Introduction to HPC

Lecture 1: INTRODUCTION TO HPC

"HPC and Cloud " course

DATA SCIENCE &
SCIENTIFIC COMPUTING

2023-2024 Stefano Cozzini

Some more information

- Slides and materials of the course available here:

https://github.com/Foundations-of-HPC/High-Performance-Computing-2023/

For any section of the course a directory has been created and information and materials will be loaded there: i.e for the first part:

- High-Performance-Computing-2023/PARALLELISM at main · Foundations-of-HPC/High-Performance-Computing-2023 (github.com)

First Section

- 28.09 Introduction to HPC
- 03.10 HPC Hardware and software
- 05.10 Parallel programming concepts

- 06.10 Tutorial Logging and using a HPC system

Agenda

- Prologue: why and where HPC ?
- What is HPC ?
- Performance and metrics
- Supercomputers and TOP500
- Parallel computers

Before starting: HPC prefix..

Factor	Name	Symbol
10^{24}	yotta	Y
10^{21}	zetta	Z
10^{18}	exa	E
10^{15}	peta	P
10^{12}	tera	T
10^{9}	giga	G
10^{6}	mega	M
10^{3}	kilo	k

- How large is your HD on your laptop ?
- How large is your RAM?
- How powerful is your CPU in your laptop ?
- How large is the L1 cache of your CPU ?
- What is the CPU frequency of your laptop?

What do they have in common ?

THEY ALL NEED COMPUTATIONAL POWER AND USE HIGH PERFORMANCE COMPUTING TO DELIVER BETTER RESULTS FASTER

Pricing shares and winning trading by millisecond arbitrage

Forecasting an hurricane and its impact with increased precision

Finding oil under a salt crust saving billions in exploration and drilling

HPC not easy to define..

High performance computing (HPC), also known as supercomputing, refers to computing systems with extremely high computational power that are able to solve hugely complex and demanding problems.

[Taken from https://ec.europa.eu/digital-single-market/en/high-performance-computing]

Complex problem 1:

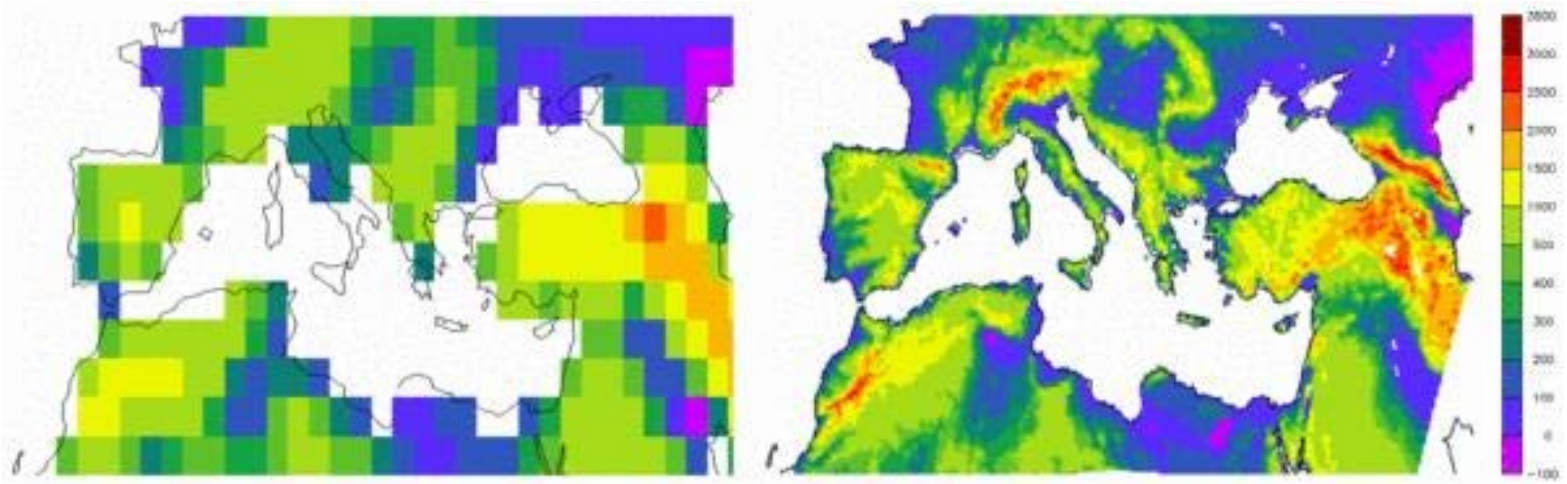
Weather forecast..

