EURO²

HPC Teaching Kit

By EuroCC Belgium

What is HPC?

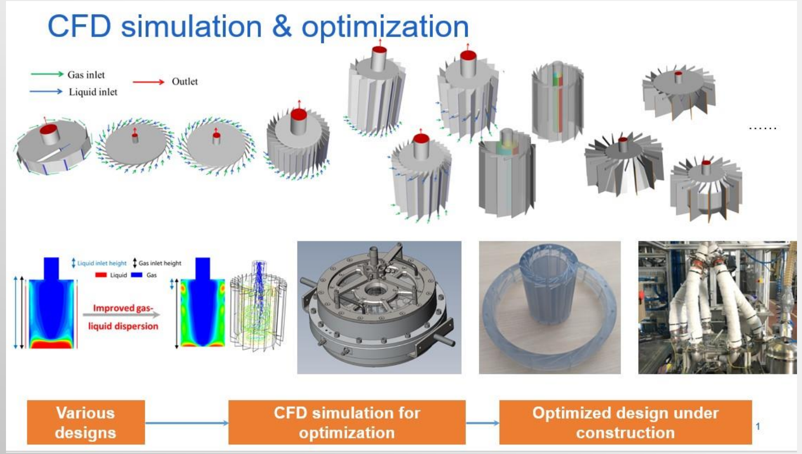
- Aggregation of computer power (in the form of supercomputer or *clusters*) to deliver high computational performances, in order to solve large problems.
- *Clusters* are linked computers (= nodes) that works together, so that, for many aspects, they look like one single computer (*more on that latter*).
- The work is distributed across workers (*more on that latter*).

Exemples of HPC uses

Have a look at www.enccb.be/stories

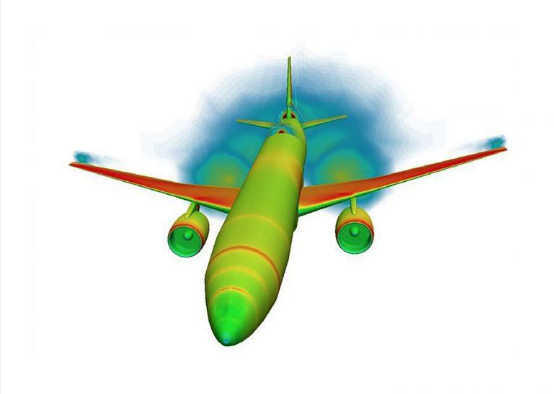
Examples: fluid dynamics

Design and optimization of a vortex unit for CO_2 capture



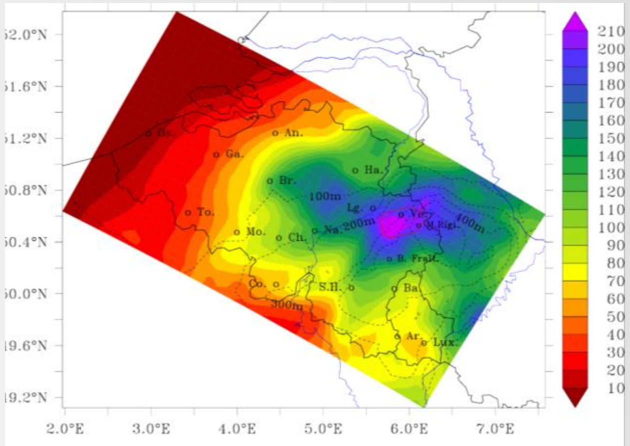
https://www.enccb.be/usvortexunit

Aircraft design



https://prace-ri.eu/automating-aircraft-design-and-optimisation/

Predicting the climate

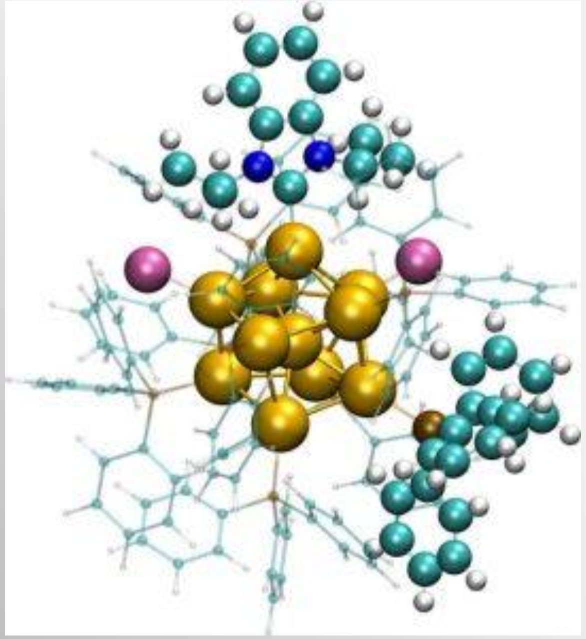


Total precipitation over 15-17 August 2033

https://www.enccb.be/usxavierfettweis

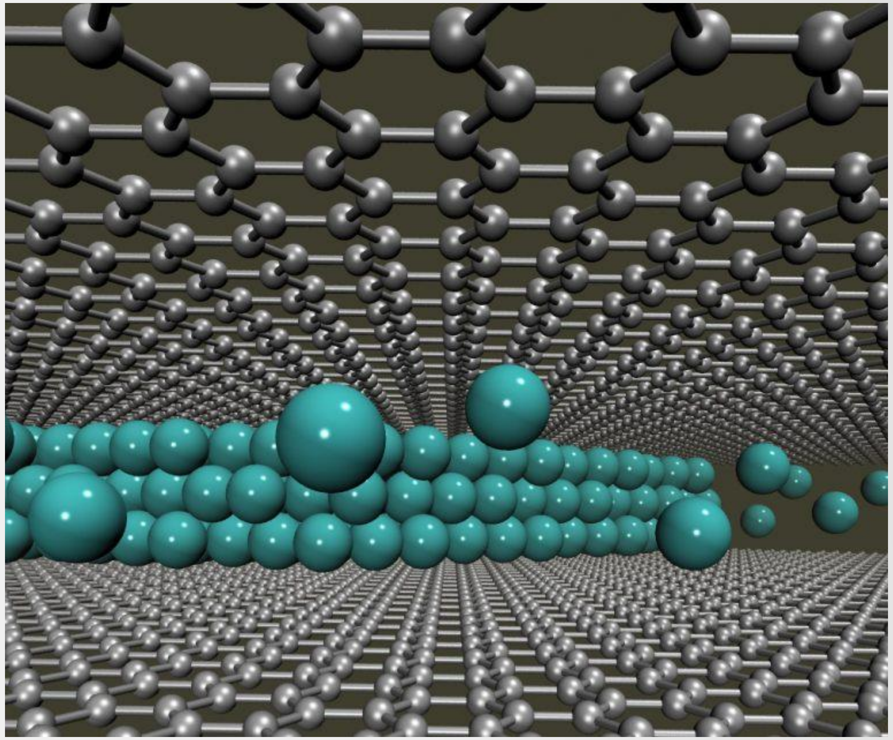
Examples: materials

Predicting the structure of gold cluster that chops carbon dioxide



https://prace-ri.eu/computer-simulations-gold-cluster/

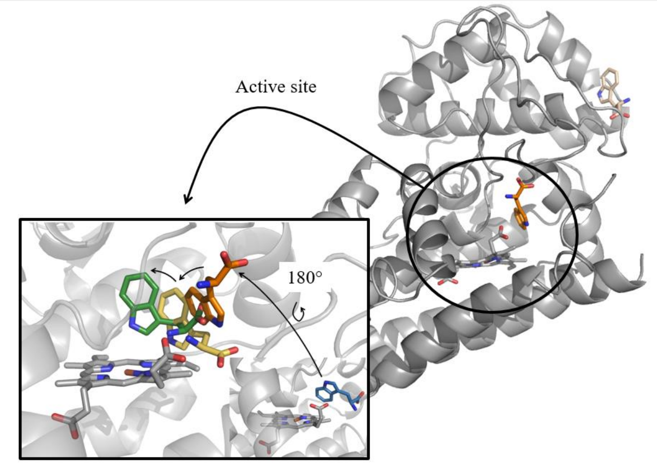
Tailoring the properties of 2D materials



