How HPC Accelerates Science

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PLAN

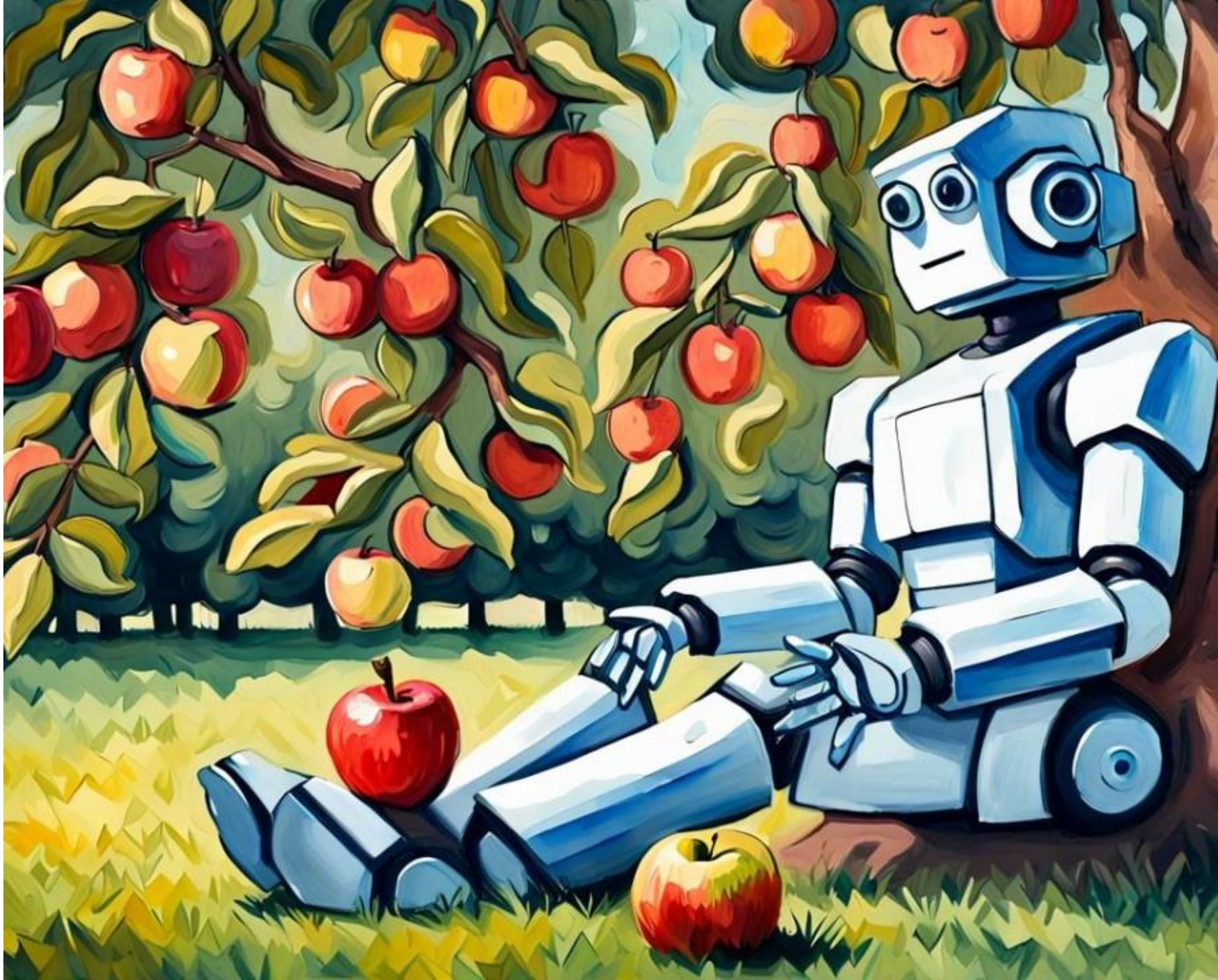
HPC concept

HPC in science

HPC definitions

HPC toys

What is HPC?



High Performance Computing

HPC (**H**igh **P**erformance **C**omputing):

- computational **challenges** beyond traditional computing capabilities
- usage of advanced computing systems:
  - **Supercomputers**
  - high-performance **clusters**
- **complex** and computationally demanding tasks
- parallel processing white **hundreds** of **processors** or cores
- key is speed, scalability, and efficiency of calculations

Supercomputer

Supercomputer - a computer with a **high level of performance** as compared to a general-purpose computer.

Supercomputers play an important role in the field of computational science, and are used for a wide range of computationally intensive tasks in various fields, including:

- quantum mechanics,
- weather forecasting,
- oil and gas exploration,
- molecular modeling,
- physical simulations,
- cryptanalysis

