



C EURO

HPC National Competence Center

Introduction High-Performance Computing - Dr. S. Bacchio



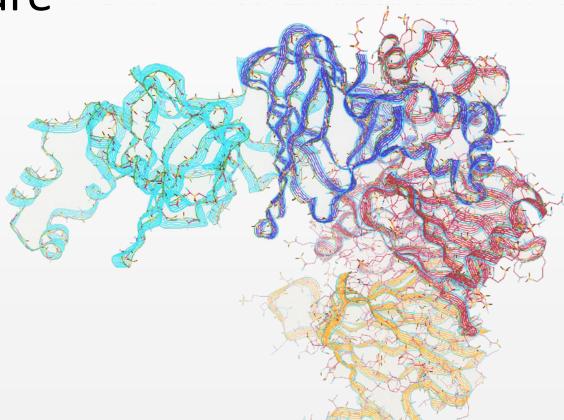
In today's talk

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



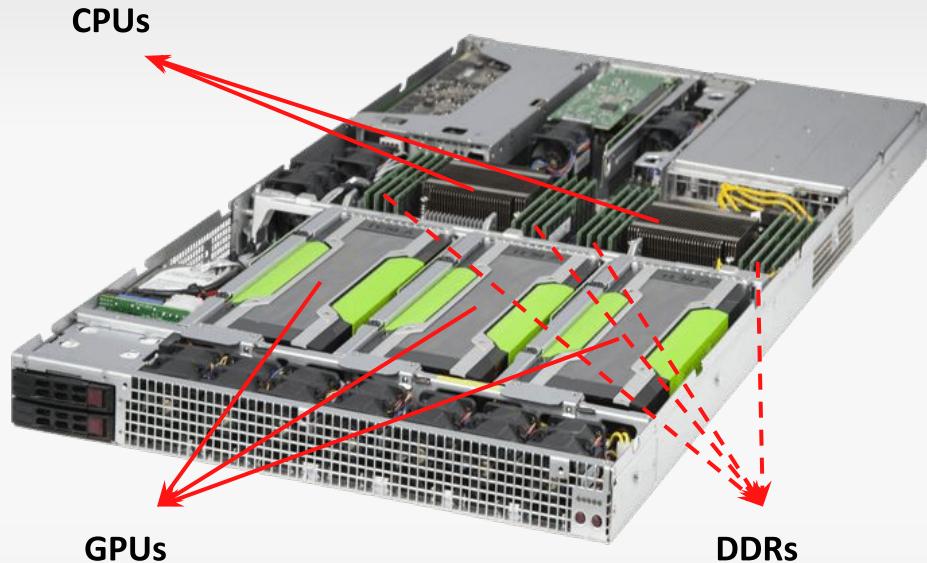
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Inside a supercomputers

