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National Competence Center in HPC - Cyprus
EURO
Introduction High-Performance Computing - Dr. S. Bacchio

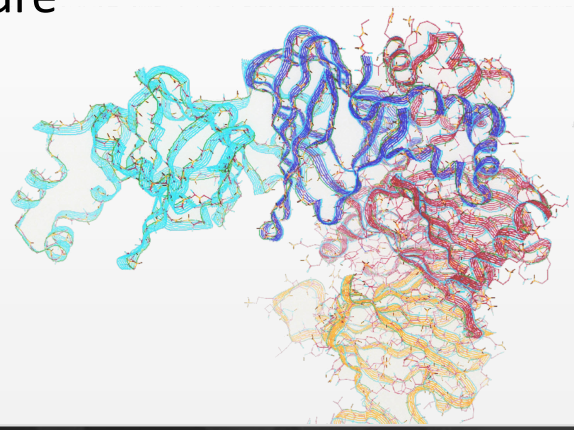
In today's talk

Introduction to High-Performance Computing

- Supercomputers in Europe, present and future
- The TOP500 list, analysis of the trends
- Co-processors: CPU vs GPU architecture
- Parallel computing

TOP500 The List.

EuroHPC Joint Undertaking



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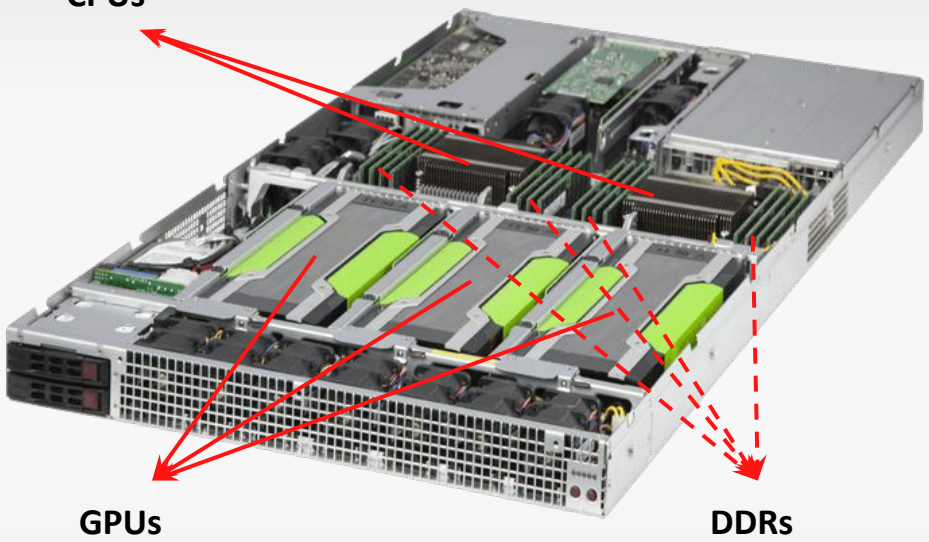
Inside a supercomputers

Computing Node

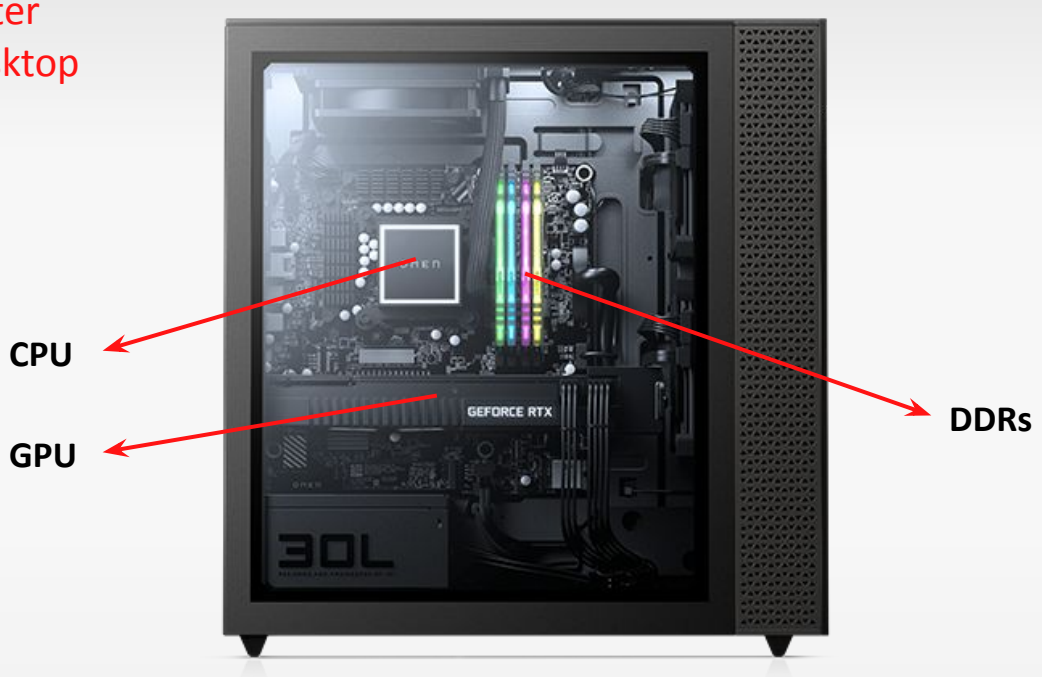


X no hard-drive and X no voltage convertor
Centralized long-term storage and power supply

VS

A node is
~5x faster
than a desktop

Desktop



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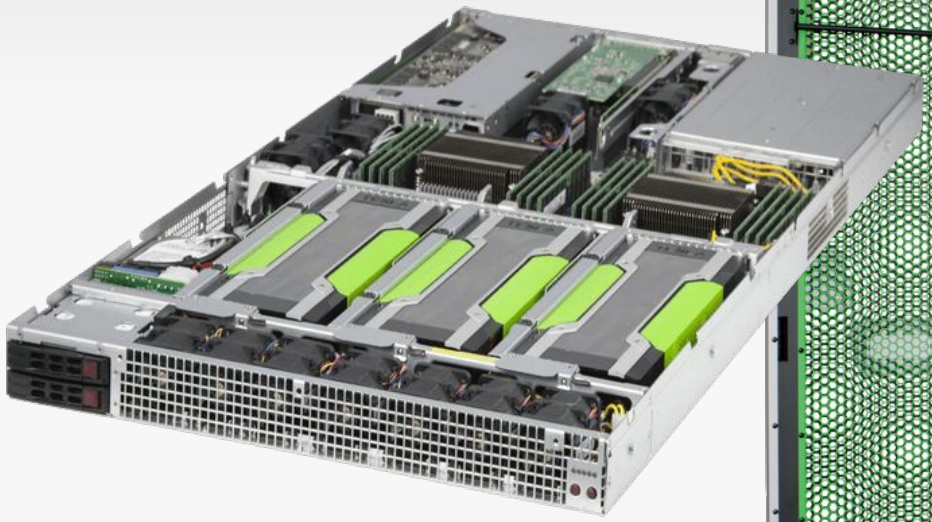
Inside a supercomputers

