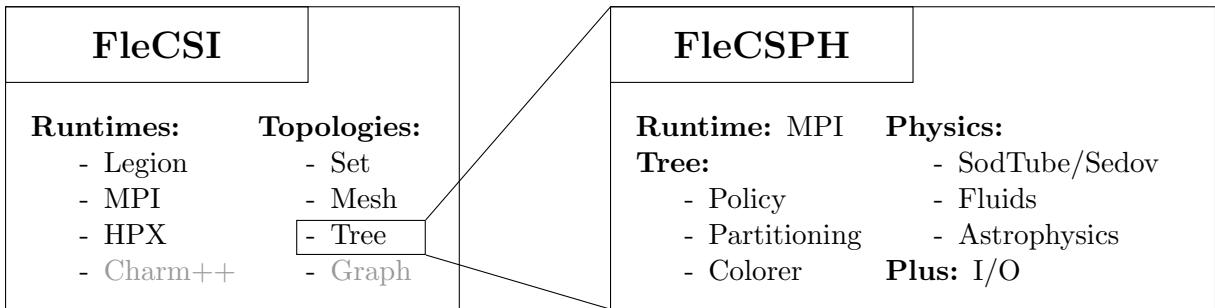


Figure 7.1: FleCSI and FleCSPH frameworks

structure and traversal and our distribution strategy. This project, in collaboration with the LANL, is named FleCSPH.

FleCSPH² is a framework initially created as a part of FleCSI. The purpose of FleCSPH is to provide a data distribution and communications patterns to use the tree topology provided in FleCSI applied to SPH. The final purpose of FleCSPH is to complement the tree topology and provide the *colorer* to FleCSI. The distribution strategies associate to a data structure. As presented in the previous sections, SPH is a very good candidate to benchmark the binary, quad and oct tree topology. The demand is high for astrophysics simulation regarding the recent discoveries of the LIGO and the SPH method allows us to generate those simulations. Figure 7.1 presents how FleCSI and FleCSPH are integrated. FleCSPH is based on the tree topology of FleCSI and follows the same structure define in FleCSI. The ideal runtime in FleCSI is Legion but this in-development code does not allow us to do more than static data distribution. This is why we decided to work with the MPI runtime in FleCSPH. Those MPI functions can then be integrated to FleCSI to generate group of particles and labeled them, the coloring.

Figure 7.2 present the file systems of the github repository. We use the tools from Cinch⁴ developed at LANL for the CMake and the makefile generation. It also provides the GoogleTests API for our unit tests. The FleCSPH code is currently public and available on github under the *laristra* (Los Alamos Ristra) project. The continuous integration is ensured by using Travis based on Docker and *Dockerfiles* provided in the Docker folder. In addition to Travis for the unit tests we use tools as CodeCov⁵ for the code coverage and SonarQube⁶ for the quality gates. In the current version we use external libraries: HDF5, H5hut and a specific library for I/O based on H5hut. Those elements are present and installed using scripts in *third-part-library* folder.

For the first implementation we present the code without considering accelerators. We intent to provide an efficient multi-CPU distributed code. The description starts with the domain decomposition strategy which is a basic element for the tree implementation. We explain the tree data structure for the construction and the search of particles along with the distribution strategy.

7.3.1 Domain decomposition

The number of particles can be high and represent a huge amount of data that does not fit in a single node memory. This implies the distribution of the particles over several computational nodes. As the particles moves during the simulation the static distribution is not possible and they have to be redistributed at some point in the execution. Furthermore, this distribution need to keep local particles in the same computation node to optimize the exchanges and computation itself.

