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# High-Performance Computing at Exascale: challenges and benefits

Mathieu Lobet, Matthieu Haefele, Vineet Soni, Patrick  
Tamain, Julien Derouillat, Arnaud Beck

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SFP Division Plasma  
June 14th 2018



# Lab and speaker presentation

## Maison de la Simulation (Saclay)

### Missions:

- Research in HPC, Applied Math, visualization
- Support to the scientific community
- Training (national, Prace)

Involved in national and European projects: EoCoE, Prace



### Mathieu Lobet:

Research Engineer in HPC at CEA Saclay

### Projects:

- Energy oriented Centre of Excellence for computing application (EoCoE)

### Applications:

- SMILEI – High performance Particle-In-Cell code for plasma simulation
- TOKAM3X - Edge turbulence fluid simulations of tokamak plasmas



# Content

I. The Exascale challenge

II. Future hardware

III. Programming challenges

Conclusion



# I. The Exascale challenge



# Exascale challenge

To Reach the **exaflop computing power** ( $10^{18}$  flop/s) level with a maximum electricity consumption of **20-40 Mwatts**

Main sources of energy consumption:

- Computing units (~50% of the total power consumption on most recent facilities)
- Interconnect
- Memory



USA – Aurora at  
Argonne  
2021



Europe  
2022



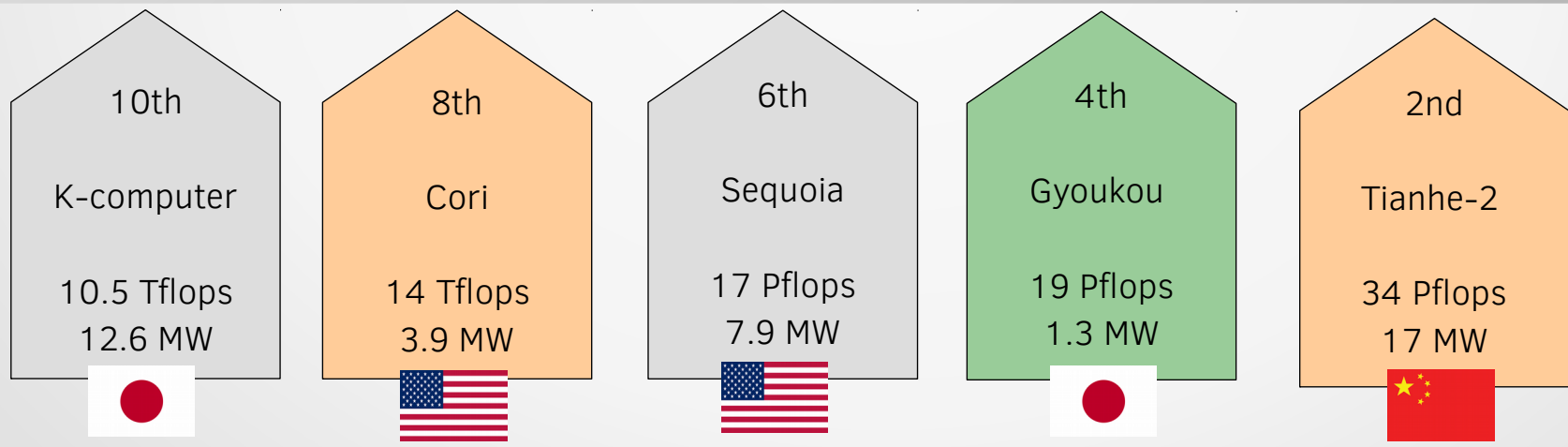
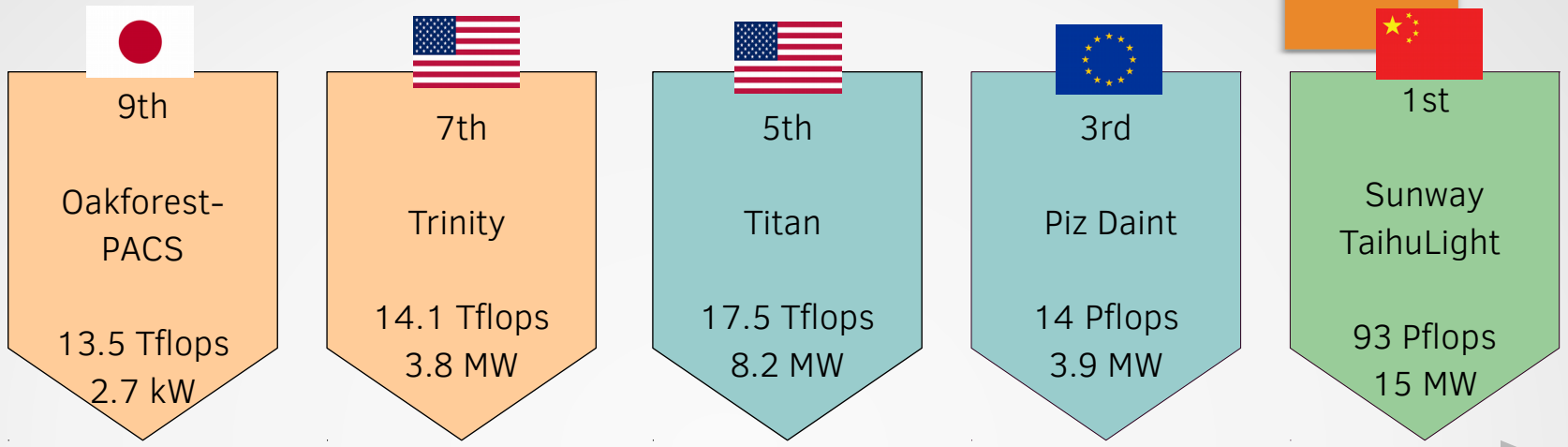
China  
2019-2020



Japan – Post-K  
computer  
2021



# Most powerful supercomputer analysis, Nov 2017

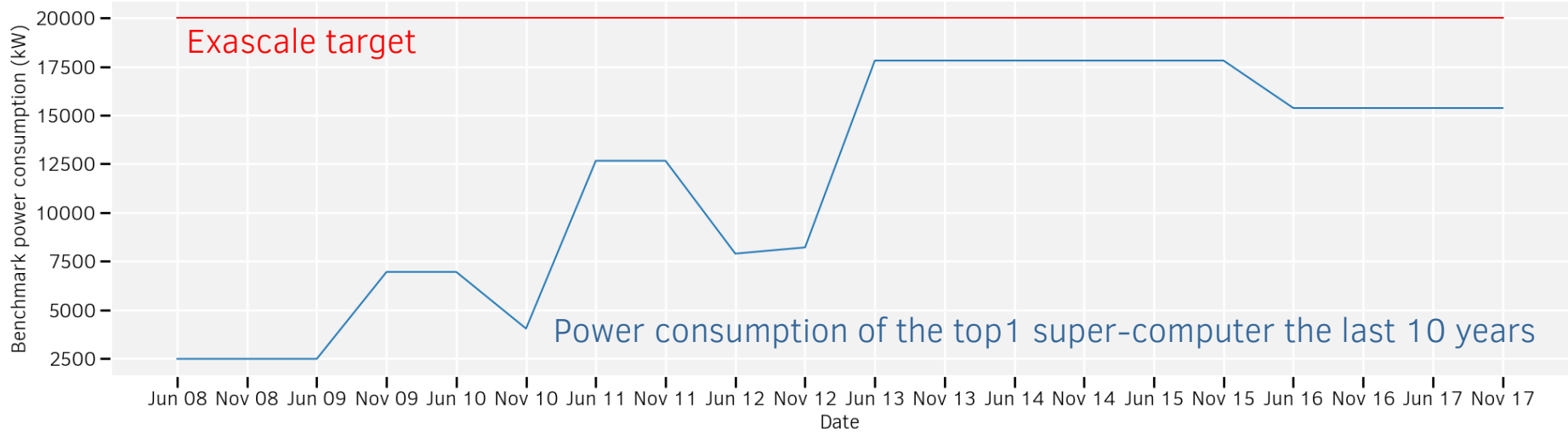
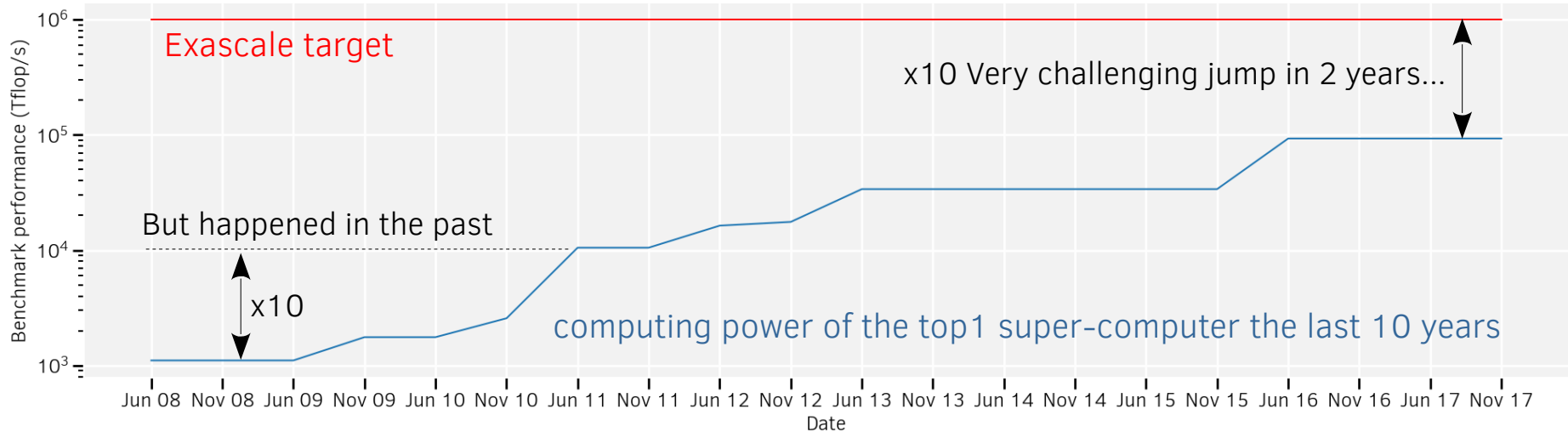