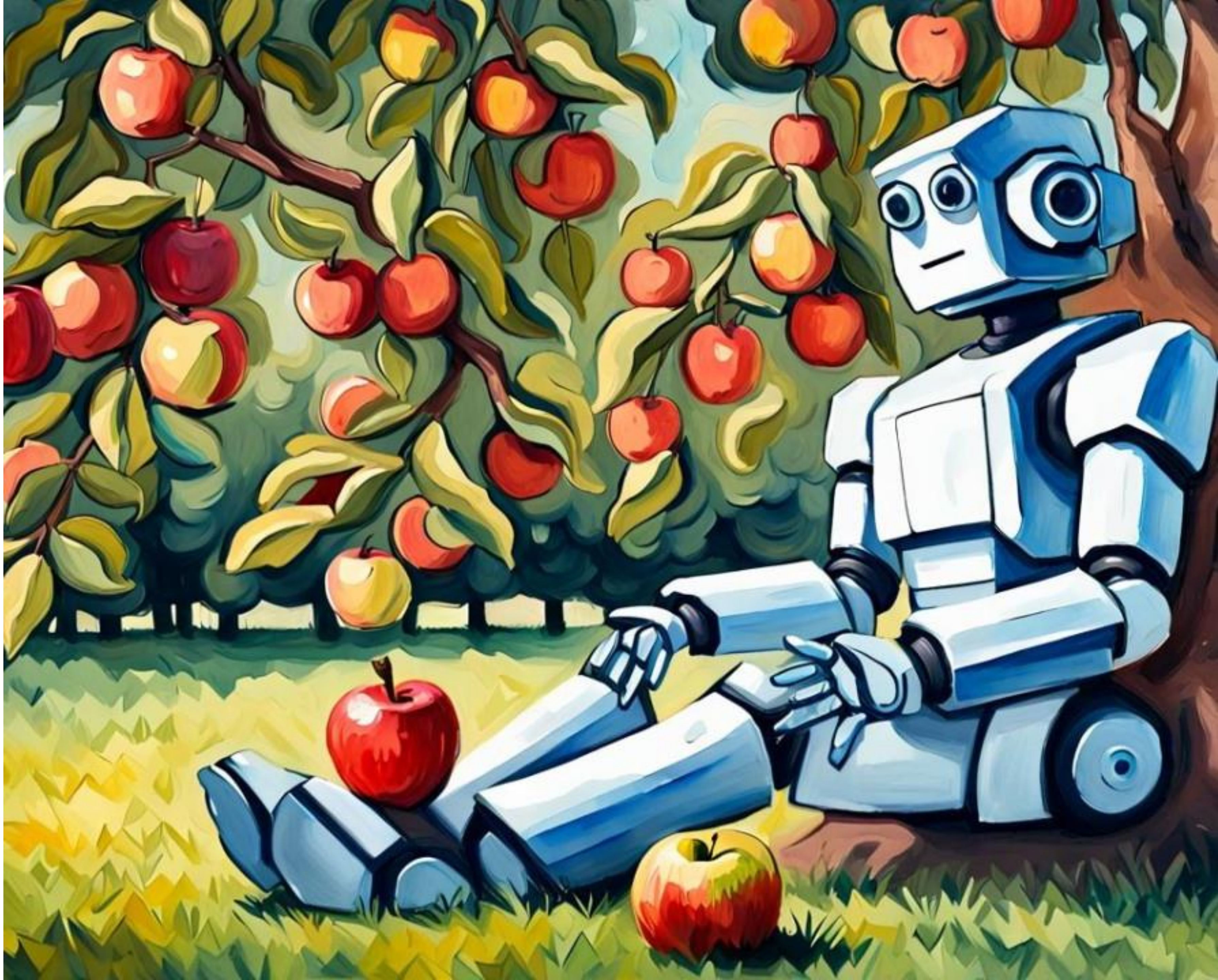
Computer cluster

A **computer cluster** is a group of interconnected computers that work together as a single system to perform tasks more efficiently than an individual computer. Each computer in a cluster is called a **node**, and they are typically linked through high-speed network connections.

Types of Clusters:

- **High-Performance Computing (HPC)** Clusters: Used for complex computations in fields like scientific research, simulations, and data analysis.
- **High-Availability (HA)** Clusters: Designed for systems that need minimal downtime, such as servers for critical applications.
- **Load Balancing Clusters**: Focused on distributing workloads evenly, commonly used in web hosting and cloud services.

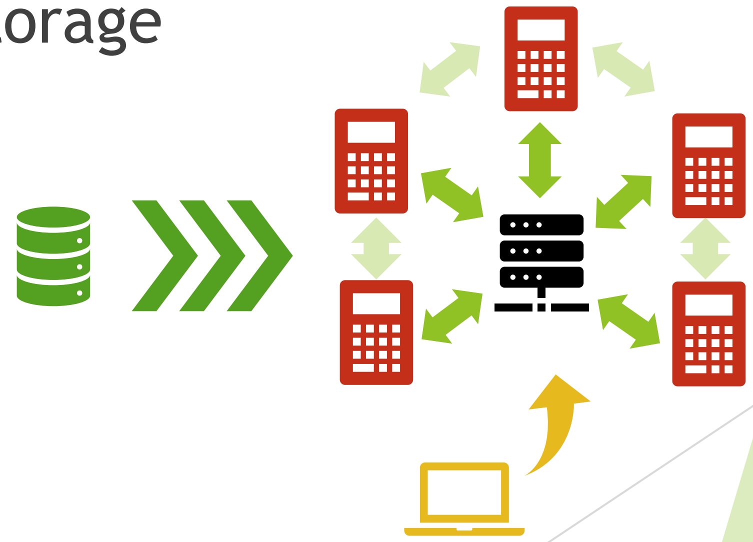
HPC hardware



Cluster architecture

A computer cluster is built of:

- **Nodes:**
  - Head nodes
  - Compute nodes
  - Service nodes
- **Interconection**
- **Shared** storage



Head node

The head node, also known as the master node, **login node** or frontend node, serves as the central control point for the cluster.

It manages the **cluster's overall** operation, including job scheduling, resource allocation, and coordination of tasks among the nodes.

The head node typically runs cluster management software and provides a user interface for **cluster administration**.

Copmute node

Compute nodes are the primary **processing units** in the cluster.

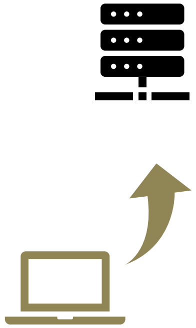
These nodes execute **computational** tasks, **simulations**, data **analysis**, or other workload-specific operations.

Compute nodes are responsible for executing the tasks assigned to them by the head node or cluster management system.