https://prace-ri.eu/simulations-help-to-tailor-the-properties-of-2d-materials/

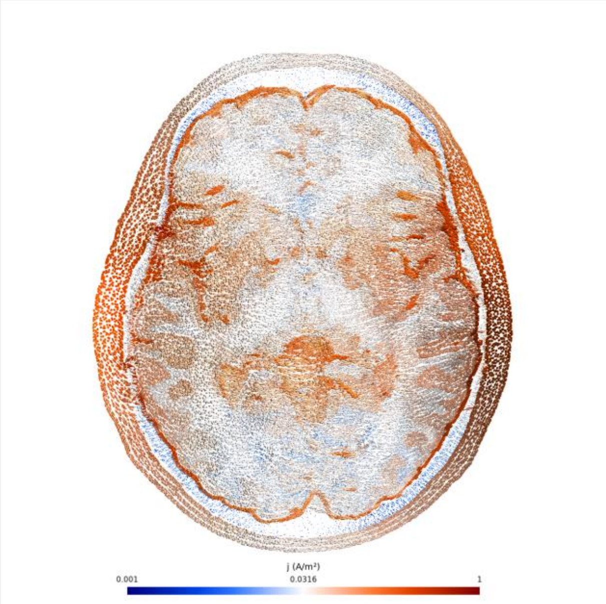
Examples: biology

Unraveling the behavior of the hIDO1 protein



https://www.enccb.be/usmanonmirgaux

Understanding how radio waves propagate in the head with Shamo



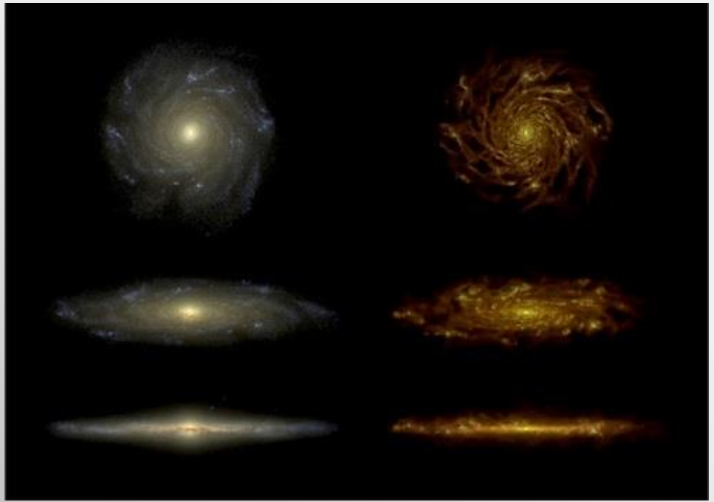
https://www.enccb.be/usshamo

Improving chocolate with supercomputing

https://www.enccb.be/uschocolate

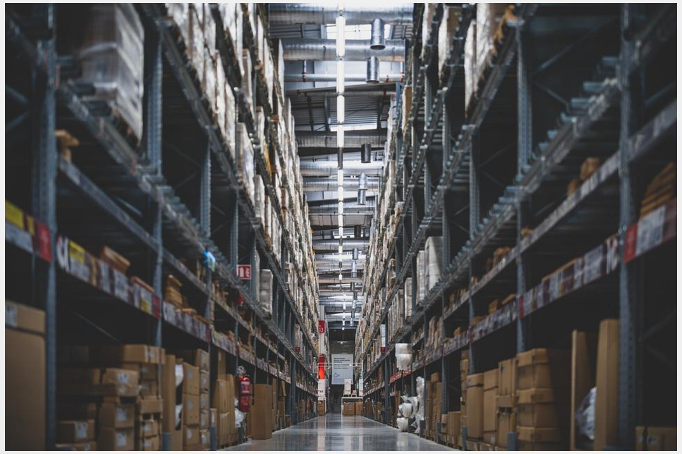
Examples: physics, mathematics, engineering,…

Simulating Galaxies



https://www.enccb.be/usuniverse

Outsmarting NP-hardness



https://www.enccb.be/uslogisticsnphardness

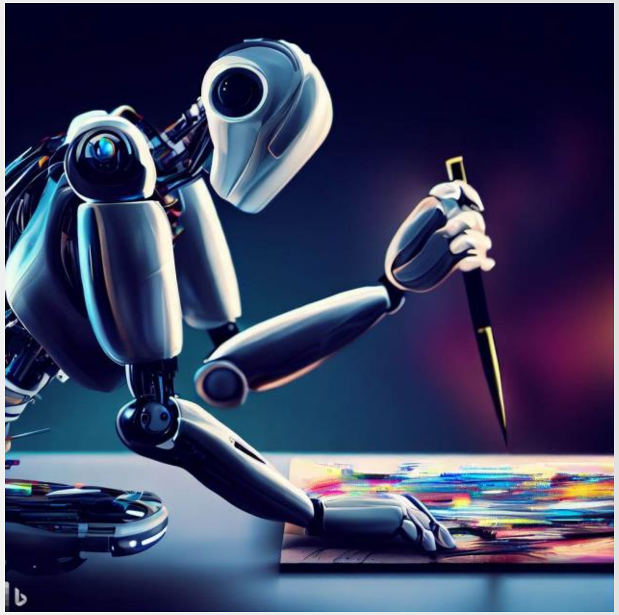
Optimizing particle processes through simulation with MPacts

https://www.enccb.be/usmpacts

Examples

But also:

- Artificial intelligence
- Machine learning
- Data analysis
- …



What is EuroCC?

- EuroHPC Join Undertaking is a joint initiative between the EU (European countries) and private partners to develop a world class supercomputing system in Europe.
- EuroCC is a project of EuroHPC-JU, which tasks each participating countries to create a national competence center (NCC) in the area of HPC. They coordinate activities in the HPC/HPDA/AI fields and serve as contact point.
  → More information on https://www.enccb.be/.
- Different missions, including contact with industry, raising awareness and organizing trainings.

Outline of this presentation

EURO²

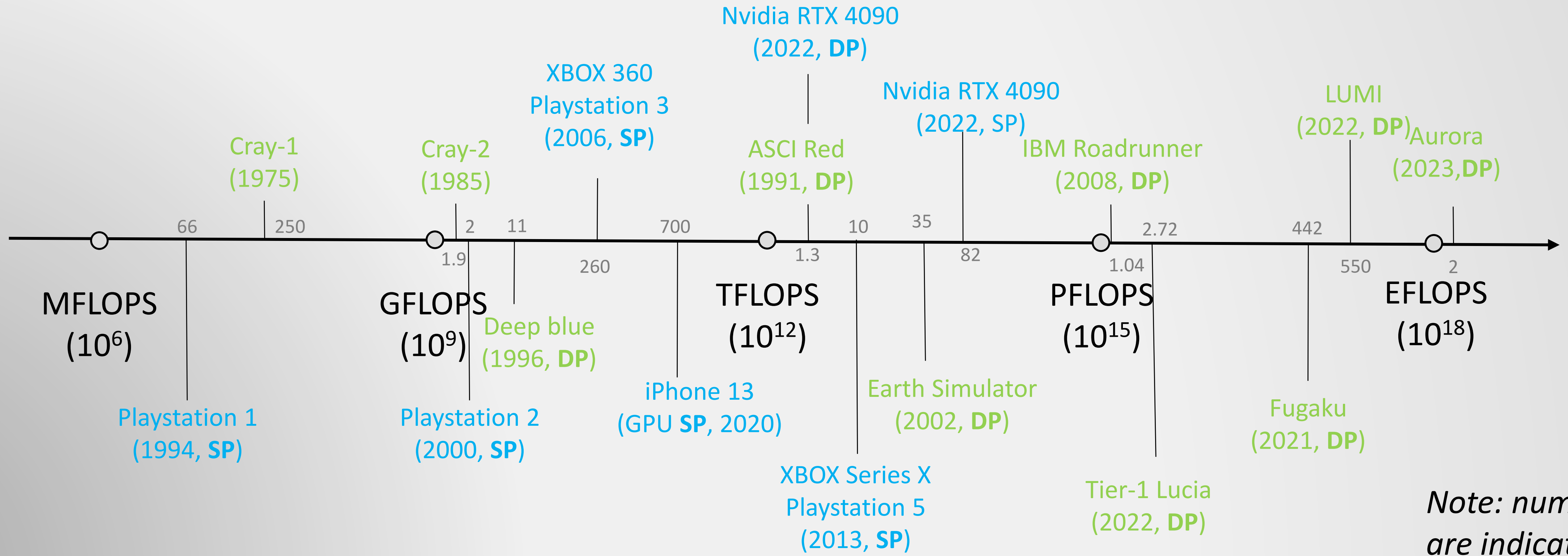
- Current status of the supercomputing infrastructures
  - Performance and the TOP500 list
  - Supercomputers in Europe
  - Supercomputers in Belgium
- Understand how a supercomputer works:
  - Architecture
  - Components
  - Interactions
- Understand how program can use such large resources, and what are the issues that needs to be overcome:
  - Parallelism
  - Parallelisation issues

Where are we today?