Recipe:

- Define a mathematical model to describe the problem
- Solve it computationally
  - Discretization over a 3d grid
  - Integrate equations
  - Check results..

Complex problem 1 : climate change over the Mediterranean sea

- What are the requirements in term of RAM to have decent results ?

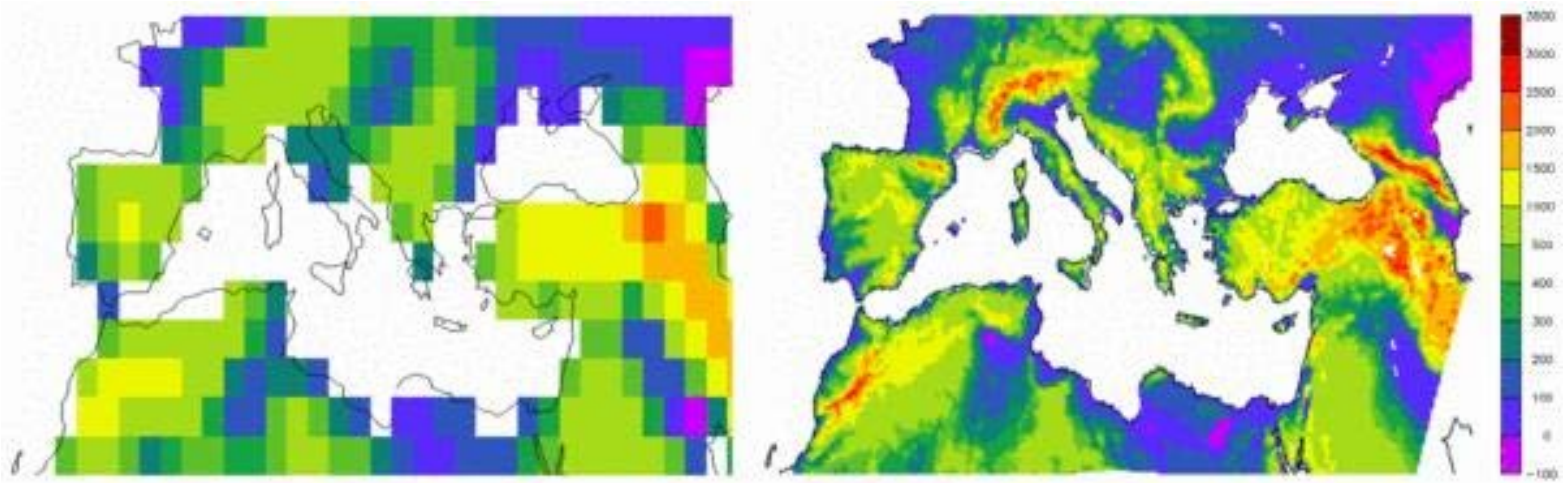


200 km

25 km

Complex problem: climate change over the Mediterranean sea

- Resolution:
  - 200km -> ~ 1GB 2km -> ? GB