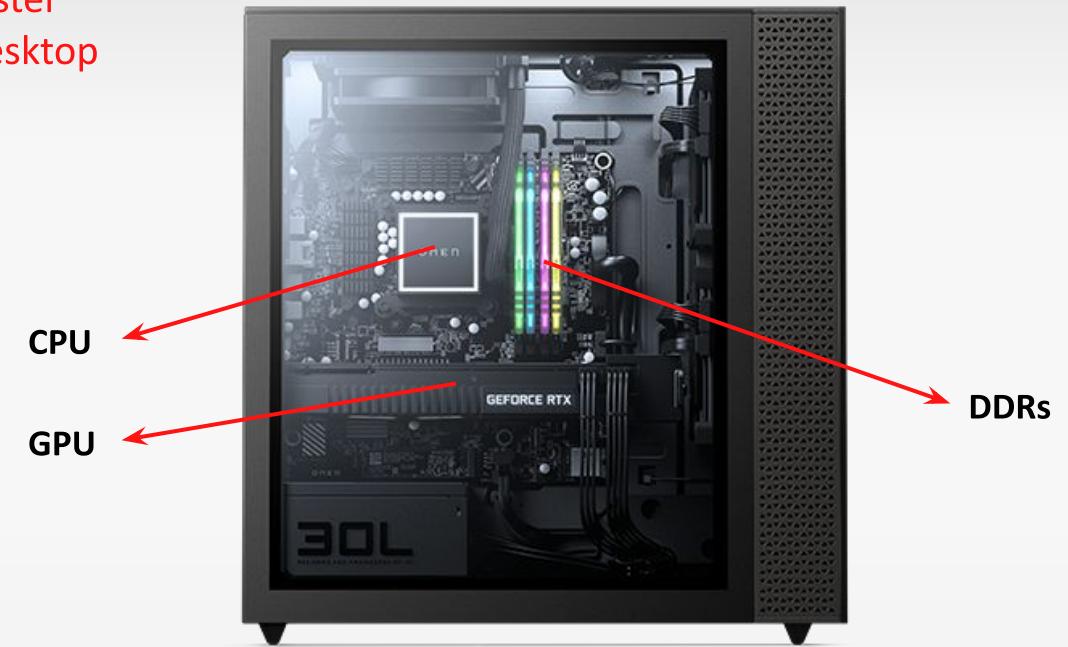
Computing Node



VS

Desktop

A node is
~5x faster
than a desktop



X no hard-drive and **X** no voltage convertor

Centralized long-term storage and power supply



Inside a supercomputers

Computing Node



Rack



Supercomputer



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



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Supercomputers in Europe

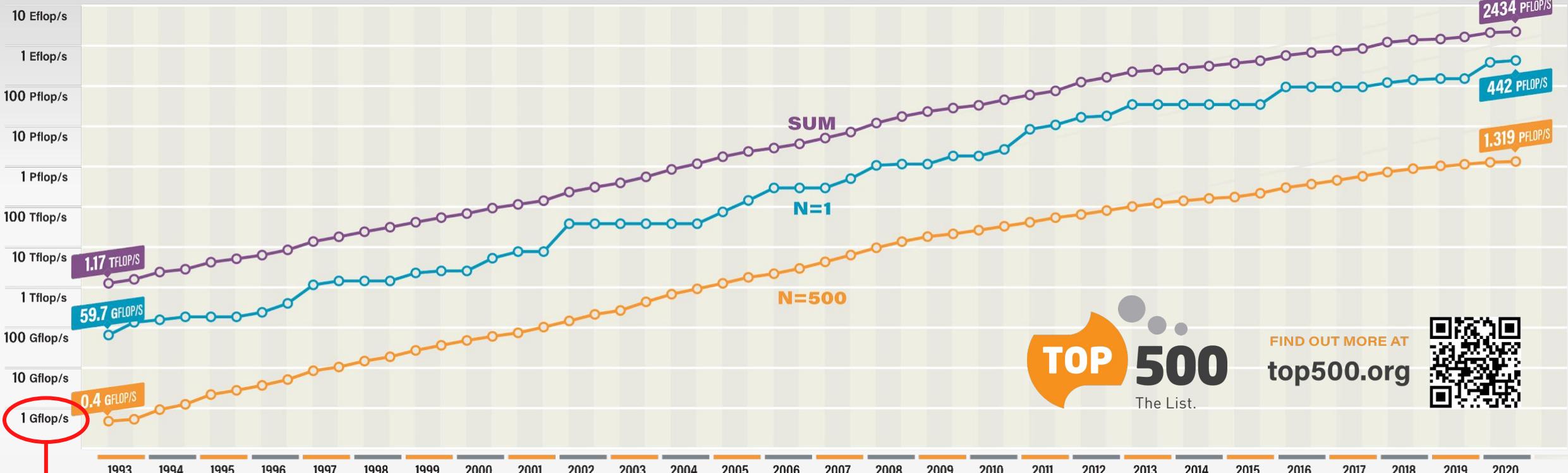


Supercomputers in Europe



TOP 500 - The List.

Performance Development



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

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

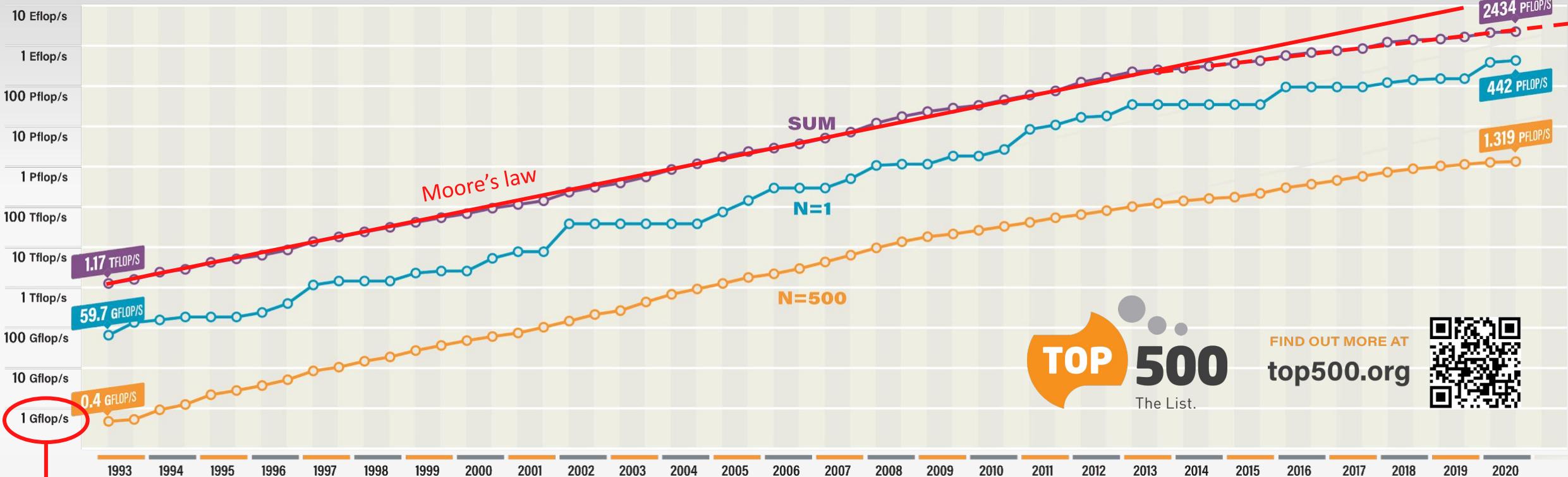


FIND OUT MORE AT
top500.org



TOP 500 - The List.