Which supercomputers for Belgium

Performances

- One of the measurement is FLOPS = floating point operations per second (≃ speed)
- Note that it depends on single (SP, 32 bits) or double (DP, 64 bits) precision!

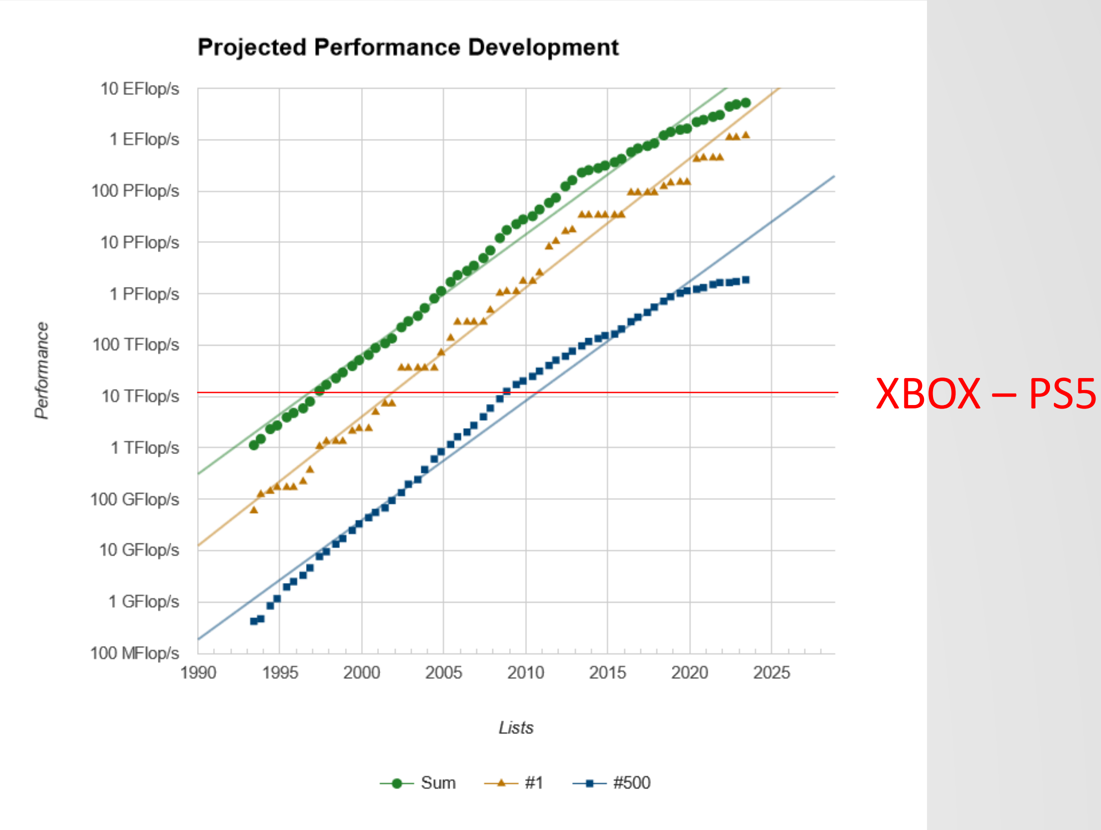


Note: numbers are indicative

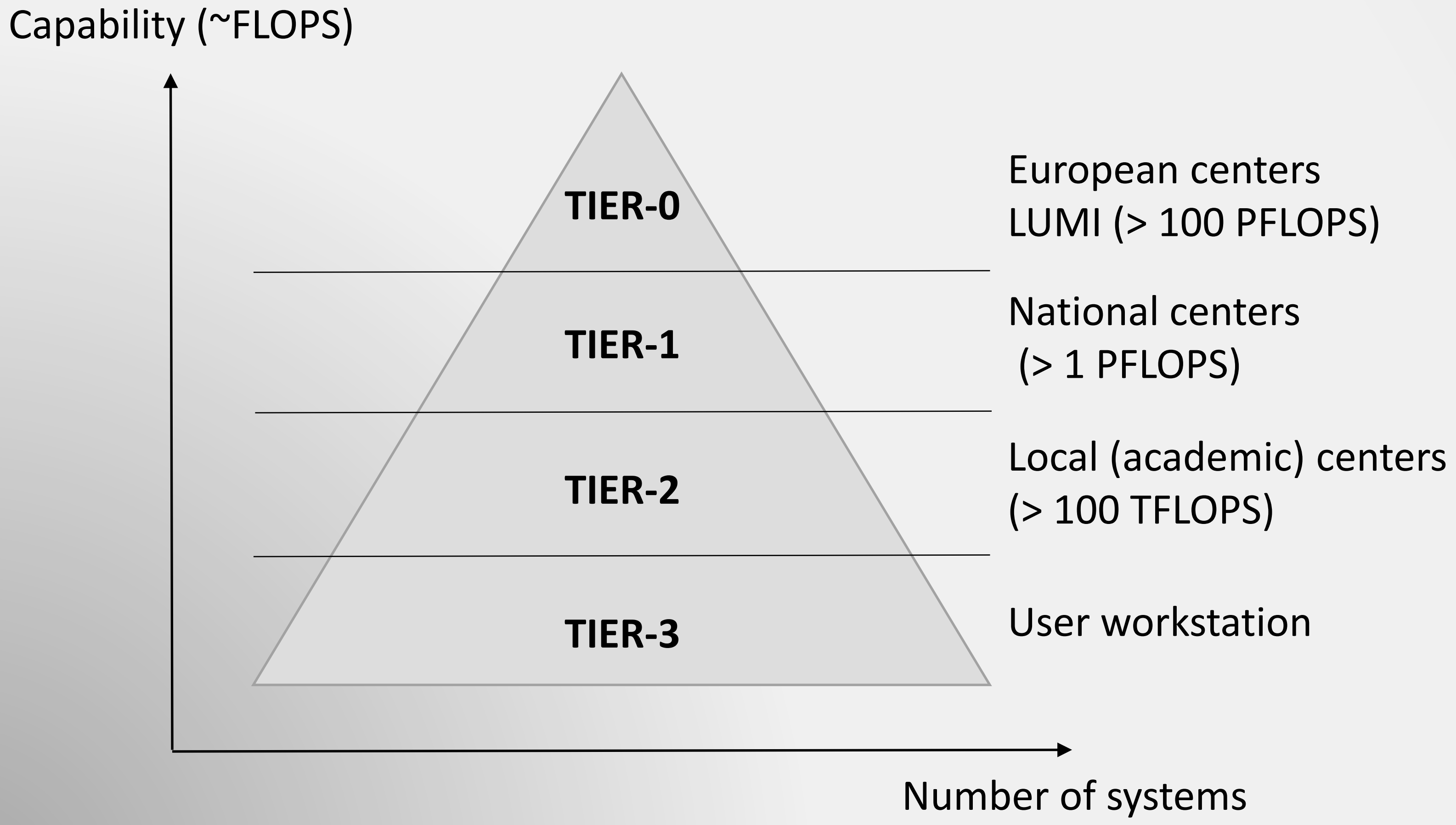
The TOP500

The TOP500 is a list of the fastest supercomputer in the world

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
2	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016
4	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404
5	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096
6	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94.64	125.71	7,438

