## Chapter 2

# Hardware in HPC

#### 2.1 Introduction

Although parallel models address most of the key points to discuss application performance it also depends on architectures hardware, which may influence the way to consider problems resolution. Thus the knowledge of hardware architecture is essential to reach performances through optimizations. Even if the nowadays software, API, framework or runtime already handle most of the optimizations, the last percents of gain are architecture's 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 keeps a focus on multi-core processors and GPUs as we based our tests on those devices.

This chapter also details the architecture of some remarkable supercomputers. This has to go 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 last released technologies. We also present the optimizations of current technologies with the arising 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 1970s single core processors to nowadays multi-core and many-core architectures that are the milestones, the basic units, to build supercomputers. We can see 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, around the 1970s, were built using a single computation core as described in the Von Neumann model. Many evolutions were made on those single core processors for the memory, the order of the instructions and the frequency increase.

#### Transistor shrink and frequency

A lot of new ways to produce smaller transistors have been discovered. Their size was about  $10\mu m$  in 1971 and reach 10nm in nowadays 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. Indeed, as the clock rate get higher, more operations can be performed on the core in the same amount of

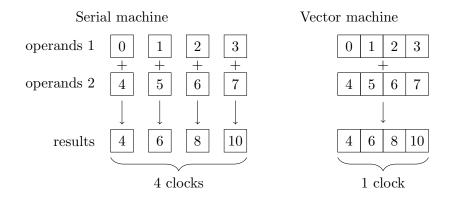


Figure 2.1: Vectorized processeur example on 4 integer addition: 128 bits wide bus

time. In 1970s the frequency was about 4 MHz allowing a maximum of 4 millions 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 next sections will show that due to power consumption and coding considerations, frequency is no more used to improve performances.

#### In/Out-Of-Order execution

In-order-process is the one described in previous chapter. The control unit fetches instructions and the operands from memory. Then the ALU computes the operation, and finally the result is stored to memory.

In this model the time to perform an instruction is the cumulation 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 (pointed out with 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. As an example we can execute operations simultaneously on 4 to 8 floats with a bus size of 128 or 256 bits. This requires specific care for coding with *unrolling* and *loop tiling* that will be addressed later in this study, and to avoid bad behavior leading to bad performances. But 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. Based on vector processor it was able to deliver up to 160 MFLOPS. 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 4 cycle and, at the opposite, 1 cycle on the right with the vectorized machine.

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

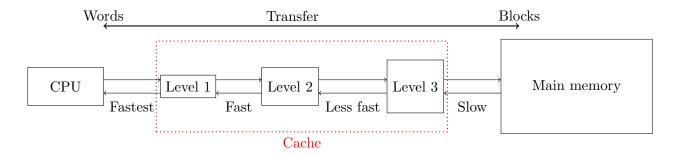


Figure 2.2: Cache memory technology on three levels L1, L2 and L3

#### Memory technology evolution

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

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

**SRAM:** The Static Random Access Memory is built using so called "flip-flop" circuits that can store data at anytime 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 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 in fact 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 1x to 4x but the limitation of those products is the price, constantly rising.

#### 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. The closer to the CPU is L1, then L2 and generally no more than L3 except on specific architectures. When looking for a data the CPU first checks if it is present in the L1 cache, otherwise 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 L2 and L1, lines of informations are exchanged usually called 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, and cache-miss when it has to be retrieved from lower levels or main memory. In a program the ratio of cache-miss has to be kept low in order to reach performance, and the impact may be very high.

#### **Pre-fetching**

Pre-fecthing was developed Based on memory optimization and especially the cache. When a data is 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-fecthing technology is a way to, knowing the next instructions operands, pre-fetch the data in closer cache before the instruction is decoded.