Performance Development



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TOP HPC systems

NOVEMBER 2020	SYSTEM	SPECS	SITE	COUNTRY	CORES	R _{MAX} 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

TOP HPC systems

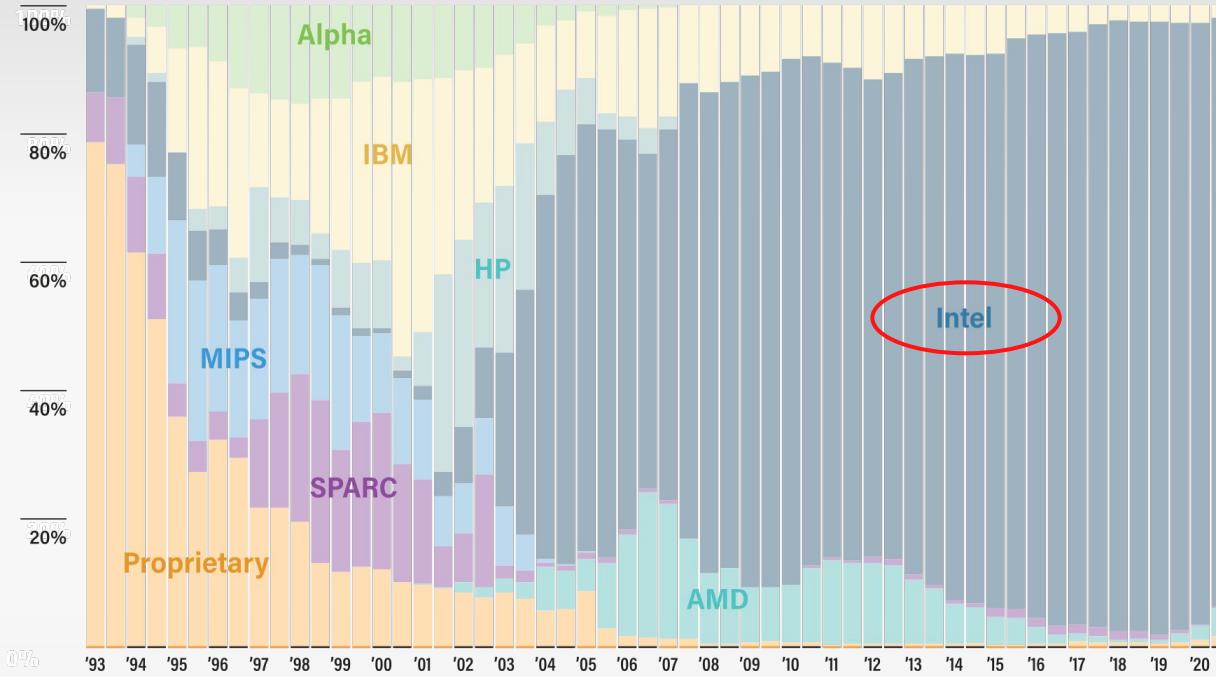
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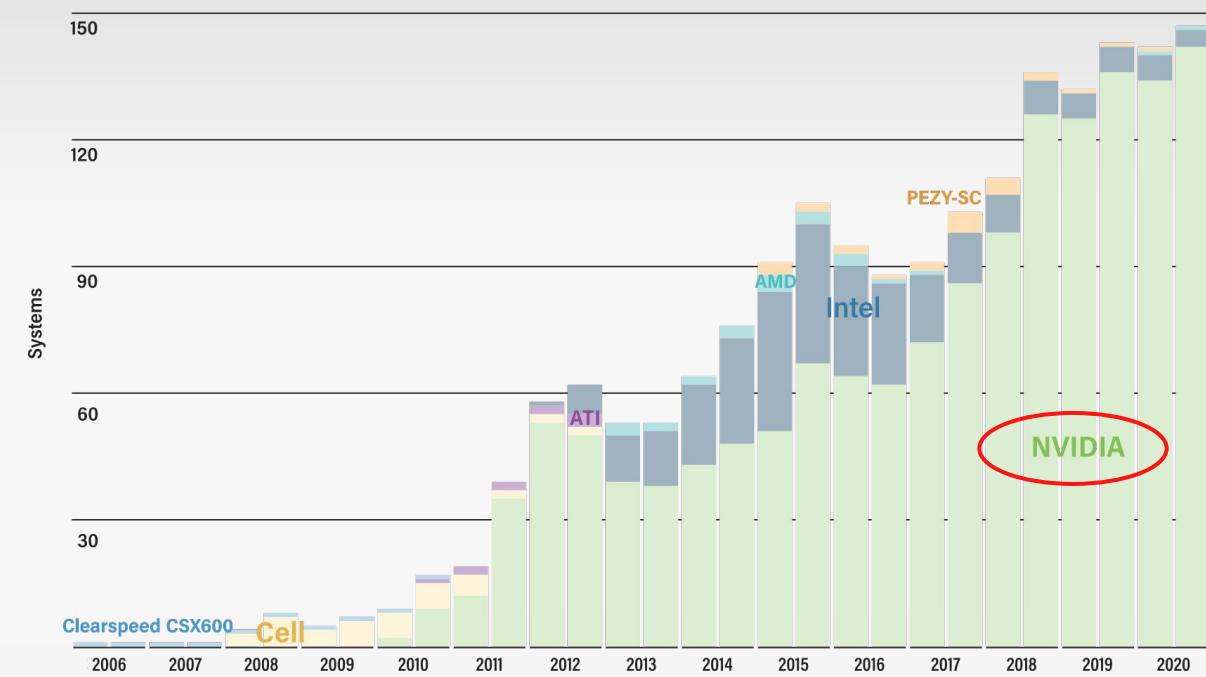
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Hardware Vendors

Chip Technology



Accelerators/Co-processors



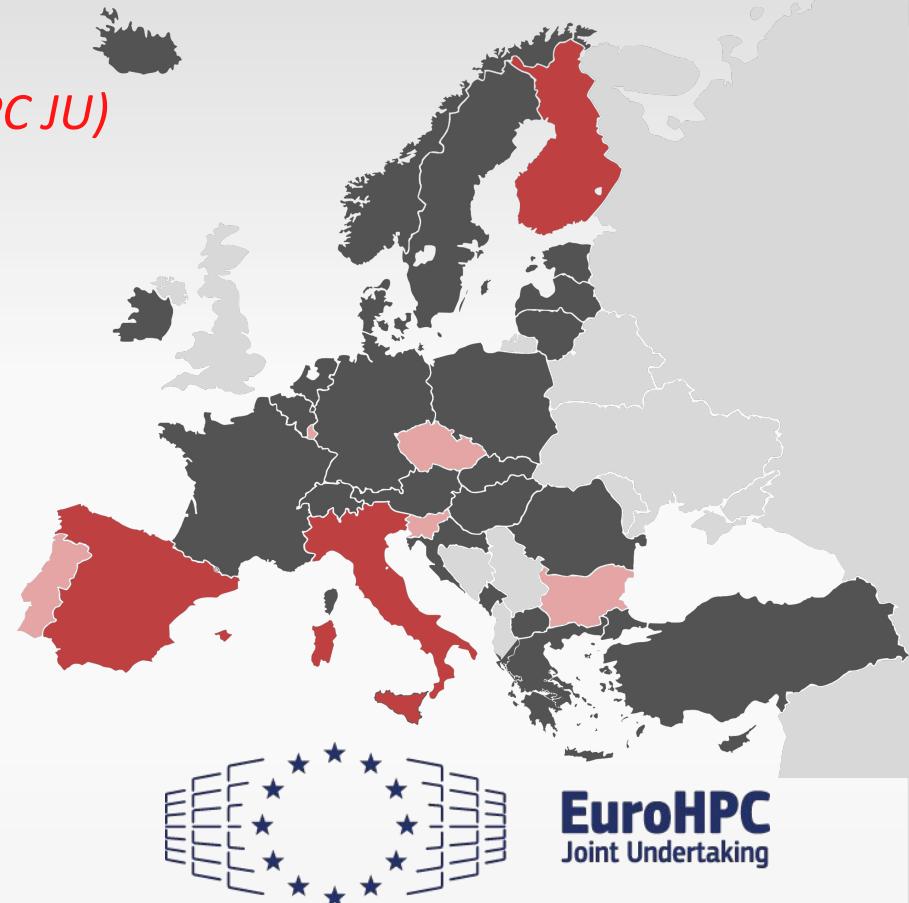
EuroHPC Joint Undertaking

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



Future Systems



EURO

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 (<i>probably</i> 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	Exascale!
2021	Frontier	AMD Epyc CPUs, AMD Instinct GPUs	OLCF	USA	1500	Expected
2022	Aurora	Intel Xeon CPUs, Intel Xe GPUs	ALCF	USA	1000	also in EU for 2023.