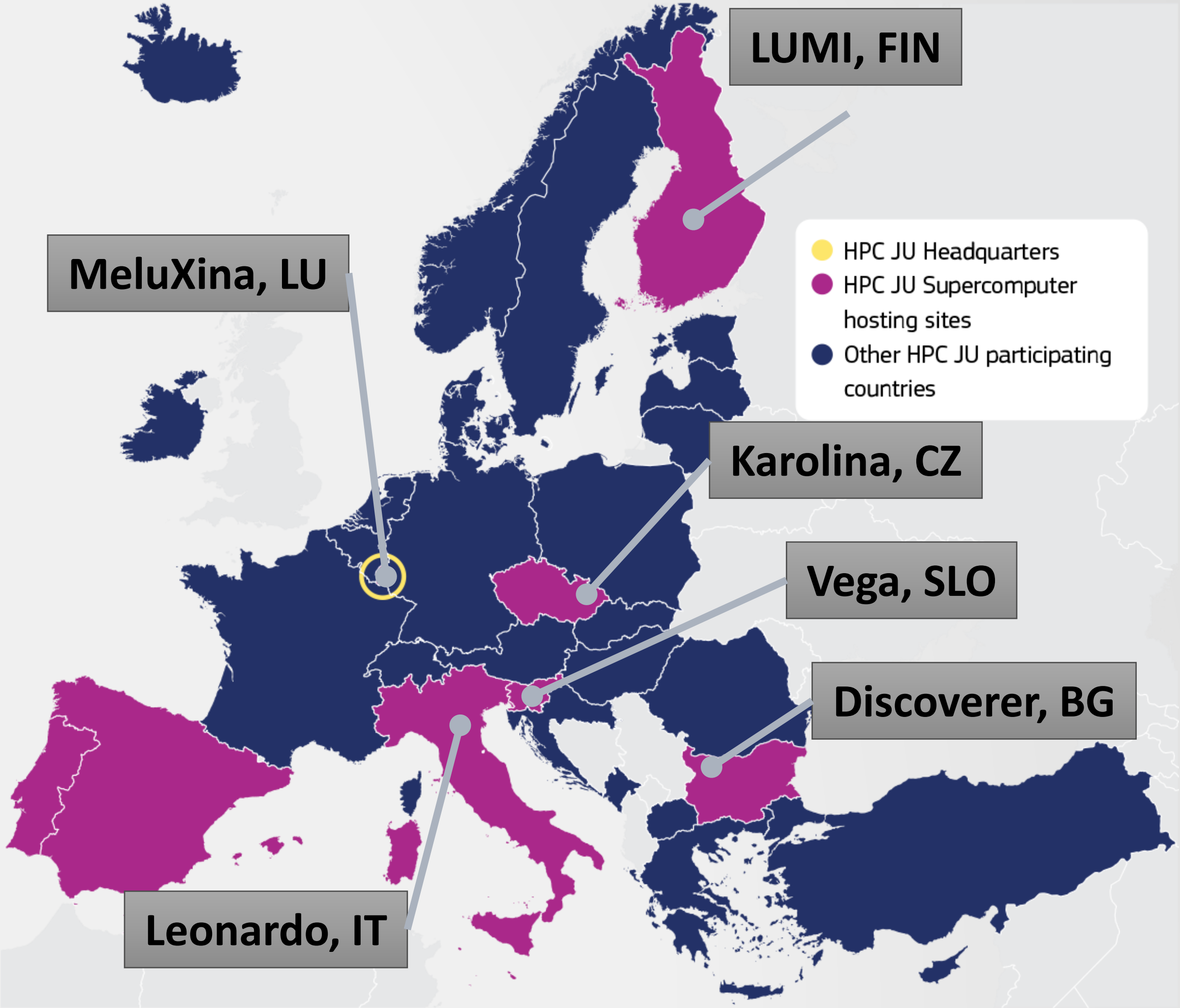


Supercomputers in Europe



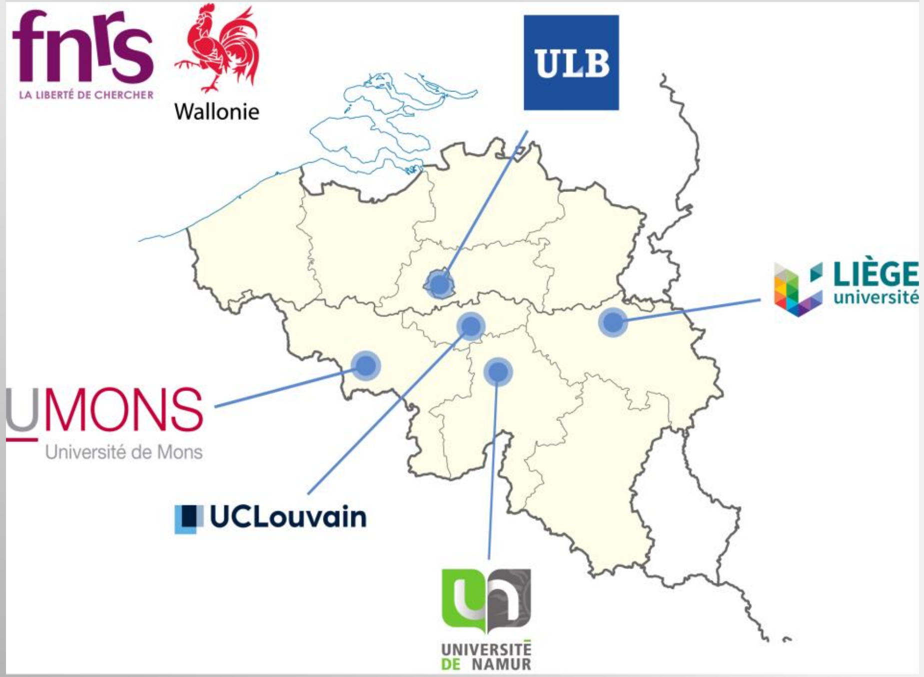
Note: getting access to the top TIER requires to demonstrate scalability on the previous ones

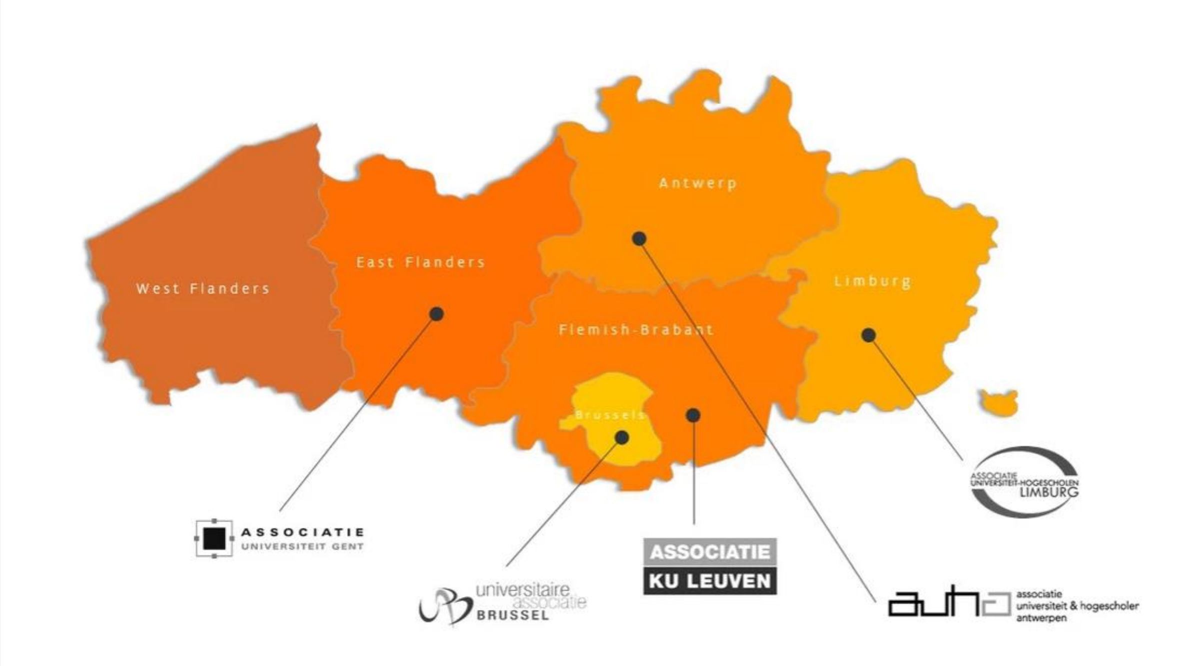
European infrastructure



TIER-2 in Belgium (academic level)