- Multi-core only (ex: Xeon, Power, SPARC)
- Many-core only (ex: Xeon Phi)
- CPU + GPU
- CPU + Acc ARM

<https://www.top500.org/lists/2017/11/>



# Is this the continuity?







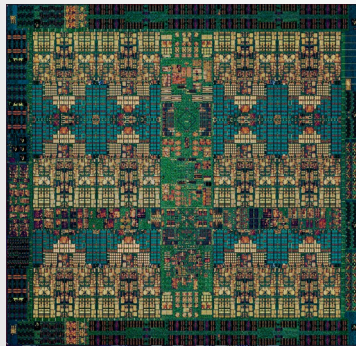
## II. Future Hardware



# X86 (Intel, AMD) and Power CPU (central processing unit)

For Intel and AMD:

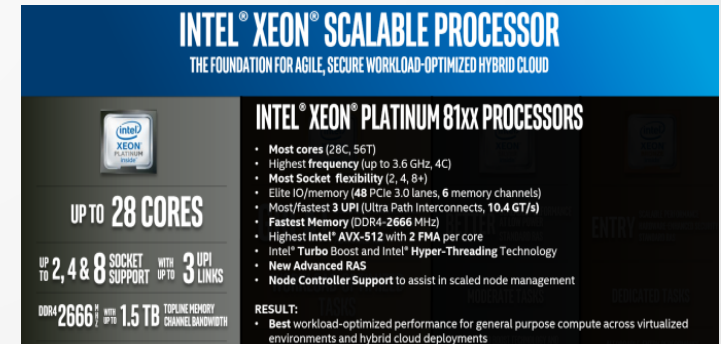
- ▶ Historically, complex processing units originally dedicated to **multiple different purposes**
- ▶ In personal computers, **a lot of silicon dedicated to complex instruction sets to be performant in major cases (operating system, web, office software, video...)**
- ▶ Disadvantage in HPC, results in a **bad energy efficiency**
- ▶ For few years now, specific processors for server and HPC purposes such as **Intel Xeon and Intel Xeon Phi** that integrates **smaller and simpler energy efficient cores with low frequency and larger vector units.**



IBM Power9  
Up to 32 cores, up to 4 Ghz, SMT4 – SMT8, 190 W



AMD Epyc 7000 series  
32 cores, base 2.2 Ghz, 180W



Intel Xeon Skylake  
28 cores, base 1.5 Hhz, 200W, AVX512

[www.microway.com/knowledge-center-articles/detailed-specifications-of-the-skylake-sp-intel-xeon-processor-scalable-family-cpus/](http://www.microway.com/knowledge-center-articles/detailed-specifications-of-the-skylake-sp-intel-xeon-processor-scalable-family-cpus/)

[www.anandtech.com/show/11544/intel-skylake-ep-vs-amd-epyc-7000-cpu-battle-of-the-decade/7](http://www.anandtech.com/show/11544/intel-skylake-ep-vs-amd-epyc-7000-cpu-battle-of-the-decade/7)

<https://www.nextplatform.com/2017/12/05/power9-to-the-people/>



# X86 (Intel, AMD) and Power CPU (central processing unit)

## Pros:

- ▲ Easy to program
- ▲ Easy to debug
- ▲ Cross-platform

## Cons:

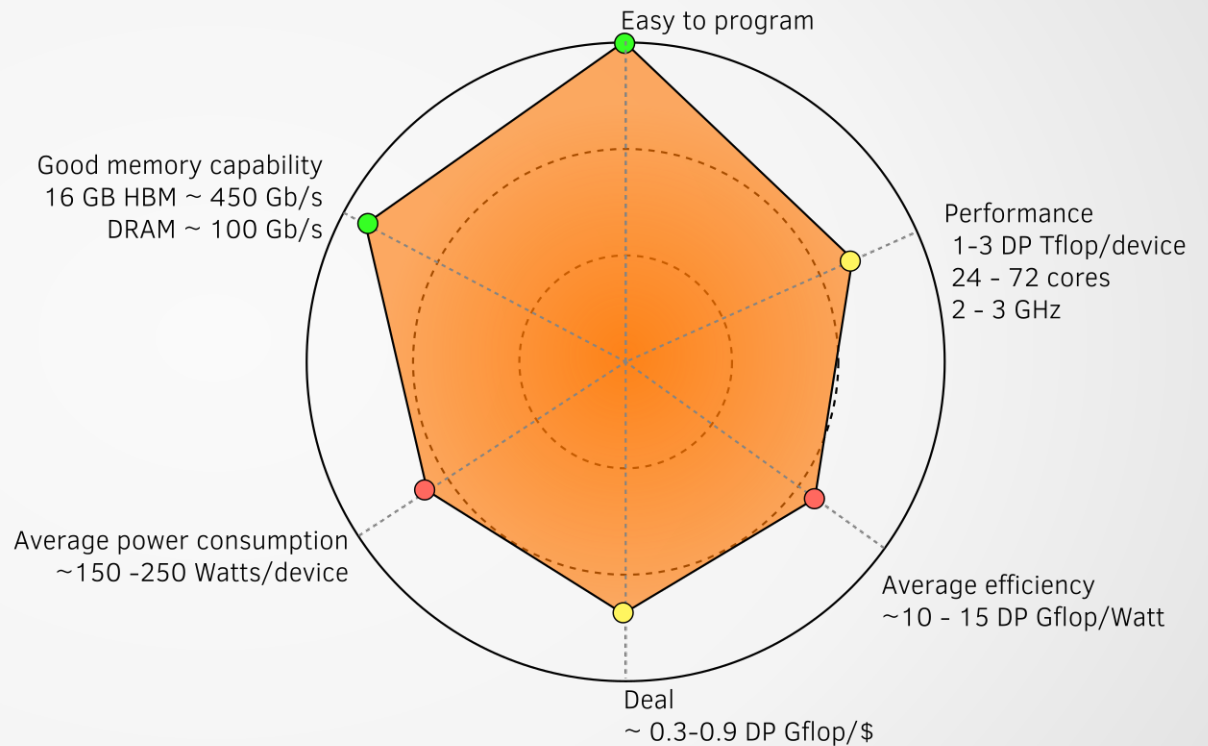
▼ For the moment, not suitable for Exascale standalone due to high energy consumption

## Configuration for HPC:

- Host
- Accelerators for Xeon Phi

## Programming models available:

- C, C++, Fortran
- Vendor compilers
- LLVM, GNU
- MPI, OpenMP, OpenCL



Based on Xeon Skylake and Xeon Phi KNL characteristics

[www.microway.com/knowledge-center-articles/detailed-specifications-of-the-skylake-sp-intel-xeon-processor-scalable-family-cpus/](http://www.microway.com/knowledge-center-articles/detailed-specifications-of-the-skylake-sp-intel-xeon-processor-scalable-family-cpus/)

[www.anandtech.com/show/11544/intel-skylake-ep-vs-amd-epyc-7000-cpu-battle-of-the-decade/7](http://www.anandtech.com/show/11544/intel-skylake-ep-vs-amd-epyc-7000-cpu-battle-of-the-decade/7)

<https://www.nextplatform.com/2017/12/05/power9-to-the-people/>



# RISC-based processors such as ARM

Historically, ARM processor uses the **light and less complex RISC architecture** (Reduced Instruction Set Computing) that does not contain complex instruction sets enabling **low energy consumption per core, less silicon and cheaper chips**.

ARM was initially designed for embedded and mobile applications.

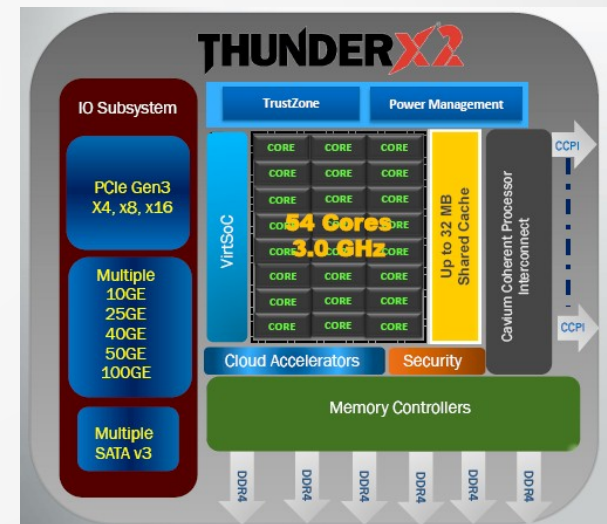
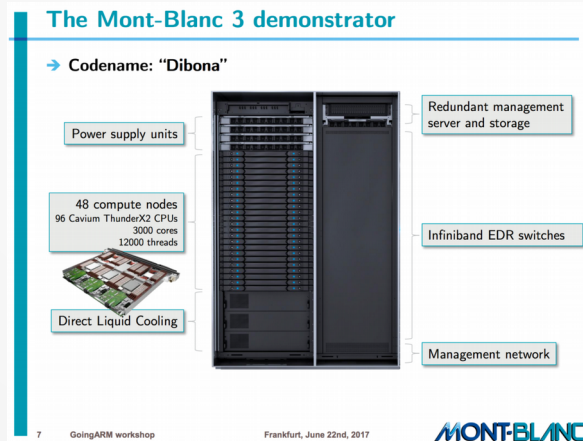
Europe (Mont-Blanc, CEA, Bull) and Japan (RIKEN) are now pushing the development of ARM super-computers.