Computing Node

Rack

Supercomputer



+ Network
+ Storage
+ Power supply
+ Cooling

Supercomputers in Europe

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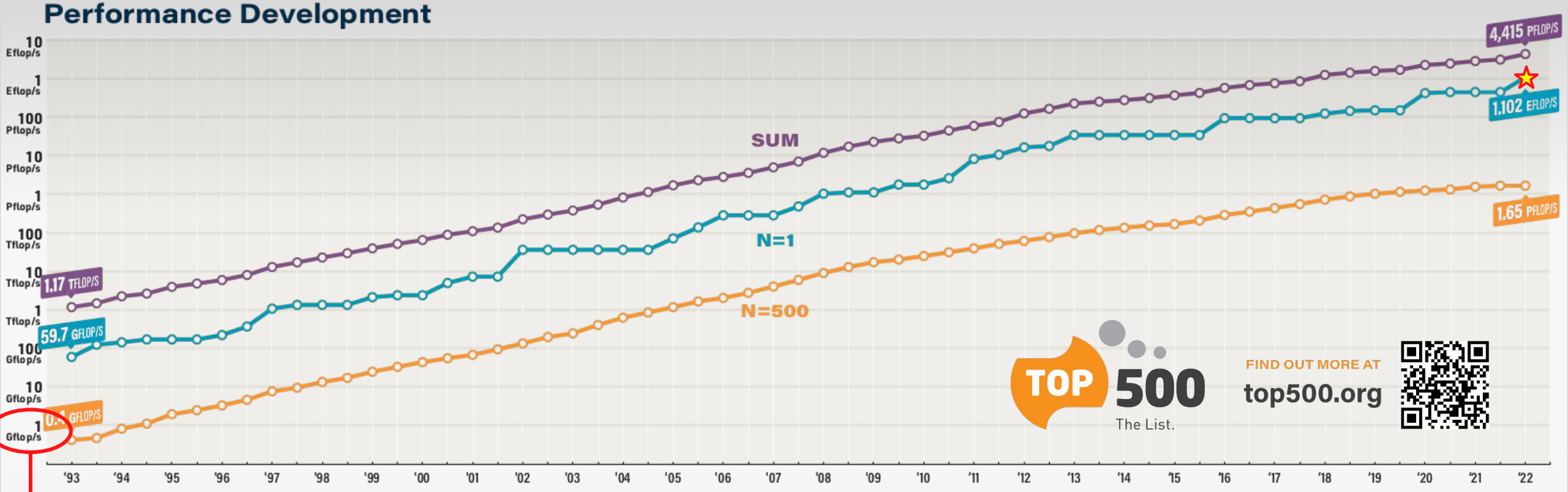
Supercomputers in Europe

TOP 500 - The List.



TOP 500 The List.

FIND OUT MORE AT top500.org

FLOP/s = Floating Point Operations per Second (in double precision)

A Standard PC does about 50 Gflops (CPU) and 1 Tflops (GPU).

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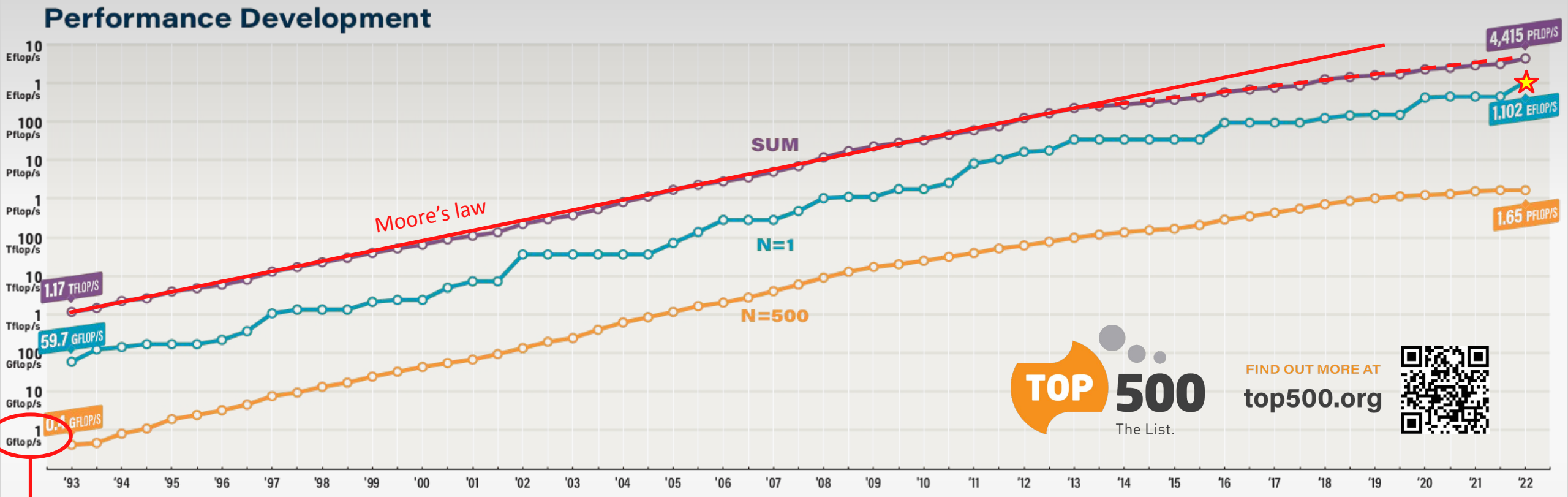
TOP 500 - The List.



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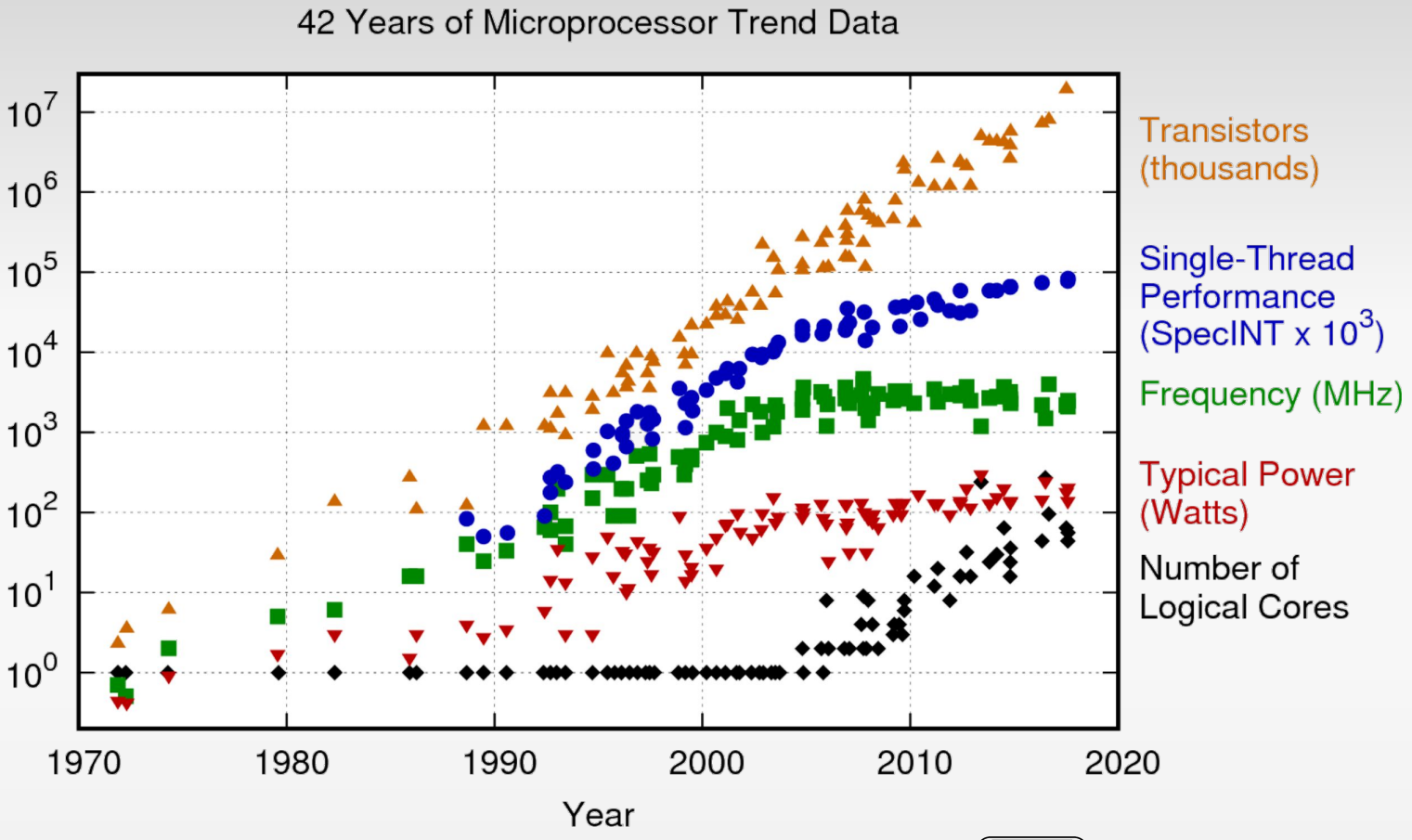
Evolution of technology

- Exascale is a milestone in HPC since 2008:
  - DARPA, US (2008), “ExaScale Computing Study: Technology Challenges in Achieving Exascale Systems”
  - Exascale systems predicted for 2015
- It has revealed to be not only an iconic milestone but a **real challenge!**