Nodes

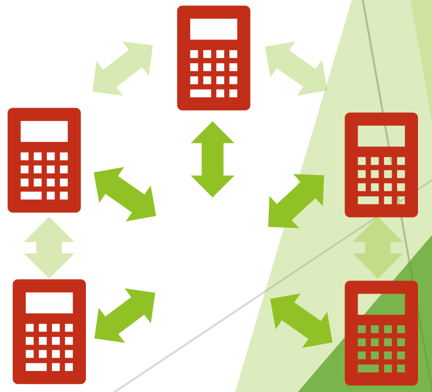
Login node:

- User **Access Point**
- Job Management
- Data Pre-/Post-Processing (small)
- Data **Transfer** (sometimes better is a bether place)
- **Limited** Computing Power



Compute node:

- Computations are performed on these
- **High** Computing Power
- No Direct Access (typically)
- **High-Speed** Interconnect



FLOPC

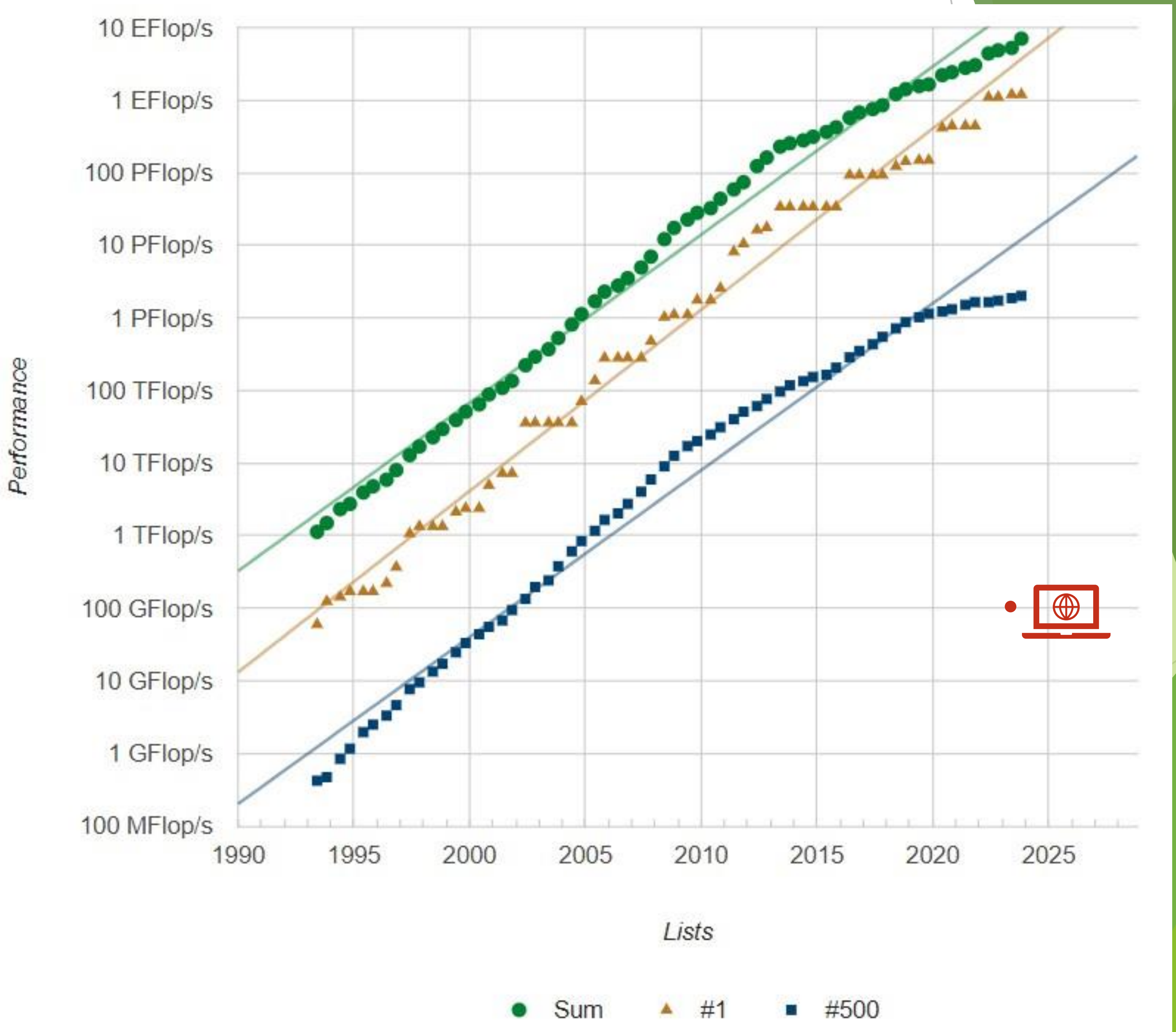
FLOPS (**F**loating **P**oint **O**perations **P**er **S**econd), is a measure of a computer's processing **speed** for **performing** floating-point arithmetic, often used to gauge the performance of high-performance computing systems.

- **GFLOPS**: 10^9 FLOPS (Giga)
- **TFLOPS**: 10^{12} FLOPS (Tera)
- **PFLOPS**: 10^{15} FLOPS (Peta)
- **EFLOPS**: 10^{18} FLOPS (Exa)

$$FLOPS = \frac{flops}{cycle} \times \frac{cycle}{second} \times \frac{cores}{socket} \times \frac{socekets}{node} \times nodes$$

https://www.nextplatform.com/2023/11/13/top500-supercomputers-who-gets-the-most-out-of-peak-performance/

