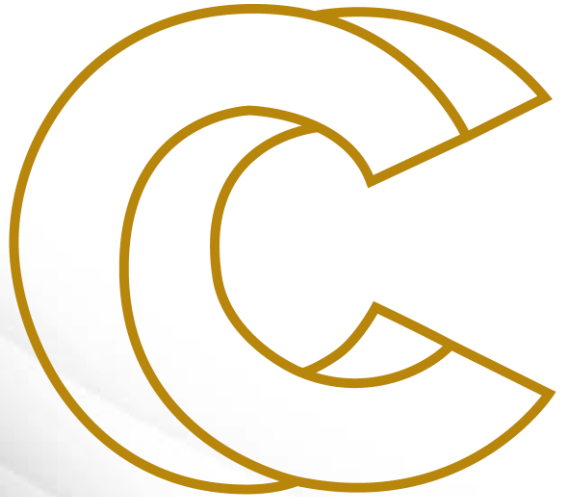


EURO^2

Introduction to HPC

By EuroCC Belgium

Outline of this presentation

EURO²

PART 1

- Introduction
  - Example of uses
  - The EuroHPC joint undertaking the EuroCC project
- Current status of the supercomputing infrastructures
  - Performance and the TOP500 list
  - Supercomputers in Europe and in Belgium

PART 2

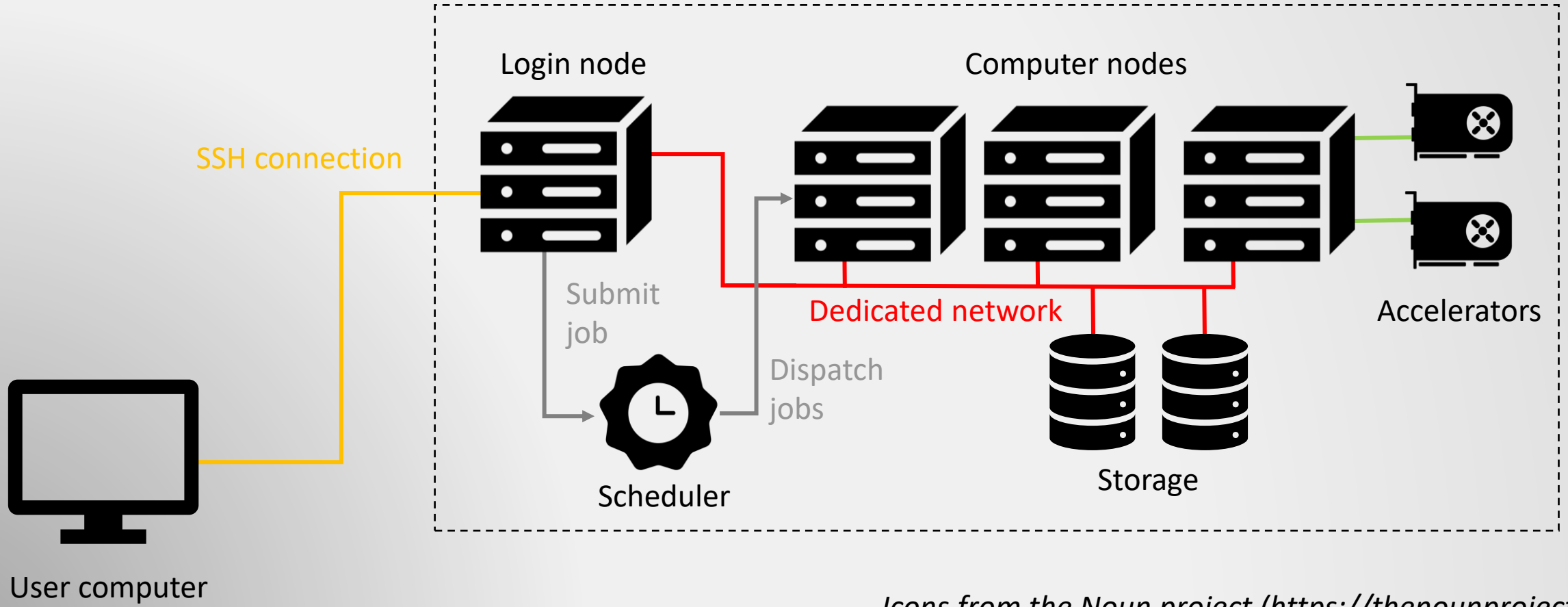
- Understand how a supercomputer works:
  - Architecture & Components
  - Interacting with supercomputers
- Understand how program can use such large resources, and what are the issues that needs to be overcome:
  - Parallelism
  - Parallelization issues

PART 2

What are supercomputers?