Future Systems

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NOTE: AMD and Intel are new enters in the list of GPUs vendors [for top HPC systems](#)

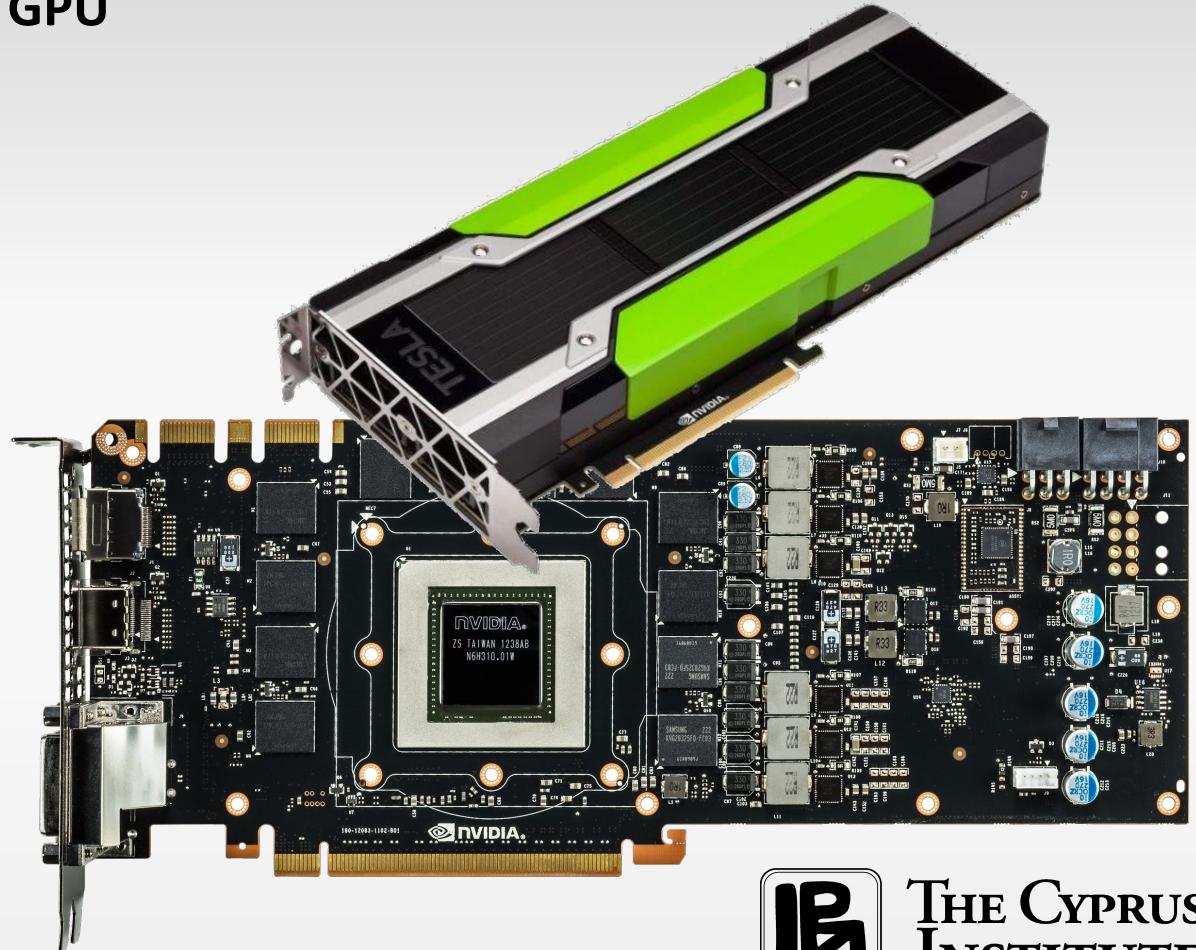


CPUs vs GPUs

CPU



GPU



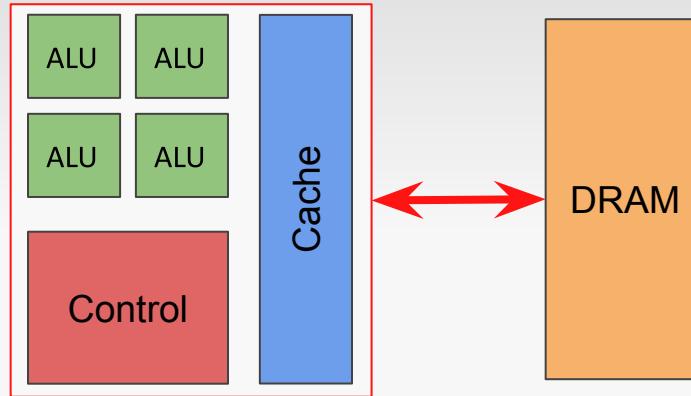
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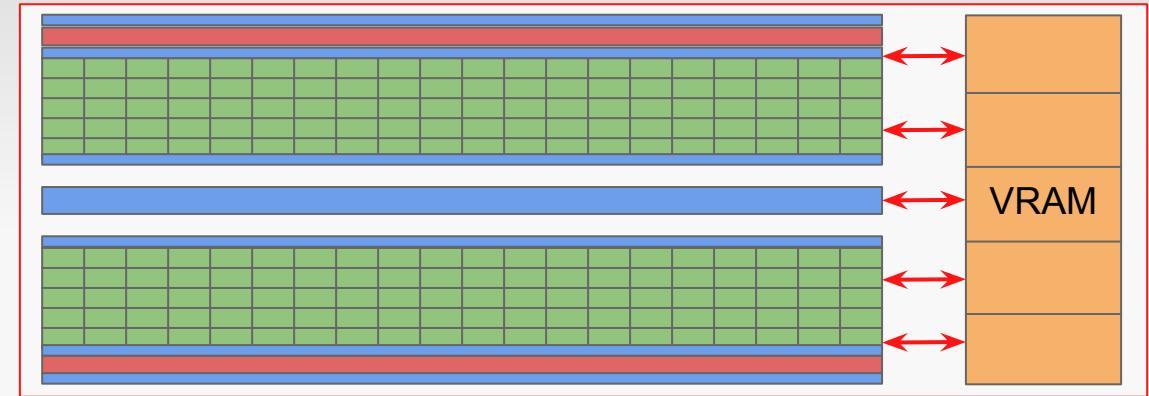


Low latency or High-throughput?