Top500



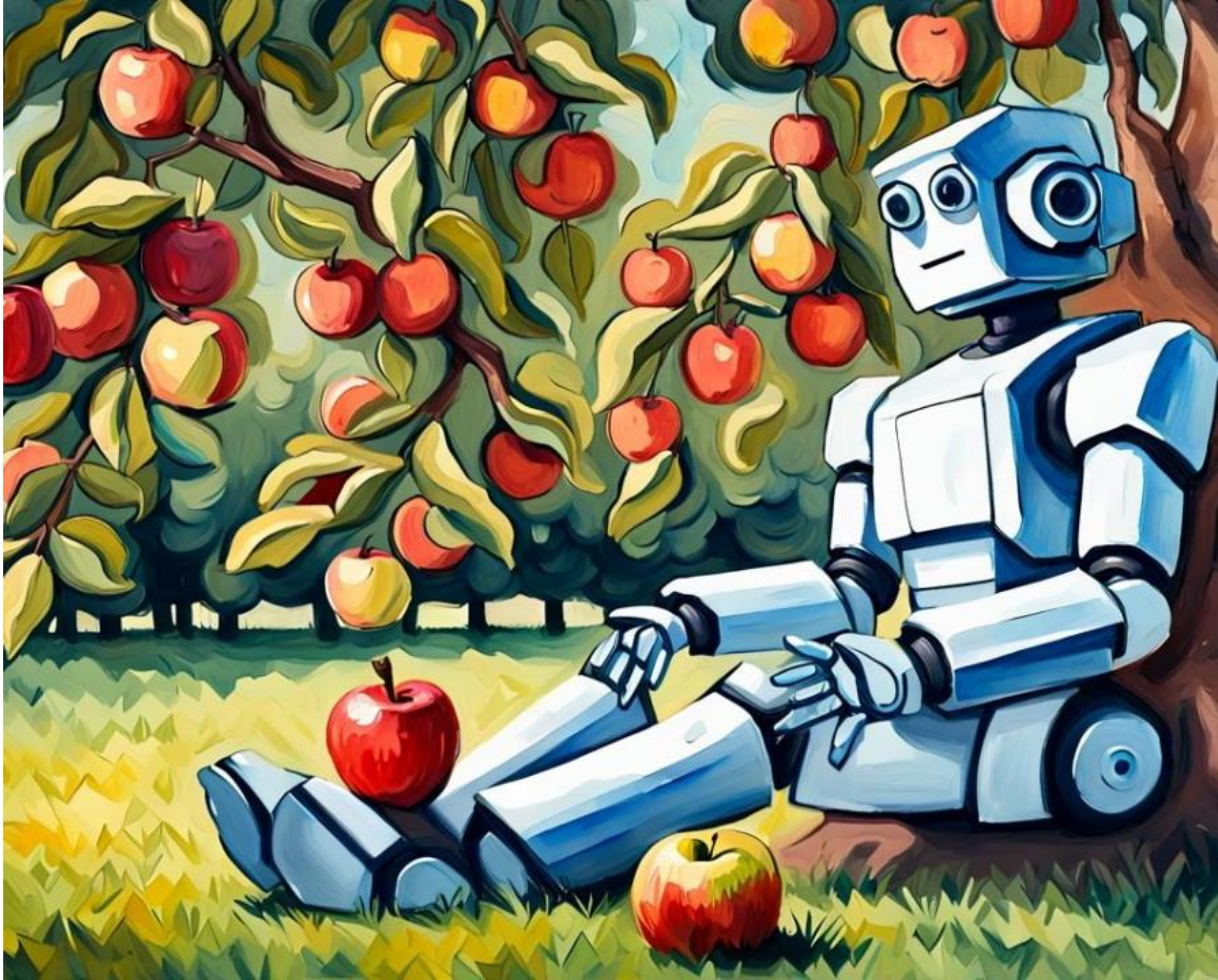
Top500

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)
1	El Capitan United States	11,039,616	1,742.00	2,746.38
2	Frontier United States	9,066,176	1,353.00	2,055.72
3	Aurora United States	9,264,128	1,012.00	1,980.01
4	Eagle United States	2,073,600	561.20	846.84
5	HPC6 Italy	3,143,520	477.90	606.97