Post-K: Fujitsu HPC CPU to Support ARM v8

Post-K fully utilizes Fujitsu's proven supercomputer microarchitecture  
 Fujitsu, as a "lead partner" of ARM HPC extension development, is working to realize an ARM Powered® supercomputer w/ high application performance  
 ARM v8 brings out the real strength of Fujitsu's microarchitecture

HPC apps acceleration feature	Post-K	FX100	FX10	K computer
FMA: Floating Multiply and Add	✓	✓	✓	✓
Math. acceleration primitives*	✓Enhanced	✓Enhanced	✓	✓
Inter core barrier	✓	✓	✓	✓
Sector cache	✓Enhanced	✓Enhanced	✓	✓
Hardware prefetch assist	✓Enhanced	✓Enhanced	✓	✓
Tofu interconnect	✓Integrated	✓Integrated	✓	✓

\* Mathematical acceleration primitives include trigonometric functions, sine & cosines, and exponential function



Post K-computer, a Japanese candidate for Exascale, will be equipped of ARMv8 with SVE ISA. (<http://www.fujitsu.com/global/Images/post-k-supercomputer-overview.pdf>)

European Bull DIBONA prototype uses Cavium ThunderX2 ARM cards in the framework of the European Mont-Blanc project. (<http://montblanc-project.eu/prototypes>)

ARM based server Cavium ThunderX2 used in DIBONA. ([www.nextplatform.com/2016/06/03/next-generation-thunderx2-arm-targets-skylake-xeons/](http://www.nextplatform.com/2016/06/03/next-generation-thunderx2-arm-targets-skylake-xeons/))

- <http://laruche.it/2014/07/05/lqt-cpu-arm-x86-differences-549851>
- <https://www.androidauthority.com/arms-secret-recipe-for-power-efficient-processing-409850/>
- <https://www.servethehome.com/cavium-thunderx2-review-benchmarks-real-arm-server-option/>



# RISC-based processors such as ARM

## Pros:

- ▲ Few code modifications from x86
- ▲ Server-oriented ARM SoC **cheaper** than Intel x86 CPUs
- ▲ Sell as licence: possibility to manufacture in Europe
- ▲ Easy to debug

## Cons:

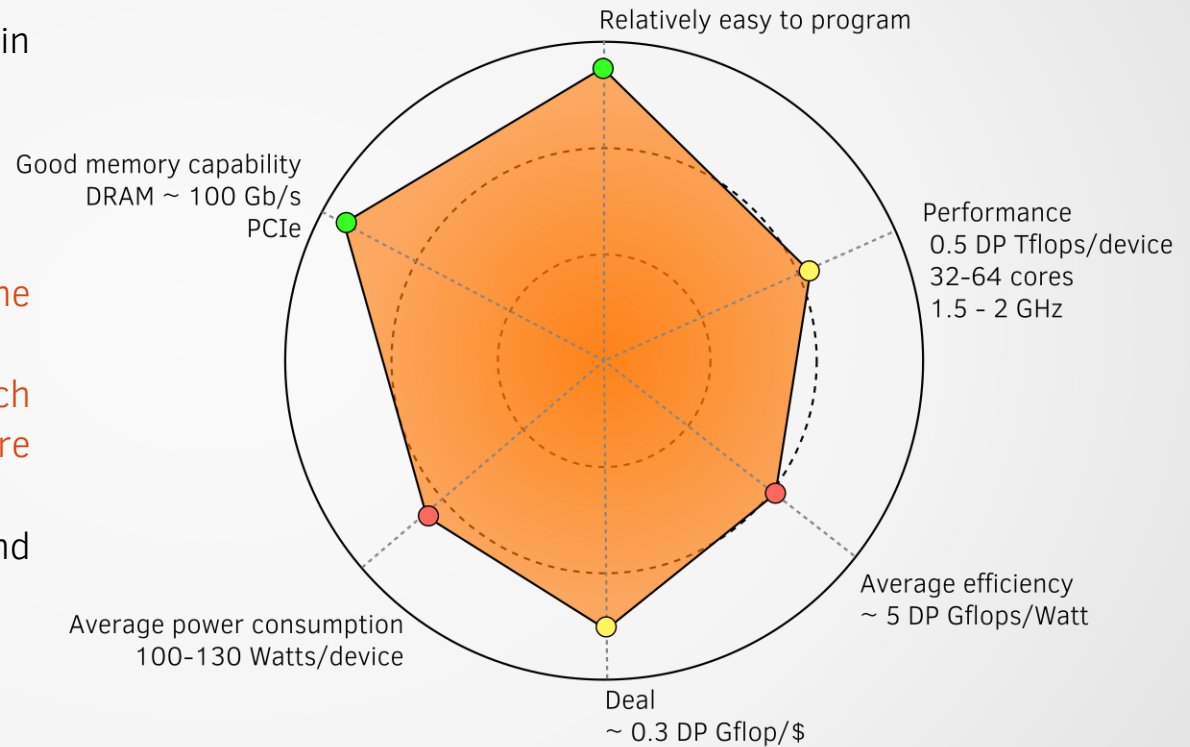
- ▼ **Not really more efficient than x86 for the moment** if strong scalable vector usage
- ▼ Server-oriented ARM **TDP tends to reach Intel x86 CPUs due to increased core complexity for HPC**
- ▼ **More optimization** let to the compilers and the developers **to get performance**

## Configuration for HPC:

- Host
- Replace the x86 CPUs

## Programming model available:

- Same as for x86 CPU architecture (C, C++, Fortran, LLVM, GNU, MPI, OpenMP...)



Based on Cavium, Ampere, Centric 2400 and Phytium Mars characteristics





# GPGPU (General Purpose Graphic Processing Units)

Historically, GPUs are used for complex graphical rendering in PC.

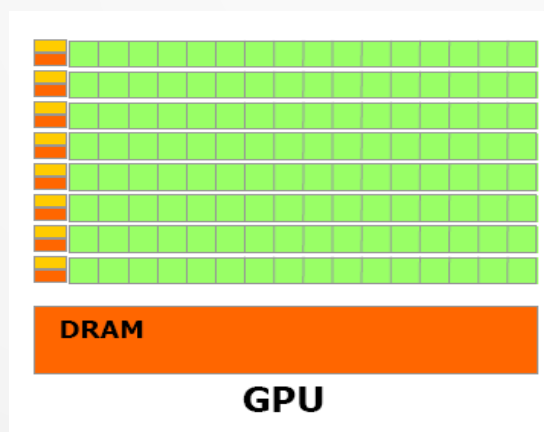
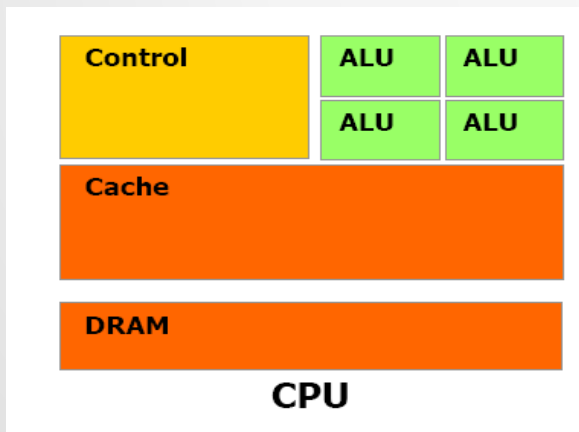
- ▶ need a lot of small simple computing units working in parallel

In the early 2000's, GPUs start to overcome CPU computational power and the gap is still increasing today.

- ▶ appeared to be excellent candidate for HPC

Today, GPUs are **massively parallel and vector devices composed of a lot of very simple and small cores (> 1000)** contrary to CPUs composed of a small number of more complex cores.

- ▶ How to parallelize an algorithm is a different way of thinking



Nvidia Tesla P100 Streaming Multiprocessor (SM) architecture

<https://images.nvidia.com/content/pdf/tesla/whitepaper/pascal-architecture-whitepaper.pdf>

<https://devblogs.nvidia.com/inside-pascal/>

[http://www.info2.uqam.ca/~makarenkov\\_v/BIF7002/Rapport\\_Arhjoul.htm](http://www.info2.uqam.ca/~makarenkov_v/BIF7002/Rapport_Arhjoul.htm)



# GPGPU (General Purpose Graphic Processing Units)

## Pros:

- ▲ Good performance in a single device (Desktop HPC application)
- ▲ Relatively easy to debug
- ▲ More and more easy to program