²<http://github.com/laristra/flecsph>

⁴<http://github.com/laristra/cinch>

⁵<http://codecov.io>

⁶<http://sonarqube.org/>

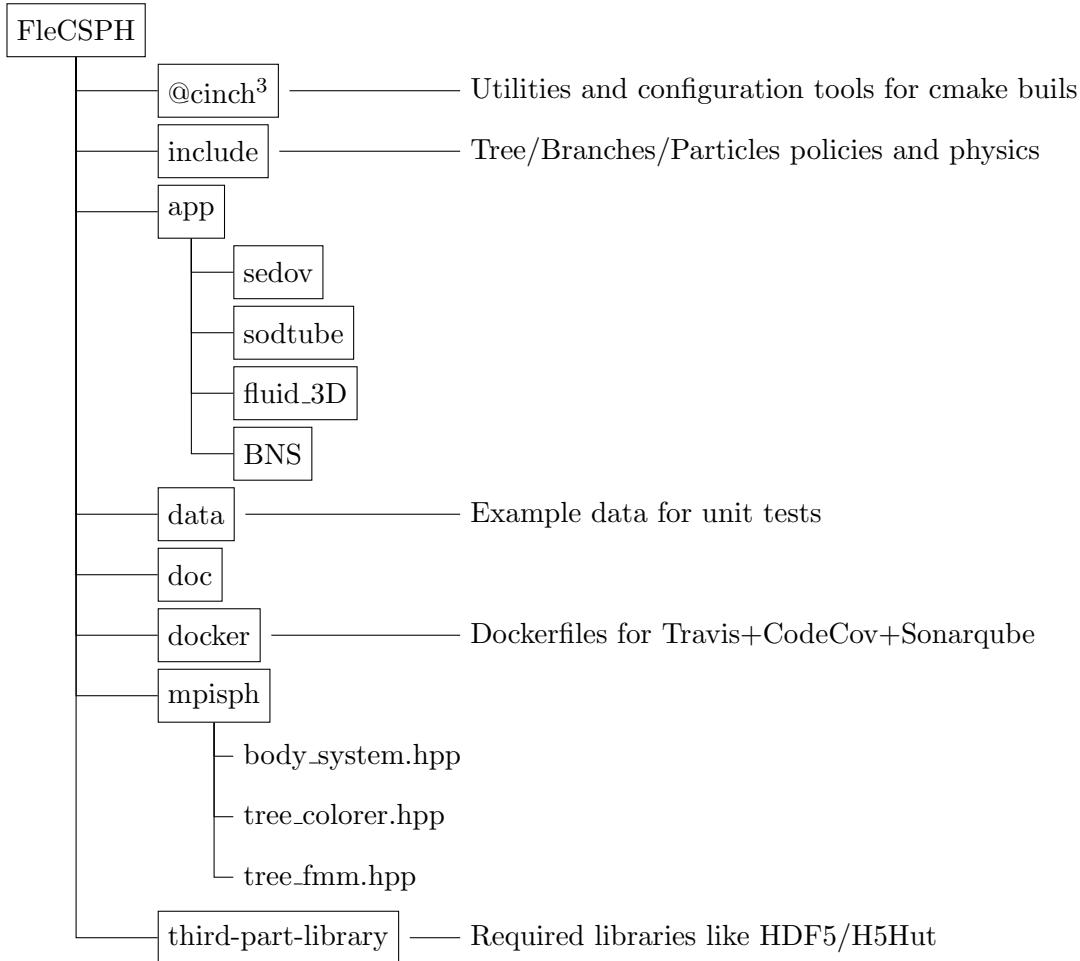


Figure 7.2: FleCSPH structures and files

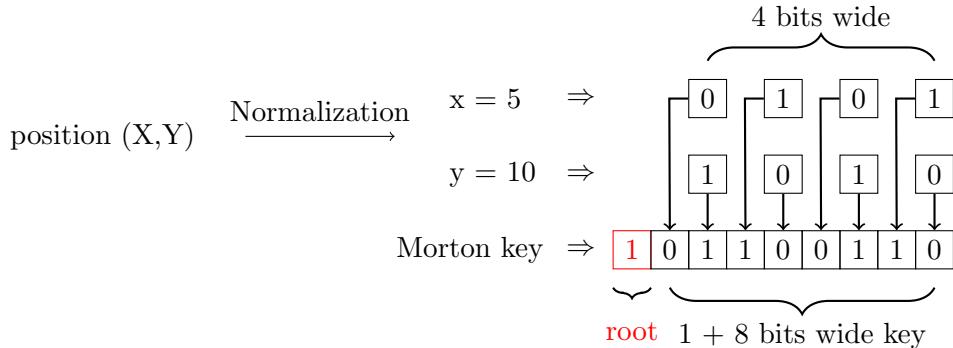


Figure 7.3: Morton order key generation

A common approach is to distribute the particles over computational nodes using *space filling curves* like in [War13, Spr05, BGF⁺14]. It intends to assign to each particle a key which is based on its spatial coordinates, then sorting particles based on those keys keeps particles grouped locally. Many space filling curves exists: Morton, Hilbert, Peano, Moore, Gosper, etc.

This domain decomposition is used in several layers for our implementation. On one hand, to spread the particles over all the MPI processes and provide a decent load balancing regarding the number of particles. On the other hand, it is also used locally to store efficiently the particles and provide a $O(N \log(N))$ neighbor search complexity, instead of $O(N^2)$, using a tree representation describe in part 7.3.2.

Several space filling curves can fit our purposes:

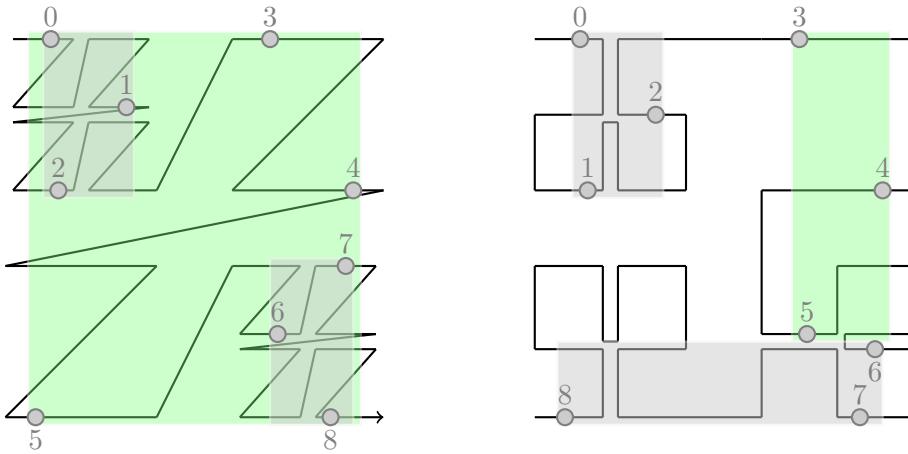


Figure 7.4: Morton and Hilbert space filling curves

The Morton curves

[Mor66], or Z-Order, is the most spread method. This method can produce irregular shape domain decomposition like shown in green on figure 7.4. The main advantage is to be fast to compute, the key is made by interlacing directly the X, Y and Z bits without rotations.

The Hilbert curves

[Sag12] are constructed by interlacing bits but also adding rotation based on the Gray code. This work is based on the Peano curves and also called Hilber-Peano. The construction is more complicated than Morton but allows a better distribution.

On figure 7.4, the Morton (left) and Hilbert (right) space-filling curves are represented in this example. The particles are distributed over 3 processes. The set of particles of the second process appears in green. As we can see there are discontinuities on the Morton case due to the Z-order "jump" over the space. This can lead to non-local particles and over-sharing of particles that will not be needed during the computation. In the Hilbert curve, the locality over the processes is conserved.

In this first implementation of FleCSPH we used the Morton ordering due to the computational cost. The next step of this work is to compare the computation time of different space filing curves.

Technically the keys are generated for each particle at each iteration because their position is expected to change over time. To be more efficient, the keys can stay the same during several steps and the final comparison can be made on the real particles positions. This increase the search time but allows less tree reconstructions.

We use 64 bits to represent the keys to avoid conflicts. The FleCSI code allows us to use a combination of memory words to reach the desired size of keys (possibly more than 64 bits) but this will cost in memory occupancy. The particle keys are generated by normalizing the space and then converting the floating-point representation to a 64 bits integer for each dimension. Then the Morton interlacing is done, and the keys are created. Unfortunately, in some arrangements, like isolated particles, or scenarios with very close particles, the keys can be either badly distributed or duplicate keys can appear. Indeed, if the distance between two particles is less than $2^{-64} \approx 1e-20$, in a normalized space, the key generated through the algorithm will be the same. This problem is then handle during the particle sort and then the tree generation. In both case two particles can be differentiate based on their unique ID generated at the beginning execution.

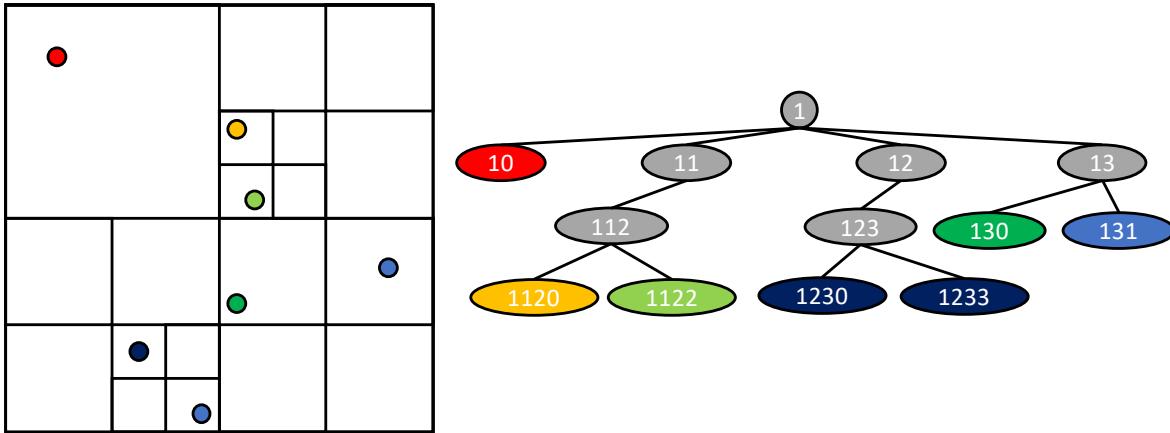


Figure 7.5: Quadtree, space and data representation

7.3.2 Hierarchical trees

The method we use for the tree data structure creation and research comes from Barnes-Hut trees presented in [BH86, Bar90]. By reducing the search complexity from $O(N^2)$ for direct summation to $O(N \log(N))$ it allows us to do very large simulations with billions of particles. It also allows the use of the tree data structure to compute gravitation using multipole methods.