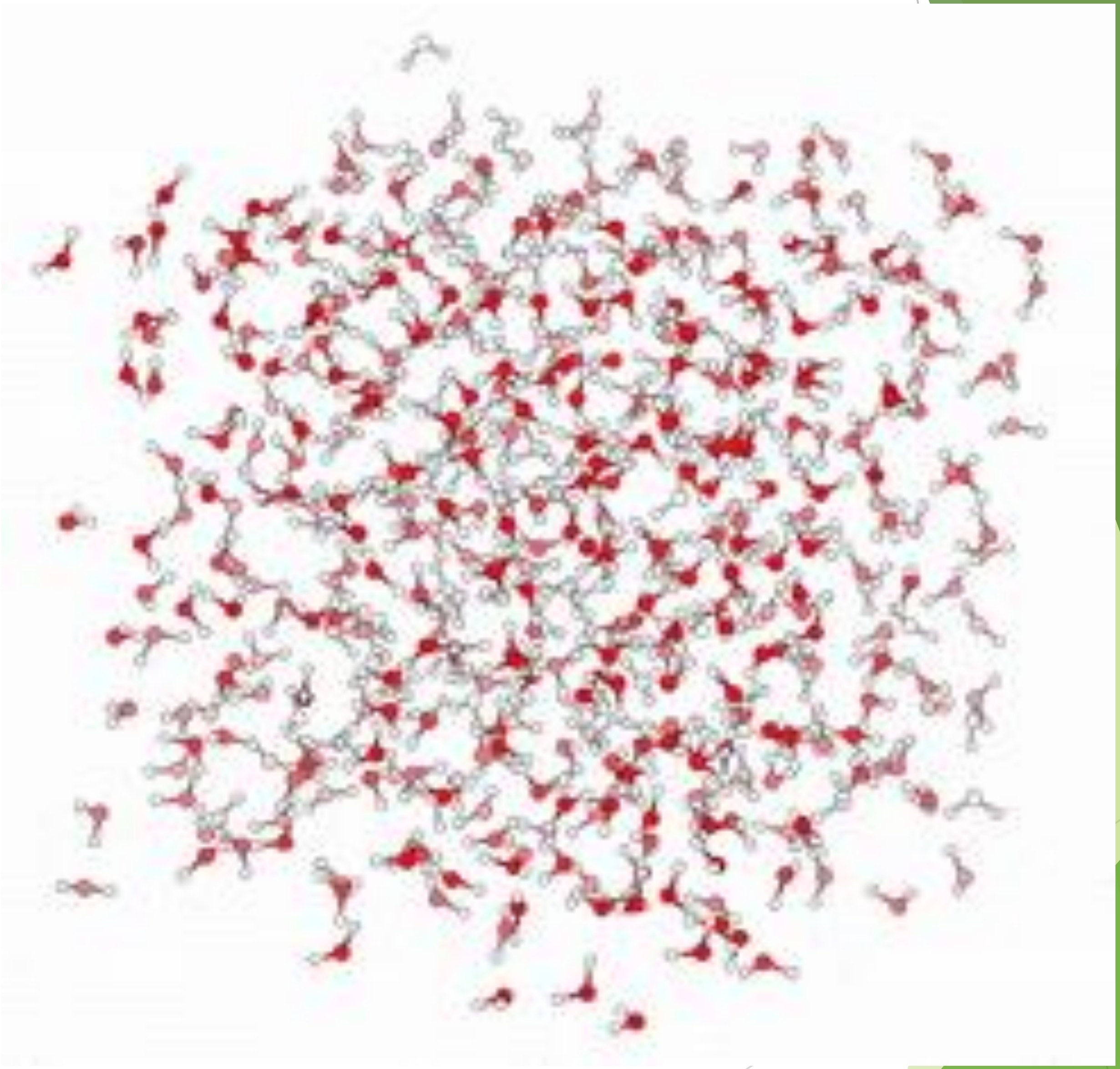
El Capitan

Site:	DOE/NNSA/LLNL
Manufacturer:	HPE
Cores:	11,039,616
Processor:	AMD 4th Gen EPYC 24C 1.8GHz
Interconnect:	Slingshot-11
Installation Year:	2024
Performance	
Linpack Performance (Rmax)	1,742.00 PFlop/s
Theoretical Peak (Rpeak)	2,746.38 PFlop/s
Nmax	25,446,528
Power Consumption	
Power:	29,580.98 kW
Power Measurement Level:	2
Software	
Operating System:	TOSS
Compiler:	g++ 12.2.1 and hipcc 6.2.0
Math Library:	AMD rocBLAS 6.0.2 and Intel MKL 2016
MPI:	HPE Cray MPI

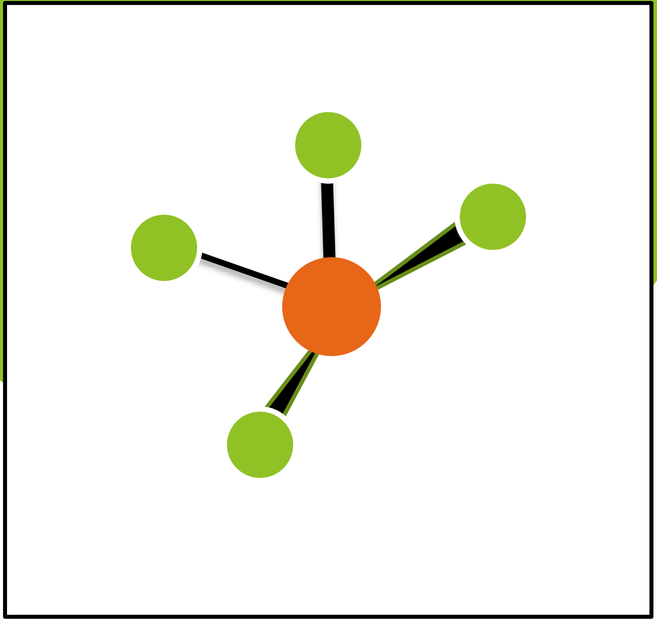
HPC for science



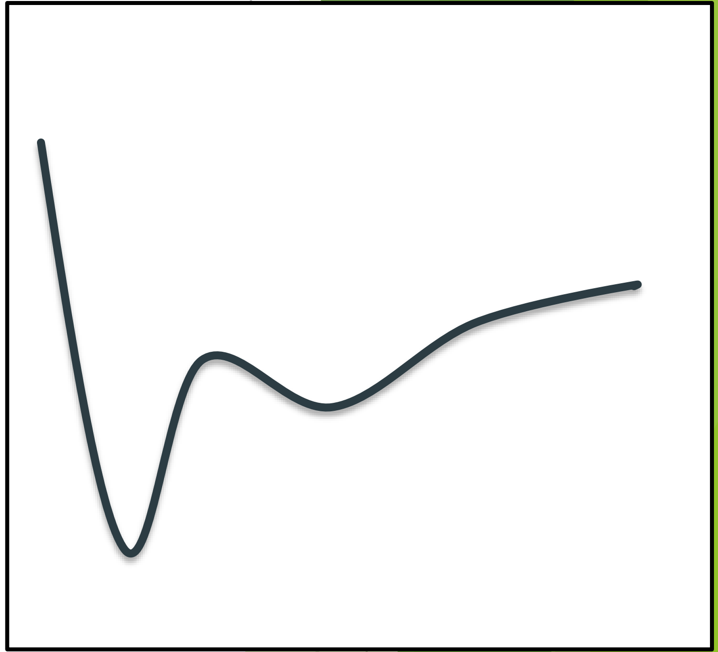
Molecular dynamic



Molecular



$$
\begin{aligned}
U(R) = & \sum_{bonds} k_r \left(r - r_{eq}\right)^2 \\
& + \sum_{angles} k_\theta \left(\theta - \theta_{eq}\right)^2 \\
& + \sum_{dihedrals} k_\phi \left(1 + \cos[n\phi - \gamma]\right) \\
& + \sum_{impropers} k_\omega \left(\omega - \omega_{eq}\right)^2 \\
& + \sum_{i<j}^{atoms} \varepsilon_{ij} \left[\left(\frac{r_m}{r_{ij}}\right)^{12} - 2\left(\frac{r_m}{r_{ij}}\right)^{6} \right] \\
& + \sum_{i<j}^{atoms} \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}
\end{aligned}
$$