*Wallonia: the **CÉCI** (http://www.ceci-hpc.be/)*



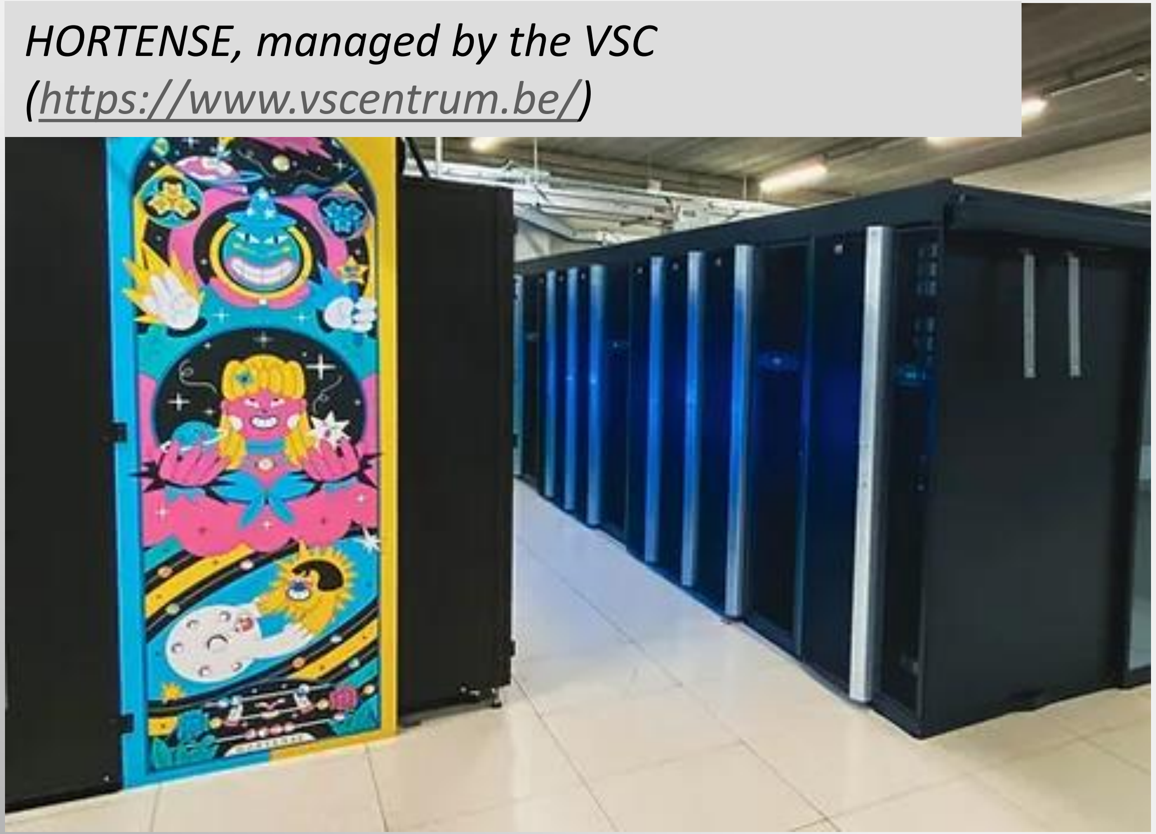


*Flanders: the **VSC** (https://www.vscentrum.be/)*

Accessible for every researchers of the corresponding universities. **Trainings** are also provided

TIER-1 in Belgium

HORTENSE, managed by the VSC
(https://www.vscentrum.be/)



Lucia, managed by Cenaero
(https://www.cenaero.be/)

Provides **access** (through calls) and **support**.

TIER-0 (LUMI)

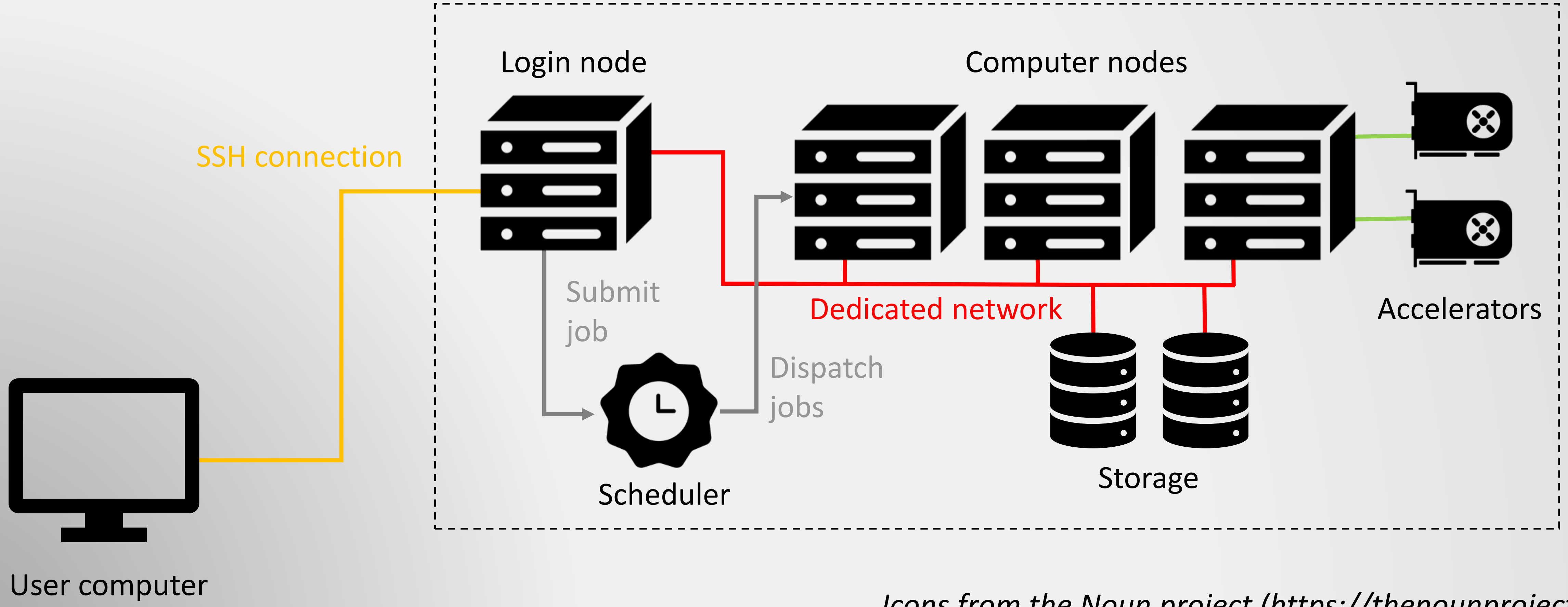
https://www.lumi-supercomputer.eu/
https://www.enccb.be/LUMI/

- First european pre-exascale supercomputer
- 100% hydropowered energy
- Regular training in Belgium

What are supercomputers?

How they work

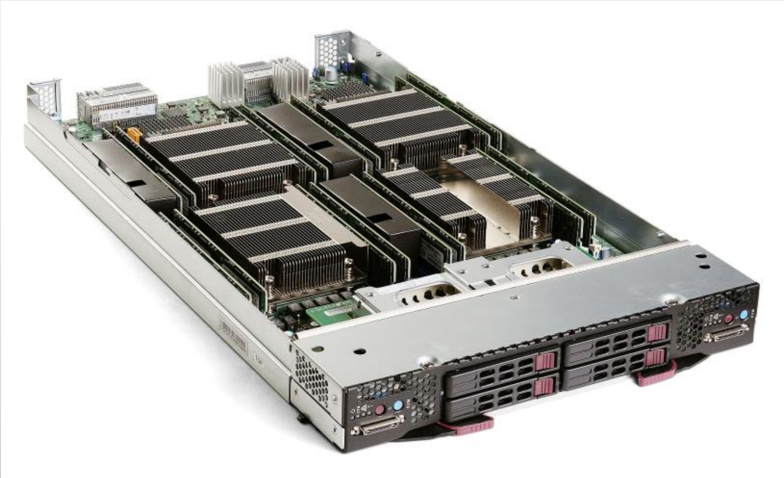
Anatomy of a cluster



Icons from the Noun project (https://thenounproject.com/)

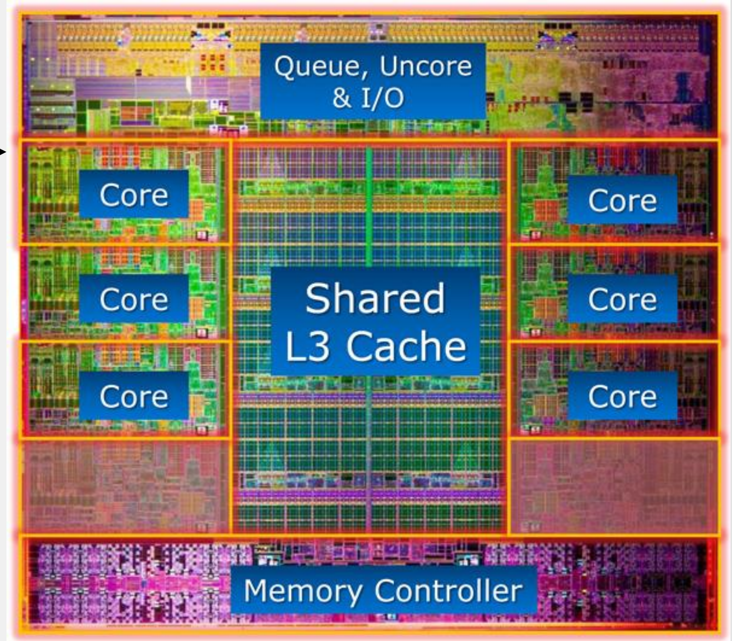
Components

EURO²



Computer node (Wikipedia)
Acts basically like a computer

- Socket (CPU)
- RAM
- Networking
- Cooling
- Local storage
- ...