We consider binary trees, for 1 dimension, quad-trees, for 2 dimensions, and oct-trees, for 3 dimensions. The construction of those trees is directly based on the domain decomposition using keys and space-filling curve presented in section 7.3.1.

As explained in the previous section, we use 64 bits keys. That gives us up to 63, 31 and 21 levels in the tree for respectively 1, 2 and 3 dimensions. As presented on figure 7.5 the first bit is used to represent the root of the tree, 1. This allows us to have up to 2^{63} different keys and unique particles.

Tree generation

After each particle gets distributed on its final process using its space-filling curve key, we can recursively construct the tree. Each particle is added, and the branches are created recursively if there is an intersection between keys. Starting from the root of key "1" the branches are added at each level until the particles are reached. An example of a final tree is shown on figure 7.5.

Tree search

When all the particles have been added, the data regarding the tree nodes are computed with a bottom up approach. Summing up the mass, position called Center of Mass (COM), and the boundary box of all sub-particles of this tree node.

For the search algorithm the basic idea would be to do a tree traversal for all the particles and once we reach a particle or a node that interact with the particle smoothing length, add it for computation or in a neighbor list. Beside of being easy to implement and to use in parallel this algorithm requires a full tree traversal for every particle and will not take advantage of the particles' locality.

Our search algorithm, presented on Algorithm 7, is a two-step algorithm like in Barnes trees: First create the interaction lists and then using them on the sub-tree particles. In the first step we look down for nodes with a target sub-mass of particles $tmass$. Then for those branches we compute an interaction list and continue the recursive tree search. When a particle is reached, we compute the physics using the interaction list as the neighbors. The interaction list is computed using an opening-angle criterion comparing the boundary box and a user-defined angle. This way we will not need a full tree traversal for each particle but a full tree traversal for

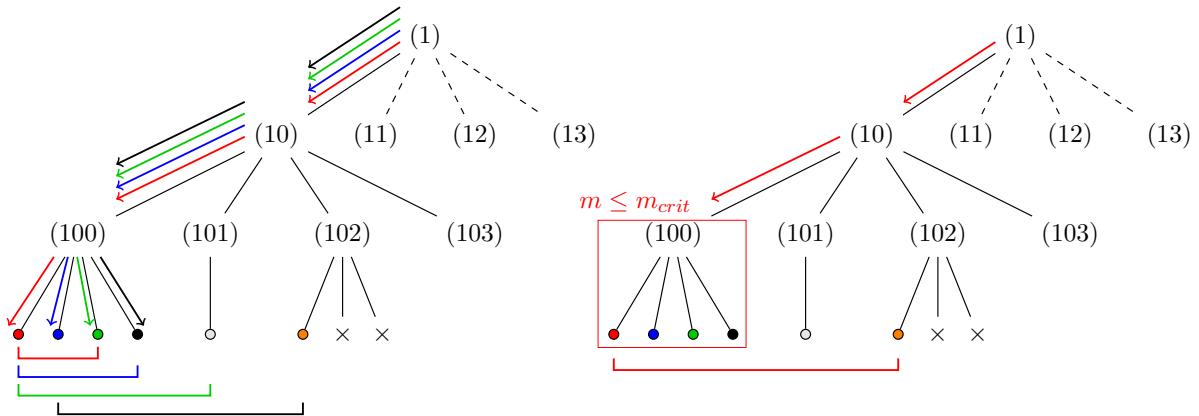


Figure 7.6: Neighbors search using a tree traversal per particle vs a group of particle and computing an interaction list

every group of particles. On figure 7.6 we present the classical and the two steps algorithm. We see that the first method, on left, force to do one walk per particle, compute the interaction list and then apply to particles. On the left, the two-step method, only perform one tree traversal for the whole block of particles, compute the interaction list and then processed to the local computation. Indeed, this implies a check of particle distance during the computation since all the particles from the interaction list are not useful for every particle.

7.3.3 Distribution strategies

The previous section presented the tree data structure that can be use locally on every node. The distribution layer is added on top of it, keeping each sub-tree on the computation nodes. The current version of FleCSPH is still based on synchronous communications using the Message Passing Interface (MPI).

The main distributed algorithm is presented on algorithm 8:

Particle distribution

The sort step, line 5, is based on a distributed quick sort algorithm. The keys are generated using the Morton order described in part 7.3.1. As we associate a unique number to each particle we are able to sort them using the keys and, in case of collision keys, using their unique ID. This gives us a global order for the particles. Each process sends to a master node (or submaster for larger cases) a sample of its keys. We determined this size to be 256 KB of key data per process for our test cases, but it can be refined for larger simulations. Then the master determines the general ordering for all the processes and shares the pivots. Then each process locally sorts its local keys, and, in a global communication step, the particles are distributed to the process on which they belong. This algorithm gives us a good partition in term of number of particles. But some downside can be identified:

- The ordering may not be balanced in term of number of particles per processes. But by optimizing the number of data exchanged to the master can lead to better affectation.
- The load balance also depend on the number of neighbors of each particle. If a particle gets affected a poor area with large space between the particles, this can lead to bad load balancing too.

This is why we also provide another load balancing based on the particles neighbors. Depending on the user problem, the choice can be to distribute the particles on each process regarding

Algorithm 7 Tree search algorithm

```

1: procedure FIND_NODES
2:   stack stk  $\leftarrow$  root
3:   while not_empty(stk) do
4:     branch b  $\leftarrow$  stk.pop()
5:     if b is leaf then
6:       for each particles p of b do
7:         apply_sub_tree(p,interaction.list(p))
8:       end for
9:     else
10:      for each child branch c of b do
11:        stk.push(c)
12:      end for
13:      end if
14:    end while
15:  end procedure
16:
17: procedure APPLY_SUB_TREE(node n, node-list nl)
18:   stack stk  $\leftarrow$  n
19:   while not_empty(stk) do
20:     branch b  $\leftarrow$  stk.pop()
21:     if b is leaf then
22:       for each particles p of b do
23:         apply_physics(p,nl)
24:       end for
25:     else
26:       for each child branch c of b do
27:         stk.push(c)
28:       end for
29:     end if
30:   end while
31: end procedure
32:
33: function INTERACTION_LIST(node n)
34:   stack stk  $\leftarrow$  root
35:   node-list nl  $\leftarrow$   $\emptyset$ 
36:   while not_empty(stk) do
37:     branch b  $\leftarrow$  stk.pop()
38:     if b is leaf then
39:       for each particles p of b do
40:         if within() then
41:           nl  $\leftarrow$  nl + p
42:         end if
43:       end for
44:     else
45:       for each child branch c of b do
46:         if mac(c,angle) then
47:           nl  $\leftarrow$  nl + c
48:         else
49:           stk.push(c)
50:         end if
51:       end for
52:     end if
53:   end while
54: end function