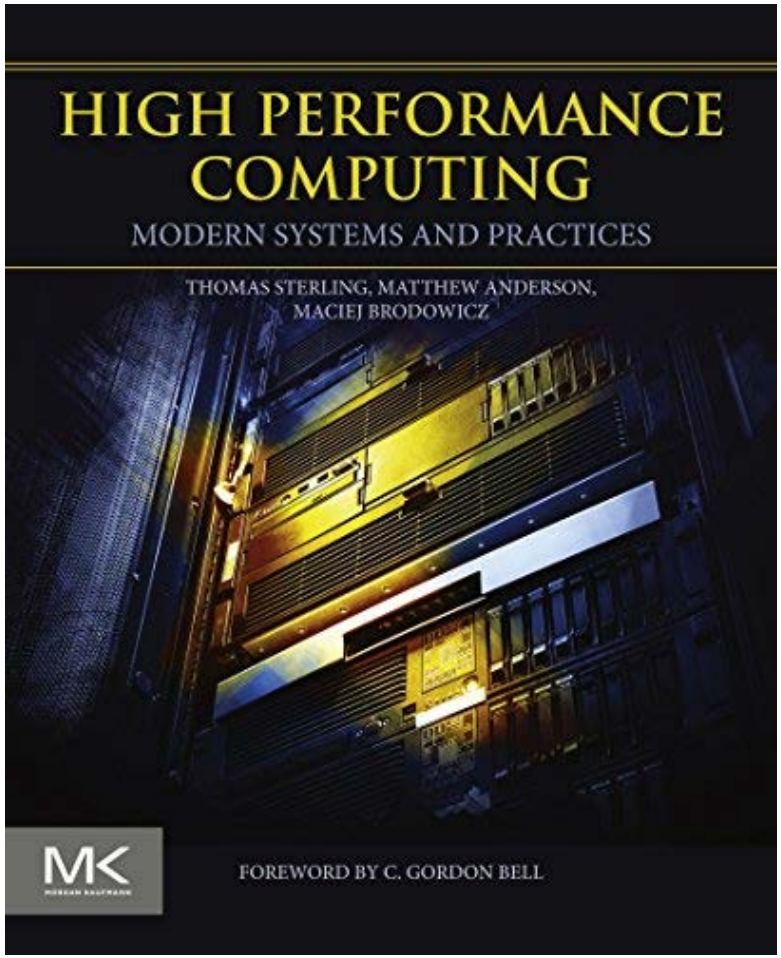
200 km 25 km

Complex problems solved by simulations

- Simulation has become the way to research and develop new scientific and engineering solutions.
- Used nowadays in leading science domains like aerospace industry, astrophysics, etc.
- Challenges related to the complexity, scalability and data production of the simulators arise.
- Impact on the relaying IT infrastructure.

Interested in more example ?