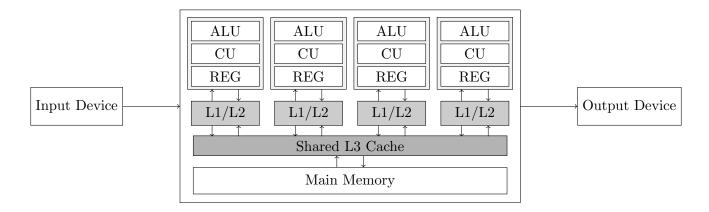


Figure 2.3: Multi-core CPU with 4 cores based on Von Neumann Model

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 2000s the limitations of single core processors were too important. The frequency was already high and requested more power consumption and caused more heat dissipation. The first idea was to provide multi-CPU devices, embedding several CPU on the same motherboard and allowing them to share memory. The evolution of that is 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 CPUs each embedding the function and units required consume n times more energy and 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, ...) and are implemented on the same due; this allows to reach the same CPU performances with less transistors and less power consumption, avoiding most of the heat 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 nowadays 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 nowadays processors. These multi-cores provide 2 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 product efficient and general purpose supercomputers.

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

#### 2.3.1 Multi-core implementations

The most world spread architecture in public and hight performance computing is the multi-core processors. Most of nowadays accelerators require a classical processor to offload tasks and data

## The Tick-Tock model through the years

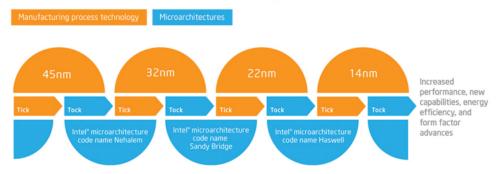


Figure 2.4: Intel Tick-Tock model

on it.

We start this presentation from the most popular processors in HPC world, the Intel company ones. We also present ARM which is another 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. Nowadays processors are mostly Intel ones, this world leader 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 its creation this model followed the same fashion: a new manufacturing technology like shrink of the chip with better engraving on a "Tick" followed by a "Tock" by the delivery of 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. Every new processor has 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 usual "Tick-Tock" process because it is just based on optimizations of the Skylake architecture. It is produced like Skylake in 14nm. The tick-tock model seems to be hard to maintain due to the difficulties to engrave in less than 10nm with quantum tunneling. This leads to using larger many-cores architecture and base next supercomputer evolutions road-map on 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 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. A lot of studies have been released on HT from Intel itself [Mar02] to other studies [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.

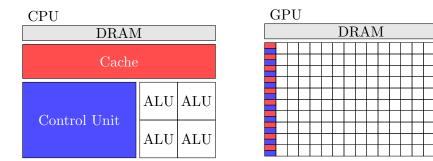


Figure 2.5: Multi-core versus Many-core architecture, case of GPUs

#### ARM

Back in 1980s, ARM stood for Acorn RISC Machine in reference to the first company implementing 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 makes them hard to create and they require way more transistor and thus energy to work. The ISA from the RISC is simpler and requires 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 would then be 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. That 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), respectively featured for highest-performances, for balancing performances and efficiency or for less power consumption.

The new ARMv8 architecture starts to provide the tools to target HPC context [RJAJVH17]. The European approach towards energy efficient HPC, Mont-Blanc project<sup>1</sup>, already constructs ARM based supercomputers. For the exascale project in Horizon 2020 this project focuses on using ARM-based systems for HPC with many famous contributors with Atos/Bull as a project coordinator, ARM, French Alternative Energies and Atomic Energy Commission (CEA), Barcelona Supercomputing Center (BSC), etc. The project is decomposed into several steps to finally reach exascale near 2020. The third 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 Many-core architecture, SIMT execution model

Several architectures can be defined as many-cores. Those devices integrate thousands of cores that are usually control by less control units. We can consider those cores as "simpler" since they have to work synchronously and under the coordination of a control unit. They are based on SIMD Flynn taxonomy. Some devices are specific like the Xeon Phi of Intel integrating a hundred of regular processor cores which can work independently.

#### **GPU**

When a CPU can usually have 2 to 32 computation cores that can operate on different instruction streams, the SIMT architecture of the GPU is slightly different. The cores are grouped and have to share the same instruction at the same clock time but all the groups can have their own instruction.

<sup>&</sup>lt;sup>1</sup>http://montblanc-project.eu/



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

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

Those devices are called General Purpose Graphics Processing Units (GPGPUs). They are derivative from classical GPUs used for graphics purpose. Pioneer shows that they can be use 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 fonded in April 1993 in Santa Clara, Carolina, by three persons in which Jensen Huang, the actual CEO. The company name seems to come from *invidia* the Latin word for Envy and vision for graphics rendering.