```

Algorithm 8 Main algorithm

```

1: procedure SPECIALIZATION_DRIVER(input data file f)
2:   Read f in parallel
3:   Set physics constant from f
4:   while iterations do
5:     Distribute the particles using distributed quick sort
6:     Compute total range
7:     Generate the local tree
8:     Share branches
9:     Compute the ghosts particles
10:    Update ghosts data
11:    PHYSICS
12:    Update ghosts data
13:    PHYSICS
14:    Distributed output to file
15:   end while
16: end procedure

```

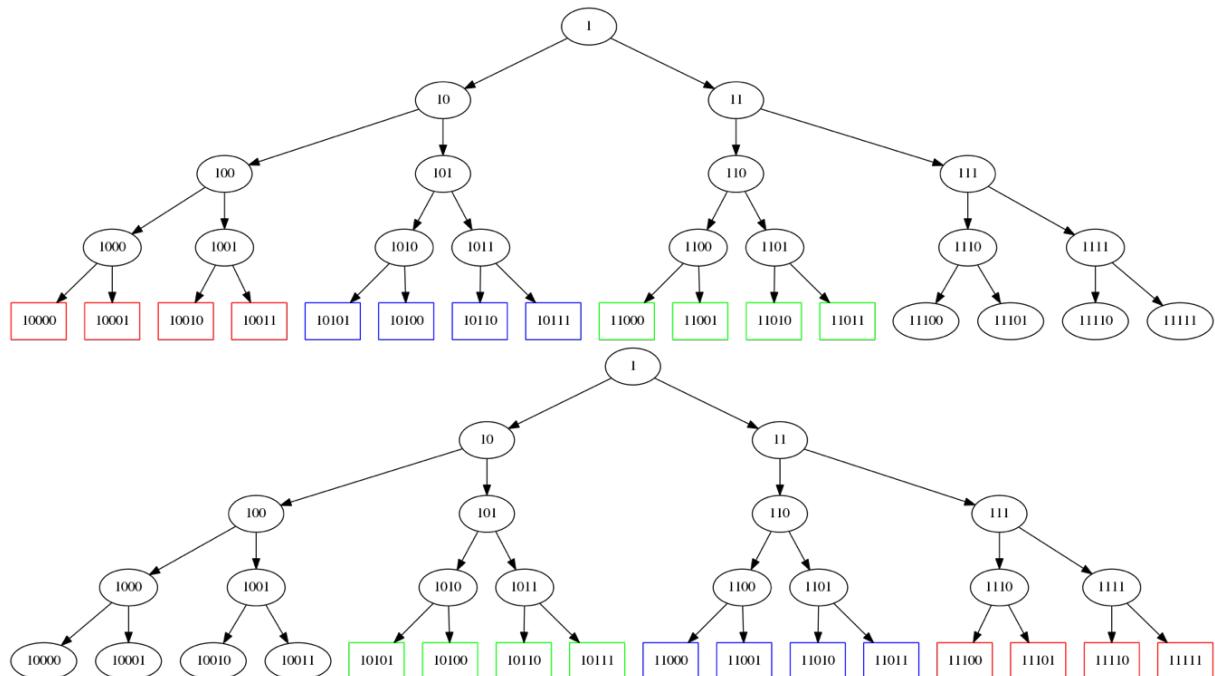


Figure 7.7: Binary tree for a 2 processes system. Exclusive, Shared and Ghosts particles resp. red, blue, green.

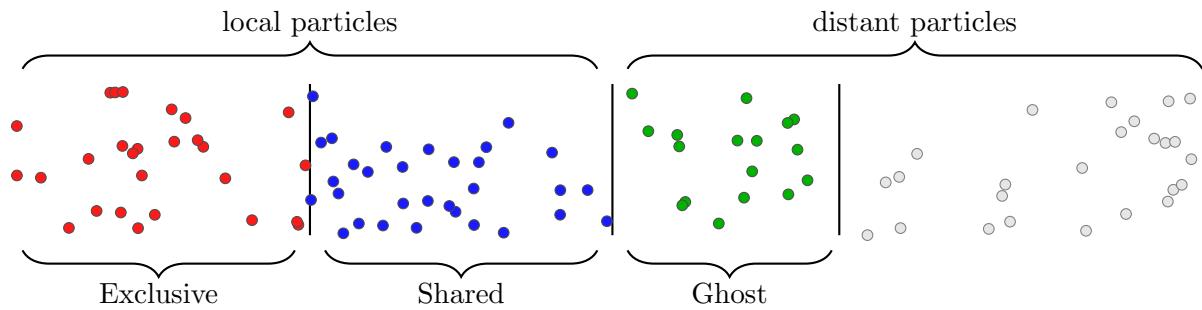


Figure 7.8: Particles "coloring" with local particles: exclusive, shared and distant particles useful during run: ghost particles

the number of neighbors, having the same amount of physical computation to perform on each process.

After this first step, the branches are shared between the different processes, line 8. Every of them send to its neighbors several boundaries boxes, defined by the user. Then particles from the neighbors are computed, exchanged and added in the local tree. Those particles are labeled as NON_LOCAL particles. At this point a particle can be referenced as: EXCLUSIVE: will never be exchanged and will only be used on this process; SHARED: may be needed by another process during the computation; GHOSTS: particles information that the process need to retrieve from another process. An example is given for 2 processes on figure 7.8 and on a tree data structure on figure 7.7.

Exchange Shared and Ghosts particles

The previous distribution shares the particles and the general information about neighbors' particles. Then each process is able to do synchronously or asynchronously communications to gather distant particles. In the current version of FleCSPH an extra step is required to synchronously share data of the particles needed during the next tree traversal and physics part. Then after this step, the ghosts' data can be exchanged as wanted several times during the same time step.

7.3.4 Fast Multipole Methods

We described in the previous chapter a method to compute gravitational interactions faster than the $O(N^2)$ n-body algorithm, the Fast Multipole Method, FMM. This allows an approach with a precision depending of a parameter called the Multipole Acceptance Criterion, MAC. This is needed for us to target binary neutron stars simulations with high number of particles.

This approach is also based on the tree topology used for the SPH method. Three main functions are used:

- **`mpi_exchange_cells`**

share the centers of mass computed in the tree up to a determined mass. By default, the program shares the lowest COM, the leaves.