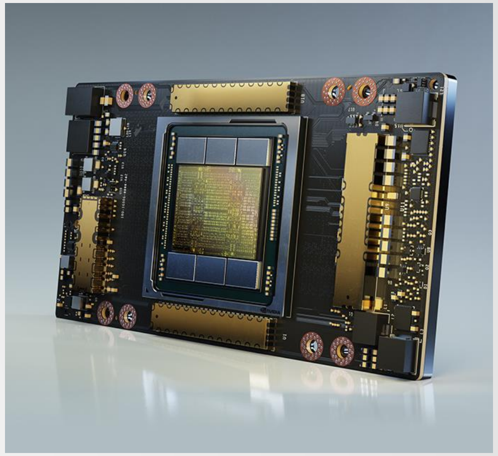


Intel sandybridge (die)
(https://www.anandtech.com/)

Components: GPU / Accelerators

- Instead of a few powerful cores, many less powerful cores
- Consumer grade GPU: provide good FLOPS for single precision operation, not for double precision
- Dedicated class of cluster grade GPU (e.g., NVIDIA Ampere or AMD Instinct)
- Future of HPC?

AMD Instinct (amd.com)



Ampere (nvidia.com)

Interaction with the supercomputer

- Generally, through command line
- Users submit jobs on the cluster, and wait for the results
- For each "job", the scheduler (e.g., SLURM) requires to know time/memory/number of processor and node and tries to fit the job when a slot is available.
- Different clusters have different purposes, e.g.,
  - High-memory application,
  - Small and fast jobs,
  - Nodes with accelerators, ...

How to use such large resources efficiently?

Solutions... and challenges

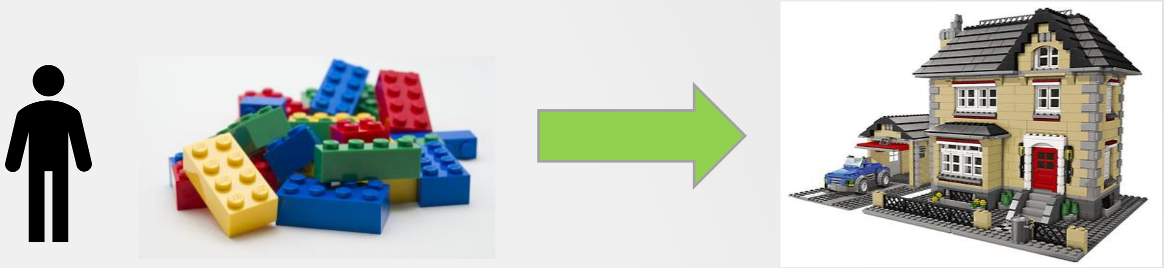
Particularities of supercomputing

- Advantage of supercomputing
  - Larger size: some problem requires large amount of memory
  - More speed: some problem requires long time to be solved
- Solution … And issues:
  - More memory (but storage hierarchy)
  - Parallelism (… has inherent difficulties)

Tackle speed: parallel computing

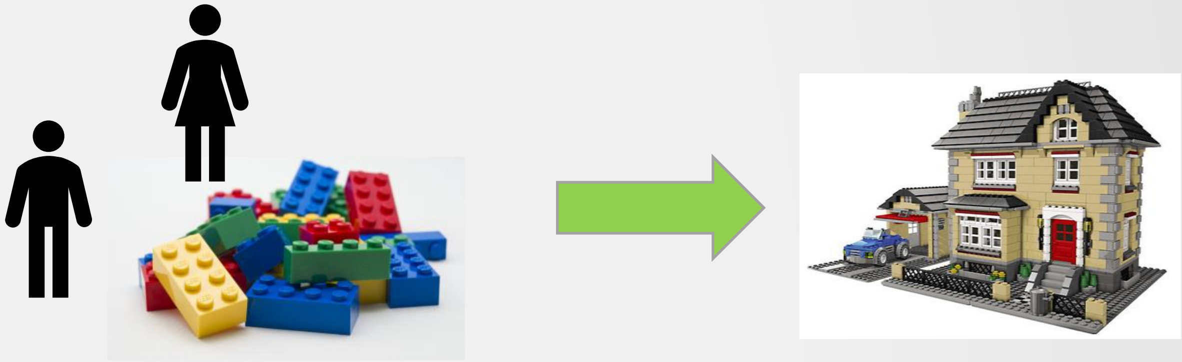
- To achieve such performances, the main idea is to rely on **parallel computing :** executing many operations in a single instance of time.
- But the program needs to be adapted for such purpose!

Serial world: 1 worker (person) to build



Images from LEGO (lego.com)

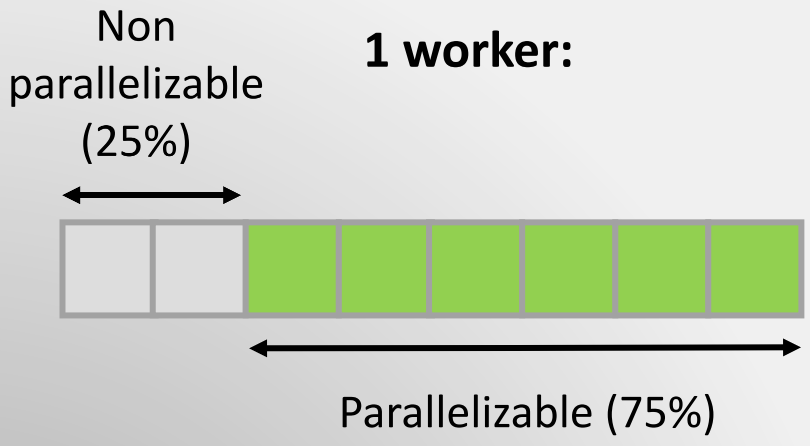
Parallel world: 2 workers to build → about 2 times faster



Speedup is never what you expect...

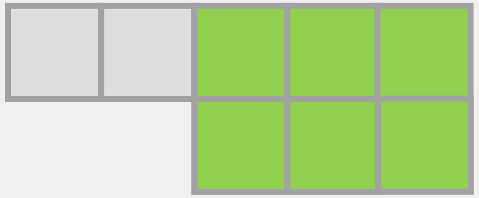
In most cases, a problem is never fully parallelizable (i.e., **embarrassingly** parallel)

1 worker:



$T_{tot,1} = 8$

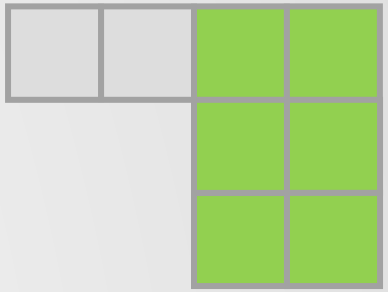
2 workers:



$T_{tot,2} = 5$

Speedup = $T_{tot,1} / T_{tot,2} = 1.6$

3 workers:



$T_{tot,3} = 4$

Speedup = $T_{tot,1} / T_{tot,3} = 2$

→ No matter how fast the parallel portion, we will always be limited by the **serial** part.

Speedup is never what you expect...