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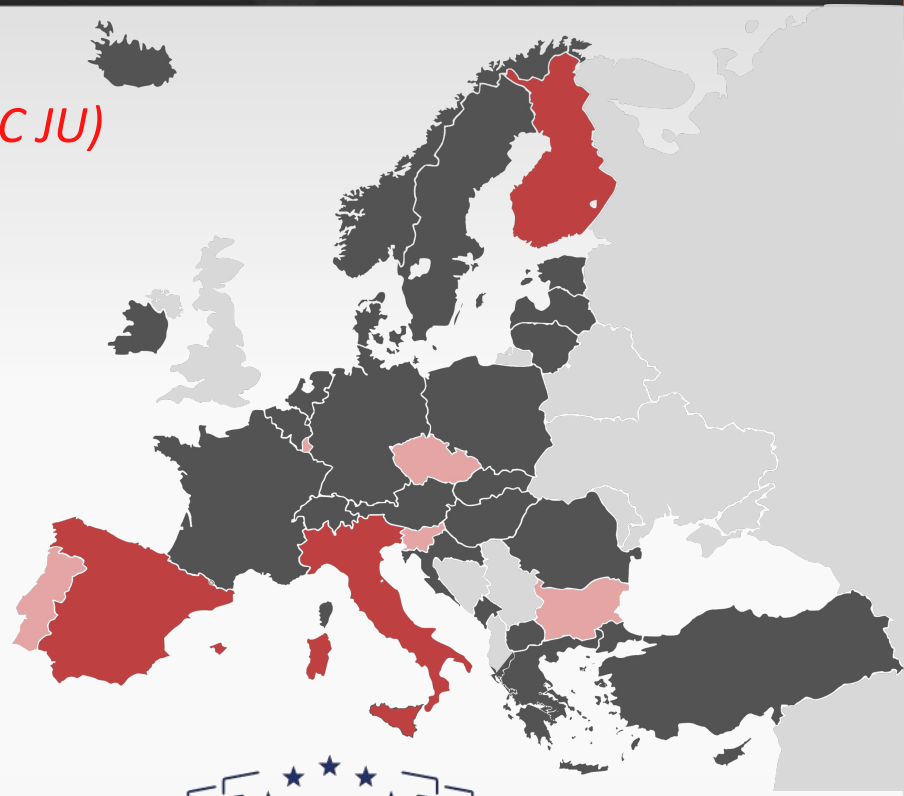
EuroHPC Joint Undertaking

The European High Performance Computing Joint Undertaking (EuroHPC JU) is pooling European resources to buy and deploy top-of-the-range supercomputers and develop innovative exascale supercomputing technologies and applications.



The JU is currently supporting two main activities:

- Developing a pan-European supercomputing infrastructure:
  - **5 PetaFlop machines** in Bulgaria, Czech, Luxembourg, Slovenia, Portugal
  - **3 Pre-Exascale machines** with over 200 PetaFlops: Lumi in Finland, Leonardo in Italy and Marenostrum 5 in Spain
  - **2 Exascale machines:** JSC in Germany, TBD

Upcoming Budget (2021 - 2033): 8 billion Euro

TOP HPC systems

JUNE 2022	SYSTEM	SPECS	SITE	COUNTRY	CORES	RMAX PFLOP/S	POWER MW
1	Frontier	HPE Cray EX235a, AMD Opt 3rd Gen EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-10	DOE/SC/ORNL	USA	8,730,112	1,102.0	21.3
2	Fugaku	Fujitsu A64FX (48C, 2.2GHz), Tofu Interconnect D	RIKEN R-CCS	Japan	7,630,848	442.0	29.9
3	LUMI	HPE Cray EX235a, AMD Opt 3rd Gen EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-10	EuroHPC/CSC	Finland	1,268,736	151.9	2.94
4	Summit	IBM POWER9 (22C, 3.07GHz), NVIDIA Volta GV100 (80C), Dual-Rail Mellanox EDR Infiniband	DOE/SC/ORNL	USA	2,414,592	148.6	10.1
5	Sierra	IBM POWER9 (22C, 3.1GHz), NVIDIA Tesla V100 (80C), Dual-Rail Mellanox EDR Infiniband	DOE/NNSA/LLNL	USA	1,572,480	94.6	7.44

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10	Adastra	AMD EPYC (64C 2GHz), AMD Instinct MI250X, Slingshot-11	GENCI	France	319,072	46.1	0.9
11	JUWELS Booster	AMD EPYC 7402 (24C 2.8GHZ), NVIDIA A100, Mellanox HDR Infiniband	Juelich	Germany	449,280	44.1	1.8
21	Marconi-100	IBM POWER9 (16C, 3GHz), NVIDIA V100, Mellanox EDR Infiniband	Cineca	Italy	347,776	21.6	1.4
23	Piz-daint	Xeon E5-2690v3 (12C 2.6GHz), NVIDIA P100, Cray/HPE	CSCS	Switz	387,872	21.2	2.4

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Future Systems

Upcoming European systems:

			SITE	COUNTRY	PFLOP/S
2024	**Jupiter**	TBD (GPU-based system, NVIDIA or AMD)	JSC	Germany	1500
2023	**MareNostrum5**	Intel Xeon CPUs, NVIDIA Ampere A100	BSC	Spain	314
2023	**Leonardo**	Intel Xeon CPUs, NVIDIA Ampere A100	Cineca	Italy	250

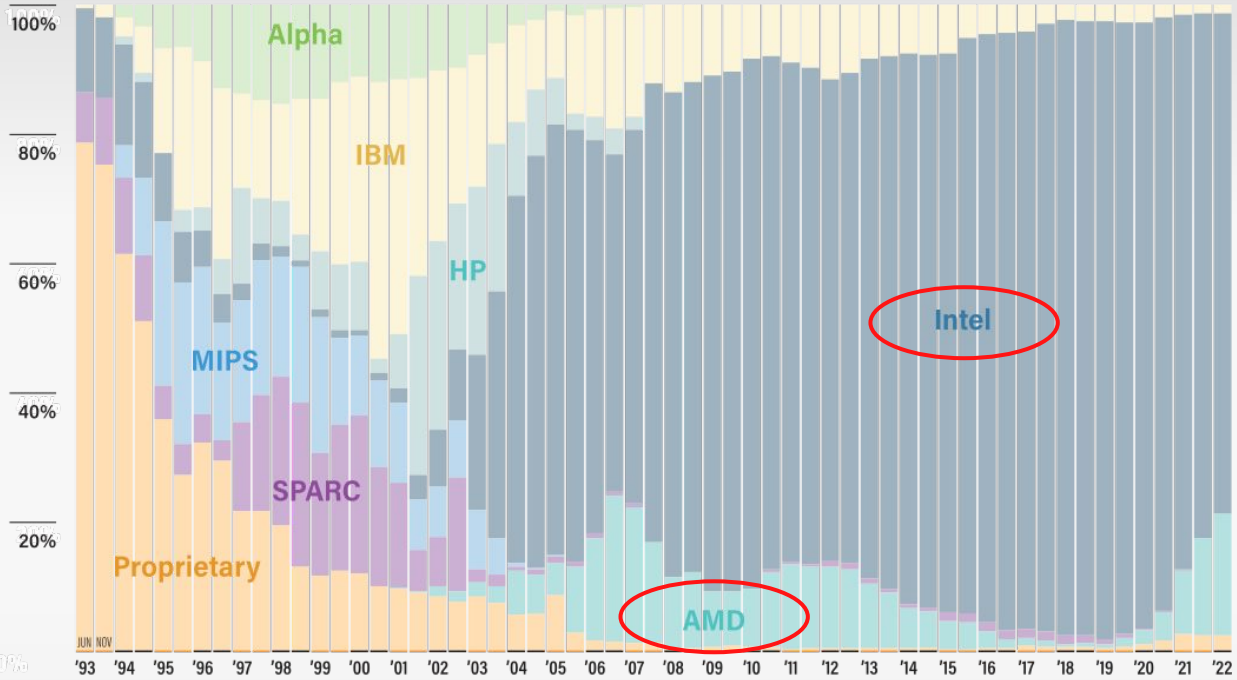
Upcoming USA systems:

			SITE	COUNTRY	PFLOP/S
2023	**El Capitan**	AMD Epyc CPUs, AMD Instinct GPUs	NNSA	USA	2000
2022	**Aurora**	Intel Xeon CPUs, Intel Xe GPUs	ALCF	USA	1000

