Foundations of High Performance Computing

Lecture 1: INTRODUCTION TO HPC

"Foundation of HPC" course

DATA SCIENCE &
SCIENTIFIC COMPUTING

2022-2023 Stefano Cozzini

First Week

- 10.10 Introduction to HPC
- 11.10 HPC Hardware and parallel computing
- 12.10 HPC Software stack and tools

- 13.10 Tutorial 1/2 Using a HPC system
- 14.10 Tutorial 1/2

Some more information

- Slides and materials of the course available here:

https://github.com/Foundations-of-HPC/Foundations_of_HPC_2022

- For any section of the course a directory has been created and informations and materials will be loaded there: i.e for the introductory part:
- https://github.com/Foundations-of-HPC/Foundations_of_HPC_2022/Basic/intro

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

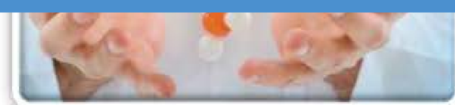
- How many data are produced daily?
- How large is your HD on your laptop ?
- How large is your RAM?
- How powerful is your CPU in your laptop ?
- How large is the L1 cache of your CPU ?

Agenda

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

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

Where and Why HPC ?

Traditionally HPC system (a.k.a supercomputers) were confined in research and academic lab…

Today they are everywhere: HPC is now an enabler not just for science but also for business

Today HPC does not necessarily means supercomputers

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:

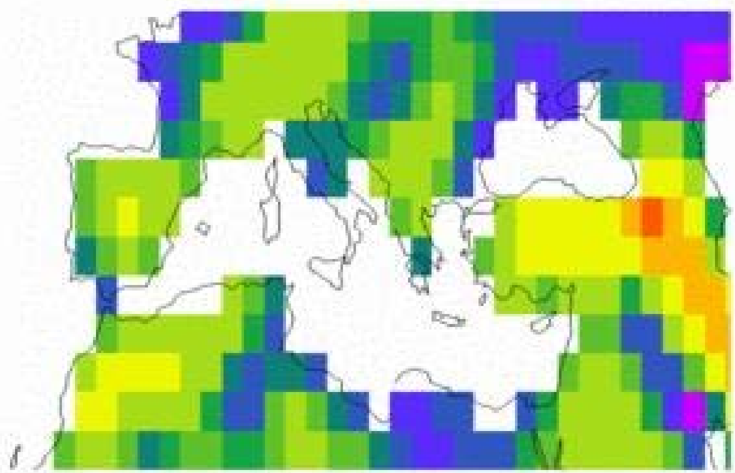
Weather forecast..

Recipe:

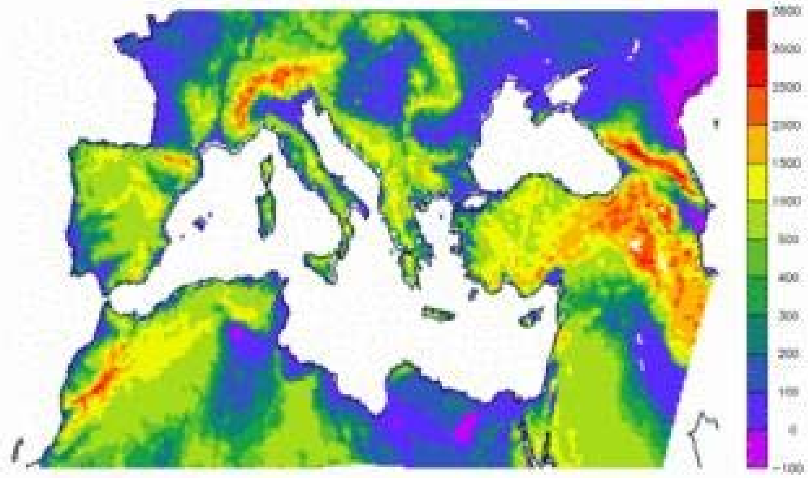
- Define a mathematical model to describe the problem
- Solve it computationally
  - Discretization over a 3d grid
  - Integrate equations
  - Check results..

