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National Competence
Center in HPC - Cyprus

EURO

Introduction High-Performance Computing - Dr. S. Bacchio

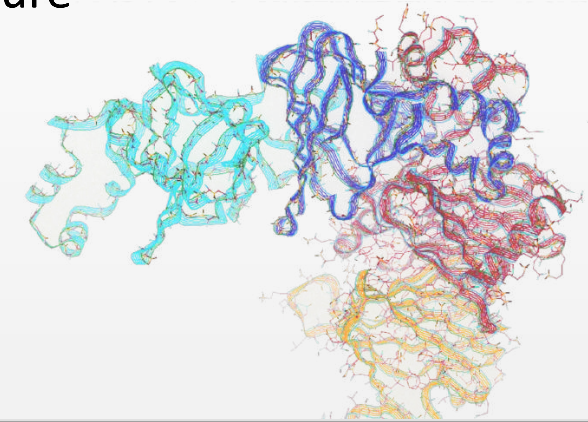
In today's talk

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

EuroHPC Joint Undertaking

TOP 500 The List.



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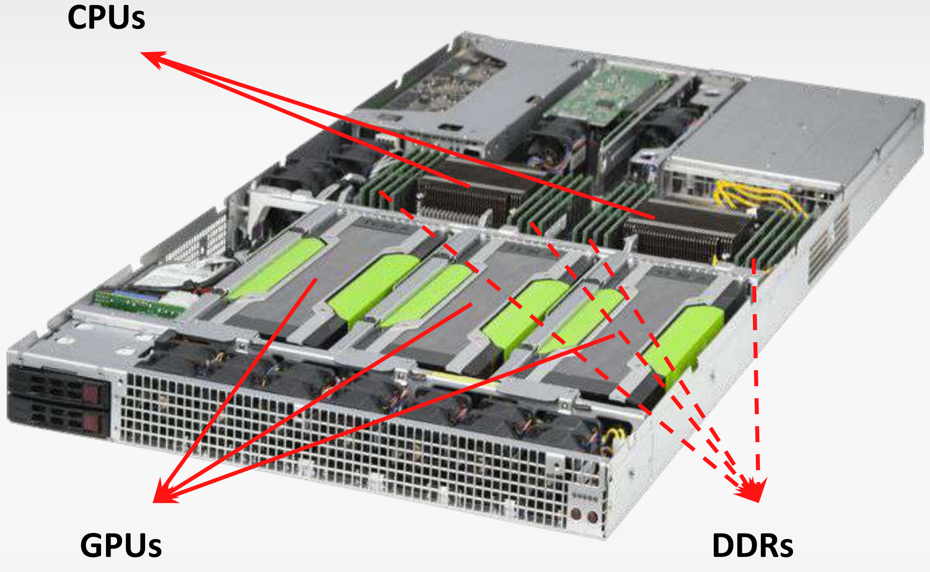
Inside a supercomputers

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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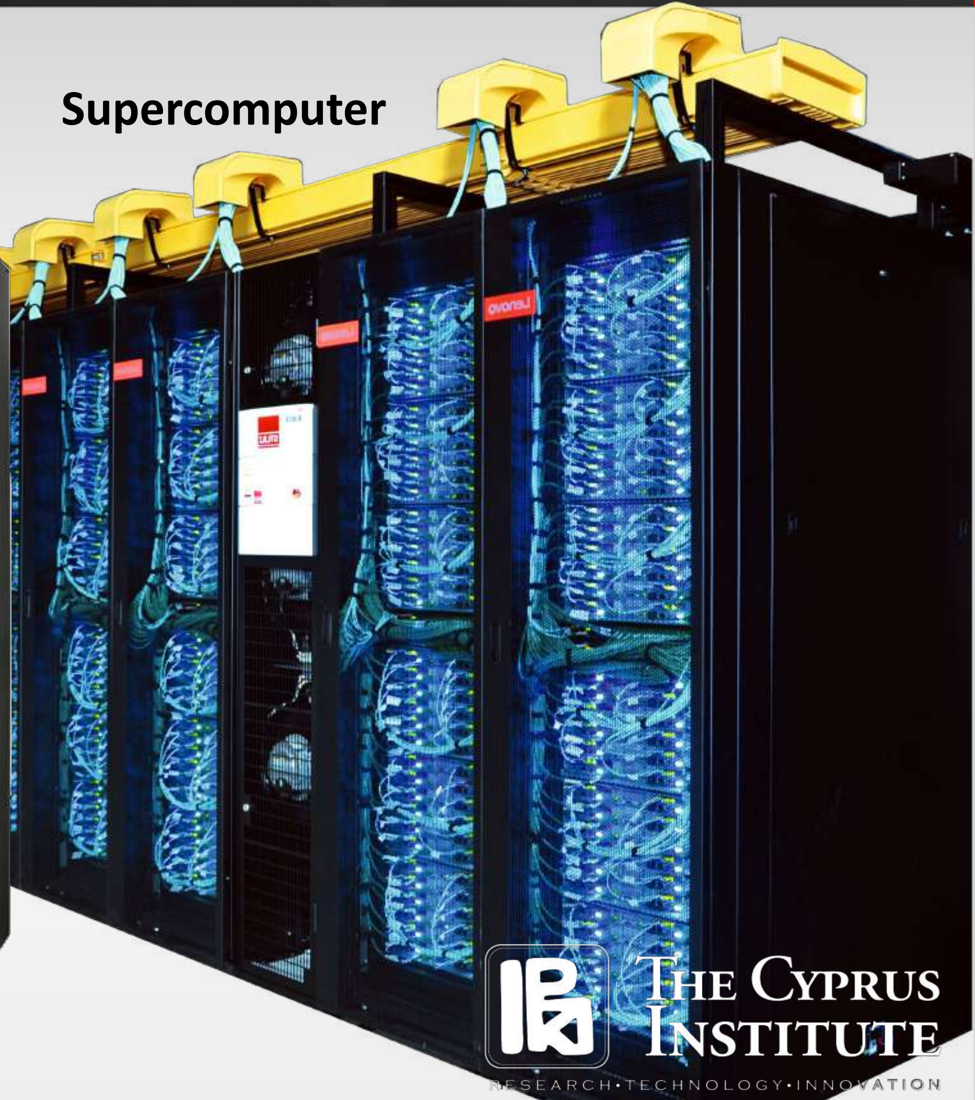
Inside a supercomputers