Known as the pioneer in graphics, cryptocurrency, portable devices and now Artificial Intelligence (IA), it seems 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 use 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 describes 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 respectively K20Xc and K20Xm. 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 precisions cores, 64 double precision cores, 32 special function units and 32 load/store units. In a SMX the memory provides 65536 32-bits registers, 64KB of shared memory L1 cache, 48KB of read-only cache The L2 cache is 1546KB shared

by the SMX for a total of 6GB 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 225W. 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 in HPC. Their HPC GPUs are called FirePro. They are targeted using a language near CUDA but not hold by a single company 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 a accord with Intel to provide dies featuring Intel processor, AMD GPU and common HBM memory. The project is call Kaby Lake-G and announce for first semester of 2018 but for public, not HPC itself.

#### 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 embedded multiple multi-cores processors interconnected. This is call Intel's Many Integrated Core (MIC). 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. We considered the Xeon Phi in the many-cores architecture despite the fact that it is composed of completely independent processors. This is due to the number of cores that is very high and the fact it can be use as an accelerator instead of the host.

#### **PEZY**

Another many-core architecture just appears 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 machine ranked in the GREEN500 list are accelerator using this many-core die. We also note that in the November 2017 list the 4th supercomputer, Gyoukou, is also powered by PEZY-SC2 cards.

#### 2.3.3 Other architectures

Numerous architecture have not been presented because out of scope in this study. We present here two technologies we have been confronted in our researches and that can be tomorrow solution for exascale in HPC.

#### **FPGA**

Field Programmable Gates Array are device that can be reprogram to fit the needs of the user after their construction. The leader was historically Altera with the Stratix, Arria and Cyclone FPGAs and is now part of Intel. With the FPGAs the user have access to the hardware itself and can design its own circuit. Nowadays FPGA can be targeted with OpenCL programming language. The arrival of Intel in this market promises the best hopes for HPC version of FPGAs. The main gap for users is the circuit building itself, perfect to respond to specific needs but hard to setup.

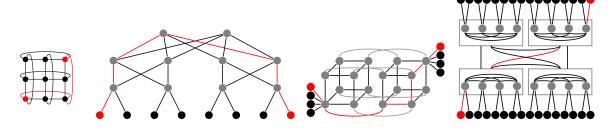


Figure 2.7: Torus, Fat-Tree, HyperX, DragonFly

#### ASIC

Application Specified Integrated Circuits are dedicated device construct for on purpose. An example of ASIC can be the Gravity Pipe (GRAPE) which is dedicated to compute gravitation given mass/positions. Google leads the way for ASIC and just created its dedicated devices to boost AI bots. We also find ASIC in some optimized communication devices like in 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 can refer to the Von Neumann model in case of core with ALU and CU. We can separate core from CPU to GPU, the first one able to be independent whereas the second ones working together and sharing the same program counter.

Socket/Host: A socket is mistakenly called a CPU in nowadays language. It is, for multicores 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. They can also share the accelerator usage.

**Computation node:** The next layer of our HPC system if the computation node. Grouping together several socket and accelerators sharing memory;

Rack: A rack is a set of computation nodes, generally a vertical stack. It can 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.

In order to connect node together and allow distributed programming an interconnect technology is required. Interconnection network is the way the nodes of a cluster are connected together.

#### 2.4.2 Interconnection topologies

Several topologies exists from point to point to multi dimensional torus. The figure 2.7 is

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

a representation of famous topologies. Each interconnect technology has its own specificity. These networks takes 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 use 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, higher the position in the tree more connection are found and the bandwidth is important. The nodes are available as the leafs, on the middle level we find the switches and on top the routers. Another topology, HyperX[ABD+09], is base on Hyper-Cube. The DragonFly[KDSA08] interconnect is recent, 2008, and use in nowadays supercomputers.

InfiniBand (IB) is the most spread technology used for interconnect with different kind of bandwidth presented in figure 2.1. It provides high bandwidth and small latency and companies like 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 came in 19th century with the first multi-core processors.