Complex problem: climate change over the Mediterranean sea

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



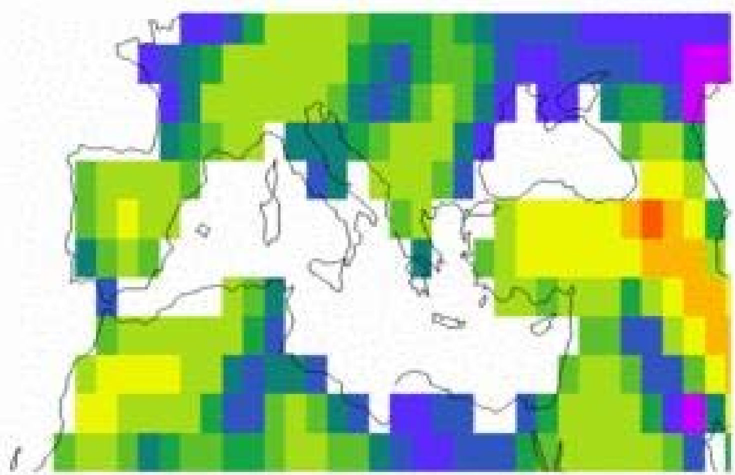
200 km



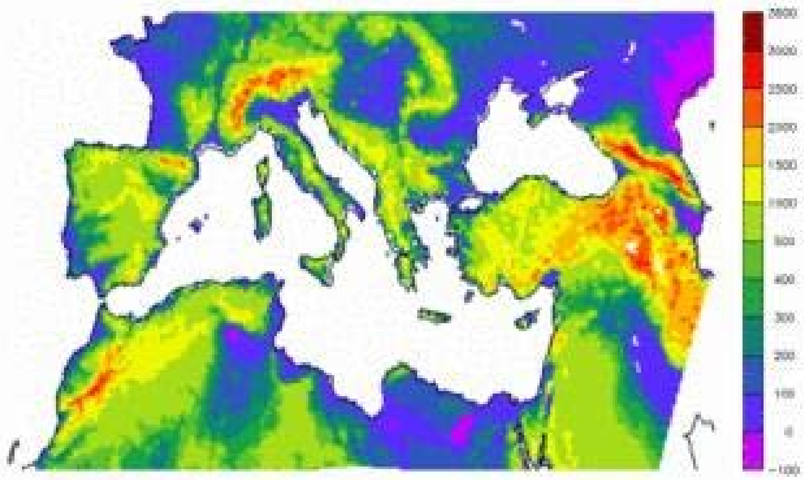
25 km

Complex problem: climate change over the Mediterranean sea

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



200 km



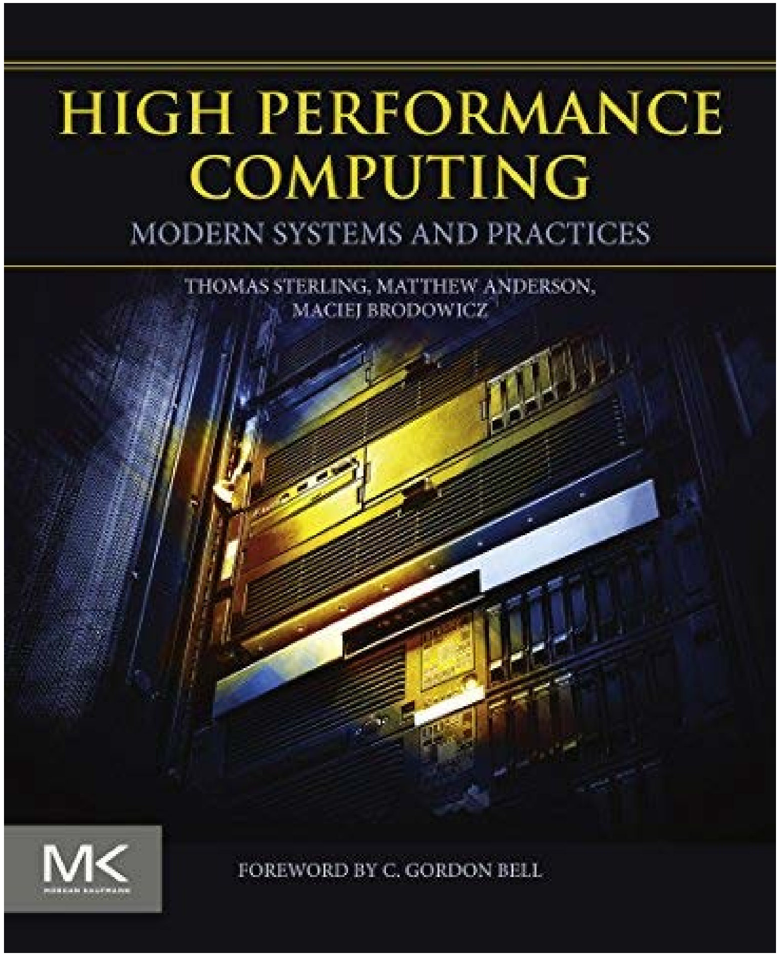
25 km

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 ?