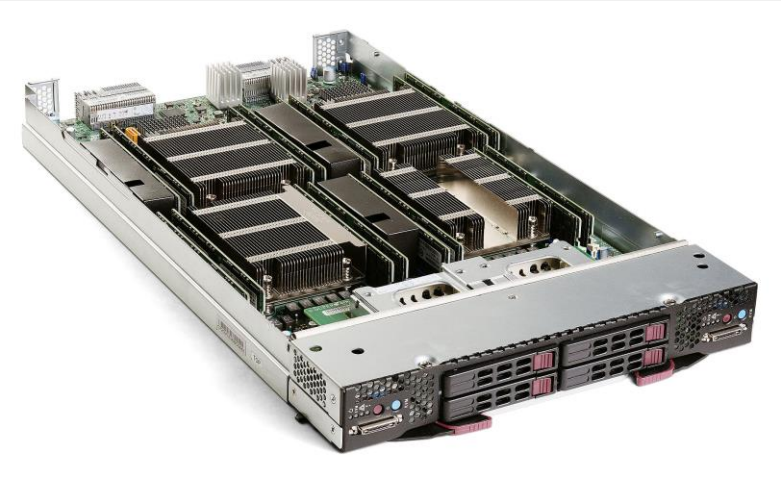
How they work

Anatomy of a cluster



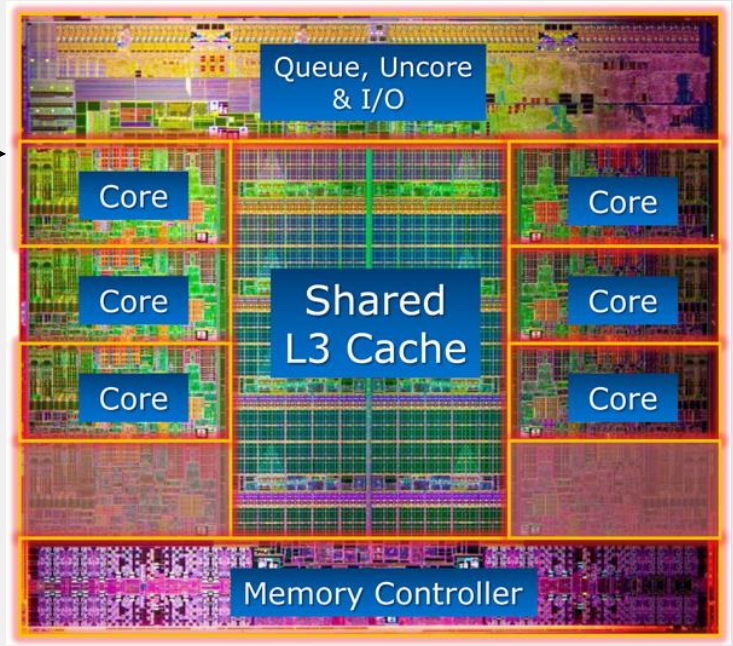
Icons from the Noun project (https://thenounproject.com/)

Components



Computer node (Wikipedia)
Acts basically like a computer

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

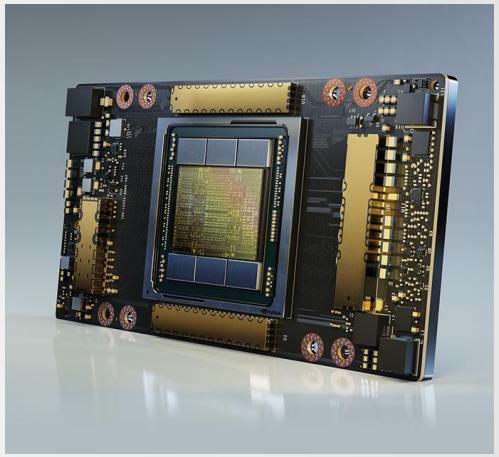


Intel sandybridge (die)
(https://www.anandtech.com/)

