

Introduction to HPC By EuroCC Belgium

## Outline

# EURO<sup>2</sup>

#### 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 1

## What is High Performance computing (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 work 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).



# Examples of HPC uses

#### Have a look at www.enccb.be/stories



## Examples: fluid dynamics (CFD)

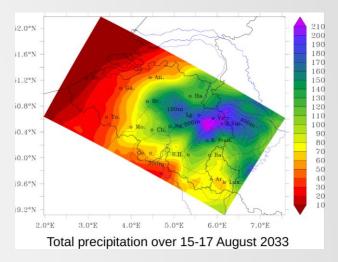


#### **Optimization of a vortex unit for CO<sub>2</sub> capture**



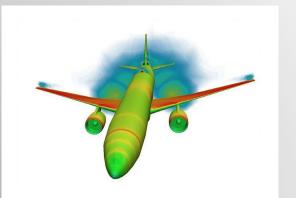
https://www.enccb.be/usvortexunit

#### **Predicting the climate**



https://www.enccb.be/usxavierfettweis

#### Aircraft design

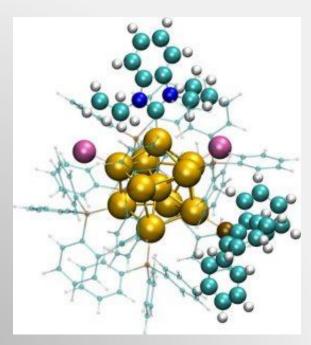


https://prace-ri.eu/automating-aircraft-design-and-optimisation/

## **Examples:** materials

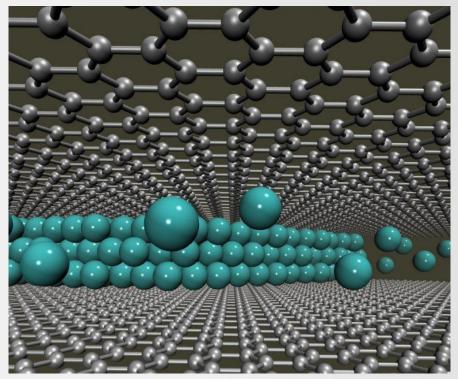


#### Predicting the structure of gold clusters that chops carbon dioxide



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

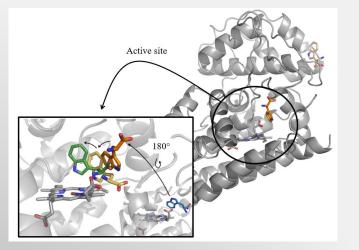
#### **Tailoring the properties of 2D materials**



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



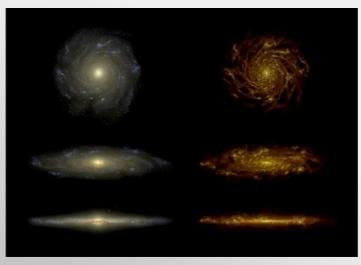
https://www.enccb.be/uschocolate



## 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

#### But also:

. .

- Artificial intelligence
- Machine learning

Examples

Data analysis







## What is EuroCC?



- EuroHPC Joint Undertaking (JU) 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 country 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.
  - $\rightarrow$  More information on <u>https://www.enccb.be/</u>.
- Different missions, including contact with industry, raising awareness and organizing trainings.





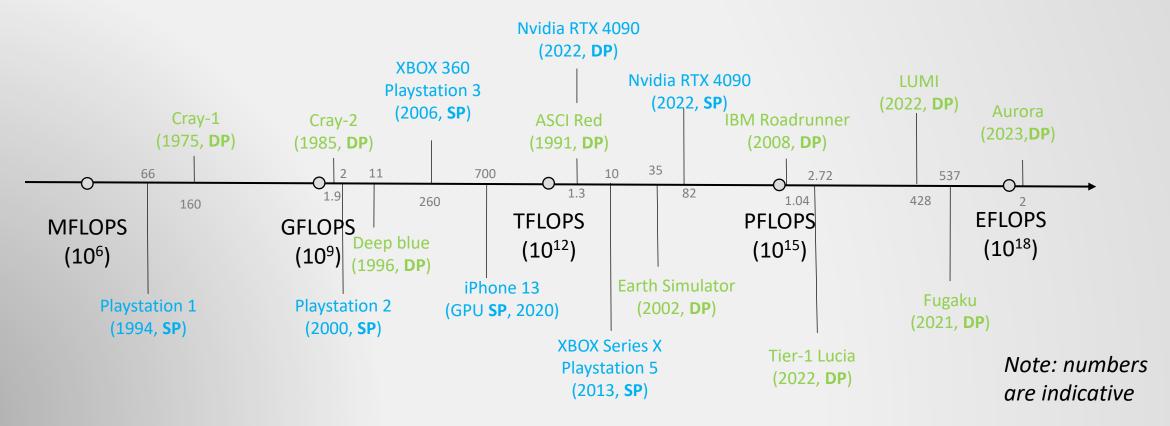
## Where are we today?