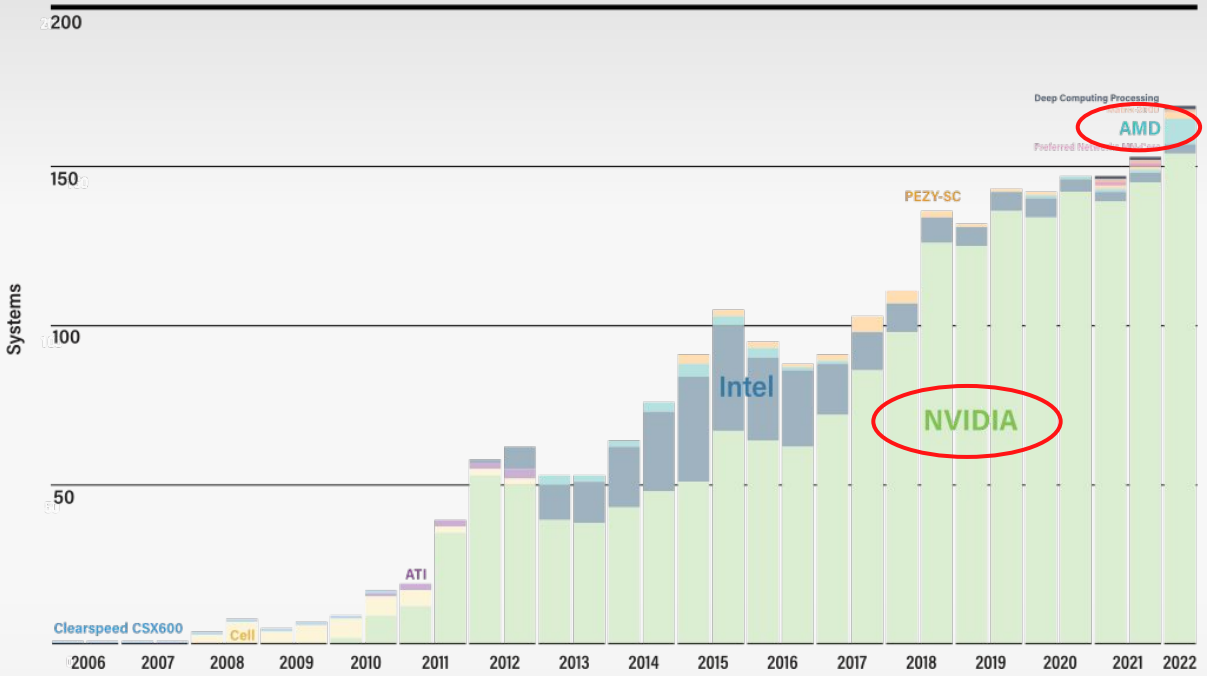
AMD and Intel have started only recently in producing GPUs for HPC systems
NVIDIA has dominated the market for more than 10 years

Hardware Vendors

Chip Technology



Accelerators/Co-processors



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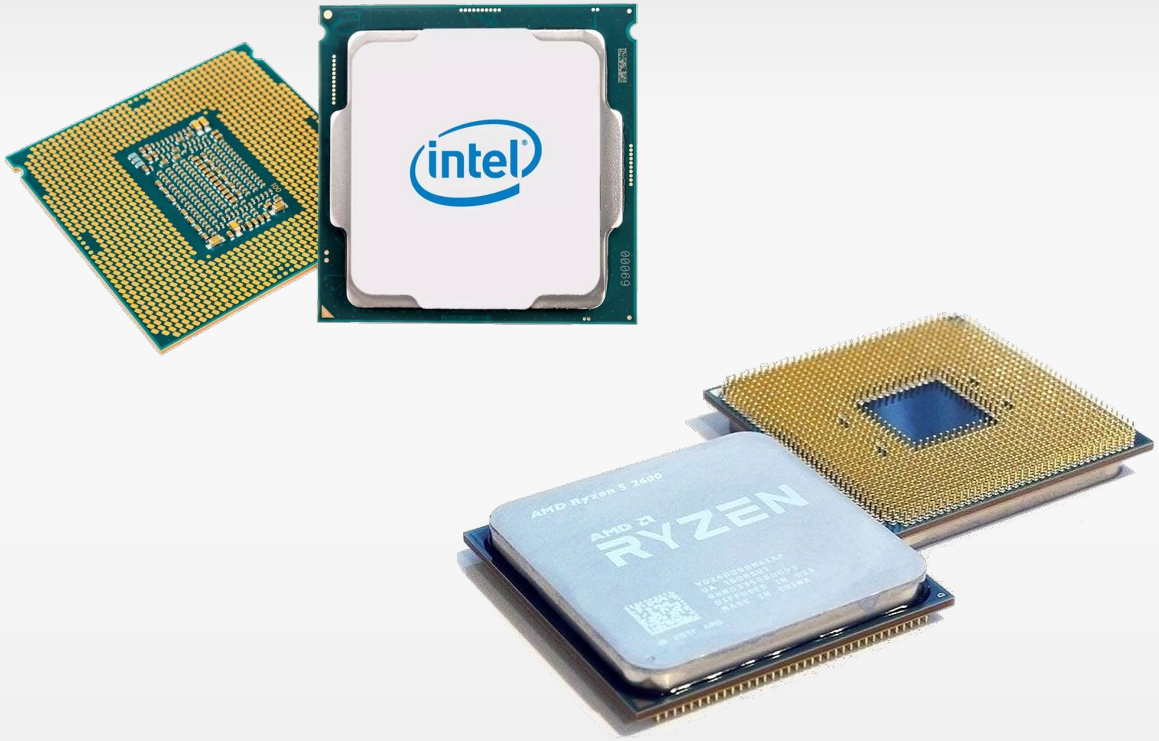
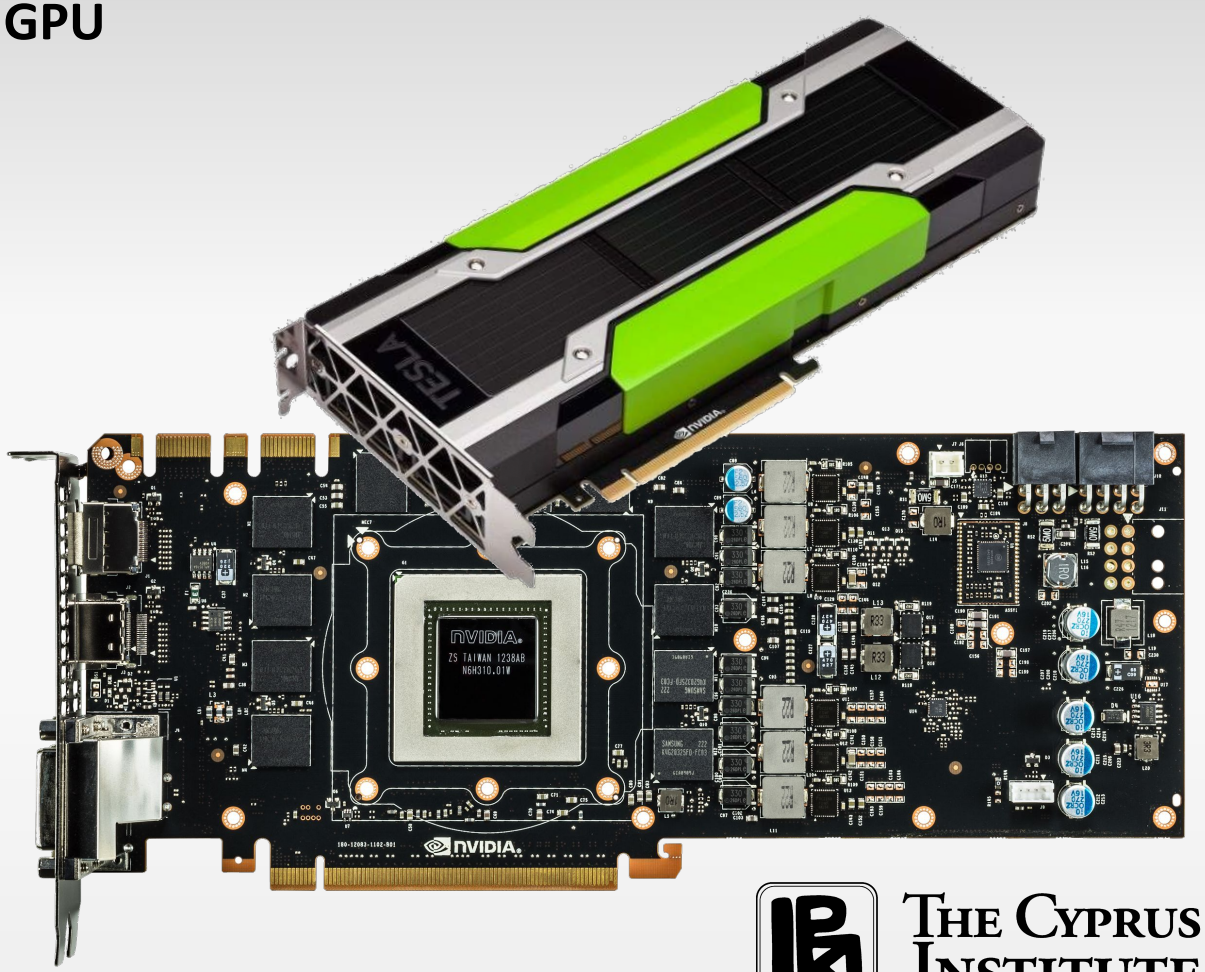
CPUs vs GPUs