Computing Node

Rack

Supercomputer



- \+ Network
- \+ Storage
- \+ Power supply
- \+ Cooling

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Supercomputers in Europe

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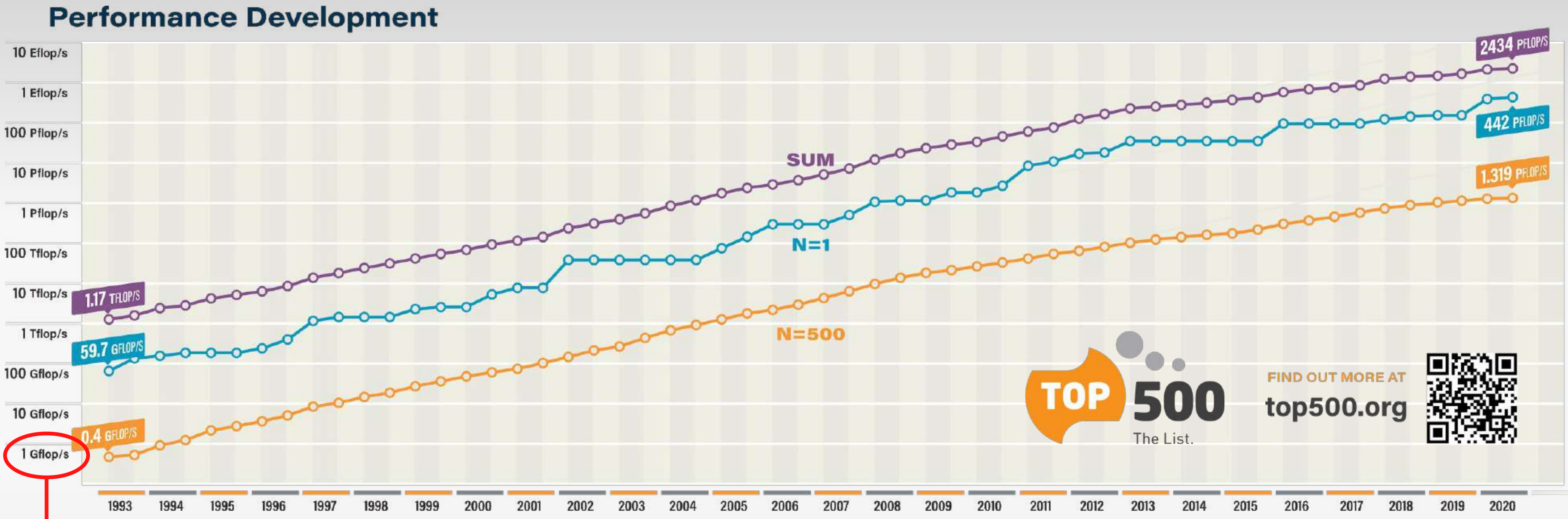
Supercomputers in Europe

TOP 500 - The List.



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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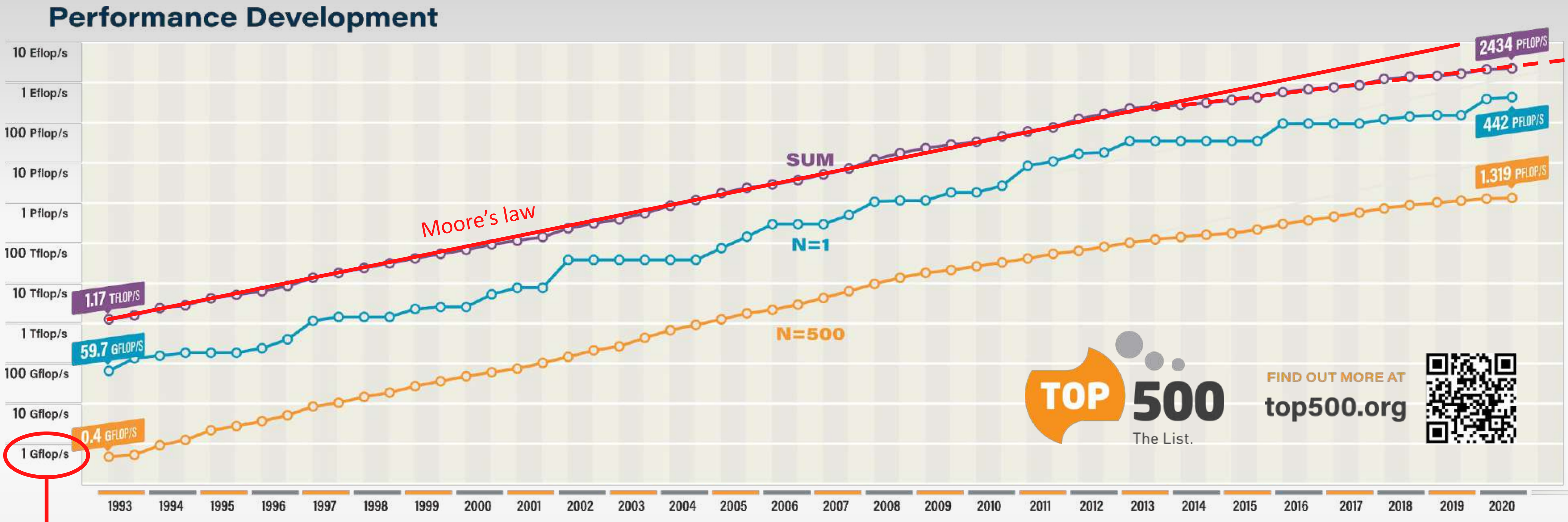
TOP 500 - The List.



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TOP HPC systems

NOVEMBER 2020	SYSTEM	SPECS	SITE	COUNTRY	CORES	RMAX PFLOP/S	POWER MW
1	Fugaku	Fujitsu A64FX (48C, 2.2GHz), Tofu Interconnect D	RIKEN R-CCS	Japan	7,630,848	442.0	29.9
2	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
3	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
4	Sunway TaihuLight	Shenwei SW26010 (260C, 1.45 GHz) Custom Interconnect	NSCC in Wuxi	China	10,649,600	93.0	15.4
5	Selene	NVIDIA DGX A100, AMD EPYC 7742 (64C, 2.25GHz), NVIDIA A100, Mellanox HDR Infiniband	NVIDIA Corporation	USA	555,520	63.4	2.65

Top European systems:

			SITE	COUNTRY	CORES	Rmax	POWER
7	JUWELS Booster	AMD EPYC 7402 (24C 2.8GHZ), NVIDIA A100, Mellanox HDR Infiniband	Juelich	Germany	449,280	44.1	1.8
8	HPC5	Xeon Gold 6252 (24C 2.1GHz), NVIDIA V100, Mellanox HDR Infiniband	Eni S.p.A.	Italy	669,760	35.5	2.3
11	Marconi-100	IBM POWER9 (16C, 3GHz), NVIDIA V100, Mellanox EDR Infiniband	Cineca	Italy	347,776	21.6	1.4
12	Piz-daint	Xeon E5-2690v3 (12C 2.6GHz), NVIDIA P100, Cray/HPE	CSCS	Switz	387,872	21.2	2.4

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HPC NCC - CaSToRC

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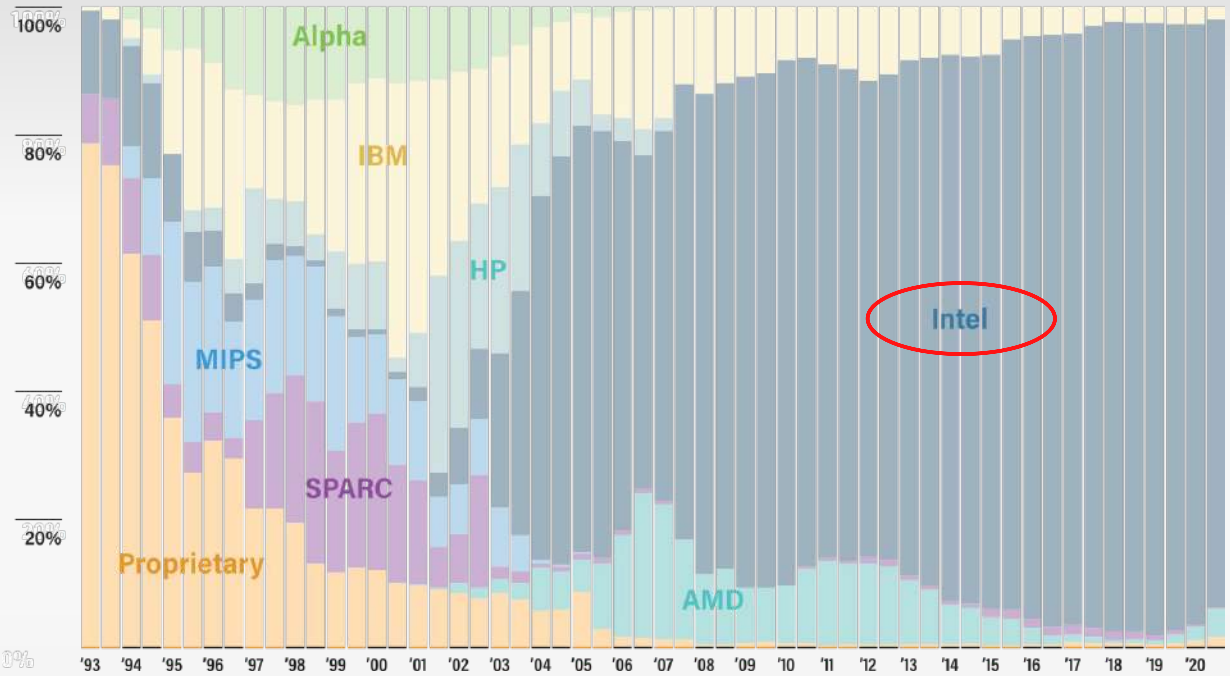
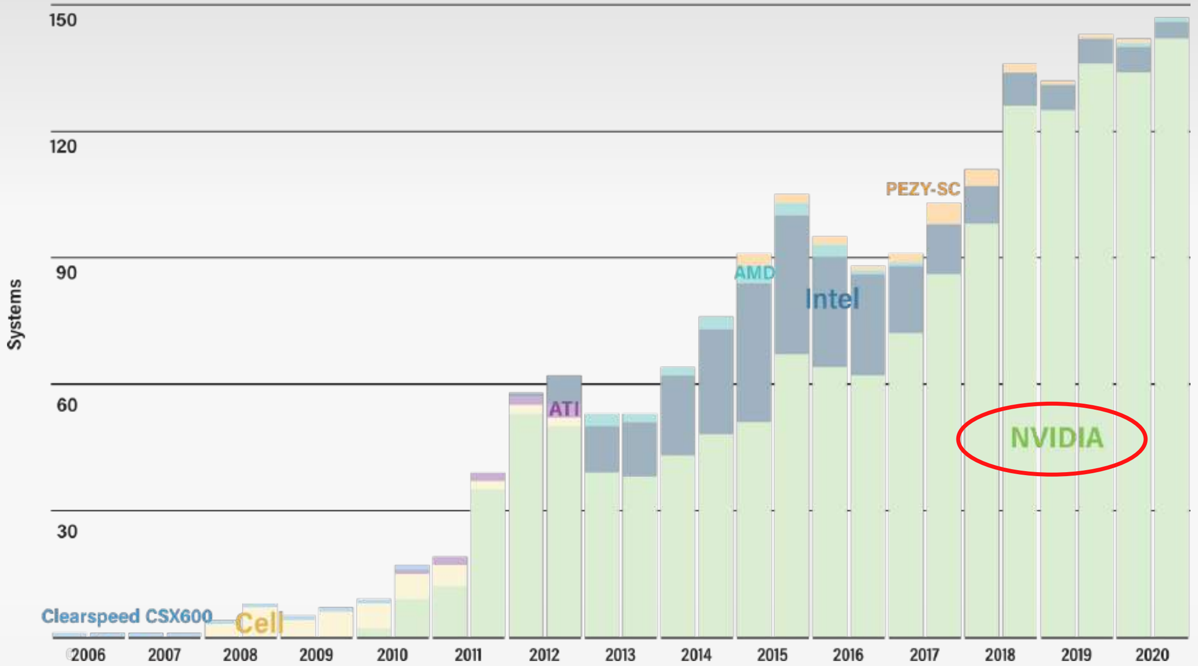
Hardware Vendors