## Cons:

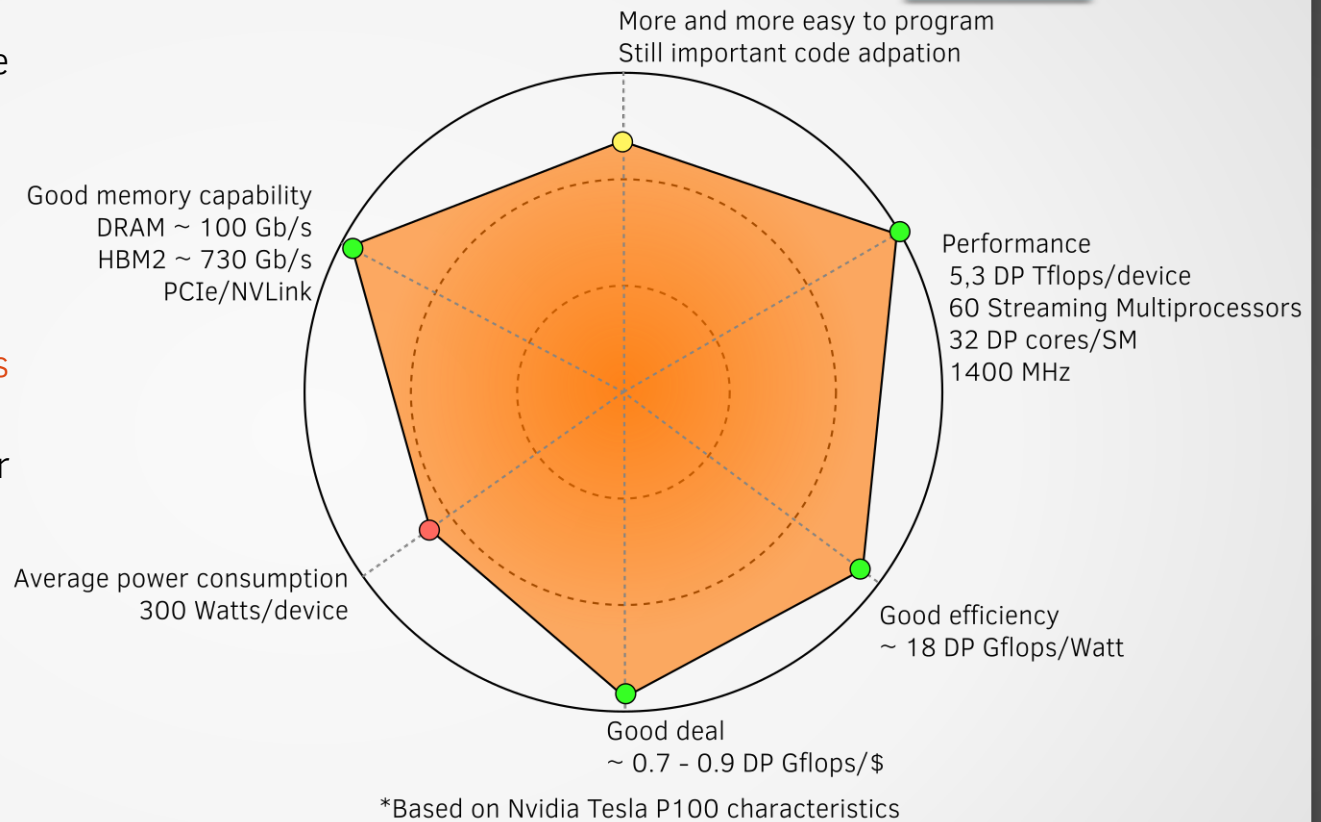
- ▼ Important adaptation efforts depending on the algorithm
- ▼ Important optimization efforts for decent performance

## Configuration for HPC:

- Accelerator

## Programming models available:

- CUDA, OpenCL, OpenACC, OpenMP



<https://images.nvidia.com/content/pdf/tesla/whitepaper/pascal-architecture-whitepaper.pdf>

<https://devblogs.nvidia.com/inside-pascal/>

[http://www.info2.uqam.ca/~makarenkov\\_v/BIF7002/Rapport\\_Arhjoul.htm](http://www.info2.uqam.ca/~makarenkov_v/BIF7002/Rapport_Arhjoul.htm)

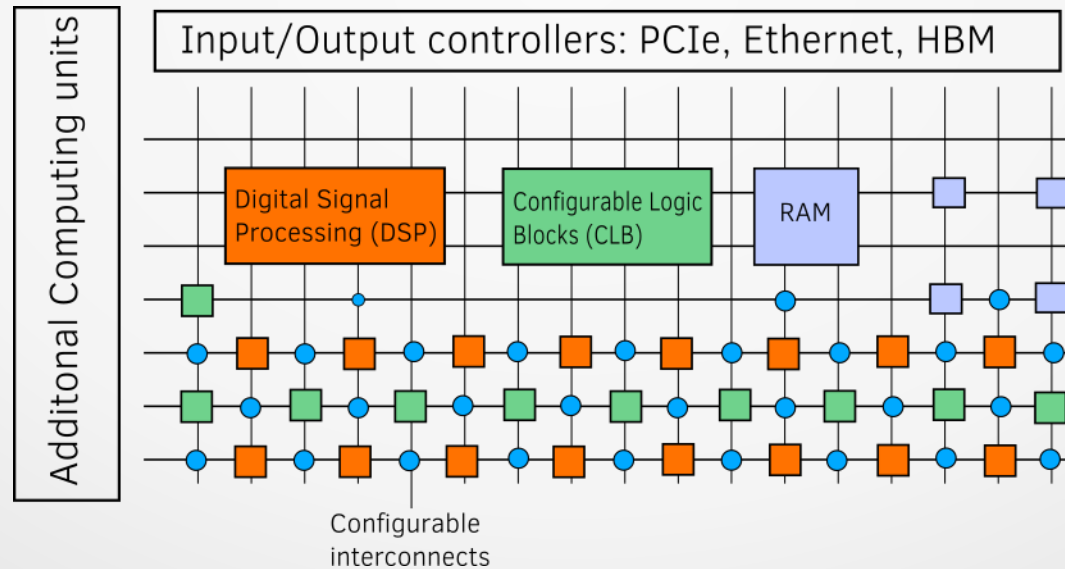


# FPGA - Field Programmable Gate Arrays

FPGA an **integrated circuit designed to be configured**: an array of programmable logic blocks and reconfigurable interconnects.

The FPGA architecture provides the flexibility to create a **massive array of application-specific ALUs** that enable both instruction and data-level parallelism.

Very high energy efficiency because of low frequency, a lot of silicon dedicated to the computation, unused blocs does not consume energy.



[https://science.energy.gov/~media/ascr/ascac/pdf/meetings/201612/Finkel\\_FPGA\\_ascac.pdf](https://science.energy.gov/~media/ascr/ascac/pdf/meetings/201612/Finkel_FPGA_ascac.pdf)  
[https://www.xilinx.com/support/documentation/white\\_papers/wp375\\_HPC\\_Using\\_FPGAs.pdf](https://www.xilinx.com/support/documentation/white_papers/wp375_HPC_Using_FPGAs.pdf)  
<https://www.altera.com/products/fpga/stratix-series/stratix-10/overview.html>





# FPGA - Field Programmable Gate Arrays

### Pros:

- ▲ Best energy efficiency (flop/Watt) on the market
- ▲ Versatile and adaptable to many kernels

### Cons:

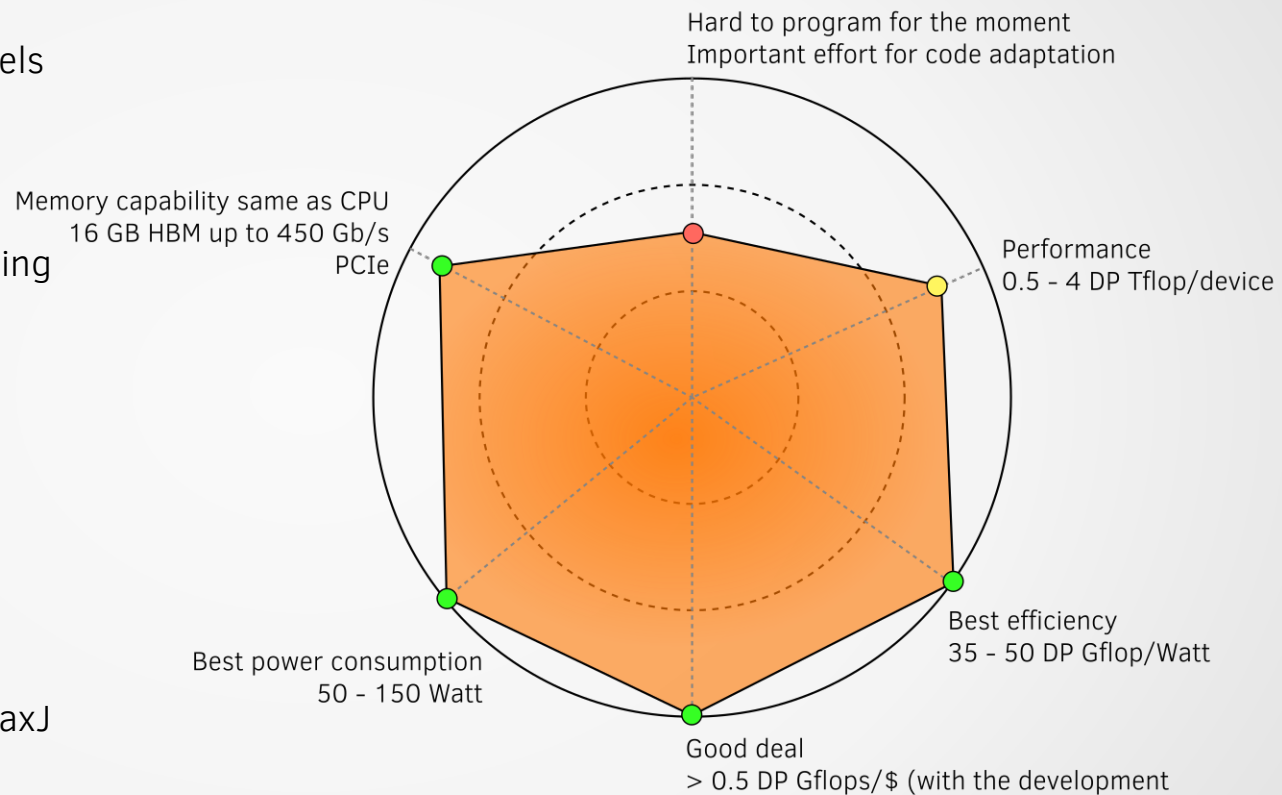
- ▼ Difficult to program today
- ▼ Low frequency (~100 MHz) ► pipelining optimization and vectorization
- ▼ Long compilation (several hours)
- ▼ Debugging ? Emulators ?