Which supercomputers for Belgium?

## Performances

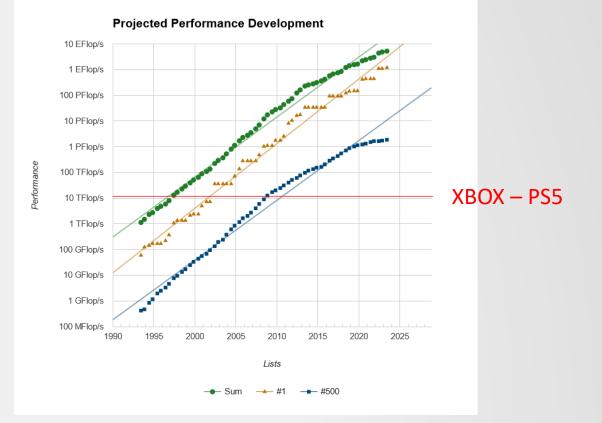


- One of the measurement is FLOPS = floating point operations per second ( $\simeq$  speed)
- Note that it depends on single (SP, 32 bits) or double (DP, 64 bits) precision!



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 2.26Hz, 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 2.66Hz, NVIDIA A100 SXM4 64 6B, 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 3.16Hz, 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



## The TOP500

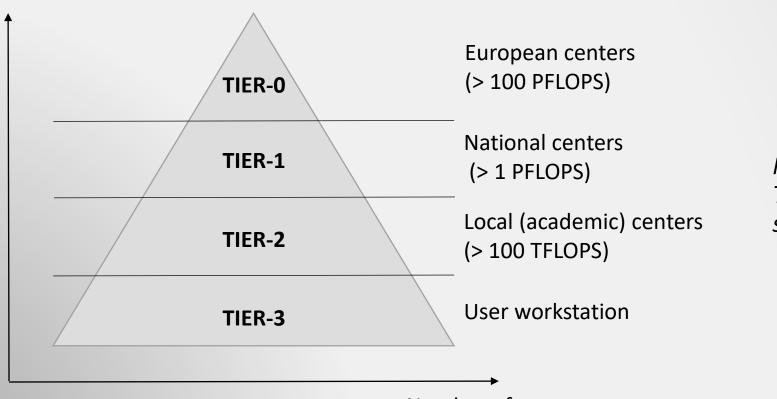
Rmax



## Supercomputers in Europe



Capability (~FLOPS)



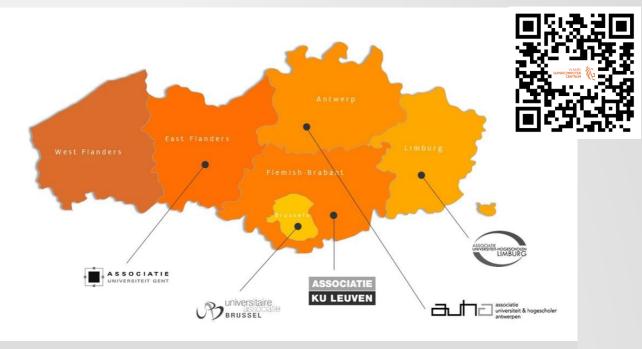
Note: getting access to the top TIER requires to demonstrate scalability on the previous ones