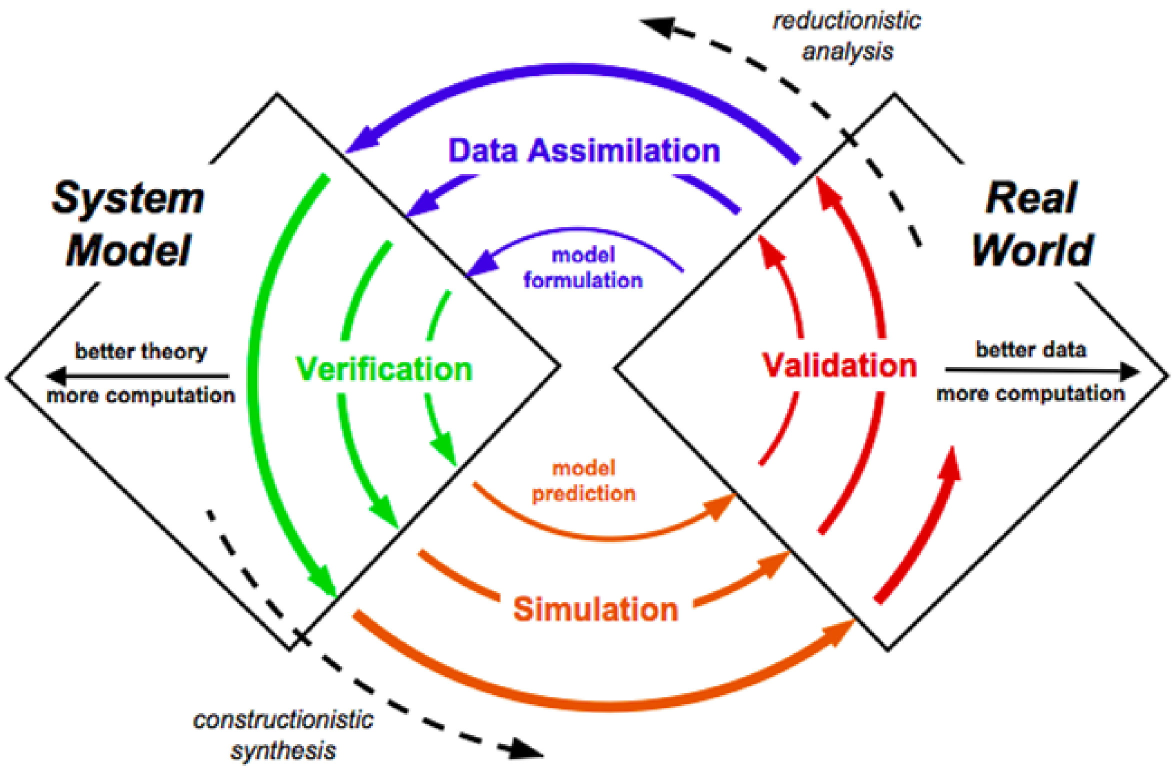
- See chapter one section 1.2 of reference 4
- Look around on the internet..



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..

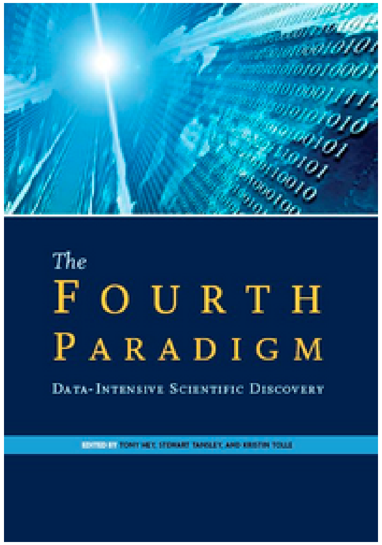
In today's world, larger and larger amounts of data are constantly being generated, from 33 zettabytes globally in 2018 to an expected 175 zettabytes in 2025). As a result, the nature of computing is changing, with an increasing number of data-intensive critical applications. is key to processing and 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