### Configuration for HPC:

- as an accelerator

### Programming model available:

- Vendor specific languages (MaxJ language for Maxeler)
- OpenCL with C/C++/Fortran (pushed by Intel)
- OpenMP/OpenACC (not mature)
- VHDL (higher difficulty)



Based on Altera Stratix 10 and Xilinx Virtex Ultrascale+ characteristics

[https://science.energy.gov/~media/ascr/ascac/pdf/meetings/201612/Finkel\\_FPGA\\_ascac.pdf](https://science.energy.gov/~media/ascr/ascac/pdf/meetings/201612/Finkel_FPGA_ascac.pdf)  
[https://www.xilinx.com/support/documentation/white\\_papers/wp375\\_HPC\\_Using\\_FPGAs.pdf](https://www.xilinx.com/support/documentation/white_papers/wp375_HPC_Using_FPGAs.pdf)  
<https://www.altera.com/products/fpga/stratix-series/stratix-10/overview.html> ; <https://indico.math.cnrs.fr/event/3435/material/slides/0.pdf>



# Processing unit general view

No miracle so far...



- Programmed FPGA
- GPGPU
- Xeon Phi Power
- Xeon SP ARMv8
- Xeon ARM
- Pentium AMD Bulldozer



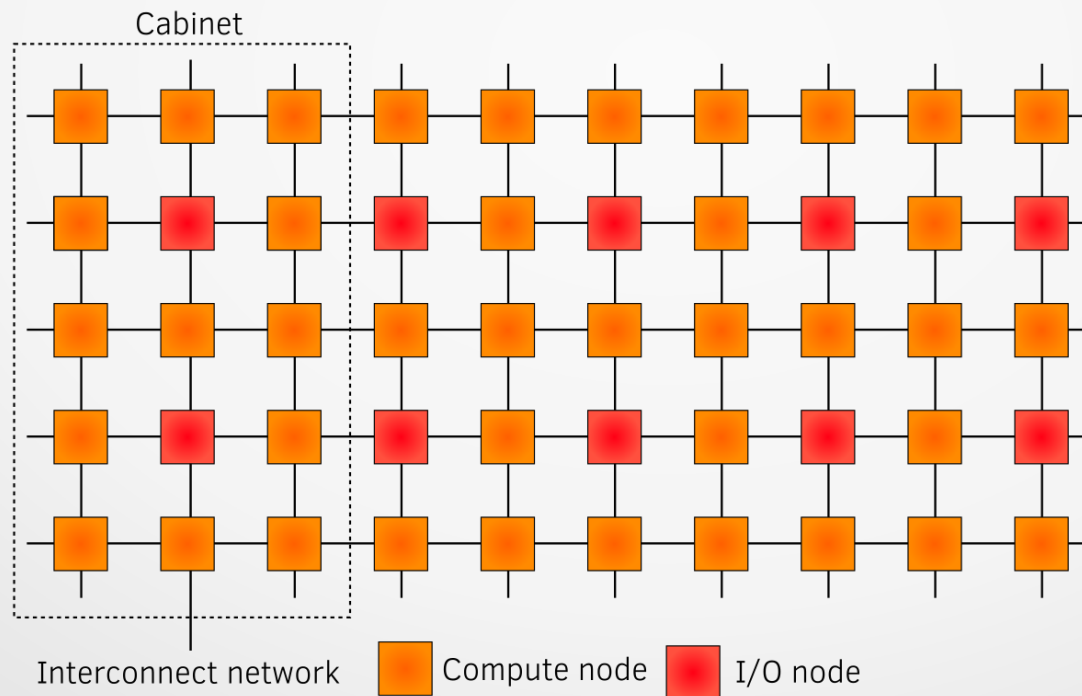
# Hardware trends: multi-level massive parallelism

Exascale supercomputers will be composed of more than 100 000 interconnected nodes (several millions cores).

Level 1 – distributed parallelism between node

↔ MPI still the considered communication model for developers

▲ Complex software stack required to handle huge traffic and failure (lossless compression, resilience, huge pages, RMA...)





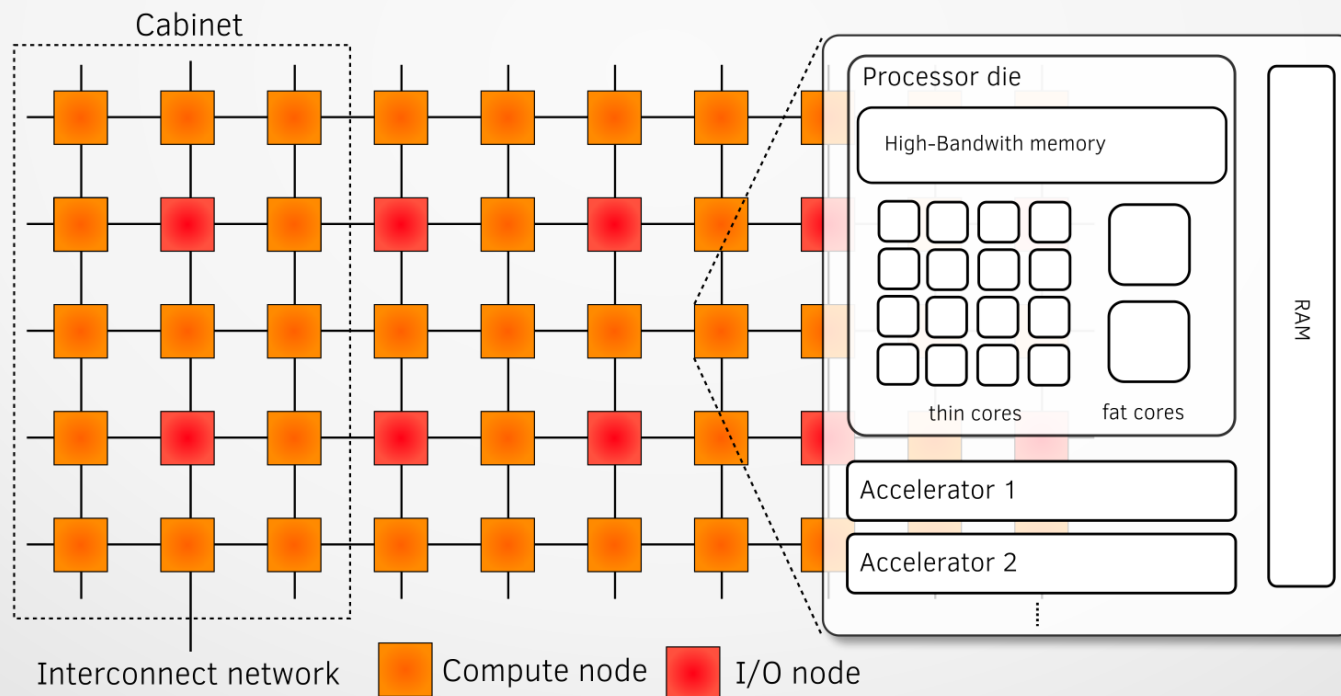
# Hardware trends: multi-level massive parallelism

Each node composed of several sockets of **several tens of cores/threads** potentially connected to **1 or more accelerators**

Level 2 – inner-node parallelism

↔ Shared parallelism with non-uniform memory access (NUMA) between cores or sockets

■ Heterogeneous computing with different accelerators, memory space and bandwidth





# Hardware trends: heterogeneity

## Frontal nodes

Role: OS

Processing units: Server x86 (Xeon), Power, ARM

## Compute node

### Host

Multi-core x86, Power, ARM CPUs

Many-core x86, Power, ARM CPUs

Skinny-Fat x86

Big.LITTLE ARM

RAM

Role: OS, computation, post-processing, software  
Programming model: MPI, OpenMP...

PCIe,  
NVLINK...

Unified  
memory

### Accelerators

Co-processors (Many-core), PEZY, MATRIX-2000

GPGPU

FPGA

HBM

Role: computation, post-processing, rendering  
Programming model: OpenCL, CUDA, OpenACC, OpenMP...