- **`mpi_compute_fmm`**

After gathering the COM this step performs the M2M computation and also isolate the particles needed for the distant P2P step.

- **`mpi_gather_cells`**

Gather The contribution of all the other processes and sum in the local branch. Then this step performs both the M2P and P2P computations. A specific P2P for distant particles is added to take in account the particles found on other processes in the M2M step.

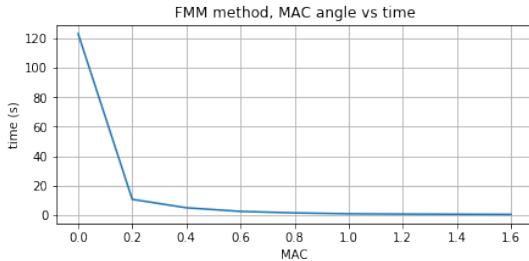


Figure 7.9: Evolution of time regarding the multipole acceptance criterion for FMM method.

The speed of computation varies with the choose of the MAC angle. An example is given on figure 7.9. It presents the time varying with the angle. We note that bigger the angle, faster the computation time. The limit of the angle is $\Theta = \frac{\pi}{2}$. The loss of precision can be quantified with the evolution of linear and angular momentum. We fixed our MAC to $\Theta = 1$.

7.3.5 Input/Output

Regarding the high number of particles, an efficient, parallel and distributed I/O implementation is required. Several choices were available, but we wanted a solution that can be specific for our usage. The first requirement is to allow the user to work directly with the Paraview visualization tool and splash⁷ [Pri07].

We base this first implementation on HDF5 [FCY99] file structure with H5Part and H5Hut [HAB⁺10]. HDF5 support MPI runtime with distributed read and write in a single or multiple file. We added the library H5hut to add normalization in the code to represent global data, steps, steps data and the particles data for each step. The I/O code was developed internally at LANL and provides a simple way to write and read the data in H5Part format. The usage of H5Hut to generate H5part data files allows us to directly read the output in Paraview without using a XDMF descriptor like requested in HDF5 format.

7.4 Distributed SPH on hybrid architectures

We constructed an efficient and reliable SPH code working on classical architecture clusters. In this section we present our multi-GPU implementation and compare it with our multi-CPU code. We kept the same data structure, distribution strategy and code architecture in the accelerator code. Several options are possible for the accelerator implementation, but we wanted to keep the code usable and working for the domain scientists. As the current version of FleCSI does not allow utilization of accelerator like GPU for the data structure, we decided to embed the GPU code directly on FleCSPH. We provided the same approach we studied in the Langford problem offloading part of the tree computation on the accelerators.

7.4.1 Distribution strategies

The FleCSPH framework provides all the tools and distribution strategies for multi-CPU and distributed computation. In order to target hybrid architectures several approaches were possible. They were identified in the previous metrics for the Langford problem. The first one is to implement the whole tree traversal and data representation on GPU. This strategy imposes several downsides especially for asynchronous communication. The data structure of FleCSI and FleCSPH does not allows the full transformation of the data structure into CUDA code and, furthermore, this would transform the framework into a problem dependent API. Even if the performances would be slightly better, the aim of this framework is to target multi-physics problems and thus general.

⁷<http://users.monash.edu.au/~dprice/splash/>

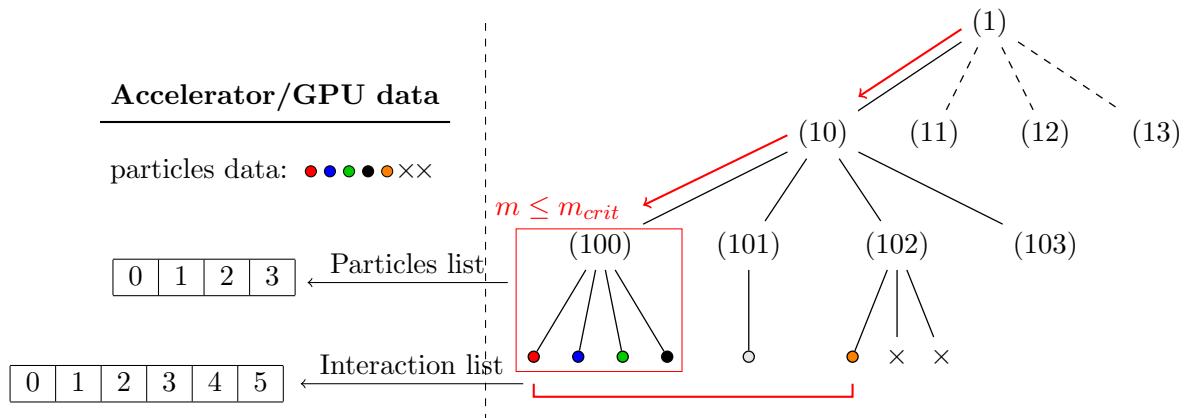


Figure 7.10: Task resolution using GPUs

The second strategy is the one used in the Langford problem case. The smoothing length computation is a tree traversal that's lead to a group of particles and their neighbors. We decided to offload the physics computation on accelerators.

Figure 7.10 presents the distribution of tasks with the accelerator. The tree traversal itself stays on the host processor and lower part of the tree are offloaded to the accelerators. The traversal is done in parallel on the host and, when a group of particles and its neighbors list is reached, the data are transferred to the GPU for computation. With this method the GPU is fully used for regularized computation and the CPU handle the data structure. When the tree traversal is done, the CPU wait for last GPU tasks to complete and can gather the result or start another traversal leaving data on GPUs.

7.4.2 Physics on accelerators

The computation of physics is also slightly different on accelerators. Indeed, the CPU send to the GPU indexes with the particles and their possible neighbors. The GPU perform a brute force computation with $O(n^2)$ algorithm. It keeps checking if the particles received are inside the smoothing length radius. The target particle is loaded in local memory and its neighbors are stored in the local memory for a WARP based computation. The threads then iterate on the local particles and output together in global memory.

7.5 Results

In this part we compare the results of the multi-GPU version and the multi-CPU version of FleCSPH. We show the benefit of using hybrid architectures even on irregular problem with high communications and computations levels.

7.5.1 Simulations

The results and tests were done on several physical and astrophysical simulations in order to check the code behavior and reliability.

The first tests, done on Sod shock tube and Sedov blast wave were presented in the previous chapter, showed perfect results.

The fluid simulation is presented on figure 7.11. On this figure we can see a 40,000 particles simulation executed on multiple nodes of the ROMEO supercomputer. This dam break simulation gave us the opportunity to represent the behavior of boundary conditions with a high number of particles.