CPU



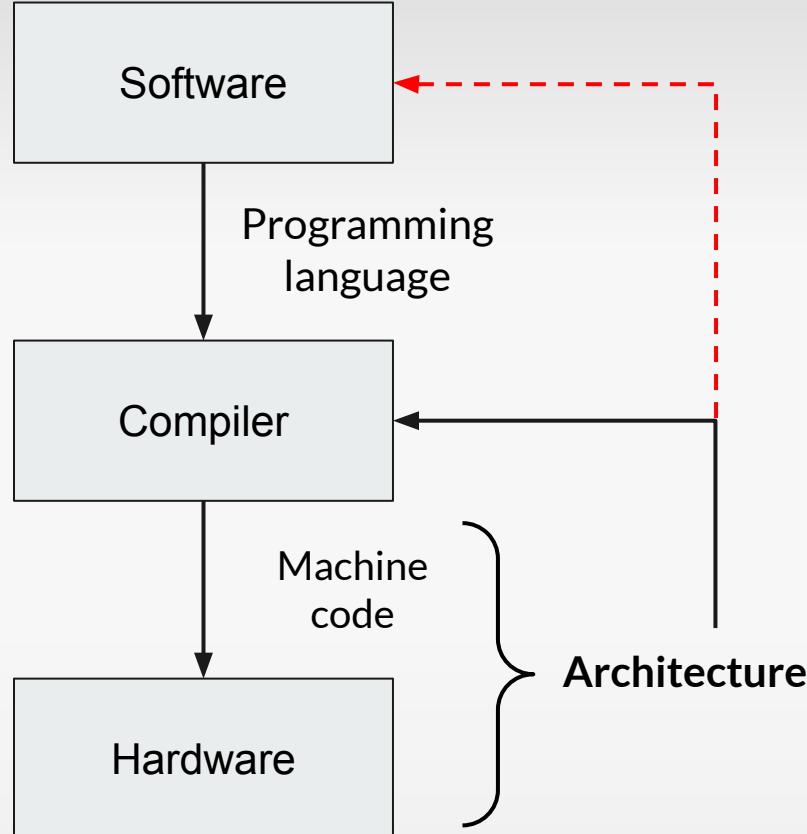
GPU



- 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**)

- 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**)

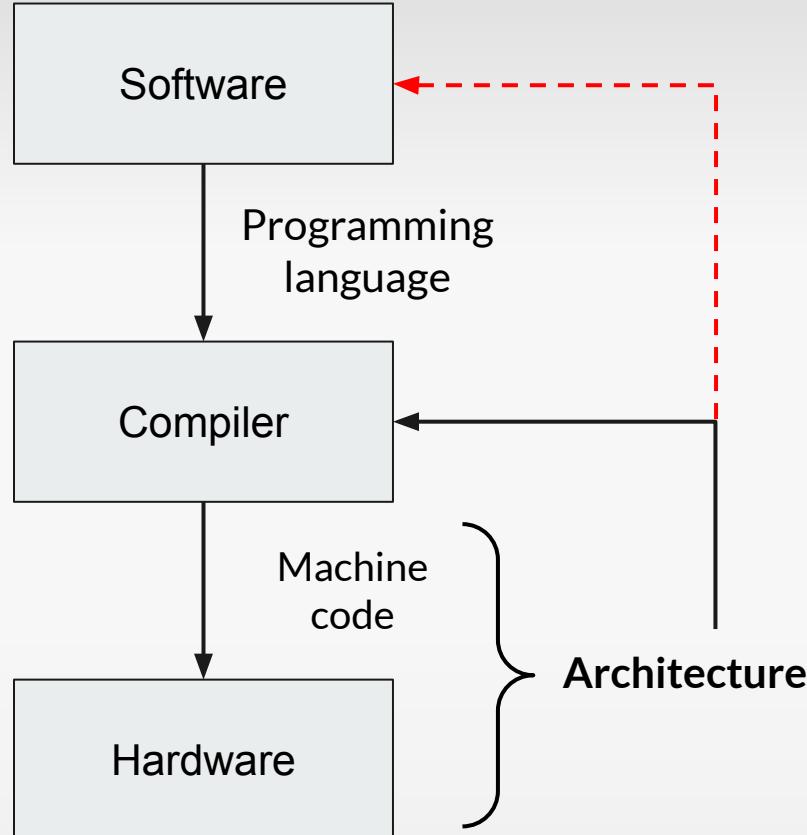
Why is the architecture important?