#### 2.4.3 Remarkable supercomputers

The TOP500 is the reference benchmarks for the world size supercomputers. Most of the TOP10 machines have specific architectures and, of course, the most efficient ones. In this section we give details on 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. A recent report from Jack J. Dongarra, a figure in HPC, decrypt the architecture of this supercomputer[Don16]. The most interesting point is the conception of this machine, completely done in China. The Sunway CPUs were invented and built in China. The Vendor is 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), 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 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. The total memory is 1.31 PB and the number of cores available is 10,649,600. The peak performance is 125.4 PFLOPS and the Linpack is 93 PFLOPS which induce 74.16% of efficiency.

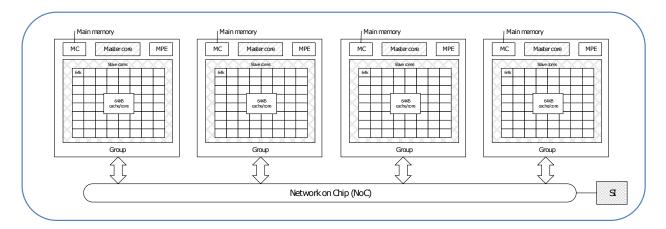


Figure 2.8: Sunway Taihulight node architecture from Report on the Sunway TaihuLight System, Jack Dongarra, June 24, 2016.

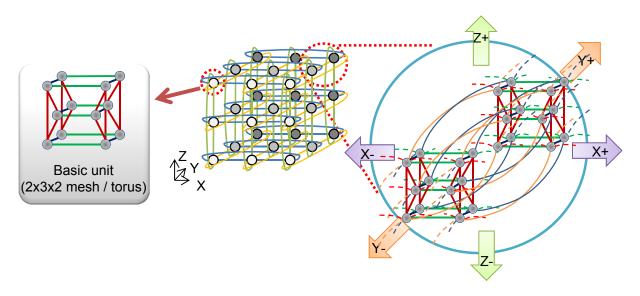


Figure 2.9: TOFU Interconnect schematic from  $\it The~K\mbox{-}Computer:~System~Overview,~Atsuya~Uno,~SC11$ 

#### Piz Daint

The supercomputer of the CSCS, Swiss National Supercomputing Center, is currently ranked 2nd of the November 2017 TOP500 list. This GPUs accelerated supercomputer is a most powerful representative of GPU hybrid acceleration. This is also the most powerful European supercomputer. He is composed of 4761 hybrids and 1210 multi-core nodes. The hybrids nodes embedded 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 and the Linpack gives 19.590 TFLOPS. The low power consumption rank Piz Daint as 10th in the GREEN500 list.

#### **K-Computer**

K-Computer was the top 1 supercomputer of TOP500 2011 list. The TOFU interconnect network makes the K-Computer unique [ASS09] and stands for TOrus FUsion. This interconnect presented in figure 2.9 mixes a 6D Mesh/Torus interconnect. The basic units are based on a mesh and are interconnected together in a 3 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

Sequoia supercomputer was top 1 of the TOP500 2012 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 notice the BlueGene architecture because even in the last GRAPH500 list, November 2017, there is 15 of these machines in the TOP20. 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 (French name for software and hardware architectures) is used for HPC for theoretic research and domain science like applied mathematics, physics, biophysics and chemistry.

This project is support by the Champagne-Ardenne region and the CEA (French Alternative Energies and Atomic Energy Commission), aim to host research and production codes of the region for industrial, research and academics purposes.

We are currently working on the third version of ROMEO, installed 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 5th in the GREEN500 list.

#### 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 have access to 16GB of memory for a total of 32GB per node, the total memory if 4.160TB. Each processor if linked, using PCIe-v3, to an NVIDIA Tesla K20Xm GPGPU. This cluster provide 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 10GB/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 always available but does not features GPUs.

The supercomputer supports MPI with GPU Aware and GPUDirect.

#### 2.5.2 New ROMEO supercomputer, June 2018

Avoir les info et decrire le nouveau ROMEO

#### 2.6 Conclusion

In this chapter we reviewed the most important nowadays 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.

2.6. CONCLUSION 13

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

We can see through the new technologies presented here that every one is moving toward hybrids architectures featuring multi-core processors accelerated by one or more devices, many-core architectures. The exascale supercomputer of 2020 will be shape with hybrid architectures and they represent the best of nowadays technology for purpose of HPC. Combining CPU and GPUs or FPGA on the same die, sharing the same memory space can also be the solution.

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