Number of systems

## TIER-2 in Belgium (academic level)





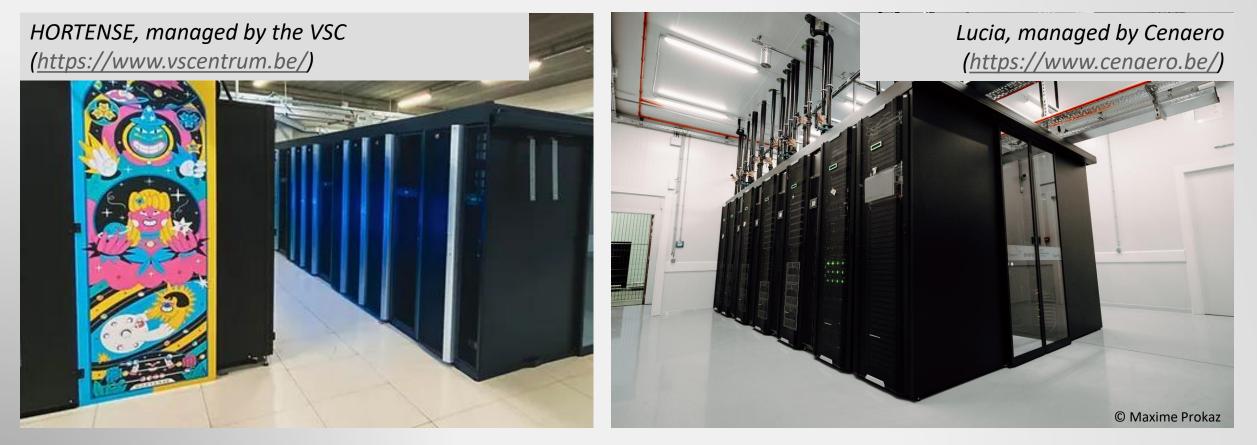


Flanders: the VSC (https://www.vscentrum.be/)

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

## **TIER-1** in Belgium

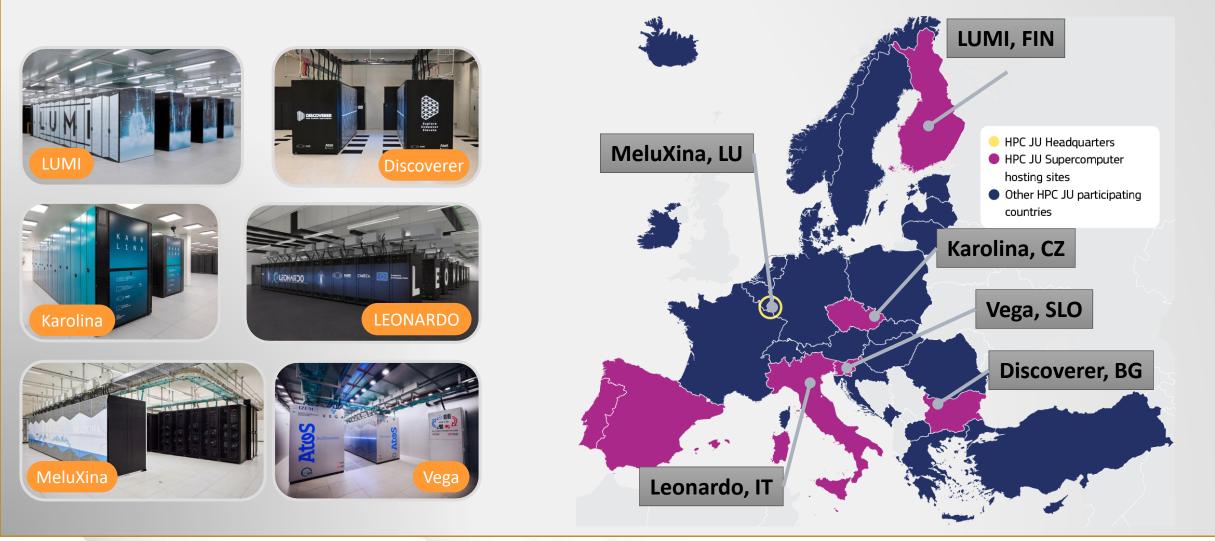




Provides access (through calls) and support.

## **European infrastructures (TIER-0)**





LUMI





- First european preexascale supercomputer
- 100% hydropowered energy
- Regular trainings in Belgium



## Conclusions





- HPC is important for actual and future research
- HPC is an active field in Belgium
- We have plenty of supercomputing resources in Belgium
- Don't hesitate to contact us, we're here to help!
- $\rightarrow$  More information on
  - https://www.enccb.be/
  - https://www.ceci-hpc.be/
  - https://www.vscentrum.be/





**Thanks!** 

Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia under grant agreement No 101101903.