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

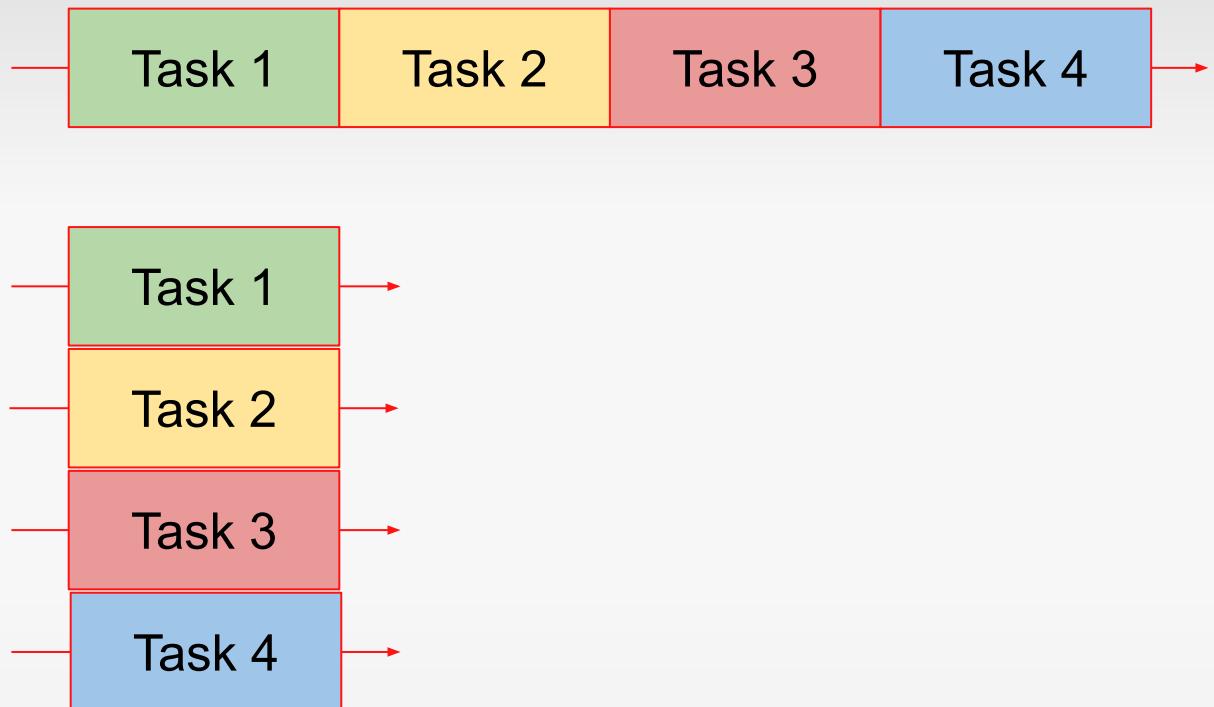
All in one solution (CPUs, GPUs, FPGAs):

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



Parallel computing

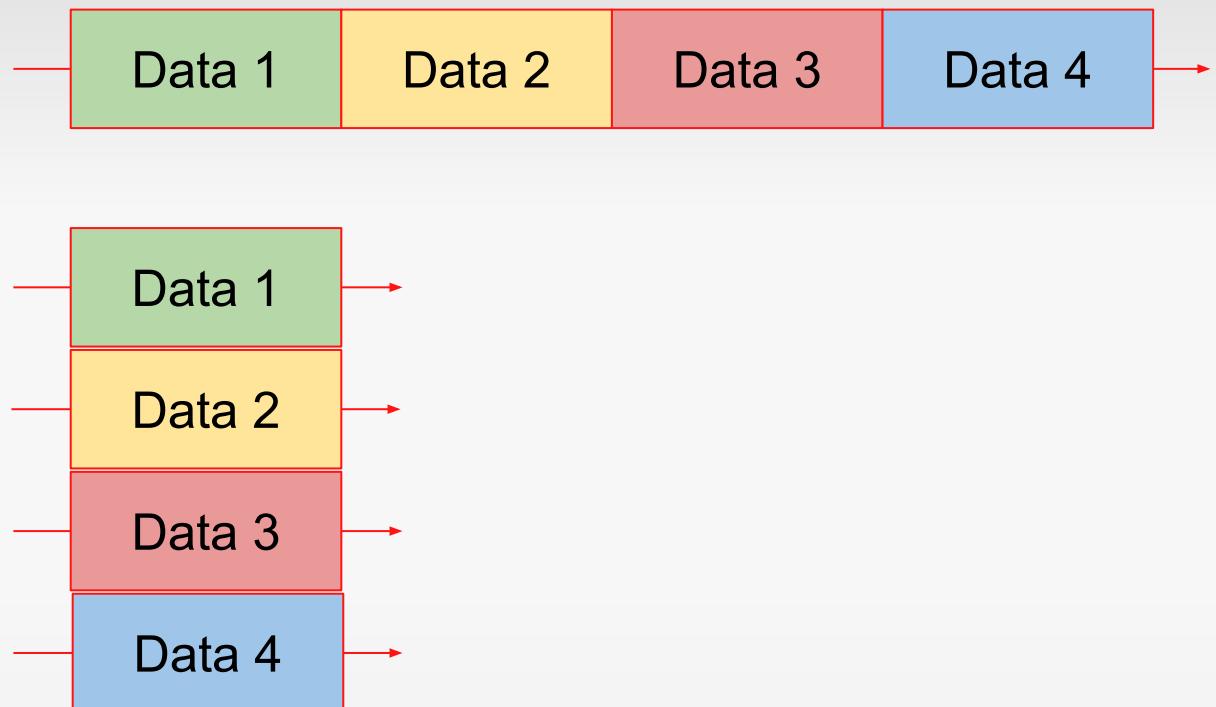
- Task parallelism:
 - Independent tasks
- Distributed Data:
 - Independent Data
- Pipeline parallelism:
 - Dependent tasks/data
- Modular computing:
 - Architecture-dependent