Chip Technology



Accelerators/Co-processors



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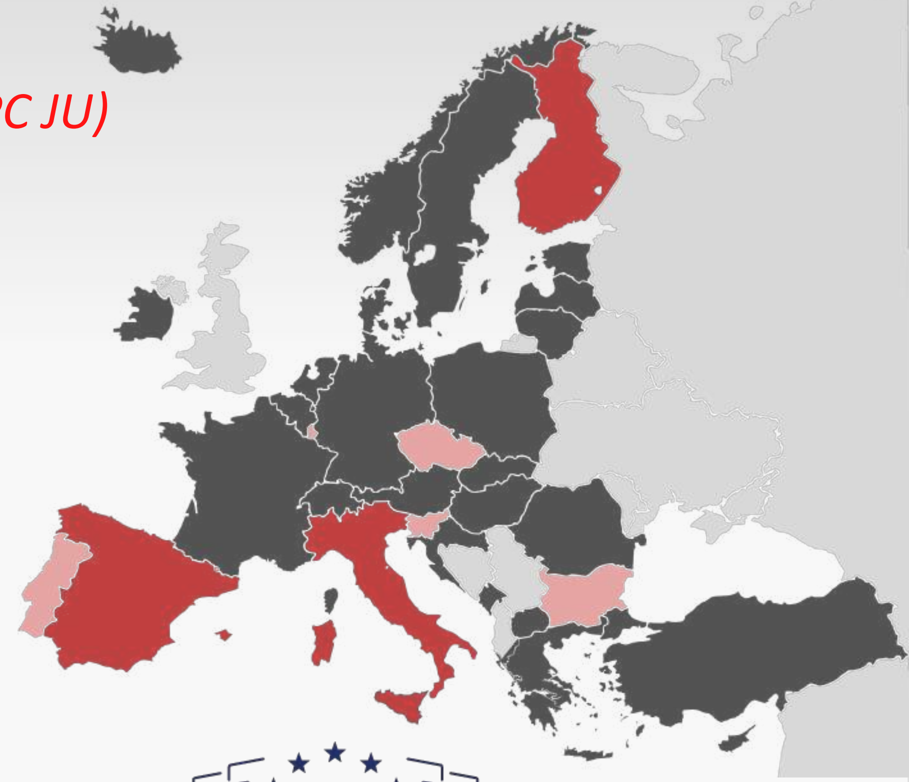
EuroHPC Joint Undertaking

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** in an upcoming call

Upcoming Budget (2021 - 2033): 8 billion Euro



EuroHPC Joint Undertaking

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Future Systems

Future European systems:

			SITE	COUNTRY	PFLOP/S
2021	**LUMI**	AMD Epyc CPUs, AMD Instinct GPUs	CSC	Finland	500
2021	**Leonardo**	Intel Xeon CPUs, NVIDIA Ampere A100	Cineca	Italy	250
2021	**MareNostrum5**	N/A (*probably* an heterogeneous system)	BSC	Spain	200

Future USA systems:

			SITE	COUNTRY	PFLOP/S
2023	**El Capitan**	AMD Epyc CPUs, AMD Instinct GPUs	NNSA	USA	2000
2021	**Frontier**	AMD Epyc CPUs, AMD Instinct GPUs	OLCF	USA	1500
2022	**Aurora**	Intel Xeon CPUs, Intel Xe GPUs	ALCF	USA	1000

Exascale! Expected also in EU for 2023.

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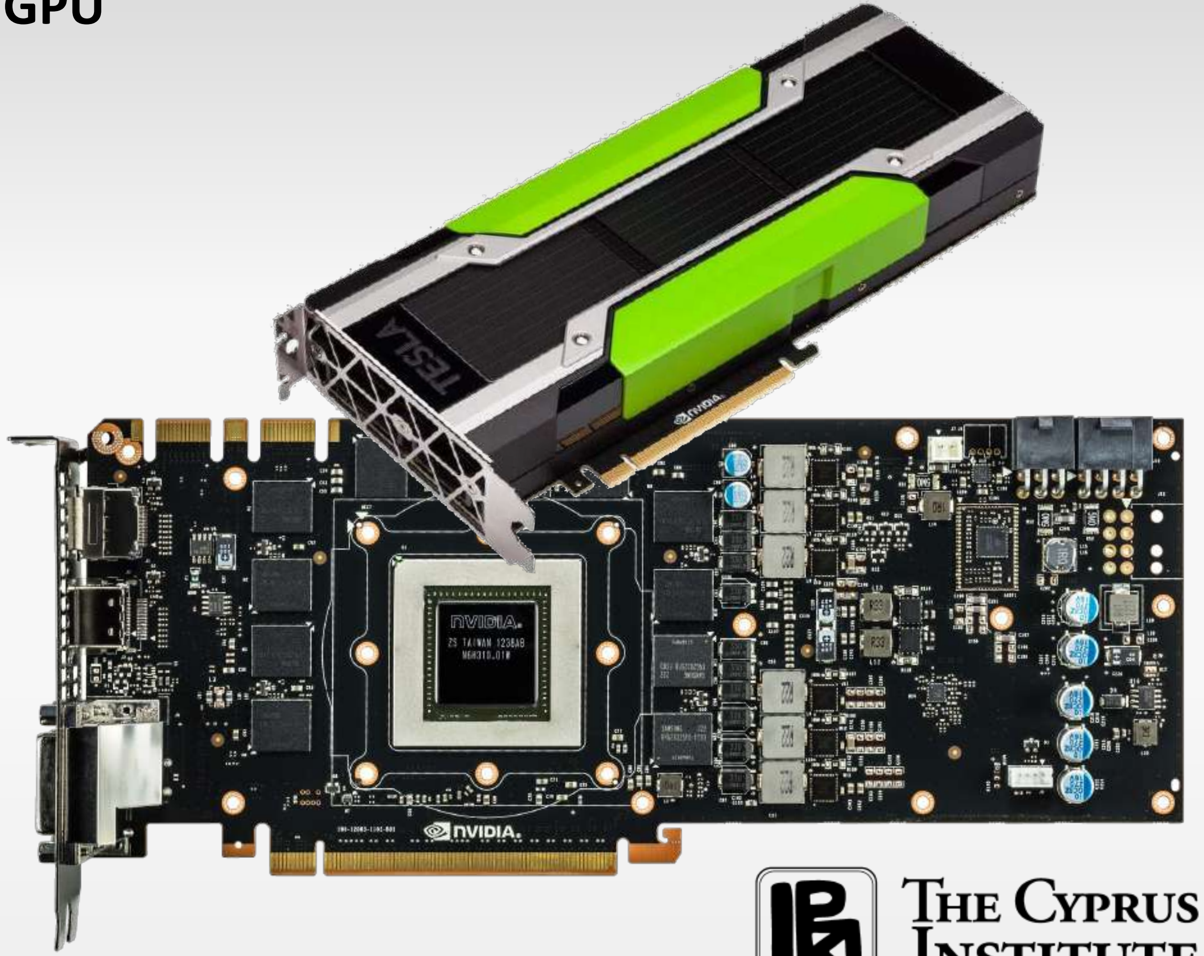
NOTE: AMD and Intel are new enters in the list of GPUs vendors for top HPC systems