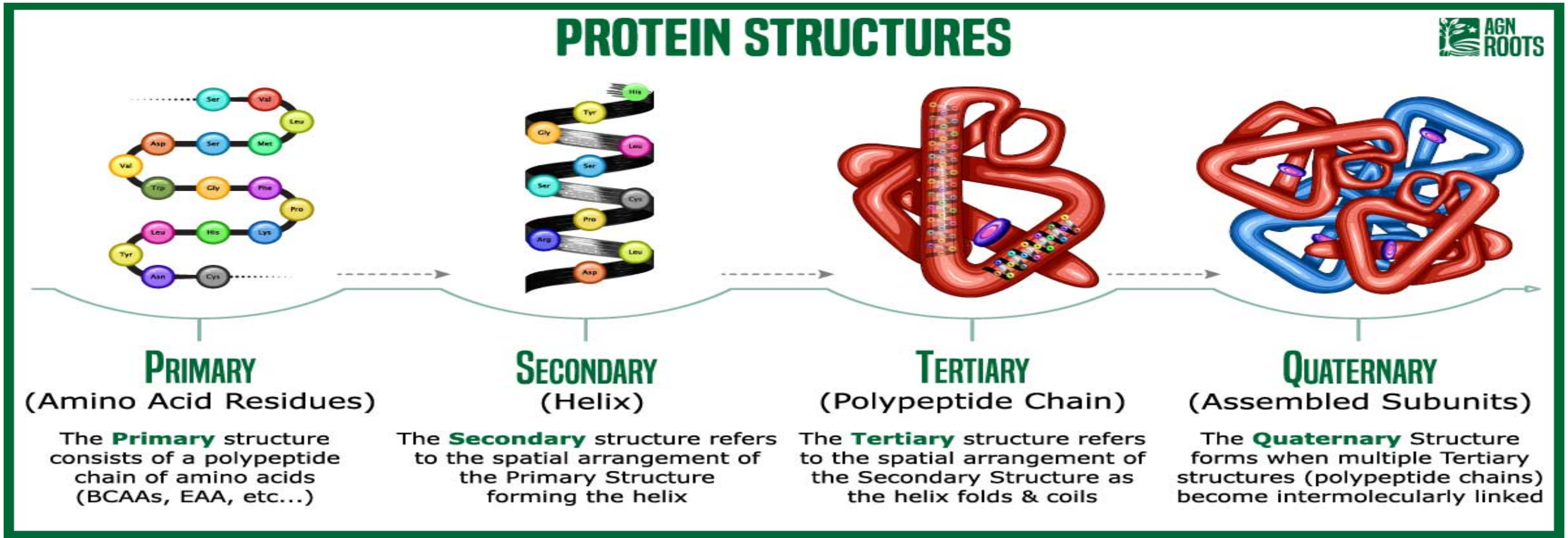
- Organizations are expanding their definitions of high-performance computing (HPC) to include workloads such as artificial intelligence (AI) and high-performance data analytics (HPDA) in addition to traditional HPC simulation and modeling workloads.

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

Complex problem 2
Protein folding..

Determine the e structure of the protein from its aminoacid sequence

- Solve it computationally..
  A. Run very long MD simulation on each sequence and wait..
  B. Predict new structures training an AI algorithm..