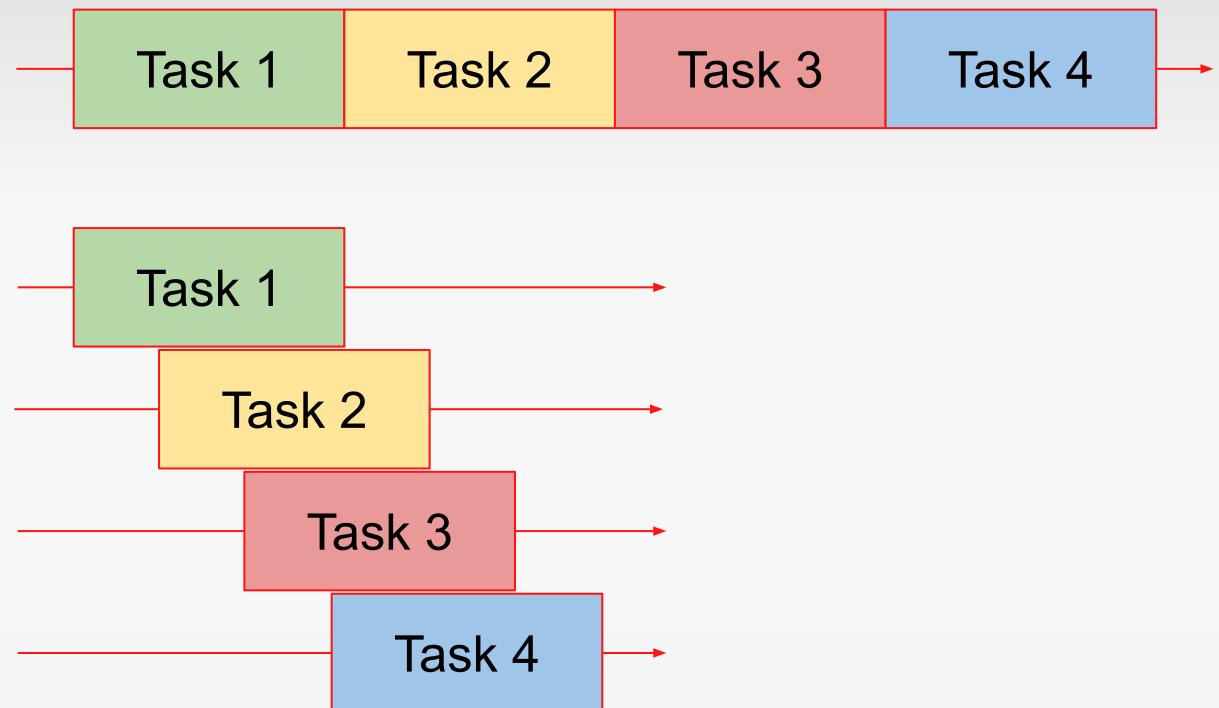
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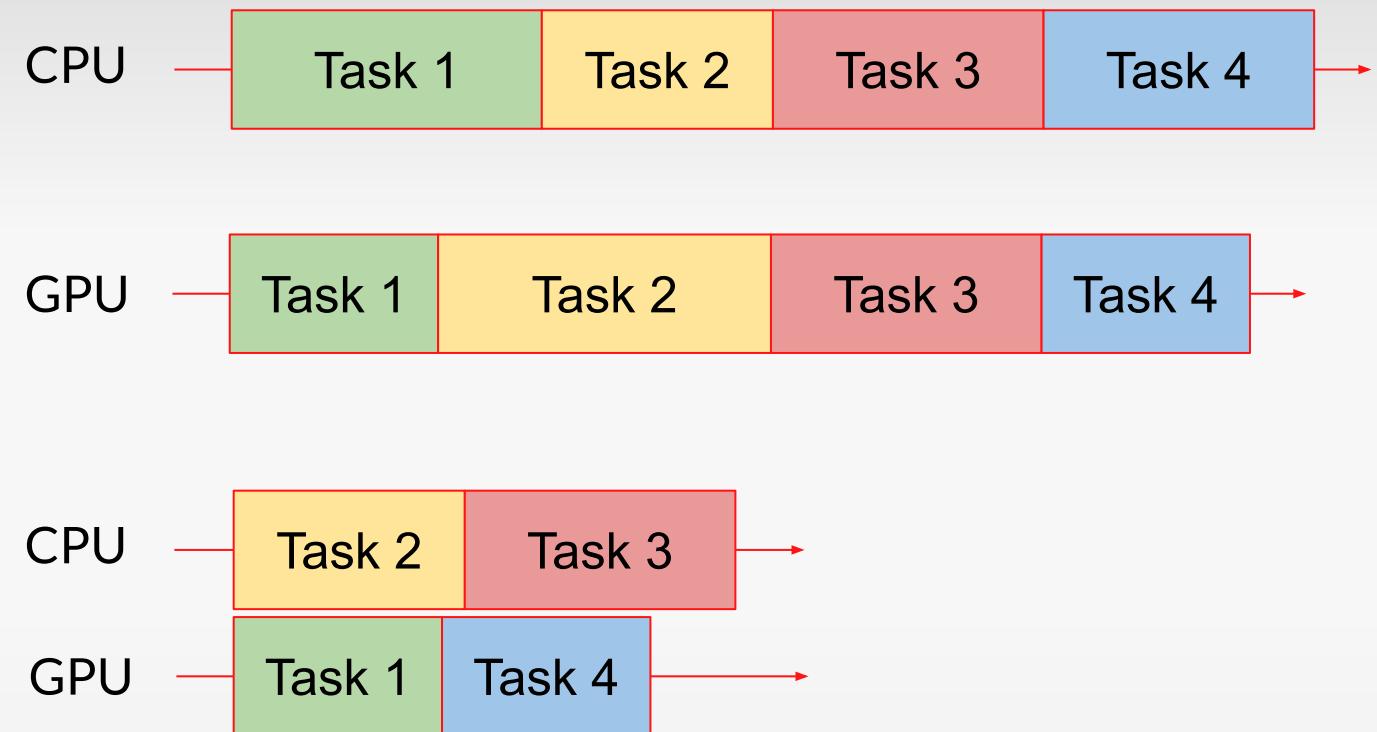
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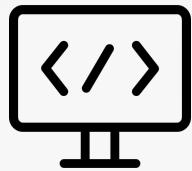
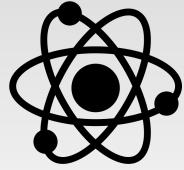
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How to research using HPC



❖ Scientific problem

- Numerical approach
- Computationally intensive
- Parallelizable (task or data)

❖ Software

- Optimized for HPC
- Scalable

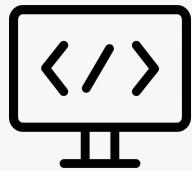
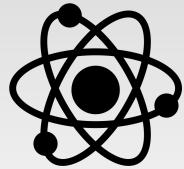
❖ Access to a Supercomputer

- Preparatory access
- Software test and benchmark
- Competitive proposal for computing time