Components: GPU / Accelerators

- GPGPU: general-purpose computing on GPU
- Instead of a few powerful cores (CPUs), 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)

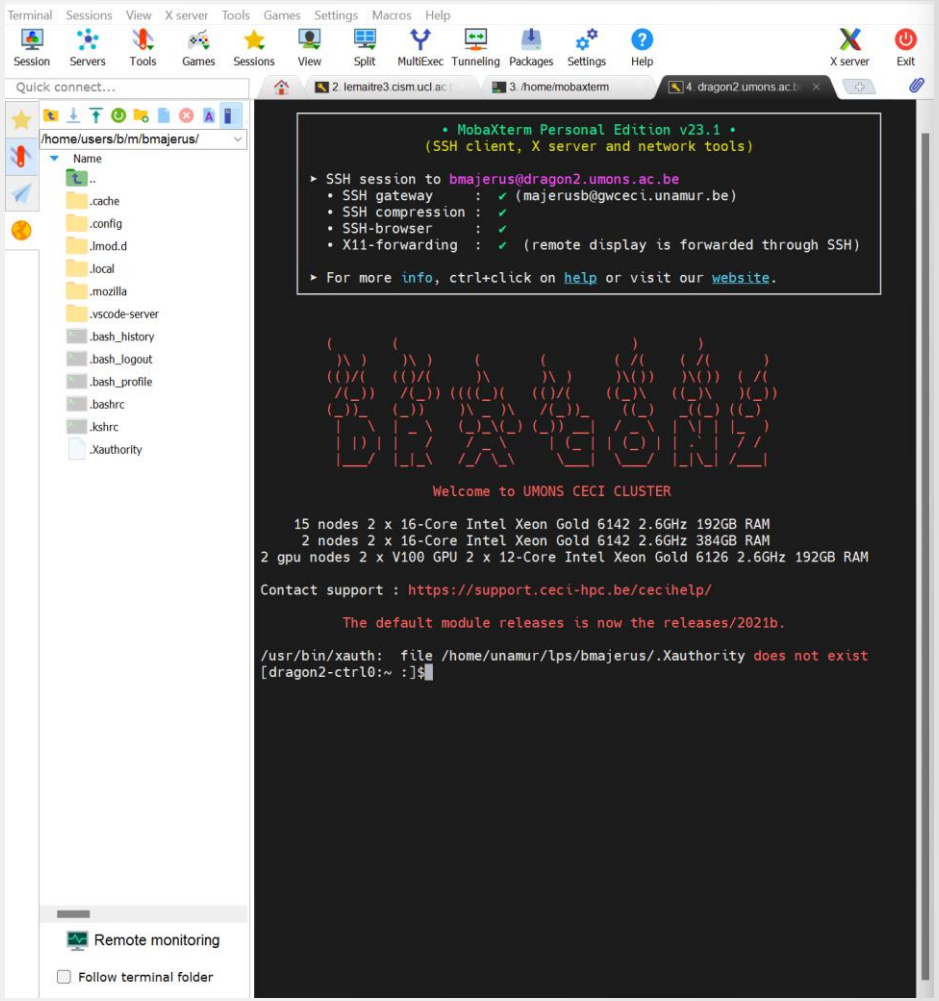


Ampere (nvidia.com)

Interaction with the supercomputer

You interact through the command line (Linux, Mac) or specific softwares (Windows, Mac).

- SSH client for connection
- Terminal for writing and receiving text
- Graphical user interface is possible (but not yet available everywhere)



The scheduler

- 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, ...

```
#!/bin/bash
#submission script for Lemaitre3
#SBATCH --job-name=CNT
#SBATCH --time=24:00:00 # hh:mm:ss
#SBATCH --ntasks=128
#SBATCH --mem-per-cpu=2000 # megabytes
#SBATCH --partition=batch


module load Python/3.6.3-foss-2017b
module load libxc

srun gpaw-python cnt_ph.py >log_ph
~
~
~
~
~
~
~
~
~
```

How to use such large resources efficiently?