CPUs vs GPUs

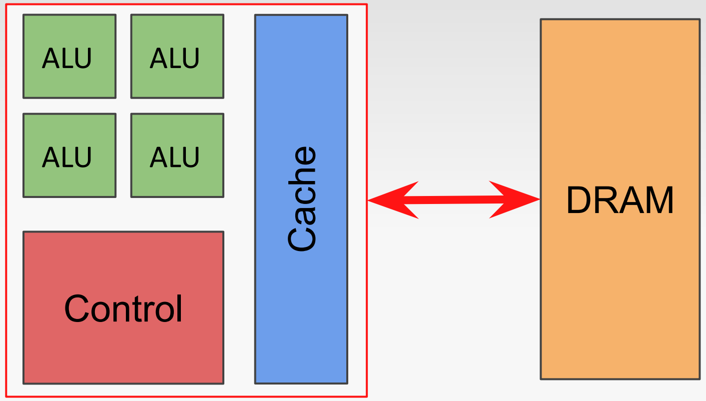
CPU

GPU



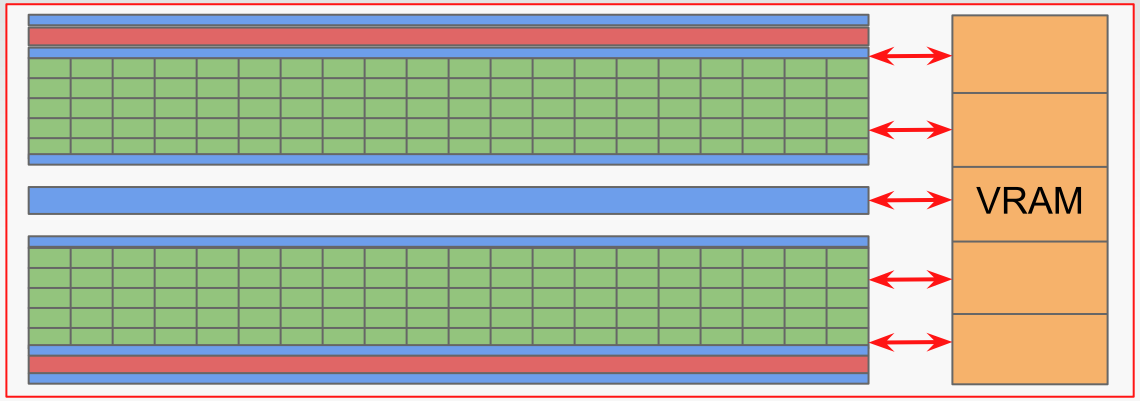
Low latency or High-throughput?

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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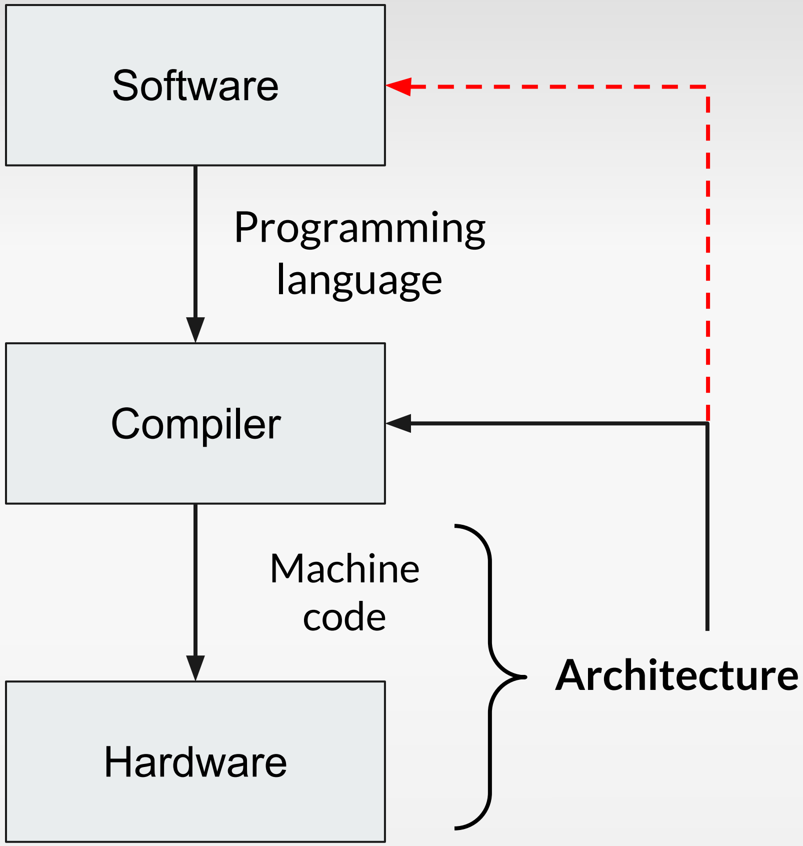
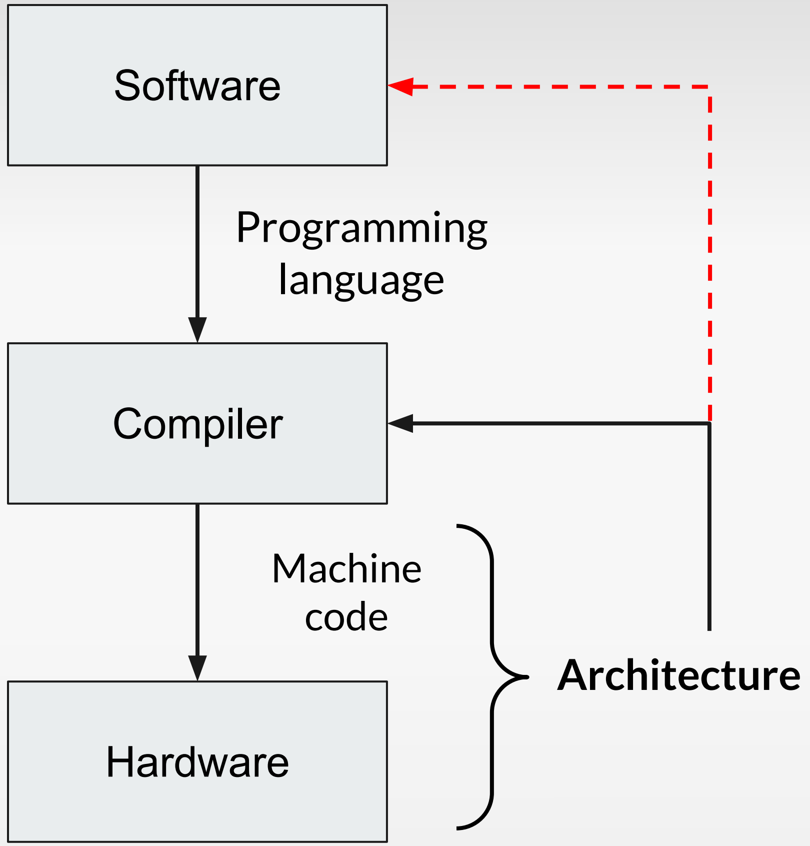
Why is the architecture important?