CPU



GPU



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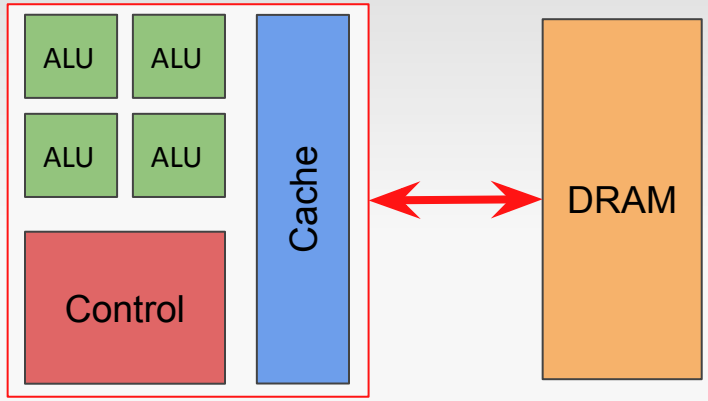
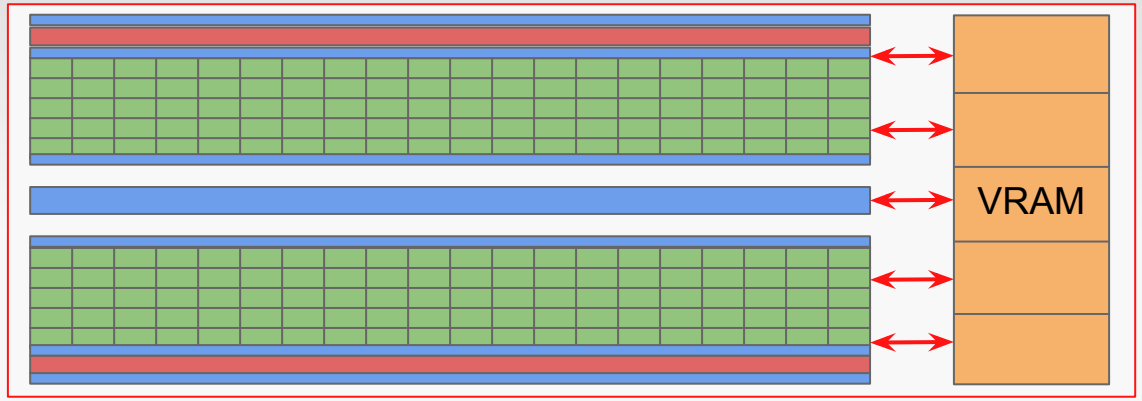
Low latency or High-throughput?

CPU



- **Optimized for low-latency access** to cached data
- Complex control logic (thousands of instructions available)
- Large caches (L1, L2, etc.)
- Optimized for serial operations
- Shallow pipelines (< 30 stages)
- Newer CPUs have more parallelism (becoming more GPU-like)

GPU



- **Optimized for data-parallel** throughput computation
- High latency tolerance
- High compute density per memory access
- High throughput
- Deep pipelines (hundreds of stages)
- Newer GPUs have better control logic (becoming more CPU-like)

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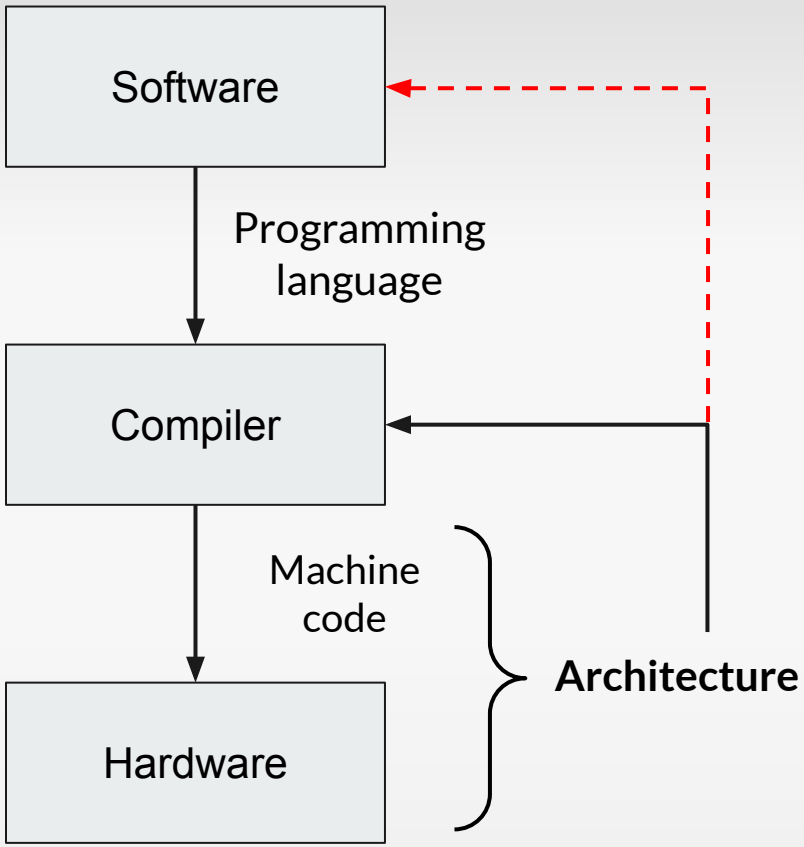
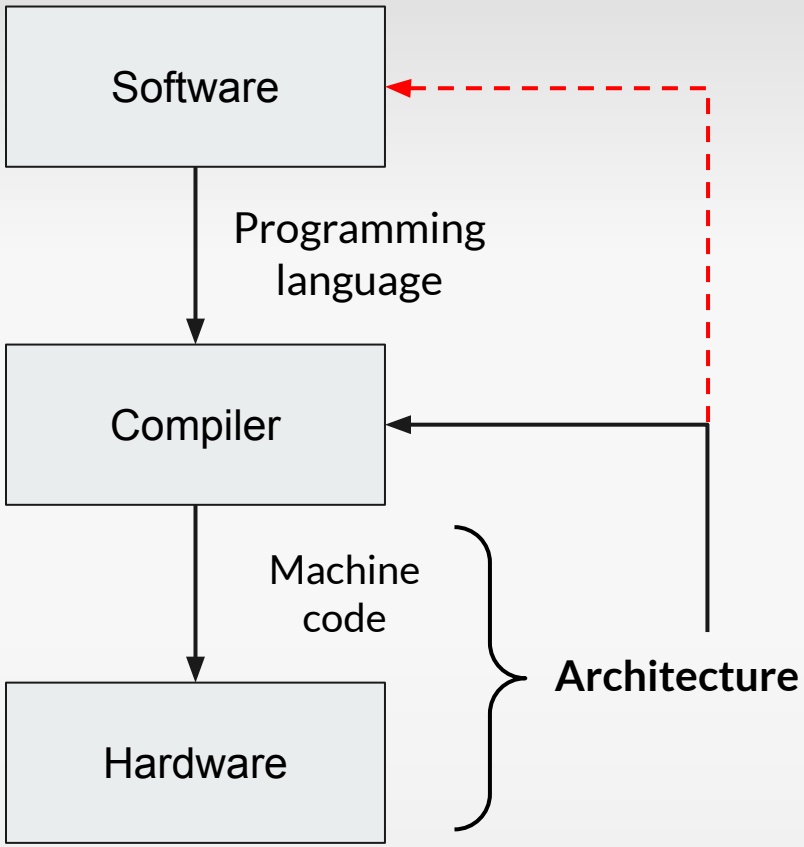
Why is the architecture important?