Solutions... and challenges

Particularities of supercomputing

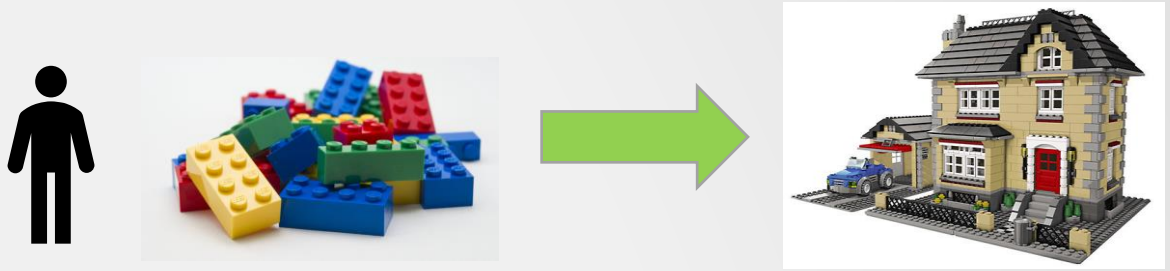
EURO²

- 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

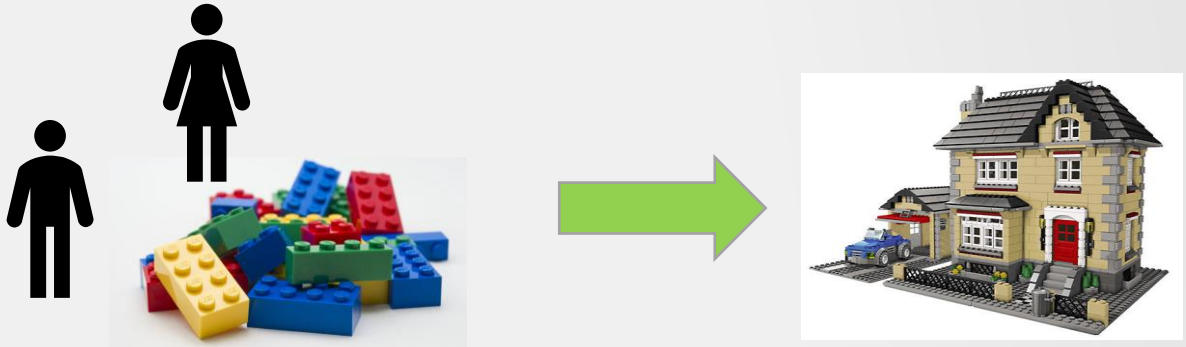
- To achieve such performances, the main idea is to rely on **parallel computing :** executing many operations in a single instance of time.
- But the program needs to be adapted for such purpose!

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)

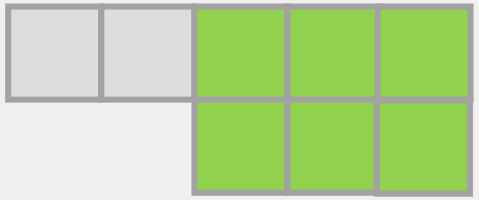
Non parallelizable (25%)

1 worker:

Parallelizable (75%)

$T_{tot,1} = 8$

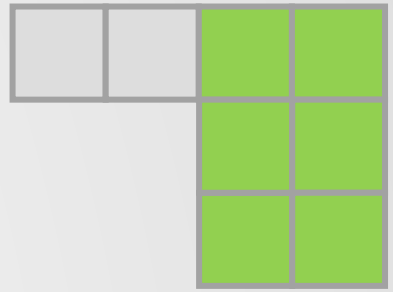
2 workers:



$T_{tot,2} = 5$

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

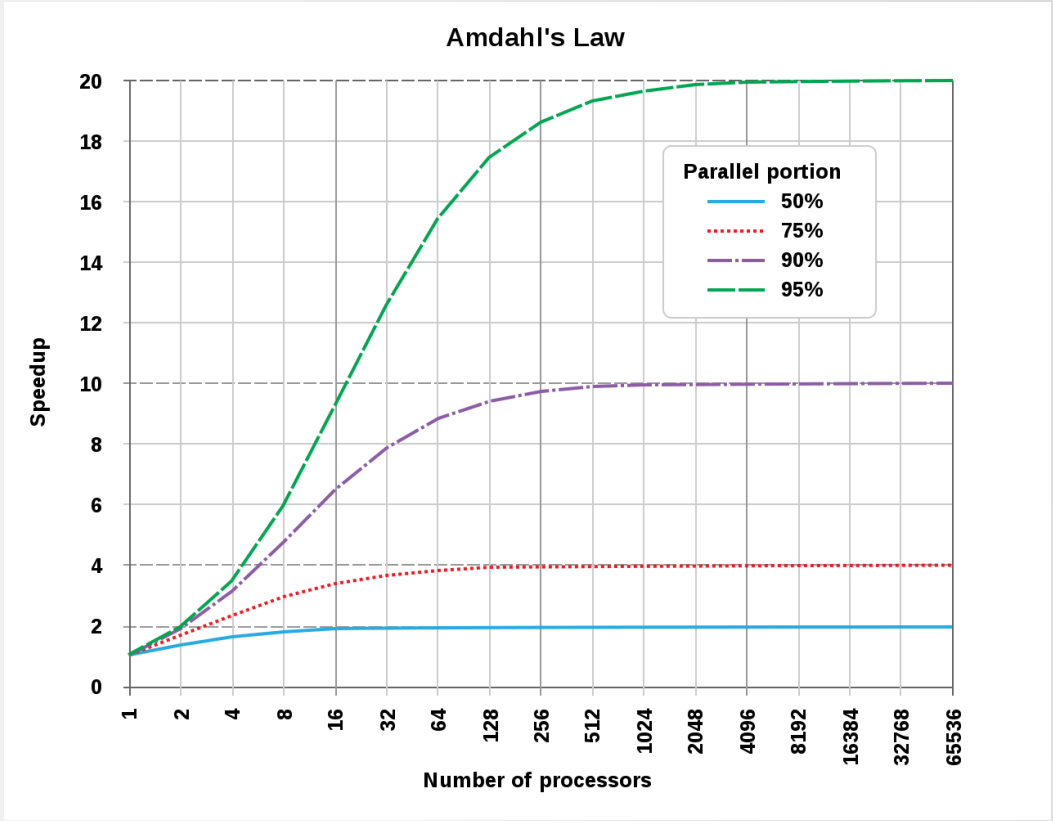
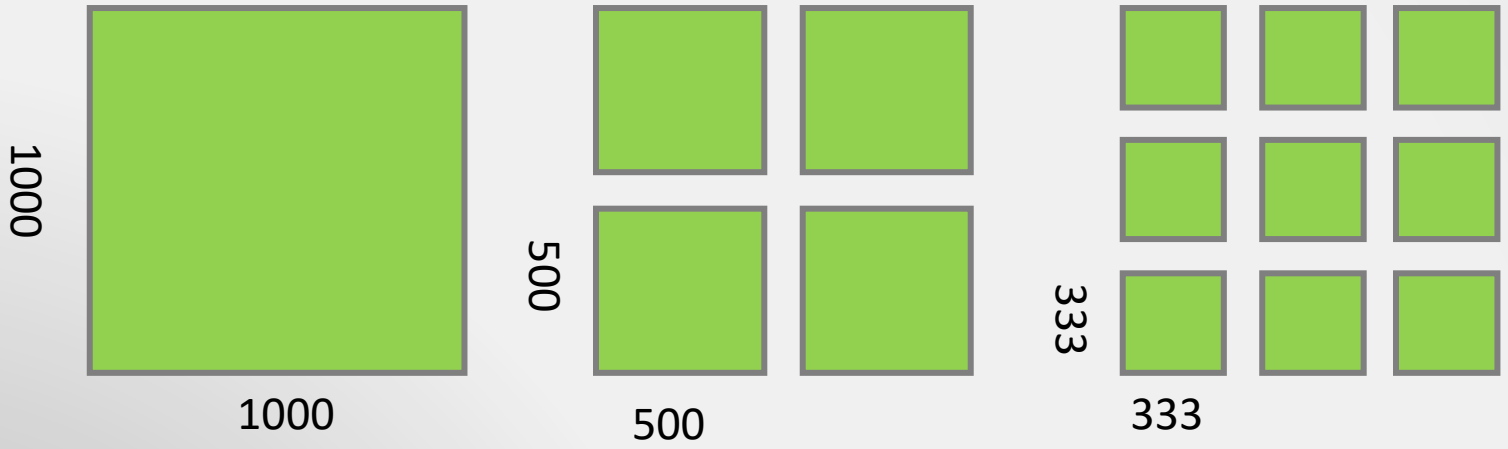