Amdahl's Law:

$$S = \frac{1}{s + \frac{P}{N}}$$

S: actual speedup

s: serial portion of the code (in %)

P: parallel portion (in %)

N: number of processors

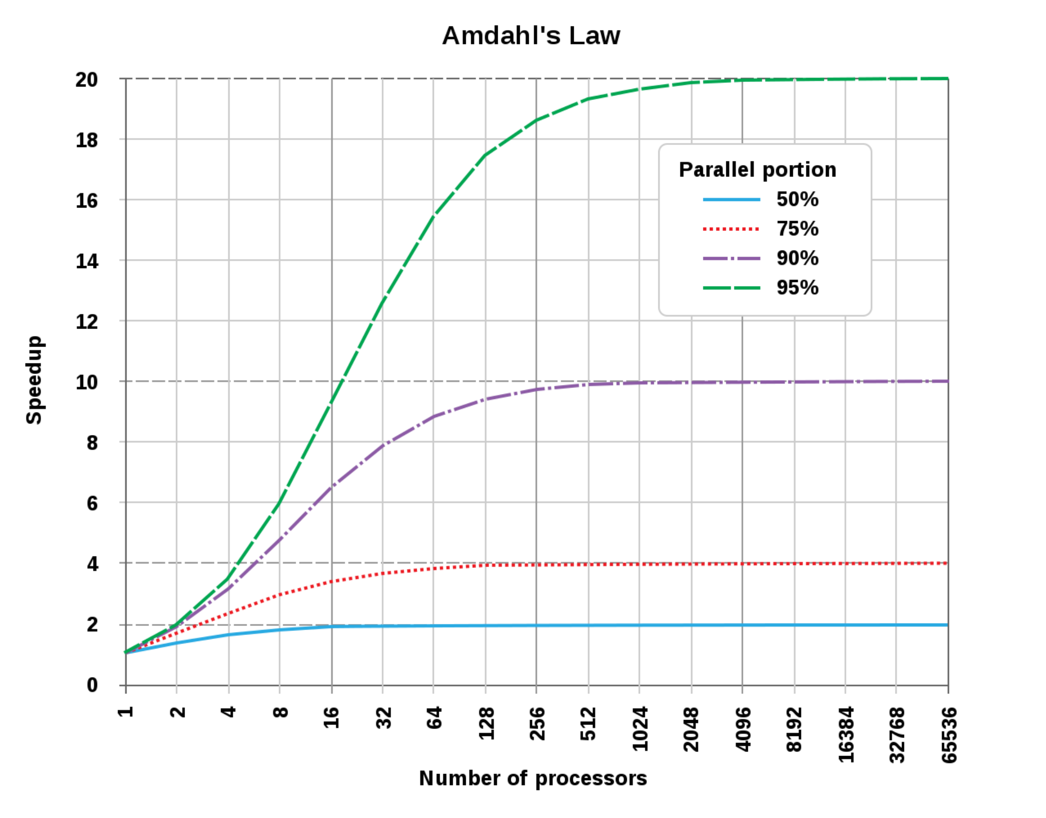


Image from Wikipedia (wikipedia.org)

This address the question "how much processors can I use for a given problem?"

On the bright side: weak scaling

If we increase the size of the problem when more processors are added,

$$S = N - s(N-1)$$

S: actual speedup

N: number of processors

S: serial fraction (in %)

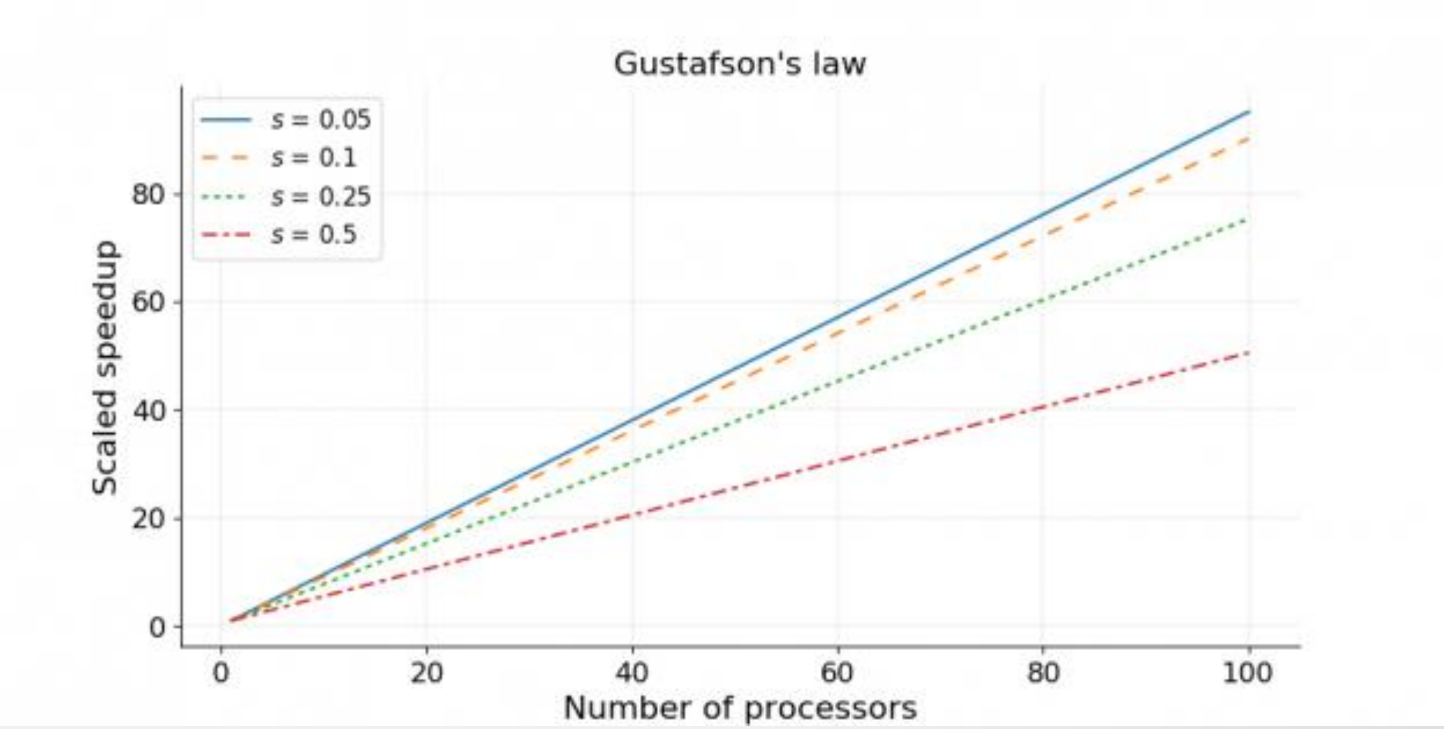
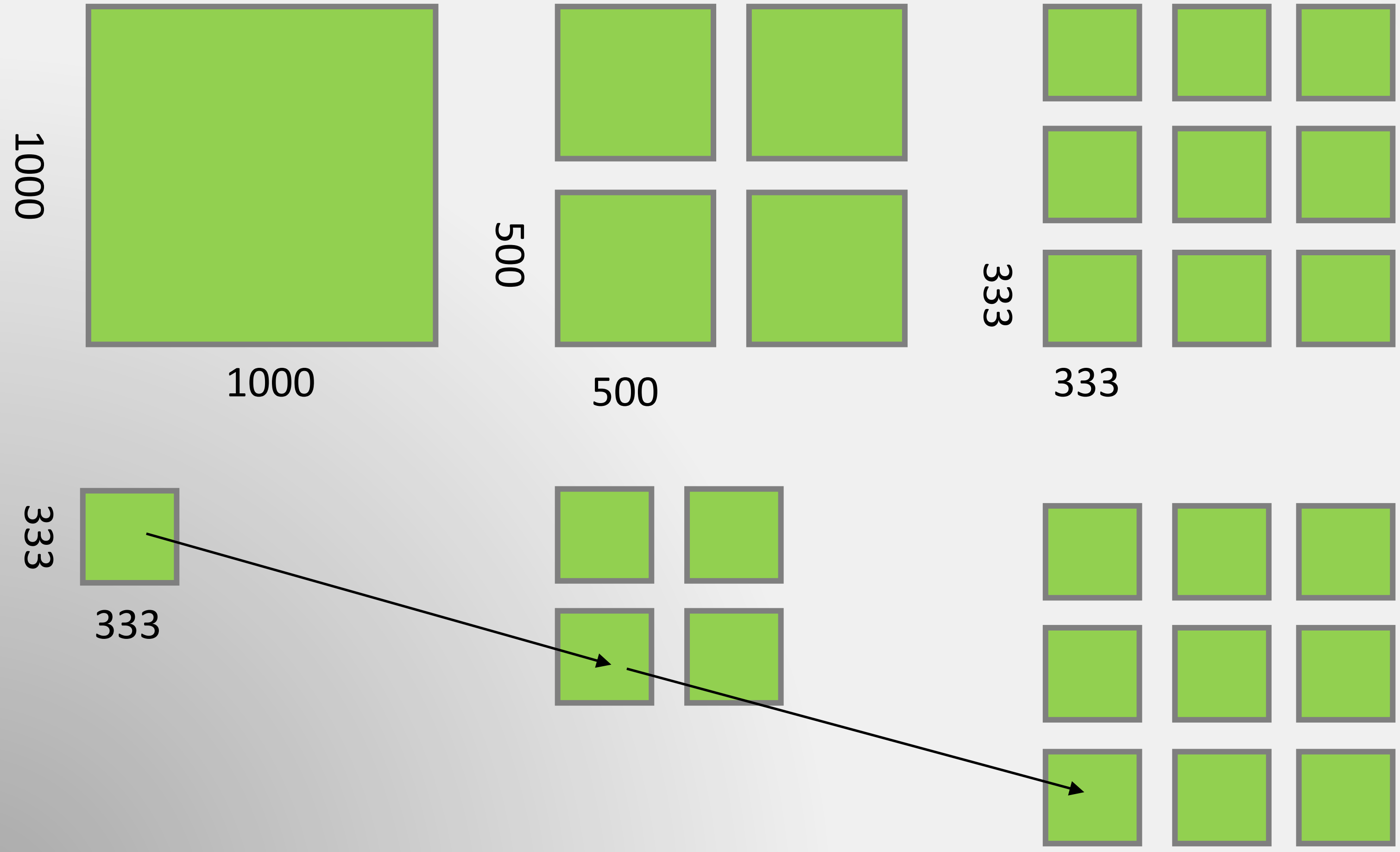