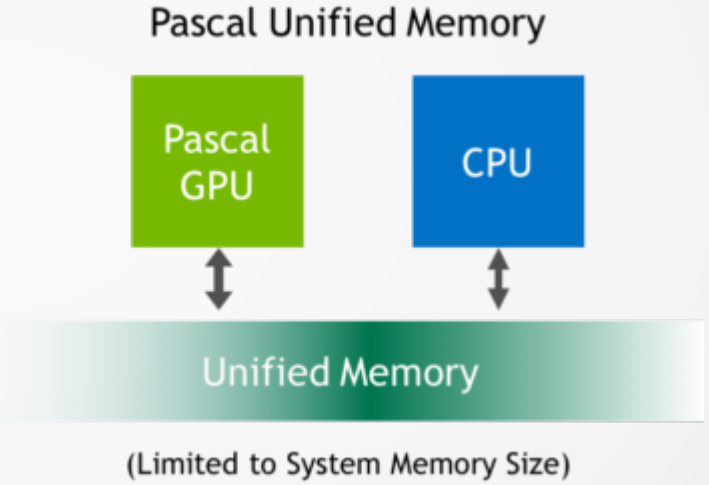
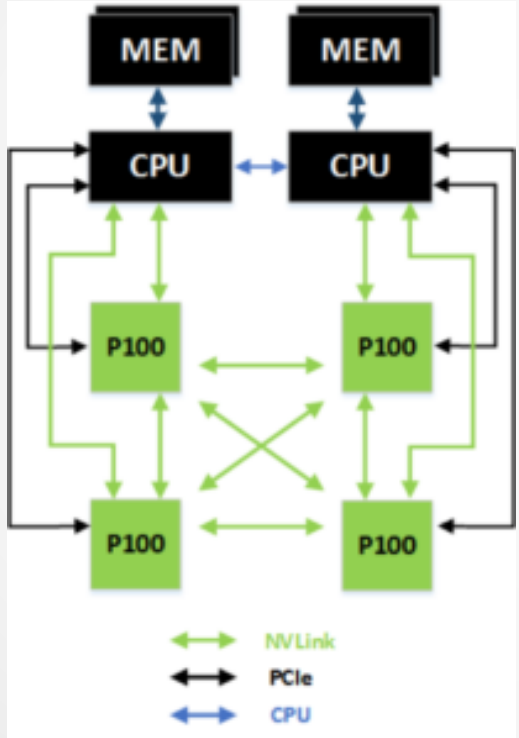
## I/O nodes

Role: OS, computation, post-processing, software, IO treatment

Programming model: MPI, IO stack



# High-speed interconnect: openPOWER example





# Hardware trends: vectorization

All computing devices can be seen as a vector machine

Level 3 – vectorization

▣ Capability to compute simultaneously a full vector of data with the same set of operations

CPU: **Single instruction multiple data** (SIMD) vectorization

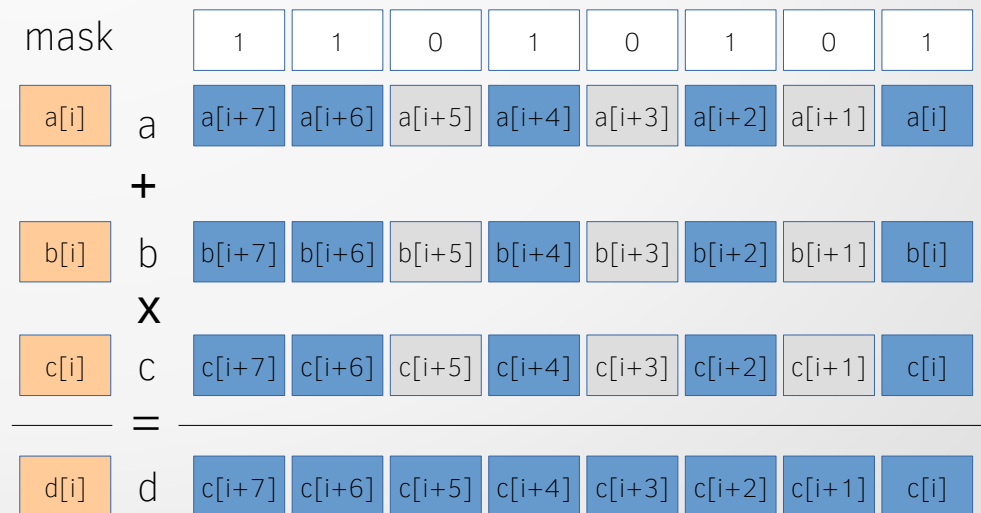
GPU: vectorization through the large number of cores working simultaneously within a SM: **Single instruction multiple thread vectorization** (SIMT)

FPGA: vectorization through kernel encoding replica: several pipelines of the same kernel working simultaneously

For i from 1 to N :

If (condition on i) :

$$d[i] = a[i] + b[i]*c[i]$$



Single Instruction Multiple Data SIMD vision as in x86 Intel



# Hardware trends: vectorization

All computing devices can be seen as vector machines

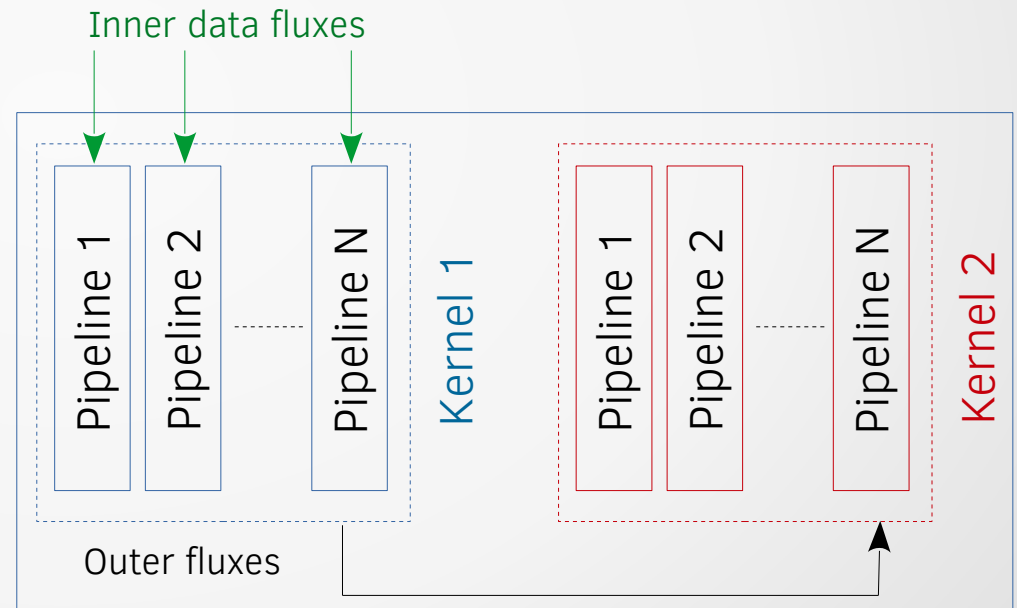
Level 3 – vectorization

▣ Capability to compute simultaneously a full vector of data with the same set of operations

CPU: **Single instruction multiple data (SIMD)** vectorization

GPU: vectorization through the large number of cores working simultaneously within a SM: **Single instruction multiple thread vectorization (SIMT)**

FPGA: vectorization through kernel encoding replica: several pipelines of the same kernel working simultaneously



FPGA pipeline vectorization by the multiplication of the a pipeline from the same kernel





# Hardware trends: I/O nodes

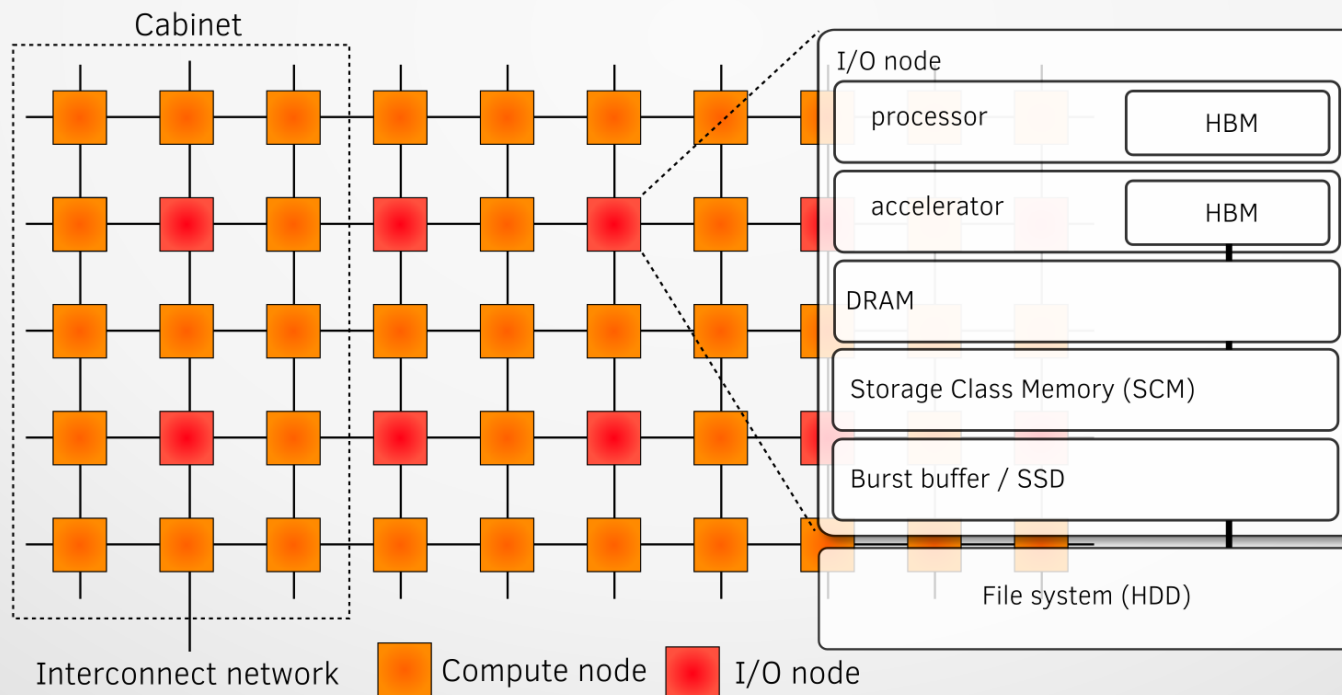
I/O nodes are specialized in fast input / output with a complex storage hierarchy

DRAM: volatile, highest bandwidth ( $\sim 100\text{Gb/s}$ ), lowest capacity ( $\sim 10\text{Gb}$ )

Storage Class Memory (SCM): volatile, lower bandwidth than DRAM ( $\sim 10\text{Gb/s}$ ) but higher capacity ( $\sim 100\text{Gb}$ )

SSD: also referred to as burst buffer, permanent, lower bandwidth ( $\sim \text{Gb/s}$ ) than SCM but higher capacity ( $\sim 500\text{Gb}$ )

HDD: permanent, lowest bandwidth ( $\sim 100\text{Mb/s}$ ), highest capacity ( $\sim \text{Tb}$ )





### III. Programming challenges



## Presentation of the codes



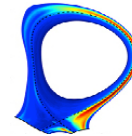
Smilei)

LULI, LLR, CEA Saclay

Smilei is a Particle-In-Cell code for plasma simulation. Open-source, collaborative, user-friendly and designed for high performances on CPU super-computers, it is applied to a wide range of physics studies: from relativistic laser-plasma interaction to astrophysics.