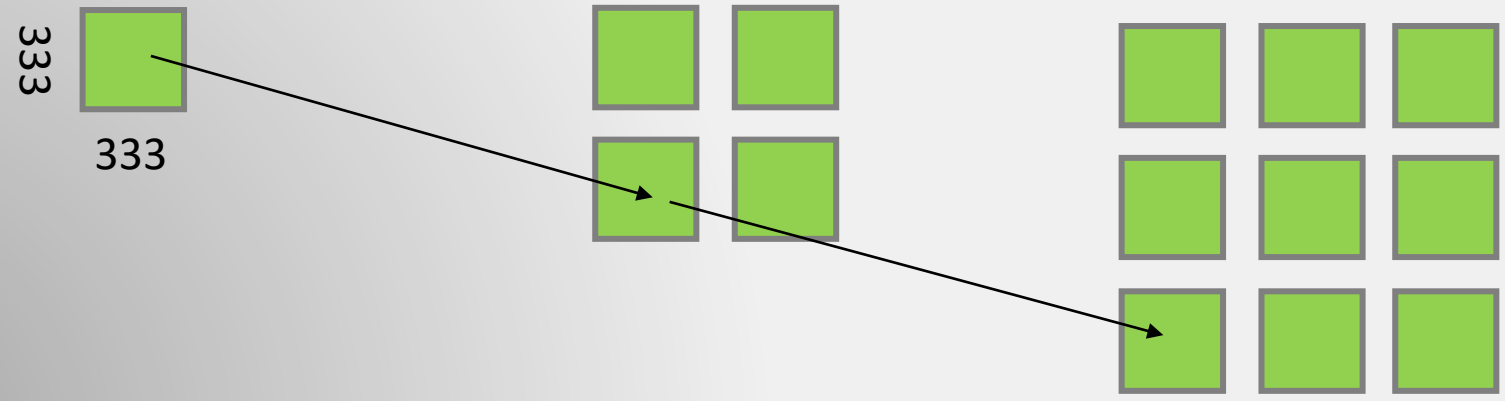
Image from Wikipedia (wikipedia.org)

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

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.

Weak scaling is great

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 %)