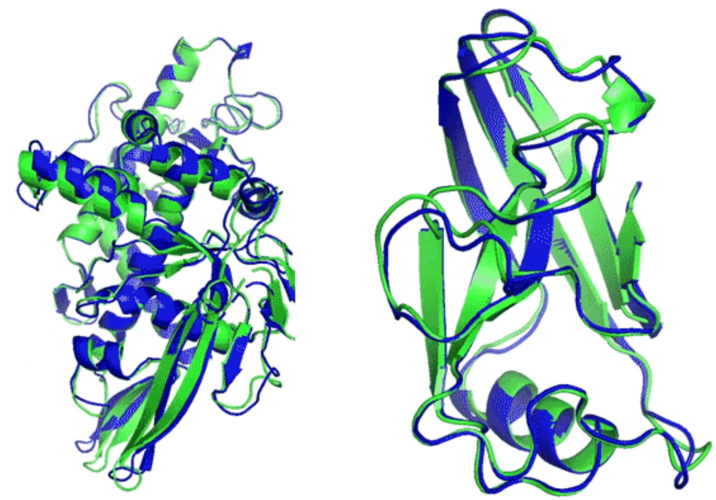
Approach A: Folding@home

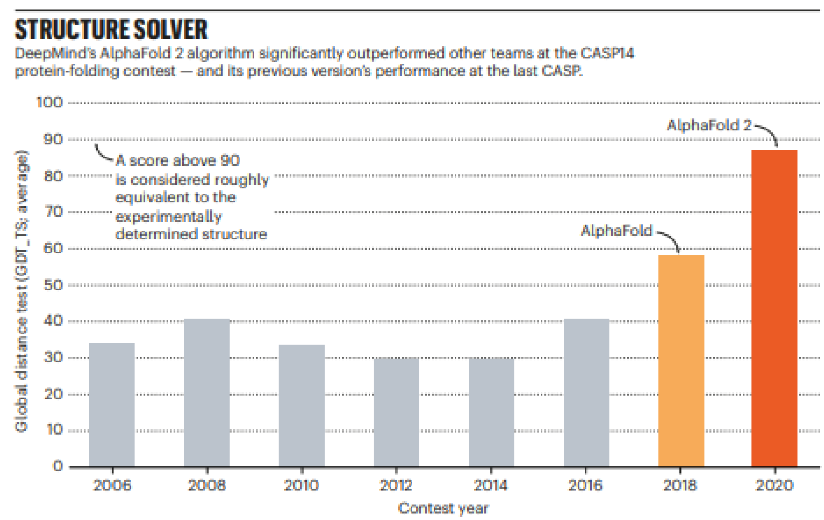
- A more than 20 year project
- It allows everybody to run an MD simulation contributing to the problem..
- Impressive distributed computational power..
- From statistics page:

OS	GPU	CPU	Tflops GPU	Tflops x86
Windows	2440+ 12864	31417	27504	55243
Linux	98 + 19257	34794	36561	72456
Total	2538+ 32121	73018	64429	128063

Approach B : AlphaFold

- AlphaFold is an AI system developed by DeepMind that predicts a protein's 3D structure from its amino acid sequence.
- Presented in 2018 and 2020 at CASP outperformed all other approaches
- Scores obtained are roughly equivalent to experimentally determined structured





AlphaFold DB

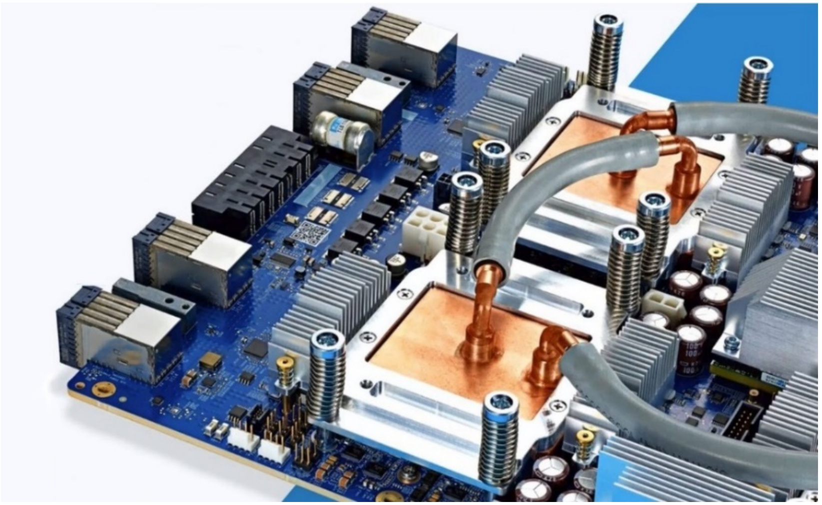
AlphaFold DB release in July 2022 open access to over 200 million protein structure predictions to accelerate scientific research.

Full dataset download for AlphaFold Database - UniProt (214M):

- The full dataset of all predictions is available at no cost and under a CC-BY-4.0 licence this by single-species for ease of downloading subsets or all of the data from Google Cloud Public Datasets. We've grouped We suggest that you only download the full dataset if you need to process all the data with local computing resources (the size of the dataset is 23 TiB, ~1M tar files).

How much power does AlphaFold

“We train the model on Tensor Processing Unit (TPU)* v3 with a batch size of 1 per TPU core, hence the model uses 128 TPU v3 cores…
The initial training stage takes approximately 1 week, and the fine-tuning stage takes approximately 4 additional days.”



* A Tensor Processing Unit (TPU) is an application specific integrated circuit (ASIC) developed by Google to accelerate machine learning. Google offers TPUs on demand, as a cloud deep learning service called Cloud TPU.