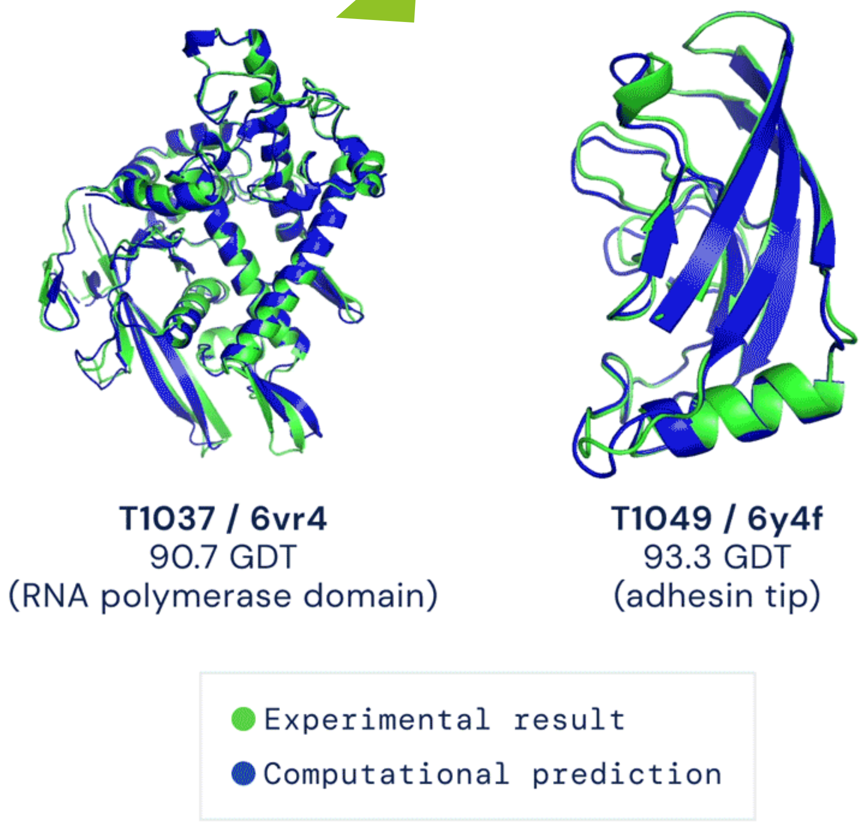
https://www.bonvinlab.org/education/molmod_online/doc

Molecular dynamic

https://github.com/google-deepmind/alphafold

Protein folding: AlphaFold

GAMGSEIEHIEEAIANAKTKADHERLVAHYEEEAKRLE
KKSEEYQELAKVYKKITDVYPNIRSYMVLHYQNLTRRY
KEAAEENRALAKLHHELAIVED



Protein folding: AlphaFold

- The total **training** time for **AlphaFold** is approximately **50,000 GPU hours**. It used processing power of 100 to 200 GPUs

https://www.biorxiv.org/content/10.1101/2022.11.20.517210v1.full

- For **RoseTTAFold** it takes about **30,000 GPU** hours to train.

https://www.marktechpost.com/2022/03/26/impressed-with-alphafold-checkout-this-protein-structure-prediction-model-fastfold-that-reduces-alphafolds-training-time-from-11-days-to-67-hours/

- Drug discovery:
  With **20^7** possible **molecules**, and each molecule taking 1 day to compute on A100 or 10 days on CPU, it would take approximately **3,506,849 GPU years**.

HPC for AI

- **GPT-4** was trained on approximately **25,000 A100** GPUs over a period of 90 to **100 days**

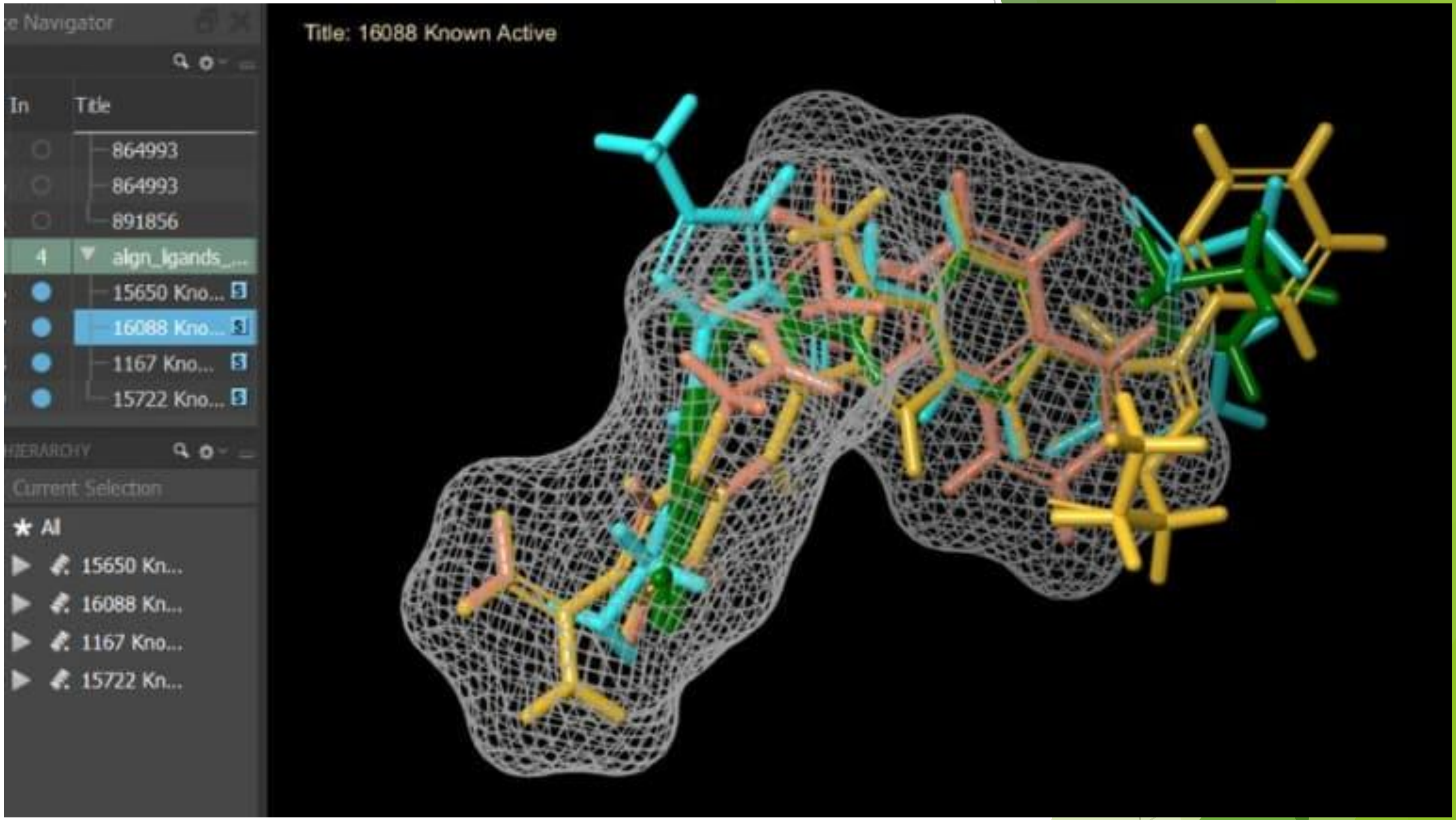
https://www.ikangai.com/the-secrets-of-gpt-4-leaked/