- ▶ Python + C++
- ▶ MPI + OpenMP
- ▶ HDF5 + OpenPMD

△ <http://www.maisondelasimulation.fr/smilei/>



Tokam3X

CEA Cadarache

The TOKAM3X code simulates both limited and diverted plasma turbulence in full torus Tokamak geometry including the open field lines of the Scrape-off Layer (SOL) and the edge closed field lines region in the vicinity of the separatrix.

- ▶ Fortran
- ▶ MPI + OpenMP
- ▶ HDF5 sequential

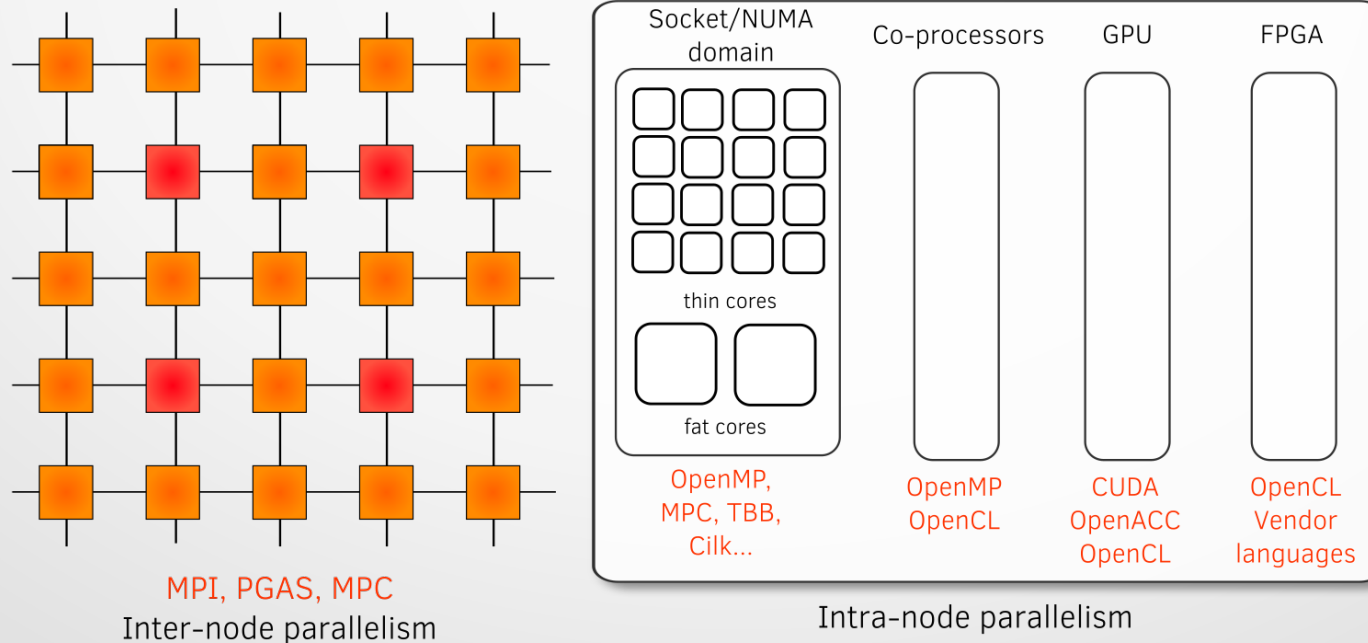


# Programming challenges – multi-level massive parallelism

Time spent in communication will overcome computational time (almost the case for SMILEI)  
Network capacity evolves less rapidly than computation power

Scalability:

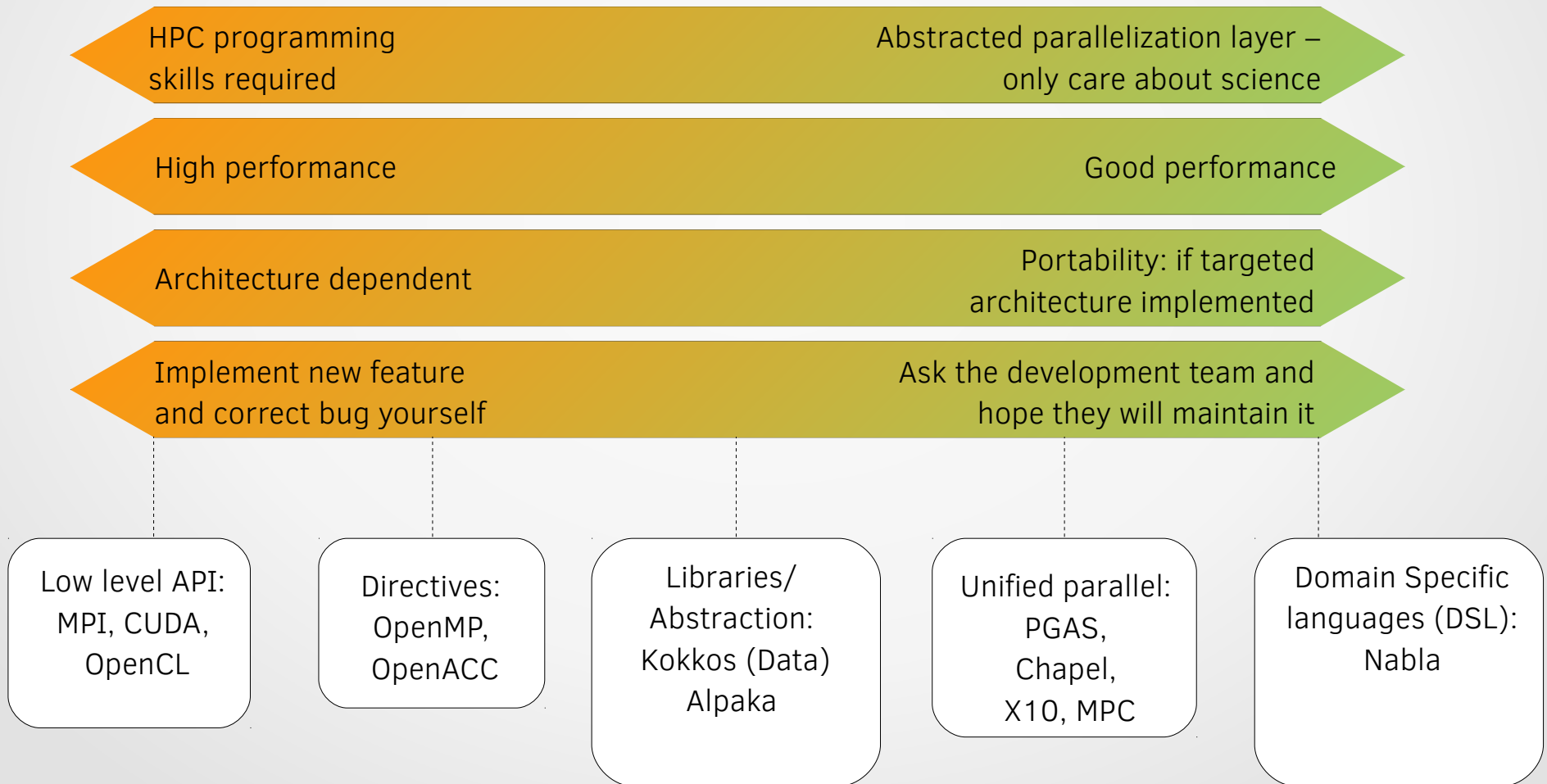
- ▶ MPI + X (OpenMP, Open ACC...)
- ▶ Limit data movements, avoid global communications, use shared memory within a node
- ▶ Use non-blocking communication with computation
- ▶ Dedicate cores to the communications, diagnostic processing, I/O
- ▶ Use accelerator in symmetric mode to exploit the full node computational power