FastFold vs. AlphaFold

FastFold: Reducing AlphaFold Training Time from 11 Days to 67 Hours

We successfully scaled the AlphaFold model training to 512 NVIDIA A100 GPUs and obtained aggregate 6.02 PetaFLOPs at the training stage. The overall training time is reduced to 67 hours from 11 days with significant economic cost savings.

TABLE IV
RESOURCE AND TIME COST COMPARE.

Implementation	Framework	Training Process	Hardward	Step Time (s)	Training Time (days)	Resource
AlphaFold	JAX [18]	Initial training Fine-tuning	128 $\times$ TPUv3	/ /	11	33792 TPU hours
OpenFold	PyTorch	Initial training Fine-tuning	128 $\times$ A100	6.186 20.657	8.39	25774 GPU hours
FastFold	PyTorch	Initial training Fine-tuning	256 $\times$ A100 512 $\times$ A100	2.487 4.153	**2.81**	**20738 GPU hours**

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

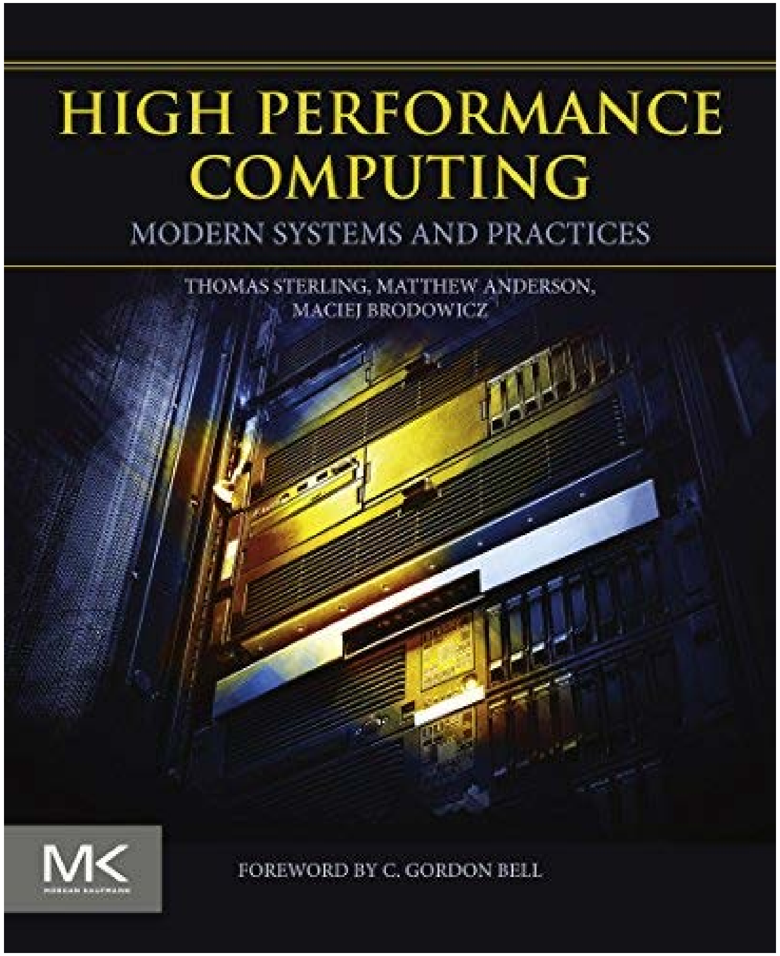
- Human capital is by far the most important aspect
- Two important roles:
  - HPC providers
    - plan/install/manage HPC resources
  - HPC user :
    - use at best HPC resource

MIXING/INTERPLAYING ROLES INCREASES COMPETENCE LEVELS

Yet another definition

- HPC incorporates all facets of three disciplines:
  - Technology
  - Methodology
  - Application

- The main defining property and value provided by HPC is delivering performance for end-user application



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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]

- P should also stand for PROFITABILITY

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.