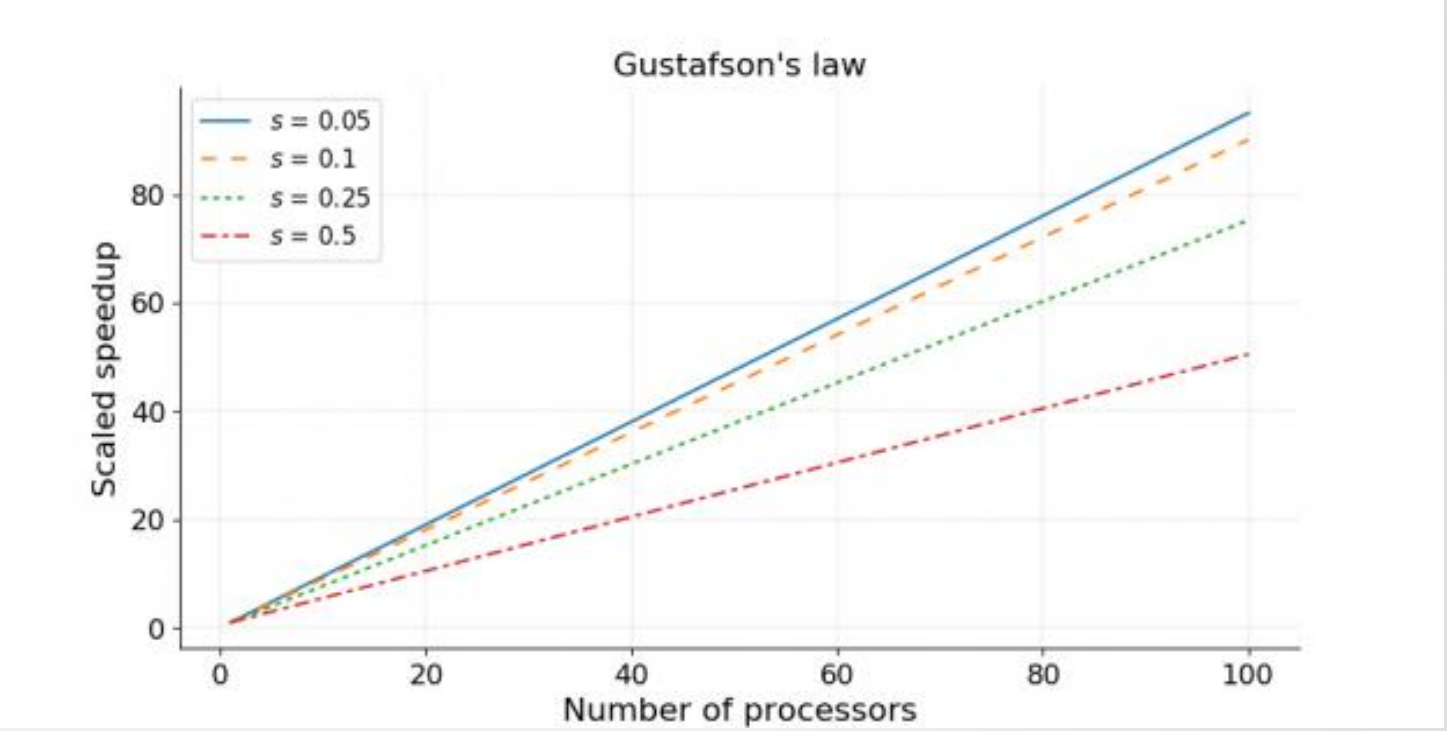
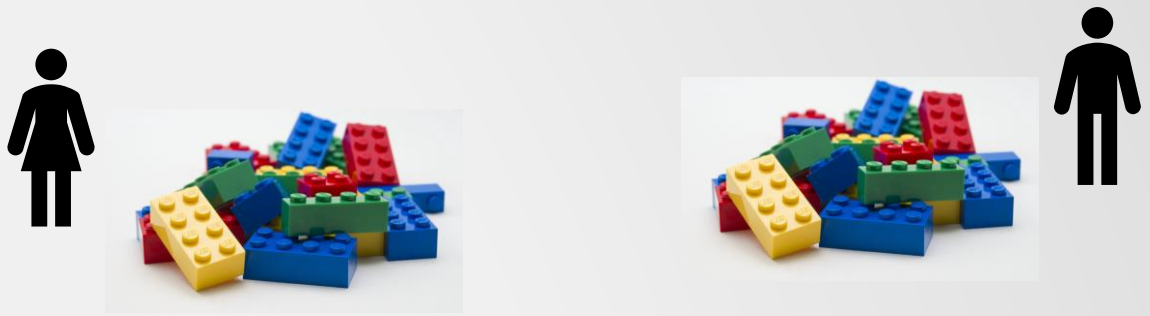


Image from Wikipedia (wikipedia.org)

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?"