The architecture **affects the design of HPC software**:

- Memory bandwidth
- Cache memory size
- Frequency
- Number of cores
- Instruction set:
  - Floating point operations (e.g. $y = a\,x + b$)
  - Single Instruction Multiple Data (SIMD)
- Architecture-specific features

Why is the architecture important?



The architecture **affects** **how we program the software**:

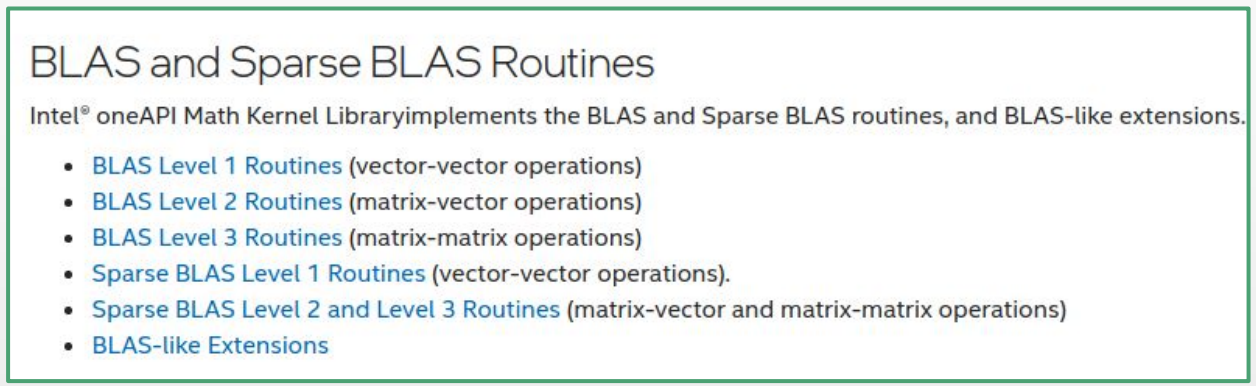
- **Intrinsic functions** in C/C++ that are architecture-dependent
- Architecture-dependent **extension of the programming lang**:
  - **CUDA** for NVIDIA GPUs -> nvcc compiler
  - **HIP** for AMD GPUs -> hipcc compiler

All in one solution (CPUs, GPUs, FPGAs):

- **OpenCL**: open-source framework in C/C++
- **OneAPI** and **DPC++**: developed by Intel, C/C++ framework and extension of the programming language

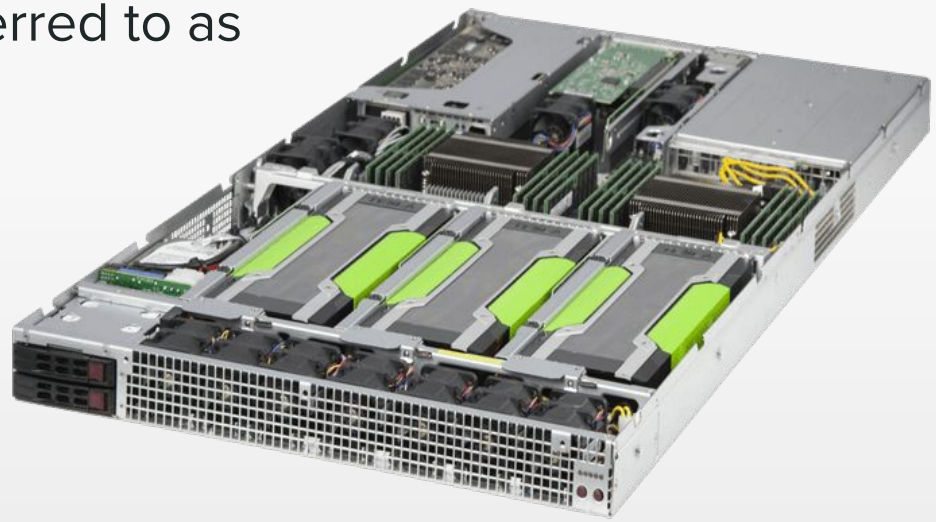
Other alternatives? Standard libraries

- Standard Software Libraries define formal APIs to be implemented and optimized on specific architectures. Examples are
  - **BLAS:** Basic Linear Algebra Subroutines
  - **LAPACK:** Linear Algebra Package
  - …
- These then have different implementations for various architectures:
  - **OpenBLAS:** Open-source library of BLAS
  - **Intel MKL:** Intel's implementation of BLAS and LAPACK
  - **cuBLAS:** NVIDIA's implementation of BLAS
  - **hipBLAS:** AMD's implementation of BLAS
- For reference see e.g.
  - shorturl.at/aOPY6



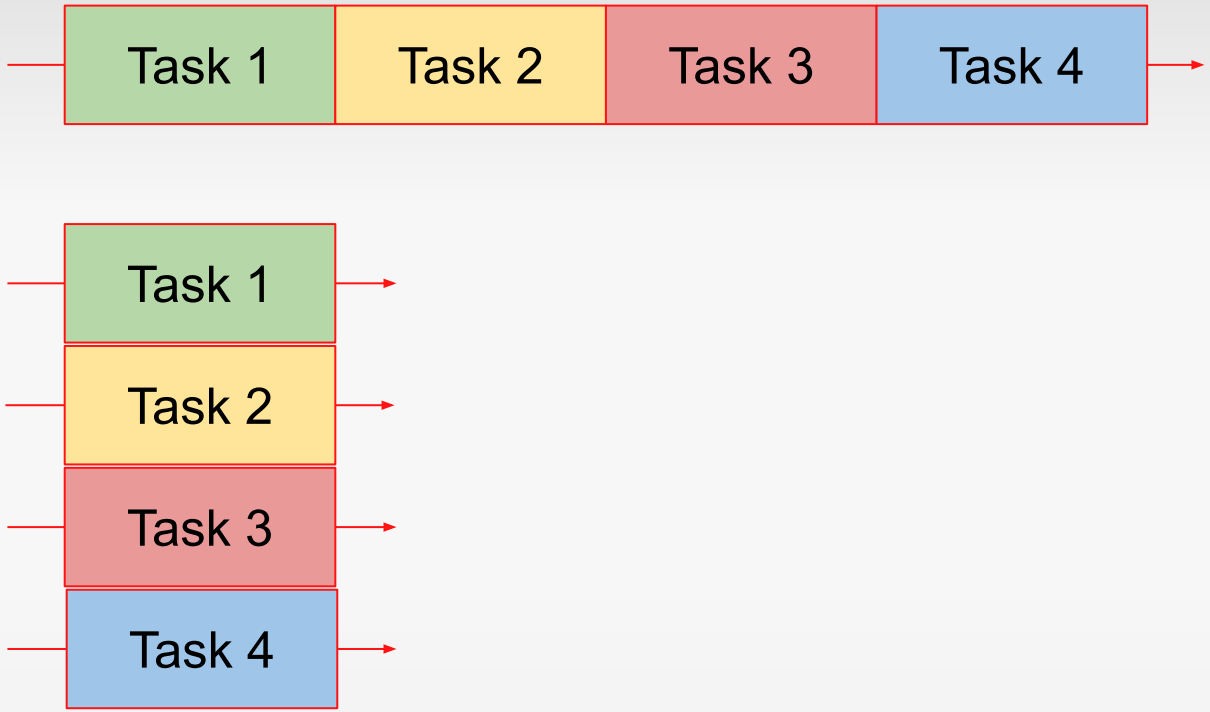
HPC is not only in-node performance

- Within a single node one can use **multithreading** and **shared memory**
  - E.g. see OpenMP
- But various nodes do not share memory and one needs to use the network to exchange data. This is referred to as **distributed computing!**
  - E.g. see MPI
- How to distribute?