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

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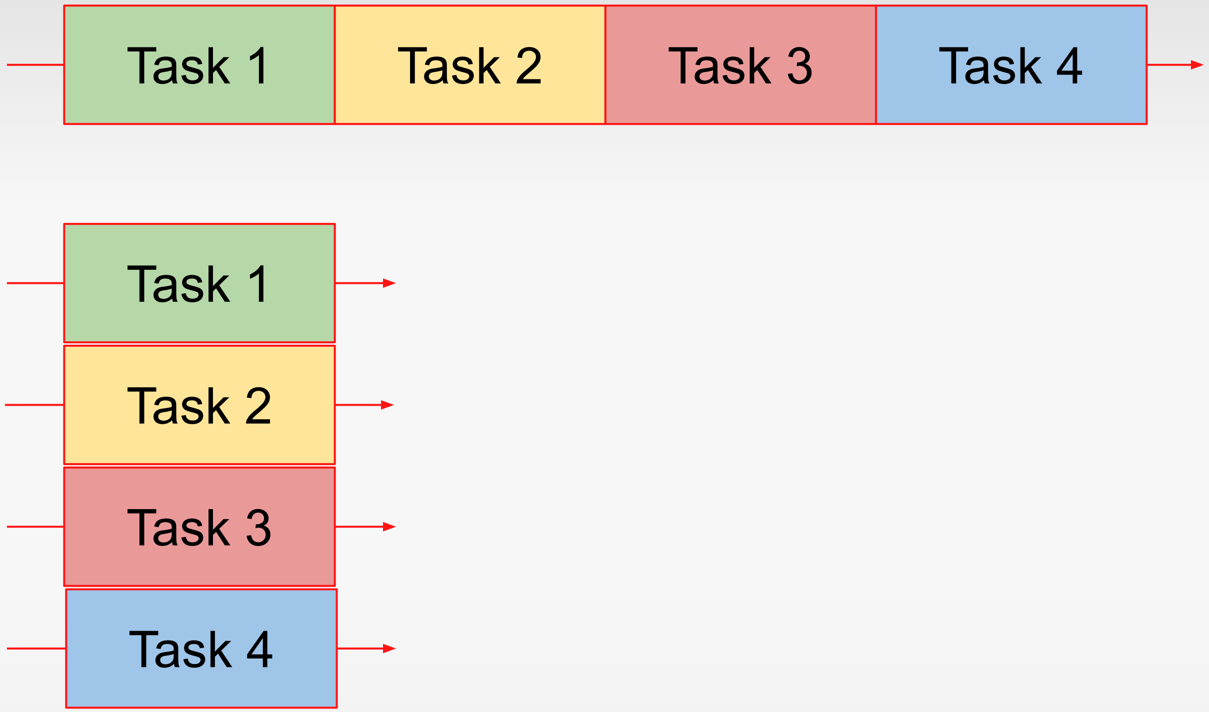
Parallel computing

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



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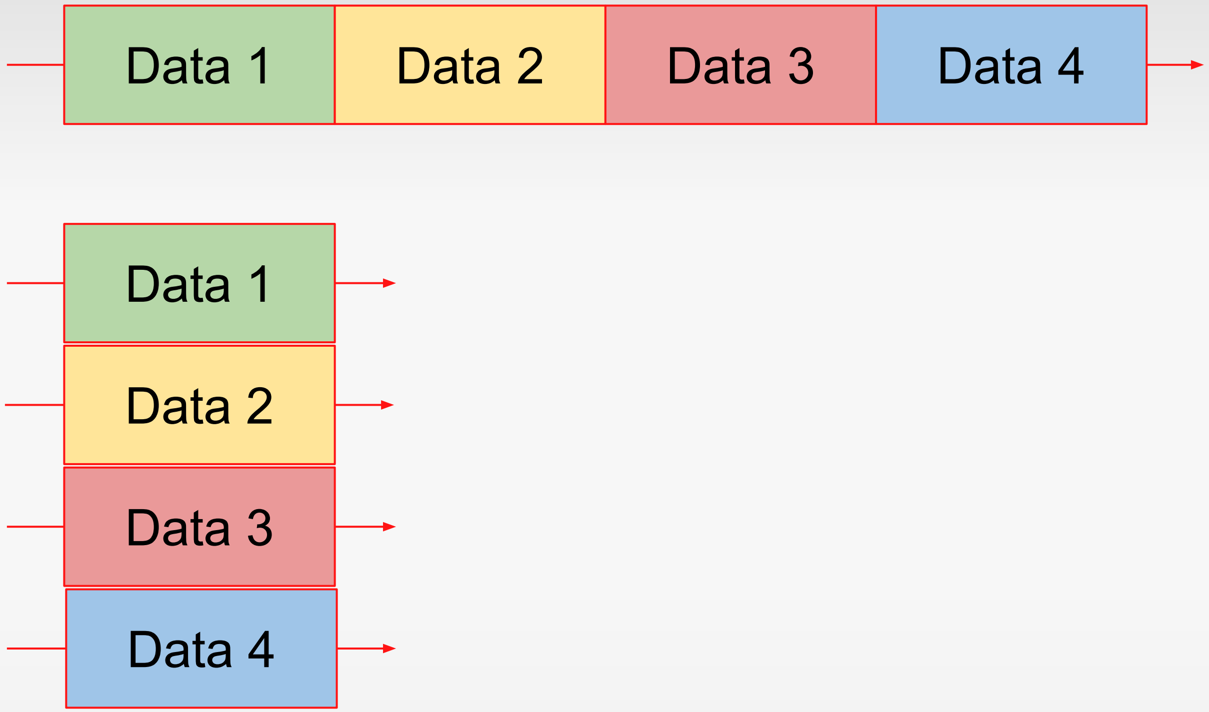