- Suggestion: Understand which kind of productivity are you interested in

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 formulafor 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:	DOE/SC/Oak Ridge National Laboratory
System URL:	https://www.olcf.ornl.gov/frontier/
Manufacturer:	HPE
Cores	
Proce	
Interc	
Instal	

Performance	
Linpack Performance (Rmax)	1,102.00 PFlop/s
Theoretical Peak (Rpeak)	1,685.65 PFlop/s
Nmax	24,440,832
Power Consumption	
Power:	21,100.00 kW (Submitted)

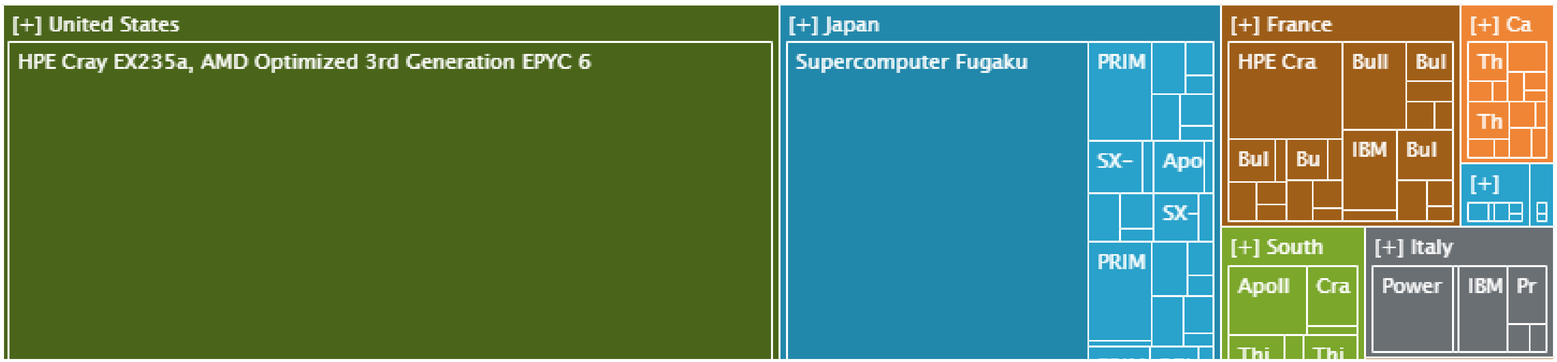
Highlights (from www.top500.org)

- the 59th edition of the TOP500 revealed the Frontier system to be the first true exascale machine with an HPL score of 1.102 Exaflop/s.
- Frontier brings the pole position back to the USA after it was held for 2 years by the Fugaku system at RIKEN Center for Computational Science (R-CCS) in Kobe, Japan.
- The Frontier has a peak performance of 1.6 ExaFlop/s and has achieved so far, an HPL benchmark score of 1.102 Eflop/s.
- On the HPL-AI benchmark, which measure performance for mixed precision calculation, Frontier already demonstrated 6.86 Exaflops!

Other highlights

- A total of 169 systems on the list are using accelerator/co-processor technology, up from 151 six months ago. 84 of these use NVIDIA Volta chips, 54 use NVIDIA Ampere, and 8 systems with NVIDIA Pascal.
- Intel continues to provide the processors for the largest share (77.60 percent) of TOP500 systems, down from 81.60 % six months ago. 93 (18.60 %) of the systems in the current list used AMD processors, up from 14.60 % six months ago.
- The average concurrency level in the TOP500 is **182,864** cores per system up from **162,520** six months ago.