Parallel computing

- Task parallelism:
  - ➢ Independent tasks
- Distributed Data:
  - ➢ Independent Data
- Pipeline parallelism:
  - ➢ Dependent tasks/data
- Modular computing:
  - ➢ Architecture-dependent



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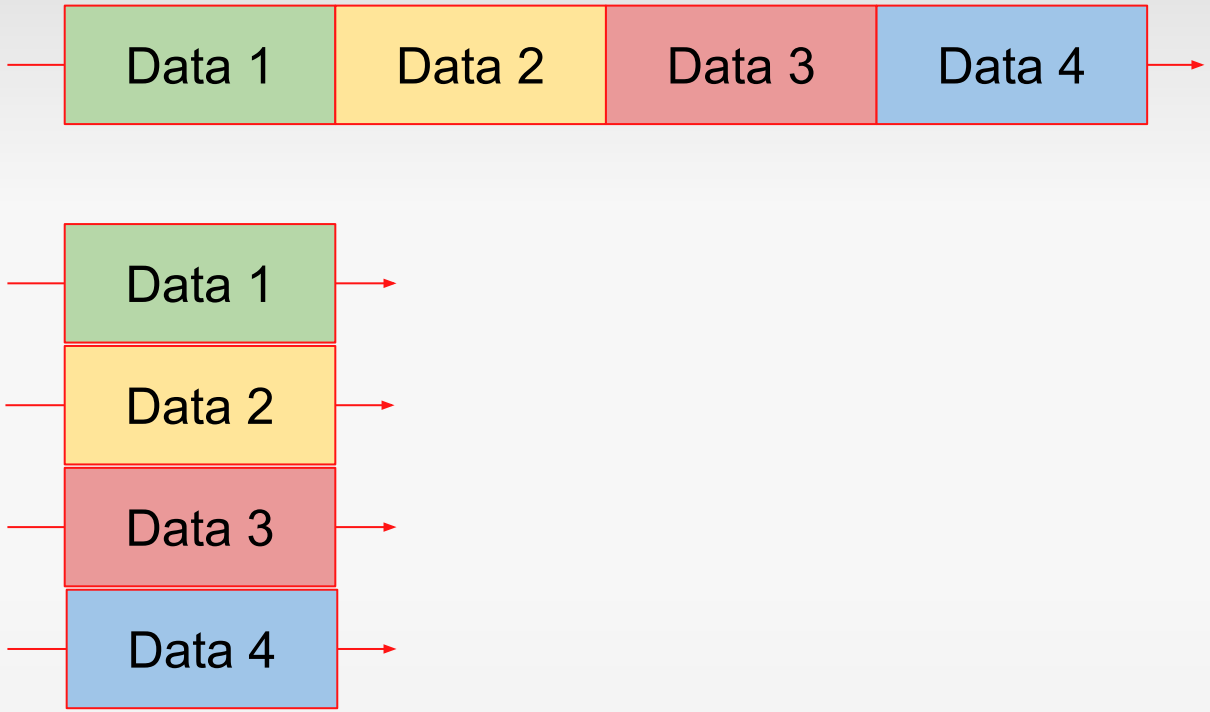

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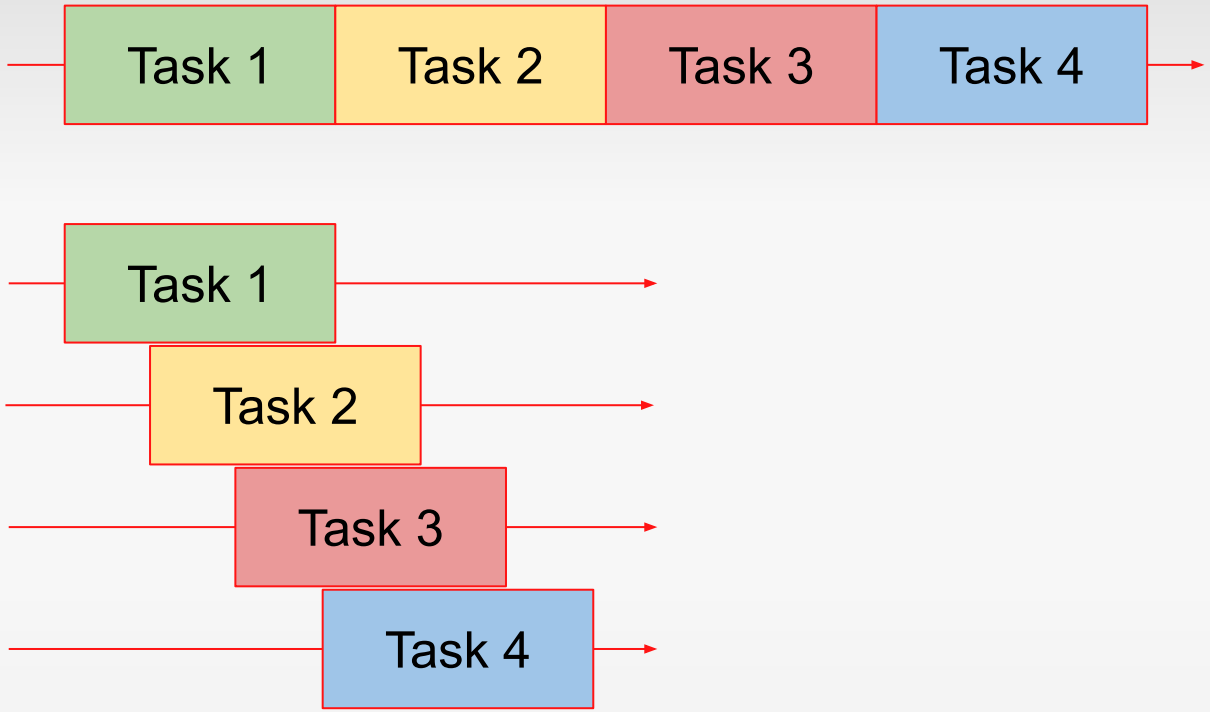

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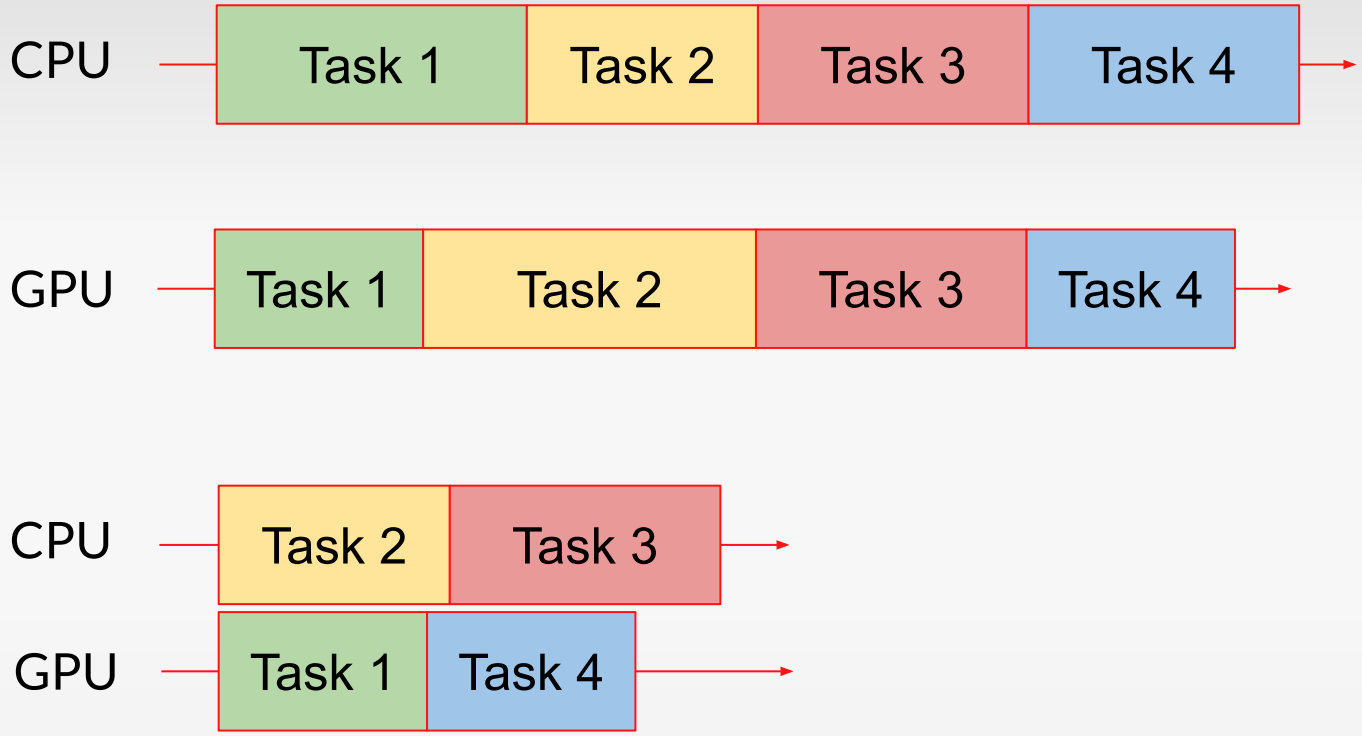
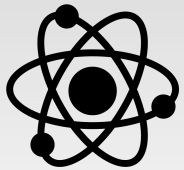
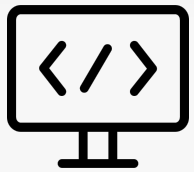