# Programming challenges – architecture dependency

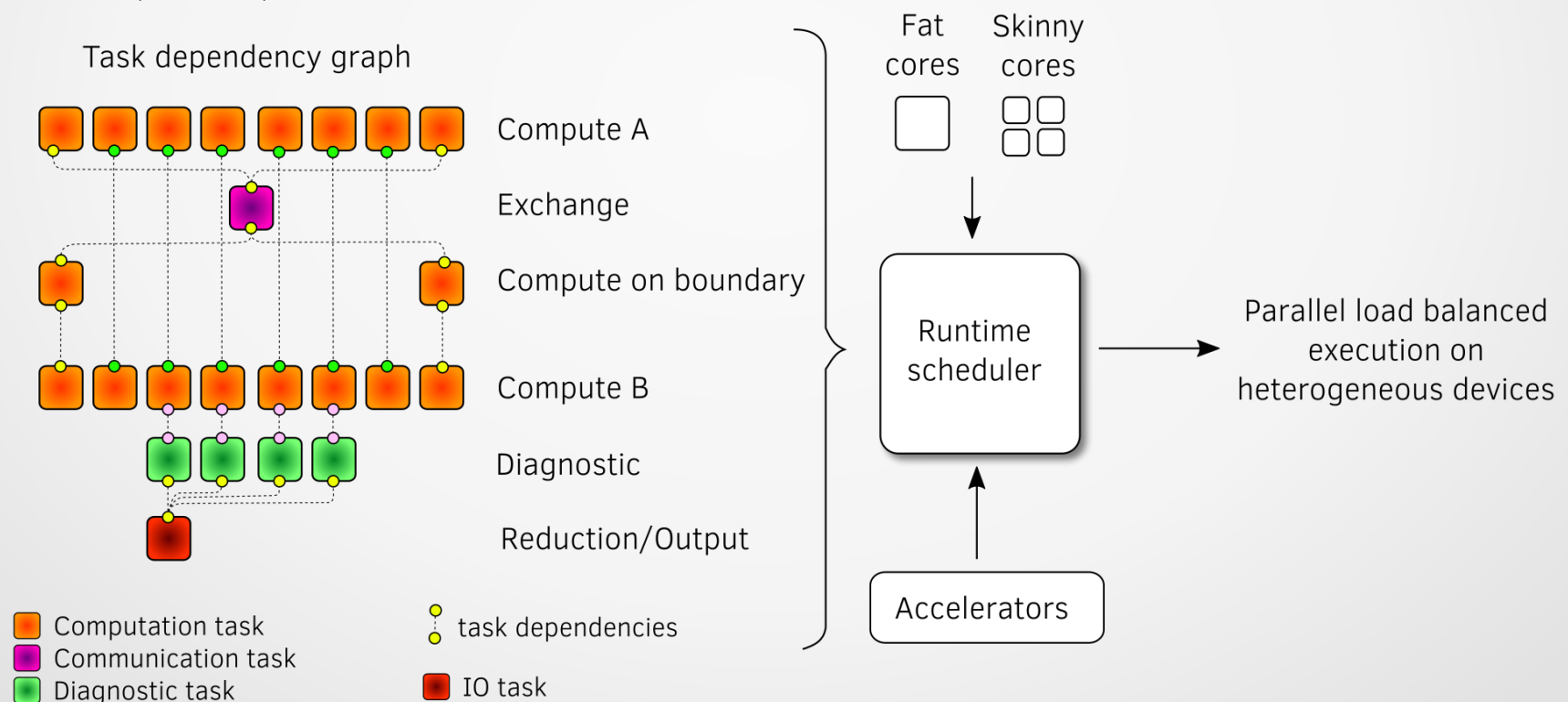
## How to deal with architecture multiplication?





# Programming challenges – Task-based approach

- ▶ An application can be divided temporally and spatially into inter-dependent tasks of different natures (computation, communication, IO)
- ▶ Using a smart runtime scheduler, tasks can then be run **concurrently/asynchronously in parallel on a large number of cores/ on several architectures.**
- ▶ To use a task-based model can speedup the code by overlapping IO and communication with computation.
- ▶ Factor of performances: grain size (fine, coarse), scheduler, dependency graph
- ▶ OpenMP task, StarPU, libKOMP...



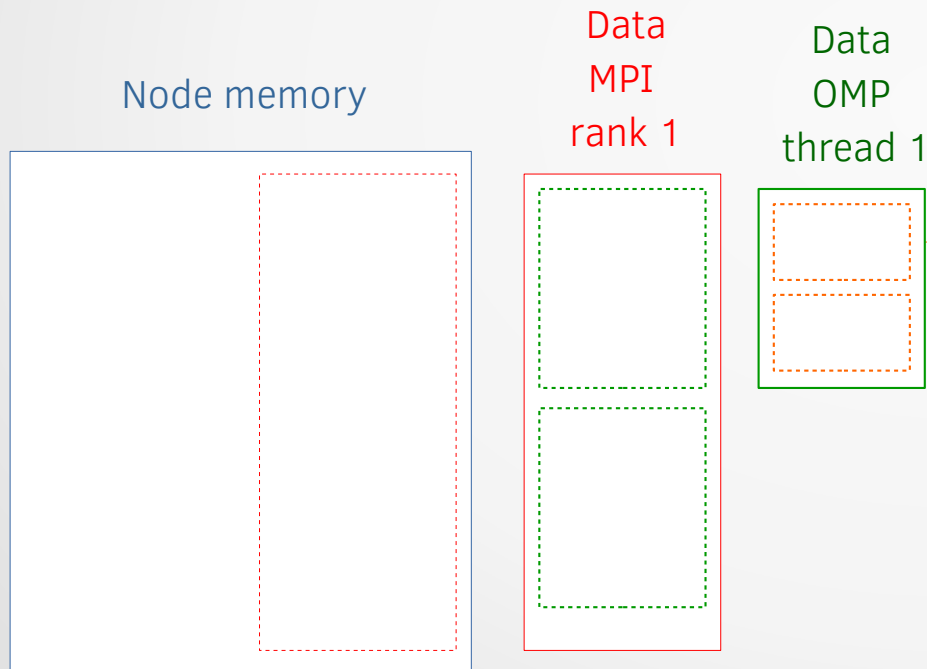


# Programming challenges – cache blocking + vectorization

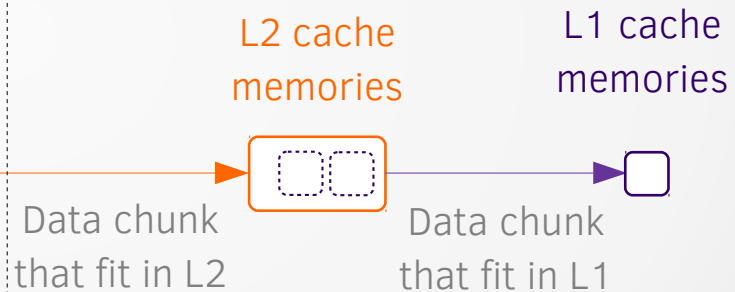
Decomposition of the workload into chunk that fit the targeted level of cache :

- ▶ Diminish number of cache misses / reuse data in cache
- ▶ Reduce memory bandwidth pressure : improve performance of memory bound algorithms

Hybrid parallel memory decomposition



Cache blocking



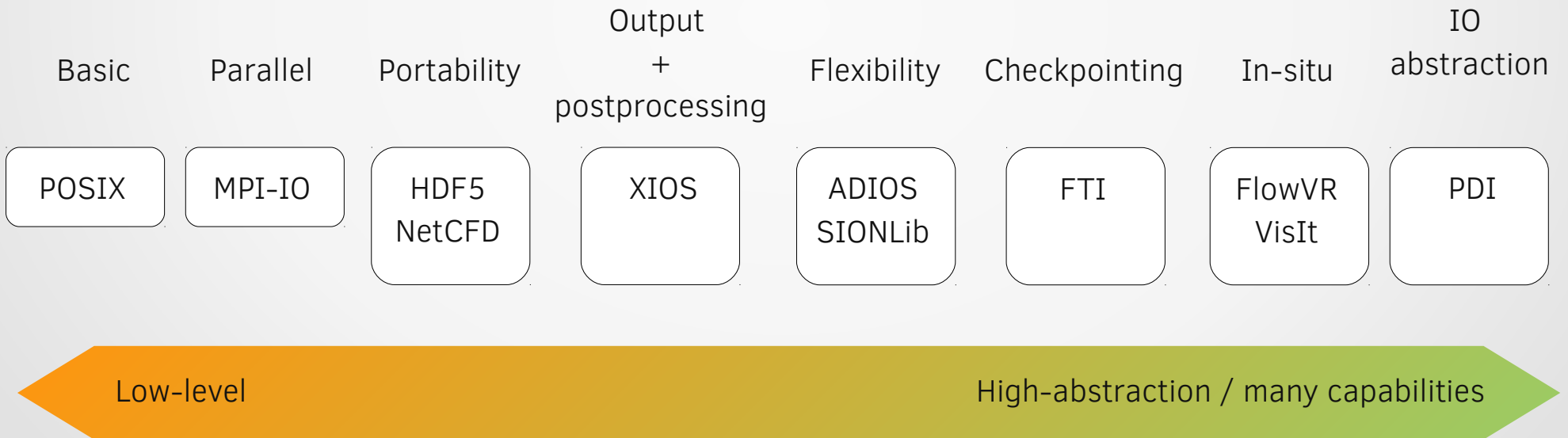
Chunk size < L2

Chunk number > number of OMP thread



# Programming challenges – IOs

- ▶ Dealing with specific IO nodes
- ▶ Dealing with complex IO hardware stack
- ▶ Scalable and concurrent reading/writing process
- ▶ Portability / Flexibility
- ▶ Checkpointing for fault tolerance
- ▶ Storage capacity increases less rapidly than computational power: data treatment on the fly, in-situ visualization, in-situ analysis via machine learning







## Additional challenging aspects not covered here

- ▶ Code output precision (how to tune precision to speed-up the code)
- ▶ Failure prediction and correction
- ▶ Code optimization to reduce energy-consumption (not just a question of computer design)



## Conclusion

- ▶ **No breakthrough expected**, forthcoming HPC hardware is the continuity or adapted from other domains such as the mobile world
- ▶ **Scalability on millions of core will be challenging**: multi-level parallelism, communication limitation, communication/computation/diagnostic overlapping, task model
- ▶ **Core optimization**: smart use of cache levels, vectorization
- ▶ **Heterogeneity will be challenging**: concurrent use of resources to reach peak performance (overlapping, task...)
- ▶ **Disk memory will be limited and IO stack more complex**: parallel use of IO nodes, dedicated resources to diagnostics and IOs, asynchronous treatment taking advantage of intermediate storages
- ▶ **Focusing on a specific architecture can be dangerous** to run efficiently on forthcoming machines
- ▶ Exascale optimization efforts useful for current architecture as well