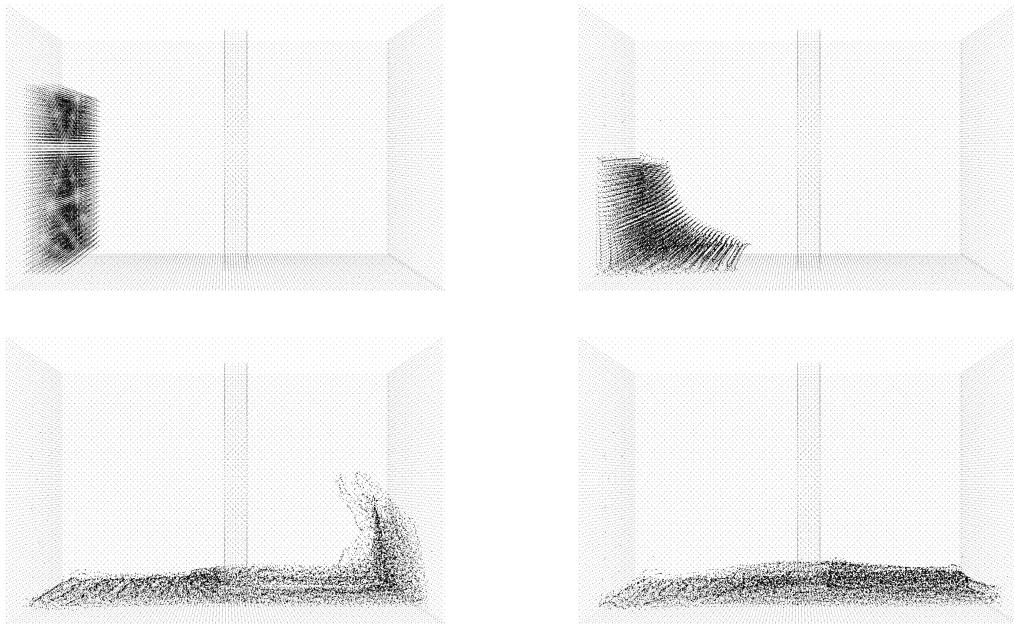


Figure 7.11: Fluid flow simulation, the dam break. For $t = 0$, $t = 0.4$, $t = 0.8$ and $t = 1$ seconds

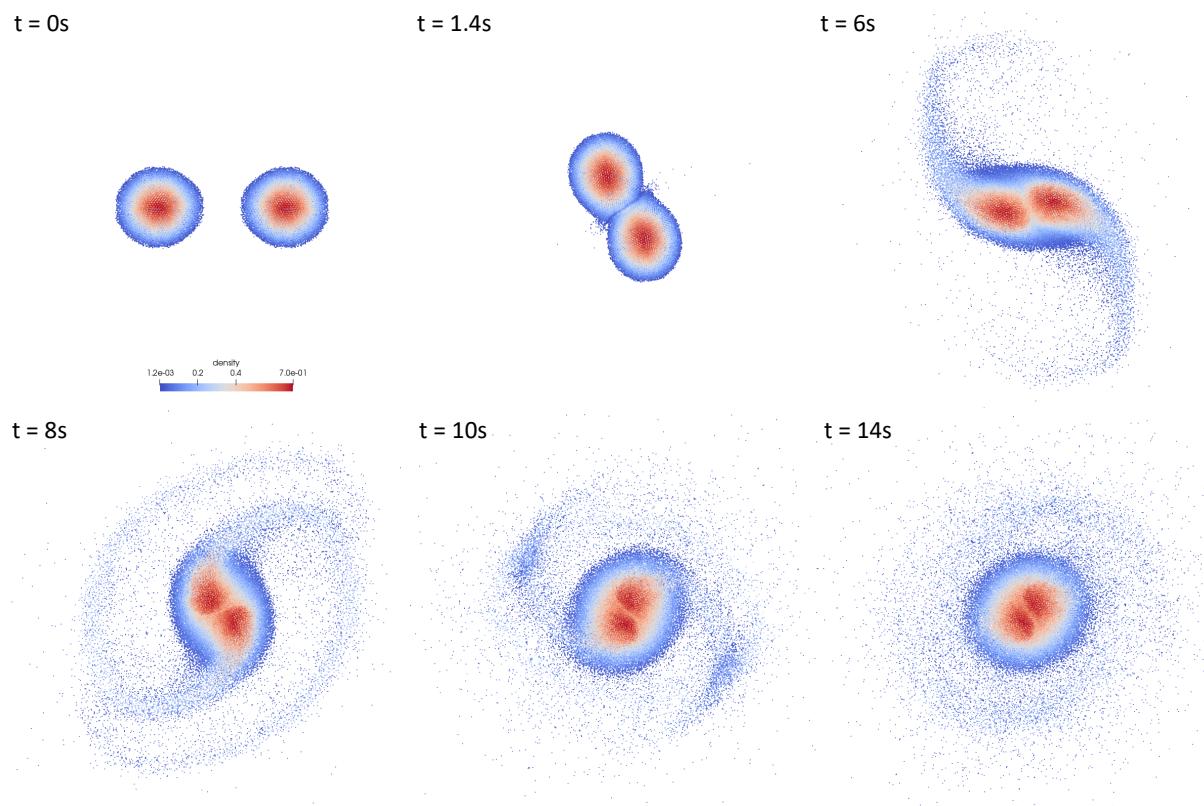


Figure 7.12: Binary Neutron Stars coalescence with 40.000 particles.

In order to target a problem with both SPH and gravitation we decided to work on Astrophysics events like Binary Neutron Stars. The initial data were generated using python 3.5 to compute the position, mass and smoothing length of every particle. A first step is done for the relaxation, so that the particles take their location. The system relaxed then evolve following the merging equations presented in the previous chapter.

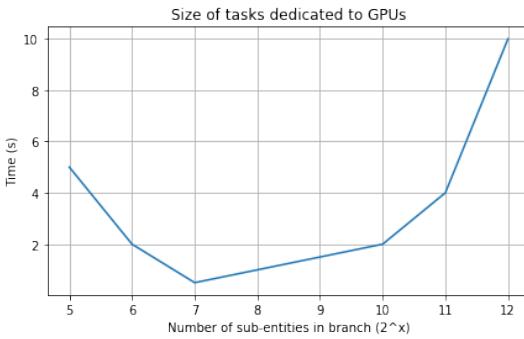


Figure 7.13: CPU-GPU tasks work balancing

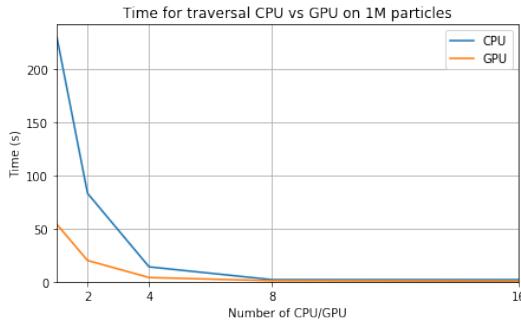


Figure 7.14: CPU vs GPU time per iteration

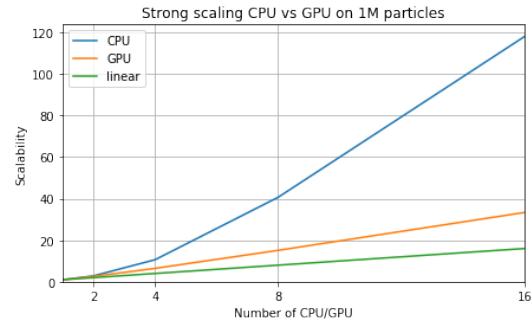


Figure 7.15: CPU vs GPU scalability per iteration

Figure 7.12 presents the binary neutron star coalescence for 40,000 particles. The computation took 5 hours on four nodes of the supercomputer ROMEO. This simulation is done with a total of 750 outputted steps with more than 100,000 iterations.