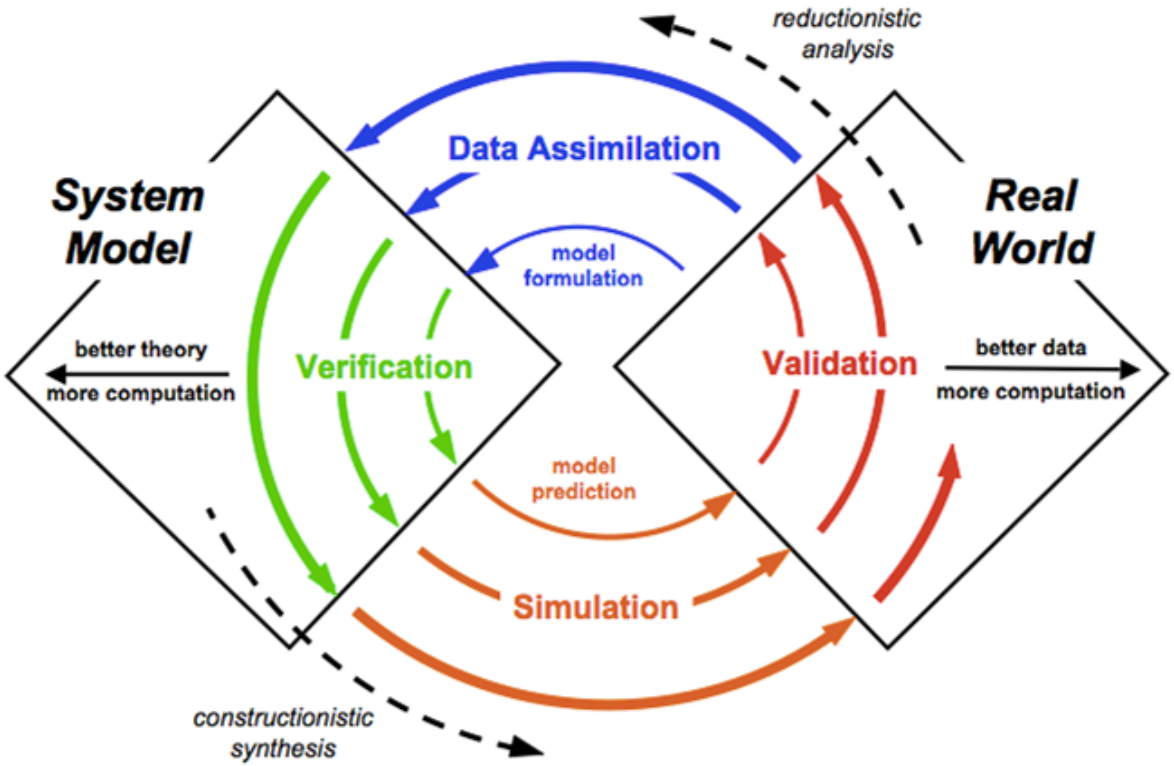
- See chapter one section 1.2 of reference 4
- Look around on the internet..



Research is changing..

- Inference Spiral of System Science

  As models become more complex and new data bring in more information, we require ever increasing computational power



Data are flooding us..

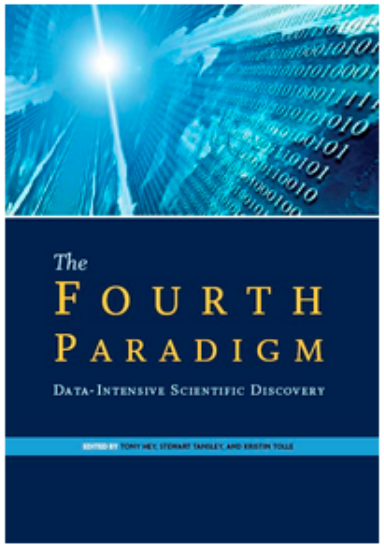
In today's world, larger and larger amounts of data are constantly being generated, from 33 zettabytes globally in 2018 to an expected 181 zettabytes in 2025). As a result, the nature of computing is changing, with an increasing number of data-intensive critical applications. HPC is key to processing and analysing this growing volume of data, and to making the most of it for the benefit of citizens, businesses, researchers and public administrations.

[Taken again from https://ec.europa.eu/digital-single-market/en/high-performance-computing]

Data intensive science

The Fourth Paradigm: Data-Intensive Scientific Discovery

Presenting the first broad look at the rapidly emerging field of data-intensive science



Increasingly, scientific breakthroughs will be powered by advanced computing capabilities that help researchers manipulate and explore massive datasets.

The speed at which any given scientific discipline advances will depend on how well its researchers collaborate with one another, and with technologists, in areas of eScience such as databases, workflow management, visualization, and cloud computing technologies.

In *The Fourth Paradigm: Data-Intensive Scientific Discovery*, the collection of essays expands on the vision of pioneering computer scientist Jim Gray for a new, fourth paradigm of discovery based on data-intensive science and offers insights into how it can be fully realized.

Critical praise for *The Fourth Paradigm*

Download

- Full text, low resolution (6 MB)
- Full text, high resolution (93 MB)
- By chapter and essay

Purchase from Amazon.com

- Paperback
- Kindle version

In the news

- Sailing on an Ocean of 0s and 1s *(Science* Magazine)
- A Deluge of Data Shapes a New Era in Computing *(New York Times)*
- A Guide to the Day of Big Data *(Nature)*

Big data challenge: from HPC to HPDA through AI

- Organizations are expanding their definitions of high-performance computing (HPC) to include workloads such as artificial intelligence (AI) and high-performance data analytics (HPDA) in addition to traditional HPC simulation and modeling workloads.