But there are always overheads

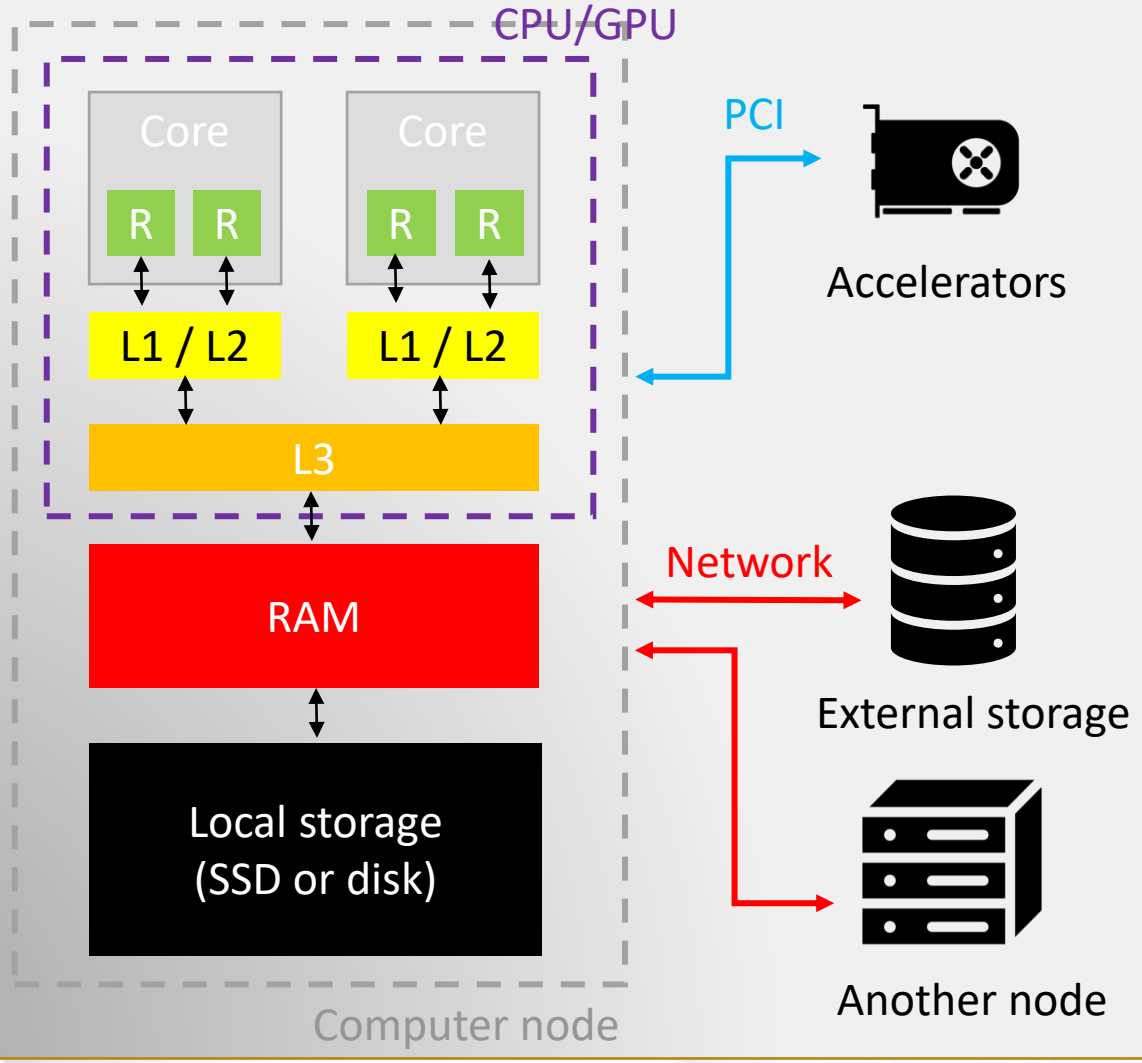
Shared memory model: all workers (or, here, person) are working on the same pool of data (or, here, lego pieces). Small overhead due to **synchronisation** (all person cannot work on the same part of the model at the same time).



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

EURO²

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)

Good news for computer rookies: Lots of scientific programs already built with parallel version and available on the supercomputers → no programming skills needed!

Conclusions

Conclusions

- Parallelization is at the core of the efficiency of supercomputers
- There are several parallelization paradigms with their own advantages and drawbacks
- You don’t need high programming skills to do supercomputing

→ More information on

- https://www.enccb.be/
- https://www.ceci-hpc.be/
- https://www.vscentrum.be/

Thanks!

Funded by
the European Union

EuroHPC
Joint Undertaking

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