7.5.2 Performances

The two metrics we worked on, in part II, gave us a hint in order to reach performances in this simulation code. The first step was to find the best repartition between the host and device.

Figure 7.13 shows the work balancing. With the smallest distribution the CPU and GPU keep exchanging data for very small amount of computation. At the opposite, if the CPU value is too high the $O(n^2)$ part is too important. We choose the value to be configured by the user and defaulted at 7.

On figure 7.14 and figure 7.15 we find the strong scaling and scalability tests for CPU and GPU versions using the empiric best depth of repartition. These tests have been led on 500,000 particles binary neutron star merging during the coalescence step, when the particles are very close. The time comparison with strong scaling shows us that the GPU version goes faster than the CPU one with a peak of 5 times faster. On the other hand, the scalability graph presents that the CPU version is more scalable than the GPU one. Indeed, the number of particles to handle by the GPUs gets too small regarding their computational power and the transfers between CPU and GPU take a more important part of time.

7.6 Conclusion

In this section we presented a tool completing our metric. This production application dedicated to smoothed particles hydrodynamics and gravitation simulation is called FleCSPH. It allows us to target both computation and communication walls in a highly irregular context.

We based our hybrid implementation on the knowledge from the two first metrics of our

benchmark. We showed the advantage of using hybrid architectures on this kind of application and this behavior can be found in many others.

It is important to notice that the GPU usage is not the best in this case. Indeed, a dedicated application for each specific SPH problem would be more efficient. The aim is to provide a framework that can be used on a large set of clusters and architectures.

In this version, the GPUs enabled us to provide an acceleration of up to 5 times faster compared to the full-CPU computation. It proves the benefit of hybrid architectures even when confronted to computation and communication wall over high irregular applications. The work is shared between host and device by sharing part of the tree of particles to the GPU.

Conclusion

This third part of the thesis highlights our study and shows the advantages of hybrid architectures compared to classical CPU centric architectures. We showed that the GPU can handle part of the computation even in the case of combined computation and communication walls with irregular behavior application. We took for this last metric a simulation problem. As the simulation is intrinsically linked with HPC for a lot of fields this application perfectly finds its place in our metric.

A huge amount of time has been spent on the comprehension and implementation of the physics itself. This was required to provide realistic test cases and show the benefit of hybrid architecture even in the most complex case. We propose simulation for classical physics problems but also complex astrophysical phenomenon's like binary neutron star merging. Based on this physics knowledge and the target of completing our metric we create a dedicated distributed application.

This application is called FleCSPH and is based on the FleCSI framework developed at LANL. The intent of this project is to provide a distributed and reliable framework for multi physics purpose to domain scientists. Indeed, with the fast evolution of technologies and the complexity of new supercomputers, new tools need to be developed. FleCSPH is a first step to reach this goal and target tree topologies. It provides a domain decomposition, a tree data structure, I/O and efficient gravitation computation.

Our hybrid version of the code is based on GPU utilization. It follows the principles we described in the second part for the Langford tree structure with GPUs. A subpart of the tree traversal is dedicated to the GPUs which handle all the physics computation.

This implementation is not the best and better results can be obtained using exclusively GPUs for the resolution. In this case we limited the code transformation to stay in a realistic usable code for the domain scientists. The overall transformation would have led to create a SPH dedicated program, but this is not the aim of this work, targeting realistic production applications.

The last version, accelerated using multi-GPUs, is confronted to both computation and communication wall with the physics computation and the particle load balancing, respectively. The irregularity is present in all the layer with the neighbors' search, the physics computation and the communication steps to share EXCLUSIVE, GHOSTS and SHARED particles. The results using classical architecture are very good and the scalability is maintained for one million particles. The multi-GPU approach gives an acceleration of at least two times faster. These results show the real benefit of hybrid architectures even in a problem representing all the limitation and walls aspects studies before in this thesis.

Conclusion and future works

The first part of this study described the tools and theories needed to understand and reach performances in HPC. We presented several architectures with their advantages and showed that the next objective for the world most powerful countries is to reach the computational power of one exaflop by the year 2020. Our belief is that these architectures will be hybrid powered by accelerators with many-cores, such as GPUs or FPGAs. We showed that the current benchmarks do not seem to represent the behavior of realistic problems with their underlying irregularities in both computation and communication.

We proposed a new metric targeting the most important walls of HPC from these observations regarding the power consumption, computation performances and communications. The intent of this metric was to confront classical and hybrid architectures to show the real benefit that can be obtained by using accelerators. This metric is separated in two parts.

In the first part, we target classical, academical and even benchmark problems as the metric. We compared the classical architectures to the hybrid counterpart using on a problem featuring heavy computations and a second one focusing heavy communications. In both cases, we wanted to fit production code and their worst behavior which is irregularity.

The first problem was the Langford pairing counting problem. This problem was studied with two different approaches based on a tree traversal and an arithmetic resolution, respectively. The tree resolution showed very good results and up to 80% of the overall work handled by the GPU with an efficient load balancing strategy. The mathematical solution was also very irregular due to the large integer arithmetic on GPUs. In this case, we showed that the GPUs were able to handle up to 65% of the computation effort. This hybrid architecture implementation allowed us to beat a timed record for the computation of the last instances using a best-effort strategy on the ROMEO supercomputer.

The second problem we address is the Graph500 benchmark. This is a perfect candidate in order to consider communication problems without heavy computation. The only operations needed were memory checking for values and copies in queues. This problem remains very irregular in both memory and communication usage. We propose an implementation based on state of the art algorithm from both NVIDIA and IBM BlueGene/Q. This allowed us to rank the ROMEO supercomputer 105th in the November 2016 Graph500 list, even though this machine was not anymore ranked in the TOP500 list. This metric showed the high level of scalability that can be reached with GPUs.