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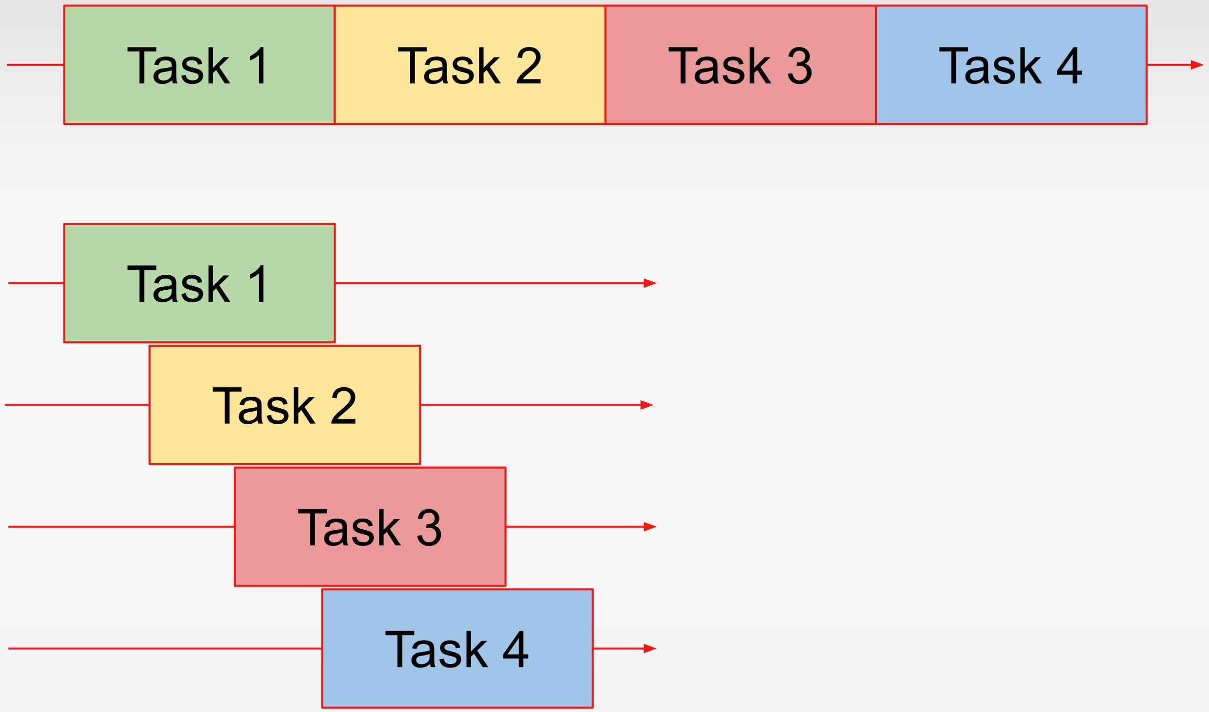

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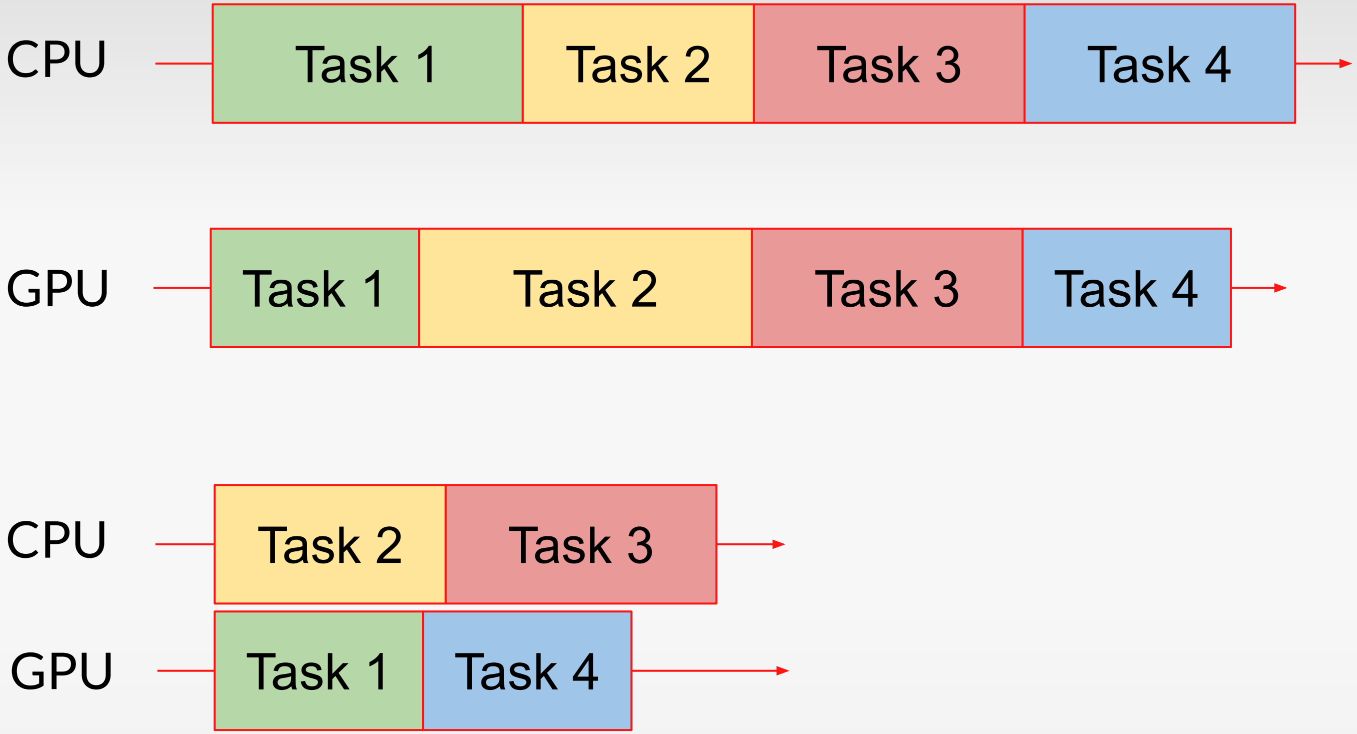