Image from Wikipedia (wikipedia.org)

This address the question "how much can I increase the size of my problem such that the execution time is the same as if I ran the problem with only one process?"

Recap of strong vs weak scaling

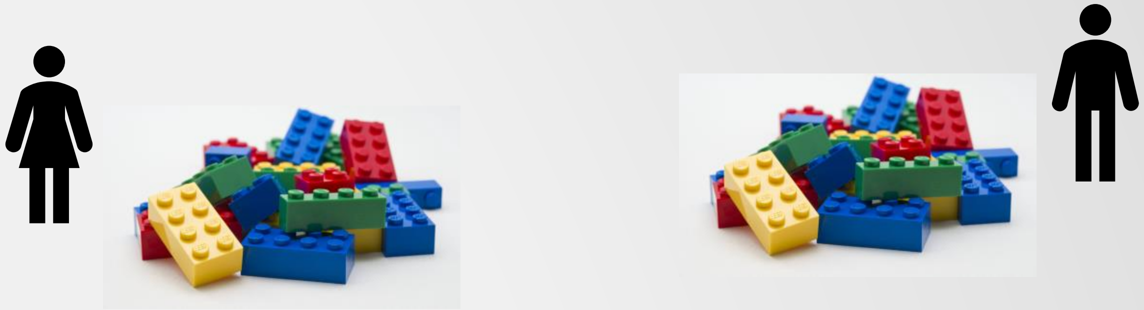


Strong scaling: size of the problem is constant and split across additional processors

Weak scaling: the size of the problem is the same for each processor.

… and there is parallel overhead!

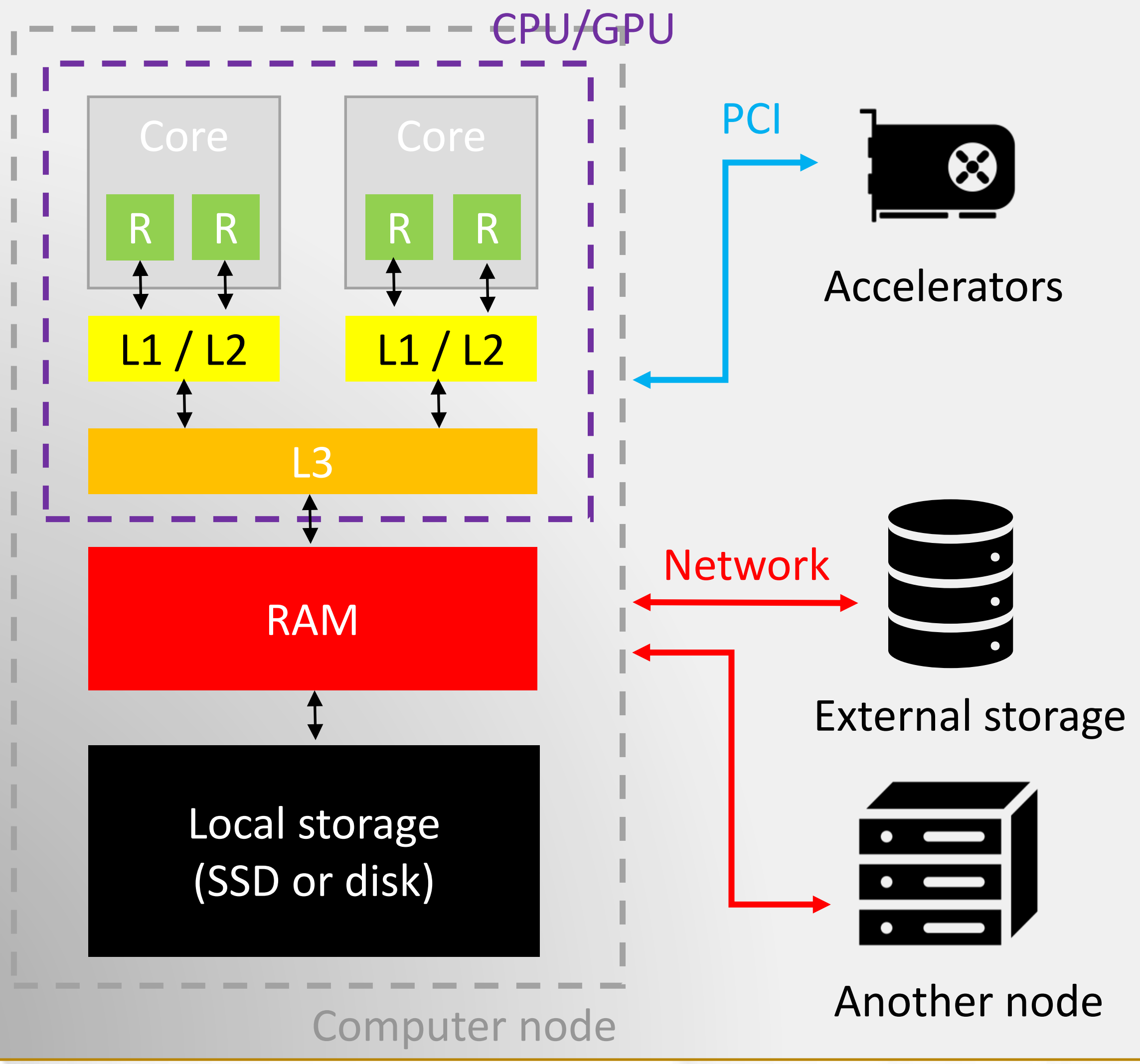
Shared memory model: all workers (or, here, person) are working on the same pool of data (or, here, lego pieces). Small overhead due to **synchronisation** (all person cannot work on the same part of the model at the same time).



Distributed memory model: each worker (or, here, person) is working on its own set of data (or, here, lego pieces). Generally, more efficient (no collaboration during work), but overhead due to **communication** (or, here, distribute pieces in the beginning and assembling the result at the end).

Generally, the two are mixed. It also requires a good **load balancing** (i.e., every person has the same amount of work to do). It is not that easy to achieve.

Also important: storage hierarchy



- The further away from the core, the slowest (but, generally, the more capacity)
- I/O may not be parallel
- Communication is a bottleneck when using multiple nodes
- Efficient movement of data to and from an accelerators

Icons from the Noun project (https://thenounproject.com/)

Tools of the trade

Parallel programming:

- Vectorization (core level)
- Threading / OpenMP (node level)
- CUDA / HIP / OpenCL / OpenACC / OpenMP (accelerator level)
- Socket / MPI / PGAS (cluster level)

Optimized libraries:

- BLAS / LAPACK / MKL (linear algebra)
- FFTW (fast-Fourier transform)
- HDF5 / netCDF (parallel I/O)

To conclude

Conclusions

EURO²

- HPC is important for actual and future research
- HPC is an active field in Belgium
- There are challenge to overcome, but tools are developed
- This was an introduction, don't be afraid to reach us if you want to know more!
  → More information on https://www.enccb.be/.

Thanks!

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the European Union

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