From https://insidebigdata.com/2019/07/22/converged-hpc-clusters/

Complex problem 2: ChatGPT…

TECH

ChatGPT and generative AI are booming, but the costs can be extraordinary

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WATCH LIVE

KEY POINTS

- The cost to develop and maintain the software can be extraordinarily high.
- Nvidia makes most of the GPUs for the AI industry, and its primary data center workhorse chip costs $10,000.
- Analysts and technologists estimate that the critical process of training a large language model such as GPT-3 could cost over $4 million.

Agenda

- ~~Prologue: why and where HPC ?~~ 
- What is HPC ?
- Performance and metrics ?
- Supercomputers and TOP500
- Parallel Computers

HPC: a ~~first~~ second definition

High Performance Computing (HPC) is the use of servers, clusters, and supercomputers – plus associated software, tools, components, storage, and services – for scientific, engineering, or analytical tasks that are particularly intensive in computation, memory usage, or data management

HPC is used by scientists and engineers both in research and in production across industry, government and academia.

[to be continued]

Elements of the HPC ecosystem..

- use of servers, clusters, and supercomputers

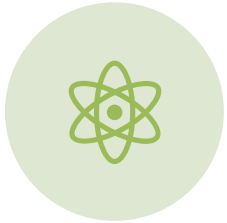
  → HARDWARE
- associated software, tools, components, storage, and services

  → SOFTWARE
- scientific, engineering, or analytical tasks

  → PROBLEMS TO BE SOLVED..

A list of HPC items

COMPUTATIONAL SERVERS



ACCELERATORS

HIGH SPEED NETWORKS

HIGH END PARALLEL STORAGE

IS ALL THIS ENOUGH ?

MIDDLEWARE

SCIENTIFIC/TECHNICAL/ DATA ANALYSIS SOFTWARE

RESEARCH/TECHNICAL DATA

PROBLEMS TO BE SOLVED

Last but not least: people

- Human capital is by far the most important aspect
- Two important roles:
  - HPC providers
    - plan/install/manage HPC resources
  - HPC user :
    - use at best HPC resource

MIXING/INTERPLAYING ROLES INCREASES COMPETENCE LEVELS

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It is all about Performance

- It is difficult to define Performance properly

  "speed" / "how fast" are vague terms
- Performance as a measure again ambiguous and not clearly defined and in its interpretation
- In any case performance it is at core to HPC as a discipline
- Let discuss it in some details

Does P stand just for Performance ?

- Performance is not always what matters..

to reflect a greater focus on the productivity, rather than just the performance, of large-scale computing systems, many believe that HPC should now stand for High Productivity Computing. [from wikipedia]

Performance vs Productivity

- A possible definition:
  - Productivity = (application performance) / (application programming effort)
- Example:
  - To speed up a code by a factor of two it takes 6 months work
  - does this deserve to be done ?
- people in HPC arena have different goals in mind thus different expectations and different definitions of productivity.

How do measure (basic) performance of HPC systems

- How fast can I crunch numbers on my CPUs ?
- How fast can I move data around ?
  - from CPUs to memory
  - from CPUs to disk
  - from CPUs on different machines
- How much data can I store ?

Number crunching on CPU: what do we count ?