How to research using HPC

- **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

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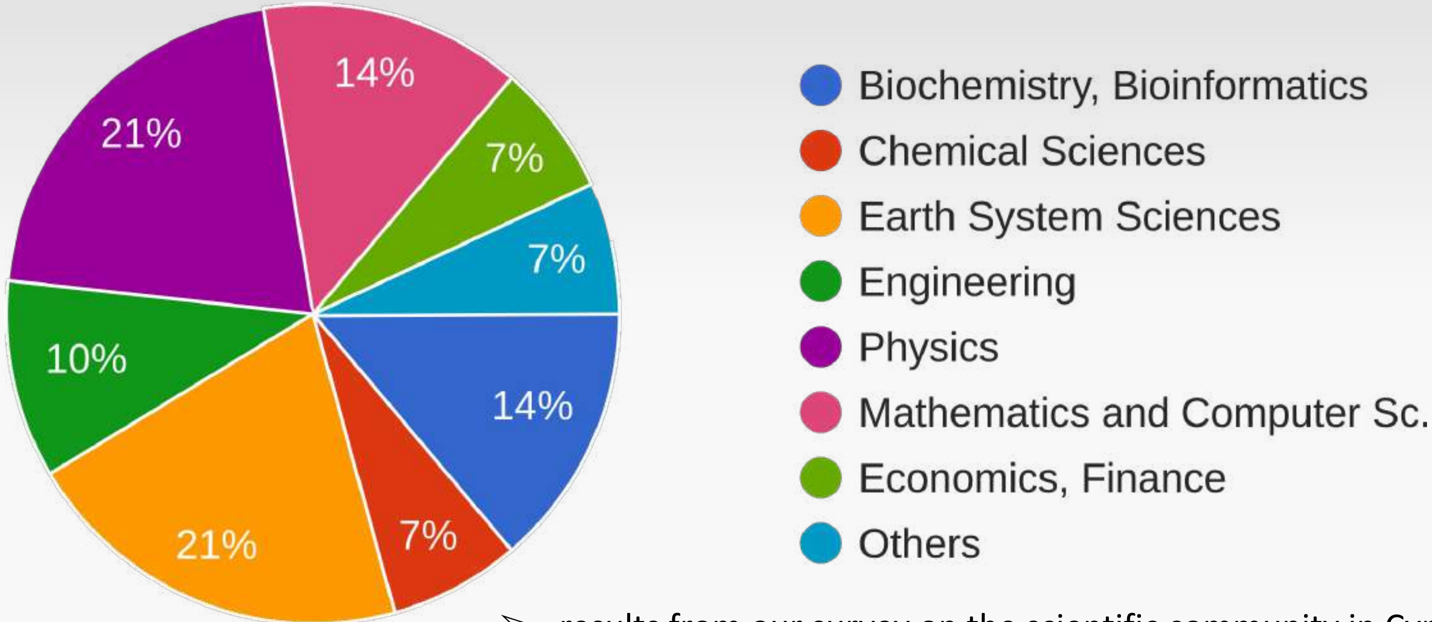
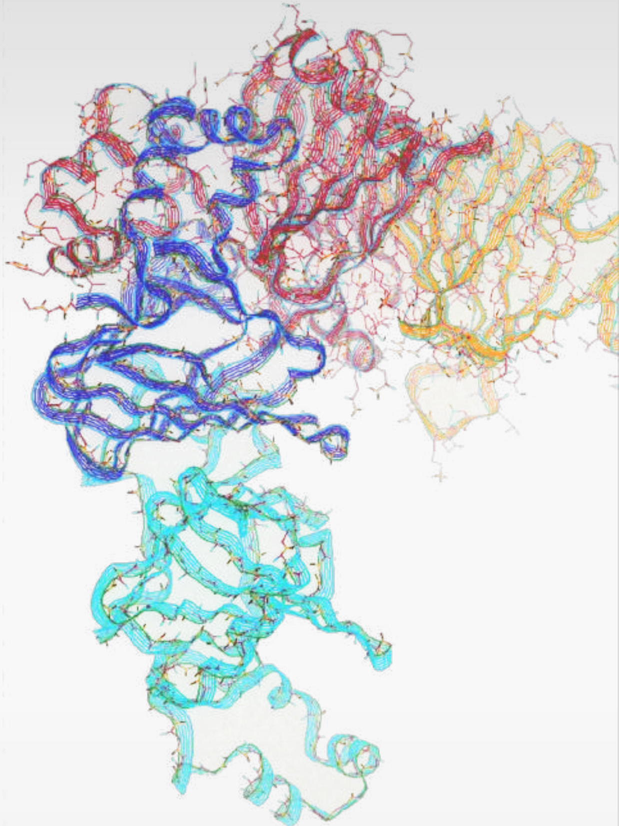
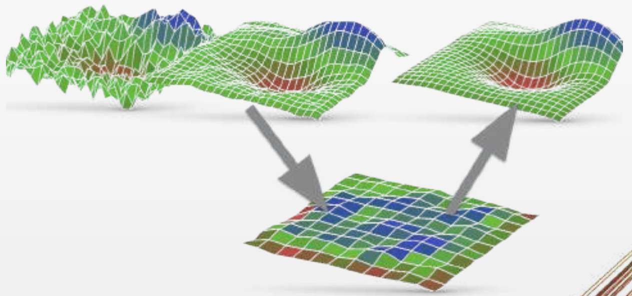
- **Extra activities:**
  - Algorithmic research
  - Numerical improvements
  - Software development
  - New methodologies
  - Machine Learning

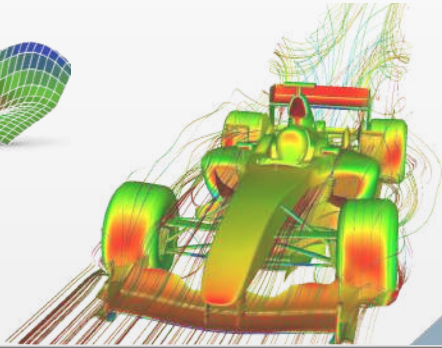
HPC research in Cyprus

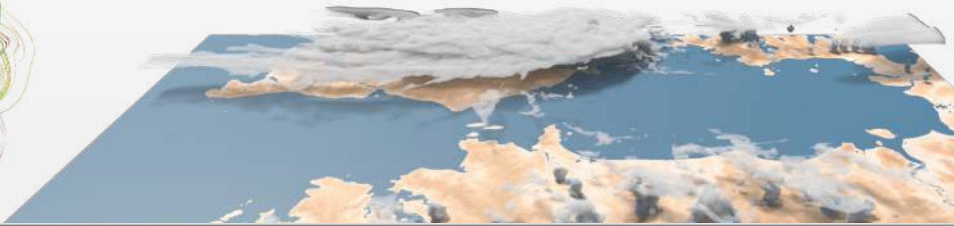


- results from our survey on the scientific community in Cyprus









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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

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Thank you!

Questions?

Thank you!

Thank you for you attention

… and talk to you later!

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