- Based on the information available, the training of OpenAI's **DALL·E 2** model is estimated to require about 100,000 to **200,000 GPU hours**, which translates to using approximately **256 V100** GPUs for a duration of 2 to 4 week

https://github.com/lucidrains/DALLE2-pytorch/issues/22

- **Converting** a text to a **Knowledge Graph** requires approximately 30 to **40 seconds** for a single page on a single GPU. A dataset consists of **100,000** page, what is 46 days.

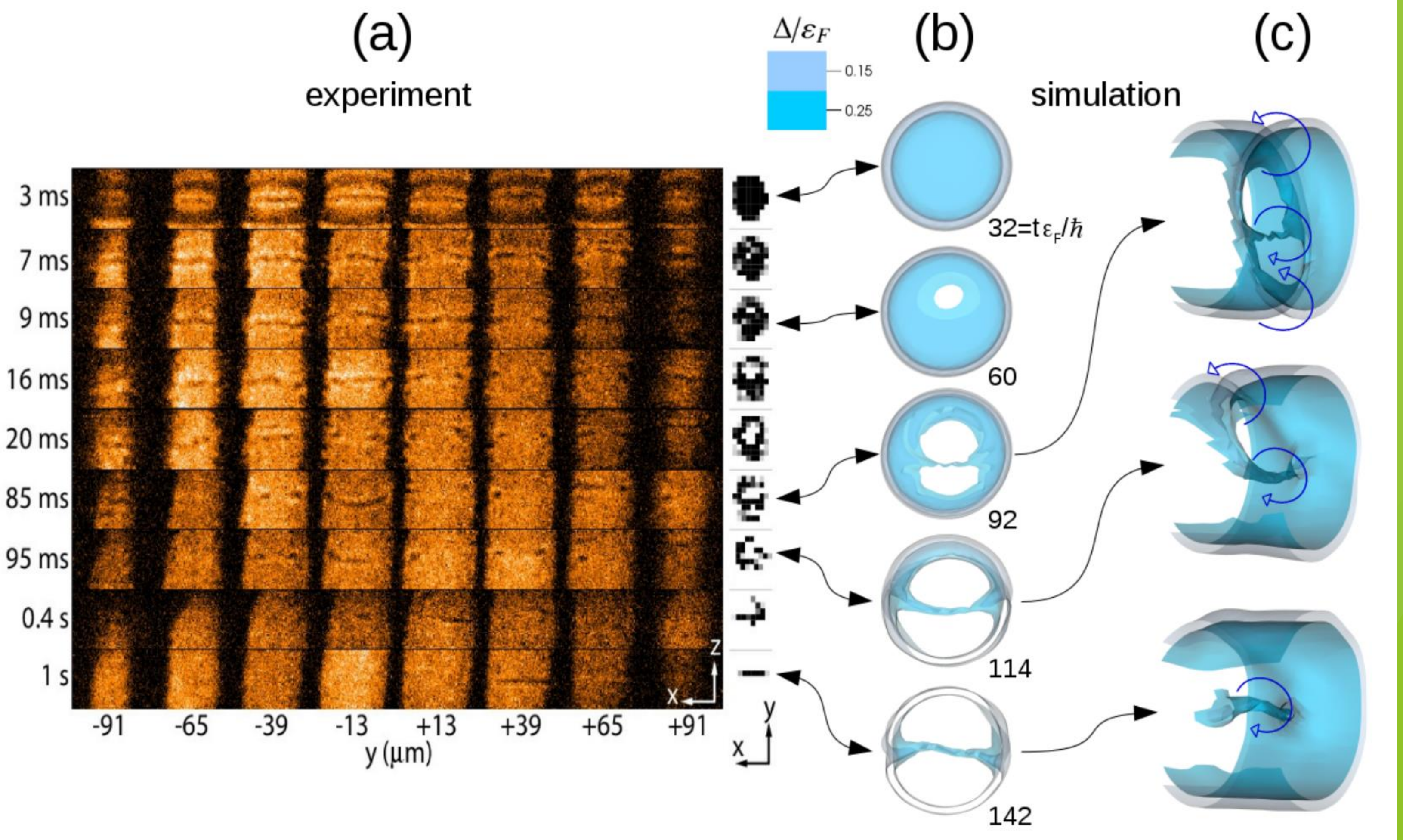
Density Functional Theory - DFT



https://www.thestreet.com/tech/news/sdgrjdm121420

a **computational quantum mechanical** modelling method used in physics, chemistry and materials science to investigate the **electronic structure** (or nuclear structure) (principally the ground state) of **many-body systems**, in particular atoms, molecules, and the condensed phases.