- Rate of [million/billions of] floating point operations per second ([M|G]flops) FLOPs/S
- Theoretical peak performance:
  - determined by counting the number of floating-point additions and multiplications that can be completed during a period of time, usually the cycle time of the machine

FLOPS=clock_rate*Number_of_FP_operation*Number_of_cores

Sustained (peak) performance

- Real (sustained) performance: a measure

FLOPS= (total number of floating point operations done by a program) / (time the program takes to run in second)

- Number_of_floating_point_operations not easy to be defined for real application
- benchmarks are available for that..
- Top500 list uses HPL Linpack:
  - Sustained peak performance is what's matter in TOP500

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TOP 500 List

- The TOP500 list www.top500.org
- published twice a year from 1993
  - ISC conference in Europe (June)
  - Supercomputing conference in USA (November)
- List the most powerful computers in the world
- yardstick: Linpack benchmark (HPL)

HPL: some details

- From http://icl.cs.utk.edu/hpl/index.html:
  - The code solves a uniformly random system of linear equations and reports time and floating-point execution rate using a standard formula for operation count.
  - Number_of_floating_point_operations = $2/3n^3 + 2n^2$ (n=size of the system)

```
================================================================================
T/V                N    NB     P     Q               Time                 Gflops
--------------------------------------------------------------------------------
WR03R2L2       86000  1024     2     1             191.06              2.219e+03
--------------------------------------------------------------------------------
||Ax-b||_oo/(eps*(||A||_oo*||x||_oo+||b||_oo)*N)=        0.0043644 ...... PASSED
```

HPL&TOP 500 List

- For each machine the following numbers are reported using HPL:
  - Rmax: the performance in GFLOPS for the largest problem run on a machine.
  - Rpeak: the theoretical peak performance GFLOPS for the machine.
  - The measure of the power required to run the benchmark

And the winner is..

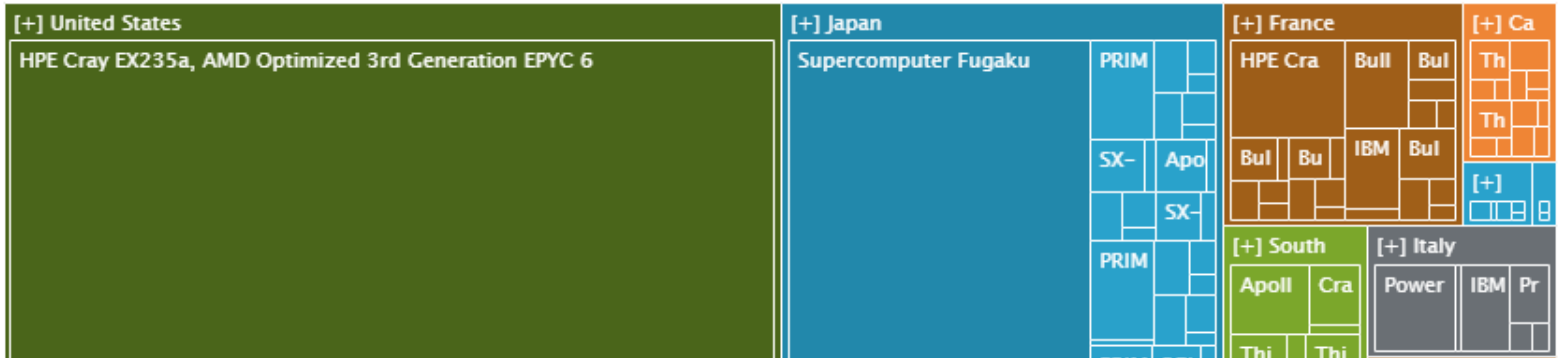
FRONTIER - HPE CRAY EX235A, AMD OPTIMIZED 3RD GENERATION EPYC 64C 2GHZ, AMD INSTINCT MI250X, SLINGSHOT-11

Site:	**Performance**	
System URL:	**Linpack Performance (Rmax)**	1,194.00 PFlop/s
Manufacturer:		
Cores:	**Theoretical Peak (Rpeak)**	1,679.82 PFlop/s
Processor:	**Nmax**	24,219,648
Interconnect:	**HPCG [TFlop/s]**	14,054.0
Installation Yea	**Power Consumption**	
	Power:	22,703.00 kW (Submitted)

Highlights (from www.top500.org)