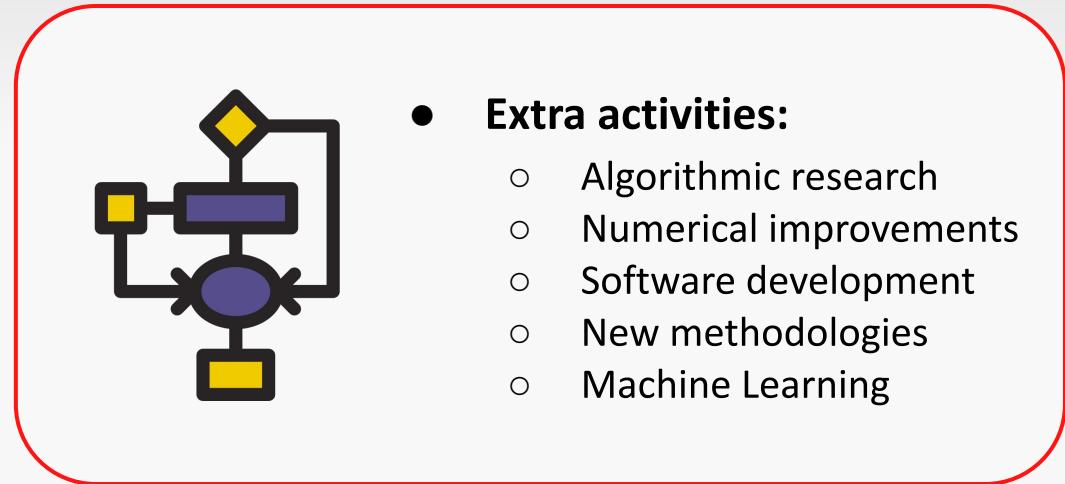
❖ Production of results and analysis

- About 1 year long or more
- Tera-/Peta-bytes of data produced
- Various publications

How to research using HPC

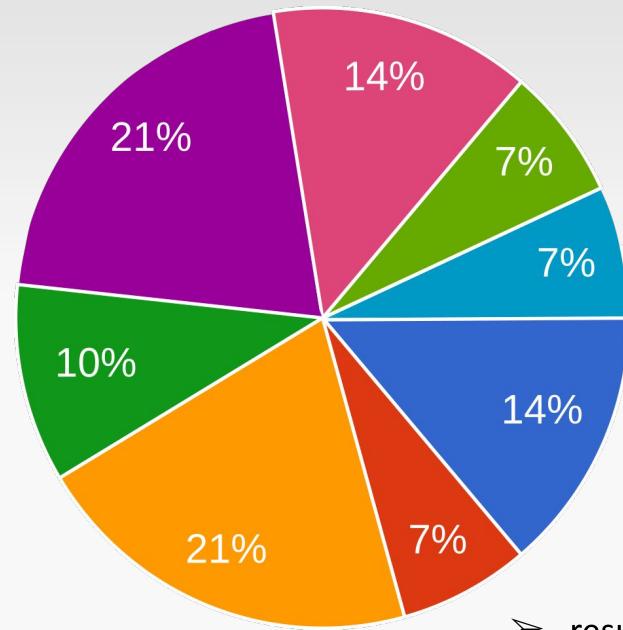


- ❖ **Scientific problem**
 - Numerical approach
 - Computationally intensive
 - Parallelizable (task or data)
- ❖ **Software**
 - Optimized for HPC
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- ❖ **Access to a Supercomputer**
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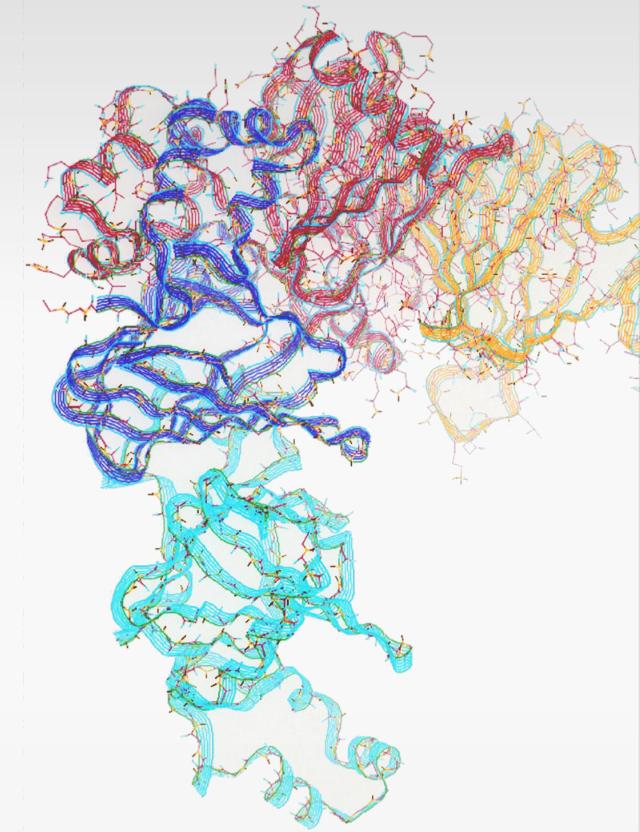
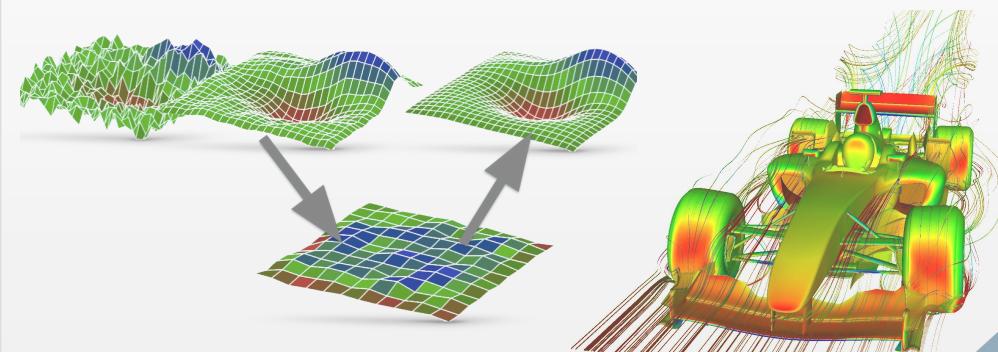
- **Extra activities:**
 - Algorithmic research
 - Numerical improvements
 - Software development
 - New methodologies
 - Machine Learning

HPC research in Cyprus



- 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 your attention

... and talk to you later!