How to research using HPC



- **Scientific problem**
  - Numerical approach
  - Computationally intensive
  - Parallelizable (task or data)

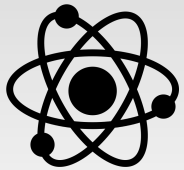


- **Software**
  - Optimized for HPC
  - Scalable

- **Access to a Supercomputer**
  - Preparatory access
  - Software test and benchmark
  - Competitive proposal for computing time

- **Production of results and analysis**
  - About 1 year long or more
  - Tera-/Peta-bytes of data produced
  - Various publications

How to research using HPC



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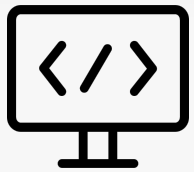

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- **Extra activities:**
  - Algorithmic research
  - Numerical improvements
  - Software development
  - New methodologies
  - Machine Learning

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HPC research in Cyprus

HPC NCC - CaSToRC

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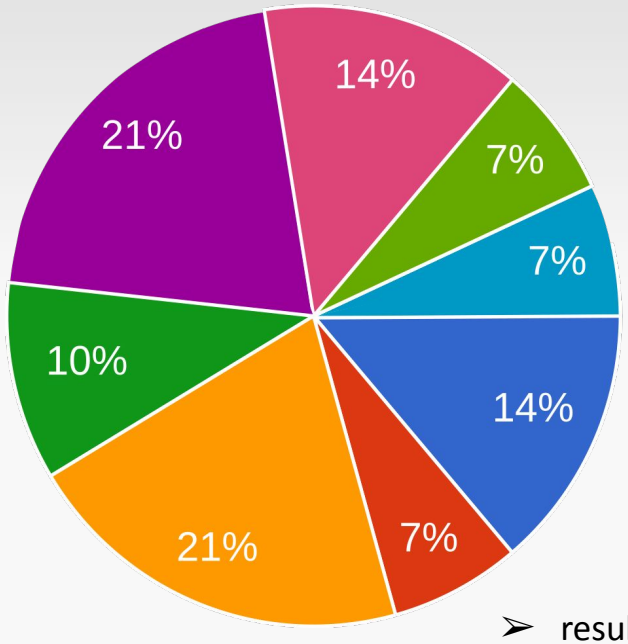
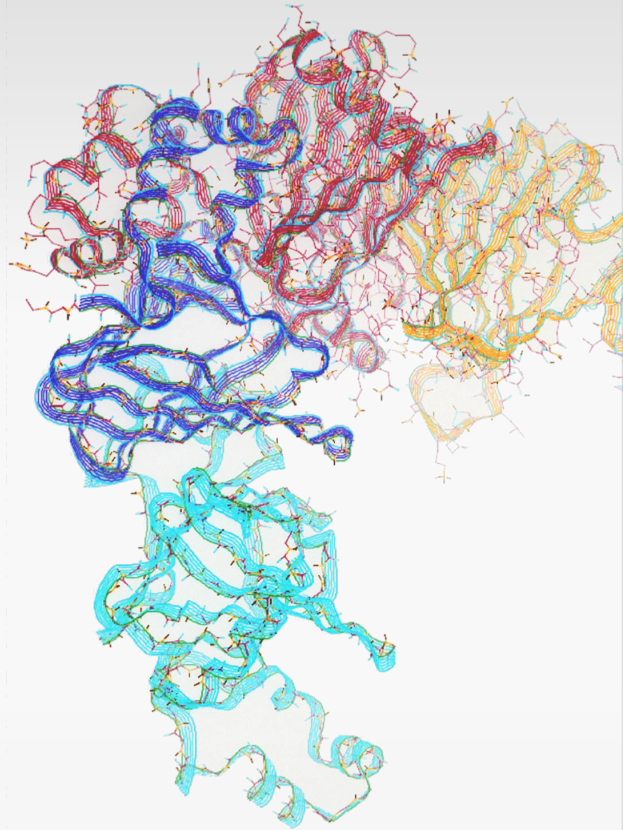
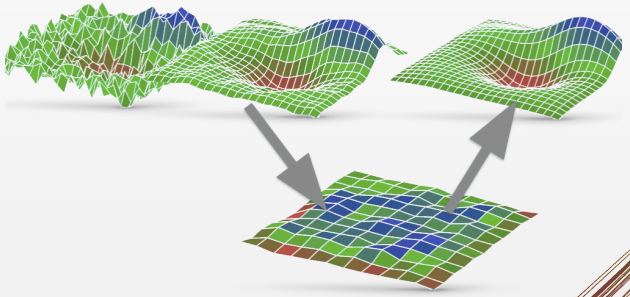
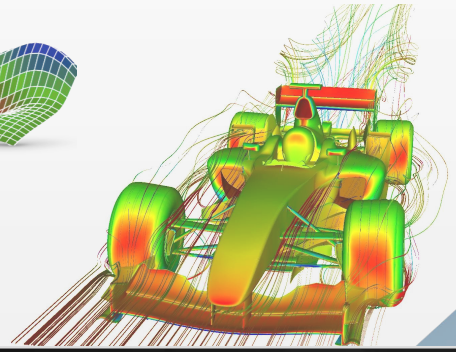


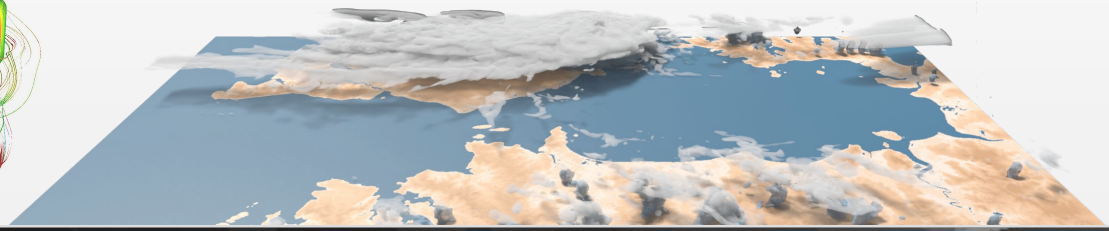
- Biochemistry, Bioinformatics
- Chemical Sciences
- Earth System Sciences
- Engineering
- Physics
- Mathematics and Computer Sc.
- Economics, Finance
- Others

➢ results from our survey on the scientific community in Cyprus









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Our HPC systems

- **Cy-Tera** (2012 - Legacy):
  - 98 nodes, 12-cores Intel Xeon CPU
  - ~300 TFlops
  - served > 480 projects

- **Cyclone** (2020 - Active):
  - 33 nodes, 2 x 20-cores Intel Xeon CPUs
  - 16 nodes with 4 x NVIDIA V100 GPUs
  - ~600 TFlops
  - Applications for access at *https://hpcf.cyi.ac.cy/apply/*

- **Upcoming** a new system for industrial applications with latest NVIDIA or AMD GPUs

- **Prototype systems:**
  - **Cyclamen** (2018): 8 nodes, 2 x 16-cores Intel Xeon CPU, 2 x NVIDIA P100 GPUs
  - **Phi** (2011): 4 nodes, 16-cores Intel Xeon CPU, 16 Xeon Phi accelerators

For more details, see https://castorc.cyi.ac.cy/infrastructure

Thank you!

Questions?

Thank you!

Thank you for you attention

… and talk to you later!

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