- **06/2023 Highlights**
- Frontier is the No. 1 system in the TOP500.
- Fugaku, the No. 2 system, is installed at the RIKEN Center for Computational Science (R-CCS) in Kobe, Japan. It has 7,630,848 cores which allowed it to achieve an HPL benchmark score of 442 Pflop/s.
- The LUMI system, another HPE Cray EX system installed at EuroHPC center at CSC in Finland is the No. 3 with a performance of 309.1 Pflop/s. The European High-Performance Computing Joint Undertaking (EuroHPC JU) is pooling European resources to develop top-of-the-range Exascale supercomputers for processing big data. One of the pan-European pre-Exascale supercomputers, LUMI, is located in CSC's data center in Kajaani, Finland.
- The No. 4 system Leonardo is installed at a different EuroHPC site in CINECA, Italy. It is an Atos BullSequana XH2000 system with Xeon Platinum 8358 32C 2.6GHz as main processors, NVIDIA A100 SXM4 40 GB as accelerators, and Quad-rail NVIDIA HDR100 Infiniband as interconnect. It achieved a Linpack performance of 238.7 Pflop/s.

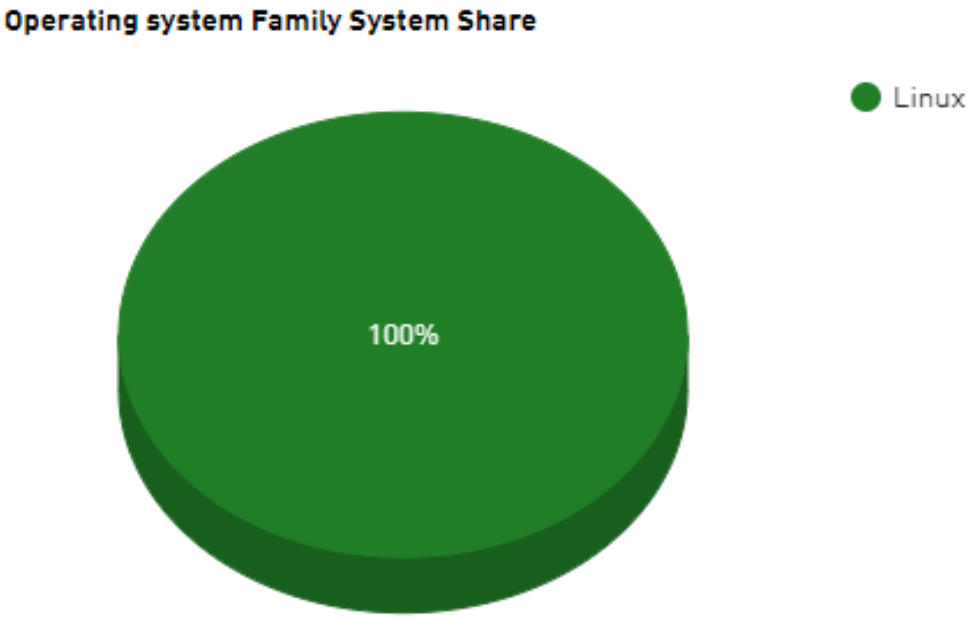
By country…



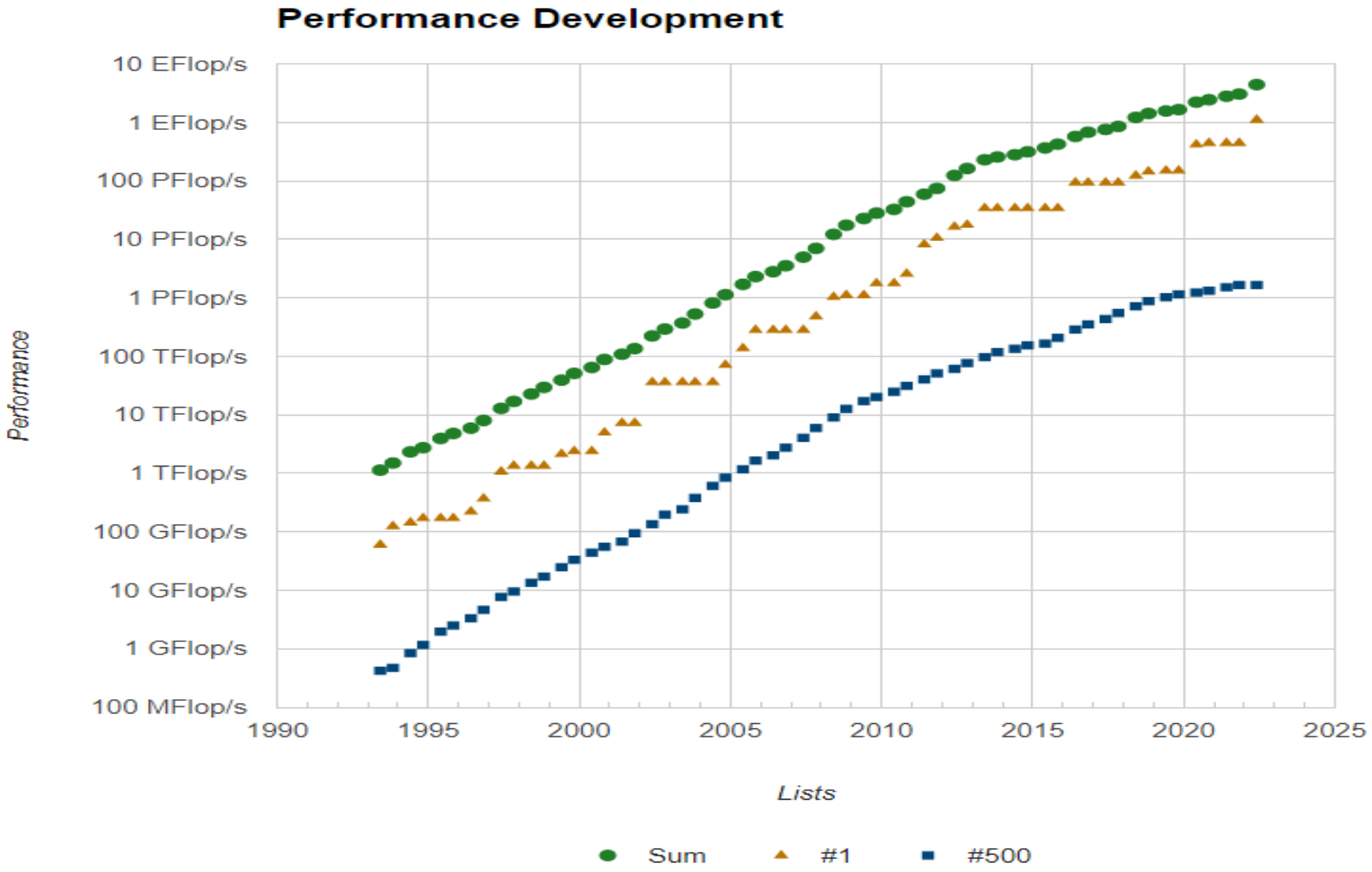
Installations by countries/regions:

		Count	System Share (%)	Rmax (TFlops)	Rpeak (TFlops)	Cores
1	China	173	34.6	530,240	1,158,771	29,413,676
2	United States	128	25.6	2,085,045	3,150,398	27,715,304
3	Japan	33	6.6	626,506	817,353	11,984,068
4	Germany	31	6.2	200,537	306,054	3,896,660
5	France	22	4.4	168,660	242,484	3,874,520
6	Canada	14	2.8	47,805	80,390	1,076,384
7	United Kingdom	12	2.4	57,018	78,629	1,779,888
8	Russia	7	1.4	73,715	101,737	741,328
9	Italy	6	1.2	78,529	114,512	1,447,536

By operating system



Performance development



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- To be continued

If time is left…

- Go here: https://bit.ly/3PAvsUb
- Let us generate and send the public key…