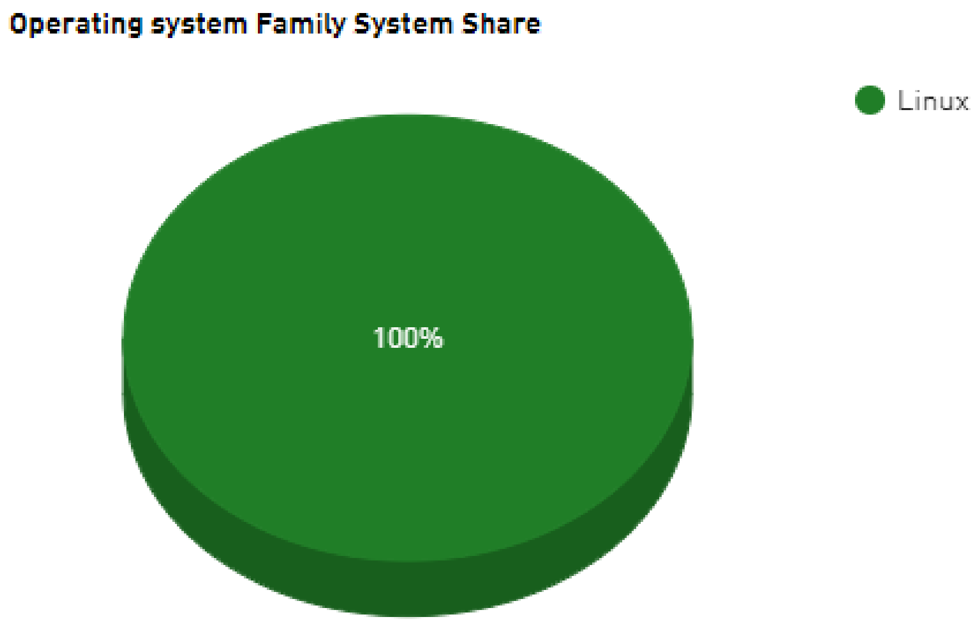
By country…



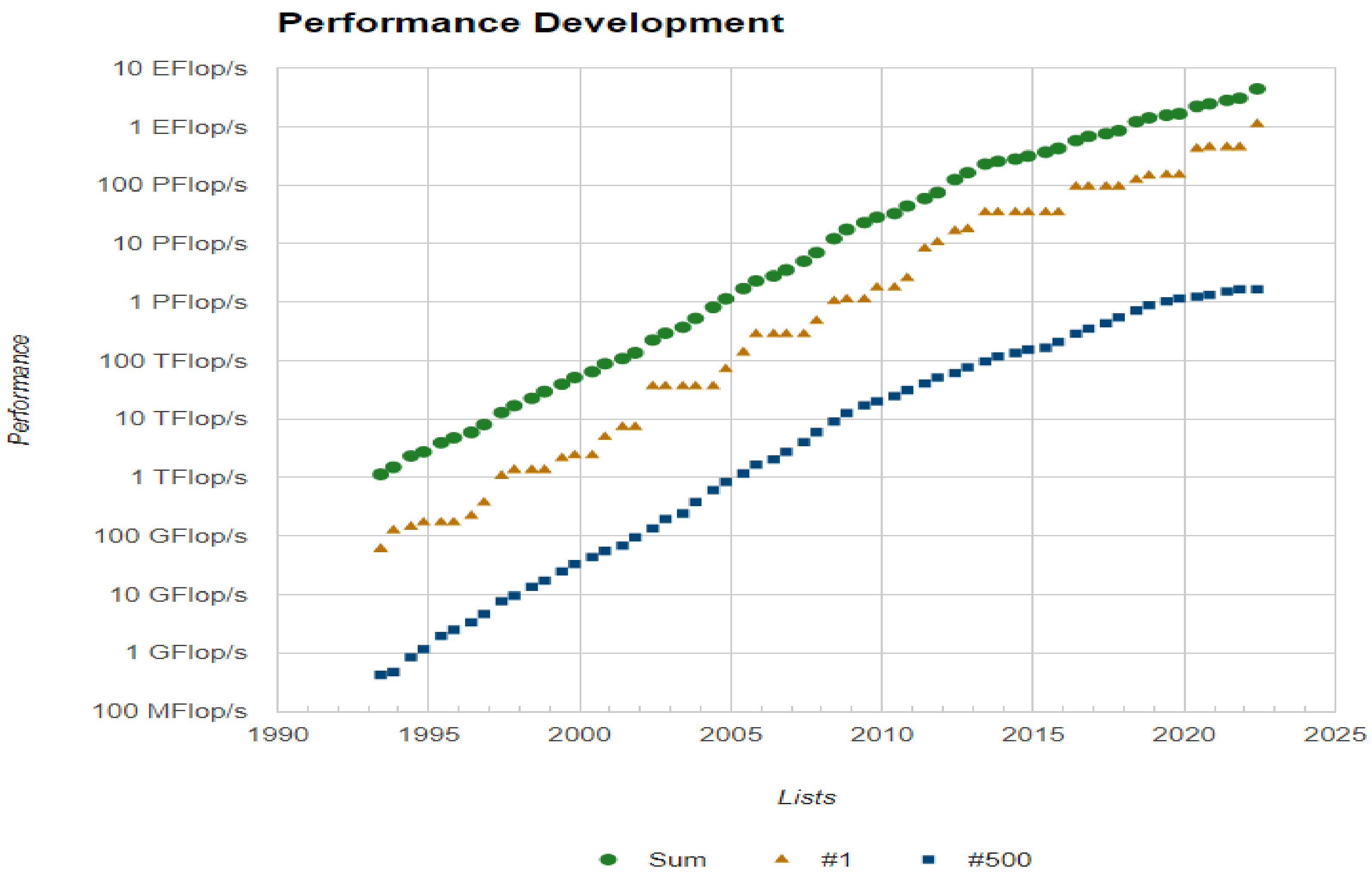
Installations by countries/regions:

		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