These first two approaches give credit to the choice of hybrid architectures on both walls separately. In order to validate our metric, we needed to evaluate the classical and hybrid architectures on a production application having both walls. We targeted a complex simulation which is representative of all these aspects. The problem we choose fitting our needs in computational and communication over irregular context was the Smoothed Particle Hydrodynamics and gravitation simulation of complex astrophysics events. We developed a framework named FleCSPH dedicated to tree topology and physics or astrophysics simulations in collaboration with the Los Alamos National Laboratory. This tool provides domain scientists a framework for tree-based simulations and gives us the opportunity to work on a production code which is still in development. We showed that our multi-GPUs implementation allows to reach performances

two times faster using hybrid architectures. Even keeping an approach not fully GPU for the production code, the performances on hybrid architectures can be greatly superior to classical CPU ones.

This study showed three basic cases proving that the hybrid architectures are the solution for Exascale supercomputers. The main walls are solved using generic strategies and new ways of thinking of the algorithms.

The Langford and the Graph500 problems are considered directly as benchmarks. Indeed, their complexity evolves with the size of the problem or instance considered. Our last metric with FleCSPH is more complex and relies on either the number of particles, their physical aspect and user's criterions for FMM.

This work led to the publication of one journal paper [KLAJ16b], many conference papers [KLAJ16a, LLB⁺18, LAJK18, LLB⁺18, LAJK18], presentations and posters [DJK⁺14, LJAK16, JDK⁺14, LAJK15, LJAK15, DBGH⁺16, LLMB17]. The goal for the future of this work will be to propose a set of initial data and settings to be able to use this kind of domain scientist application as a benchmark on its own. This will allow us to have a generic benchmark representing all the aspects of modern applications.

Hybrid architectures appear to be the only approach for building Exascale supercomputers, but computer science is a very fast evolving field of research. The release of a new technology can change the cards and lead to better, alternative solutions. The main proposal, beside classical architectures and hybrid ones, is the ARM powered supercomputers. We presented the Montblanc project, the European effort to reach Exascale with reduce instruction set processors enabling low energy consumption. Other groups are also interested in this type of ARM architecture. The Japanese supercomputer center, K computer with RIKEN, is known to integrate a very efficient interconnect with a 6-dimensional torus. The next generation of this project, the post-K⁸ computer, will keep the same TOFU interconnection topology, but provide ARMv8 processors. The metric proposed in this study relies on generic tools and data structures which allow us consider ARM architectures for later architectures tests or benchmarking.

Currently, another solution for specific problems seems to be resolved in so called Quantum Computing. The *bits* of classical processors are replaced by *qubits*, quantum bits, and can provide more states than the usual 0 - 1 of bits. These specific machines are based on quantum properties of particles and seem to target very specific applications. Quantum Computers are always in development but some centers, like the ROMEO supercomputer center, provide simulations of quantum computers behavior in order to learn about their utilizations.

This study focuses on the ways to reach the necessary computational power for the Exascale. Indeed, the main limitations are the computation and communication walls which we targeted with hybrid architectures on irregular behavior problems. As these modern architectures, such as GPU, are the less power consuming regarding their efficiency, the power consumption wall is also studied. We know that other issues will rise at the Exascale. We cited in the introduction the interconnect wall, interconnecting efficiently billions of nodes will be very expensive to keep the bandwidth high enough between them. On the other hand, the error made by environmental reasons, like magnetism, or bugs in computation is around one per week at Petascale, this error will rise to one per hour at the Exascale. We will need to create new ways to ensure the computation correctness and on-the-fly verifications. We have the same idea for component failure. The resilience wall, the way to recover faster after a crash or loss of computation element. This will need robust algorithm and task-based parallelism to ensure the computation.

The last one is the complexity wall. The evolution of hardware will lead to larger and more complex supercomputers. Computer scientists need to consider new ways to think of algorithms and implementation. On one hand, the tools like APIs and frameworks have to be able to target all the architectures and topologies. On the other hand, algorithms have to be thought

⁸<http://www.fujitsu.com/global/Images/post-k-supercomputer-overview.pdf>

natively for massive parallel architectures and most of the existing ones changed. As an example, stochastic approaches can be a way to reach the results faster with an error determined by the user, perfect for computations based on Monte Carlo or current fields, such as AI.

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Titre français: Le choix des architectures hybrides, une stratégie réaliste pour atteindre l'échelle exaflopique

La course à l'Exascale est entamée et tous les pays du monde rivalisent pour présenter un supercalculateur exaflopique à l'horizon 2020-2021. Ces superordinateurs vont servir à des fins militaires, pour montrer la puissance d'une nation, mais aussi pour des recherches sur le climat, la santé, l'automobile, physique, astrophysique et bien d'autres domaines d'application. Ces supercalculateurs de demain doivent respecter une enveloppe énergétique de 1 MW pour des raisons à la fois économiques et environnementales. Pour arriver à produire une telle machine, les architectures classiques doivent évoluer vers des machines hybrides équipées d'accélérateurs tels que les GPU, Xeon Phi, FPGA, etc.

Nous montrons que les benchmarks actuels ne nous semblent pas suffisants pour cibler ces applications qui ont un comportement irrégulier. Cette étude met en place une métrique ciblant les aspects limitants des architectures de calcul: le calcul et les communications avec un comportement irrégulier.

Le problème mettant en avant la complexité de calcul est le problème académique de Langford. Pour la communication nous proposons notre implémentation du benchmark du Graph500. Ces deux métriques mettent clairement en avant l'avantage de l'utilisation d'accélérateurs, comme des GPUs, dans ces circonstances spécifiques et limitantes pour le HPC. Pour valider notre thèse nous proposons l'étude d'un problème réel mettant en jeu à la fois le calcul, les communications et une irrégularité extrême. En réalisant des simulations de physique et d'astrophysique nous montrons une nouvelle fois l'avantage de l'architecture hybride et sa scalabilité.

Mots clés: Calcul Haute Performance, Architecture Hybrides, Simulation

English title: The choose of hybrids architectures, a realistic strategy to reach the Exascale

The countries of the world are already competing for Exascale and the first exaflopics supercomputer should be release by 2020-2021. These supercomputers will be used for military purposes, to show the power of a nation, but also for research on climate, health, physics, astrophysics and many other areas of application. These supercomputers of tomorrow must respect an energy envelope of 1 MW for reasons both economic and environmental. In order to create such a machine, conventional architectures must evolve to hybrid machines equipped with accelerators such as GPU, Xeon Phi, FPGA, etc.

We show that the current benchmarks do not seem sufficient to target these applications which have an irregular behavior. This study sets up a metrics targeting the walls of computational architectures: computation and communication walls with irregular behavior. The problem for the computational wall is the Langford's academic combinatorial problem. We propose our implementation of the Graph500 benchmark in order to target the communication wall.

These two metrics clearly highlight the advantage of using accelerators, such as GPUs, in these specific and representative problems of HPC. In order to validate our thesis we propose the study of a real problem bringing into play at the same time the computation, the communications and an extreme irregularity. By performing simulations of physics and astrophysics we show once again the advantage of the hybrid architecture and its scalability.

Key works: High Performance Computing, Hybrid Architectures, Simulation

Discipline: Informatique

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