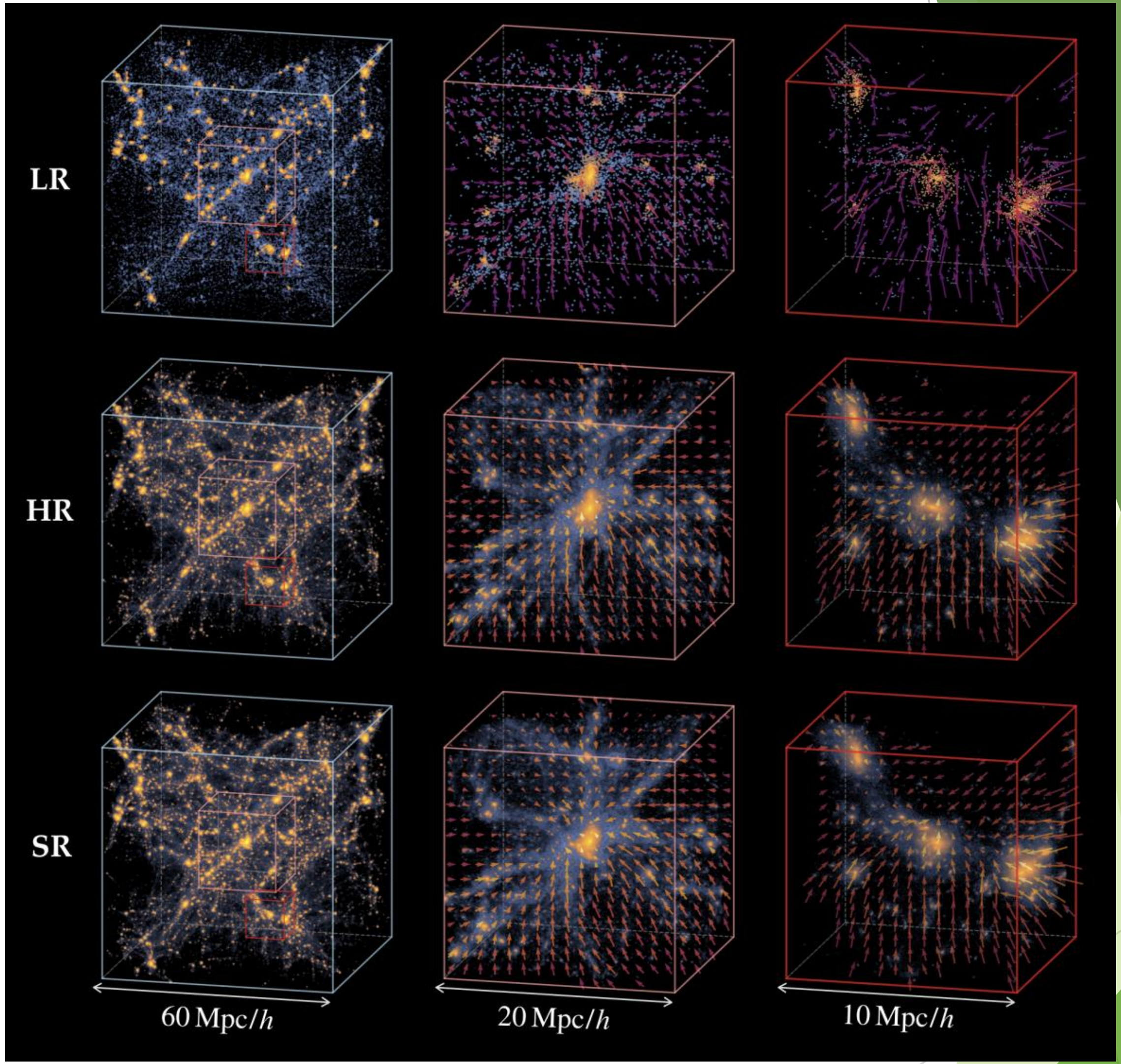
Density Functional Theory - DFT



DFT methods can also be used for really big systems like neutron **stars**. However doing these calculations requires a lot of resources. This calculations have been done using >**500 GPUs** and took several **weeks**.

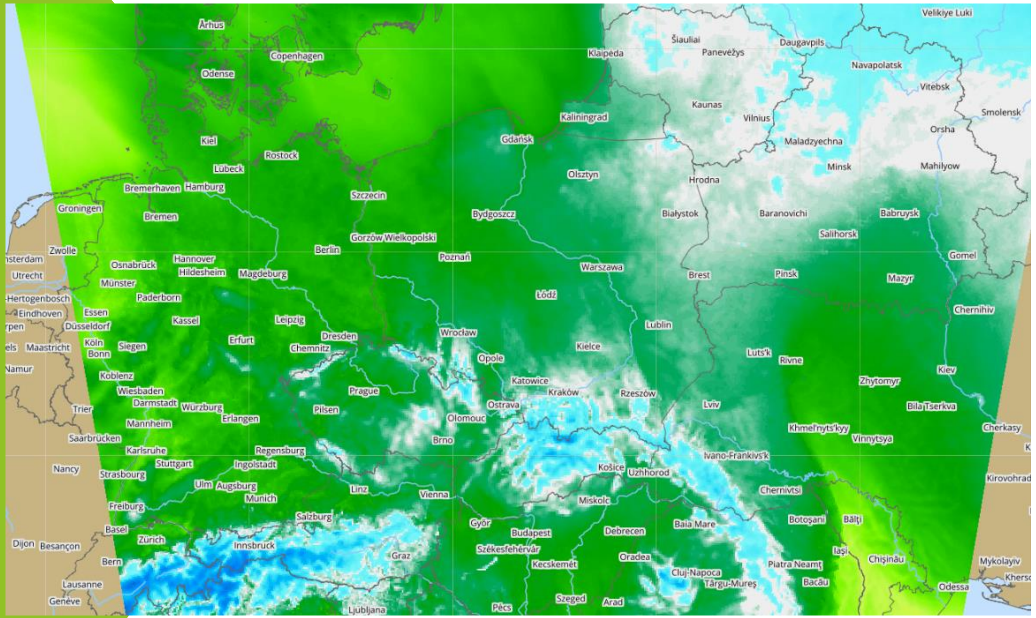
G. Wlazłowski, K. Sekizawa, M. Marchwiany, P. Magierski, Suppressed solitonic cascade in spin-imbalanced superfluid Fermi gas, Phys. Rev. Lett. 120, 253002 (2018)

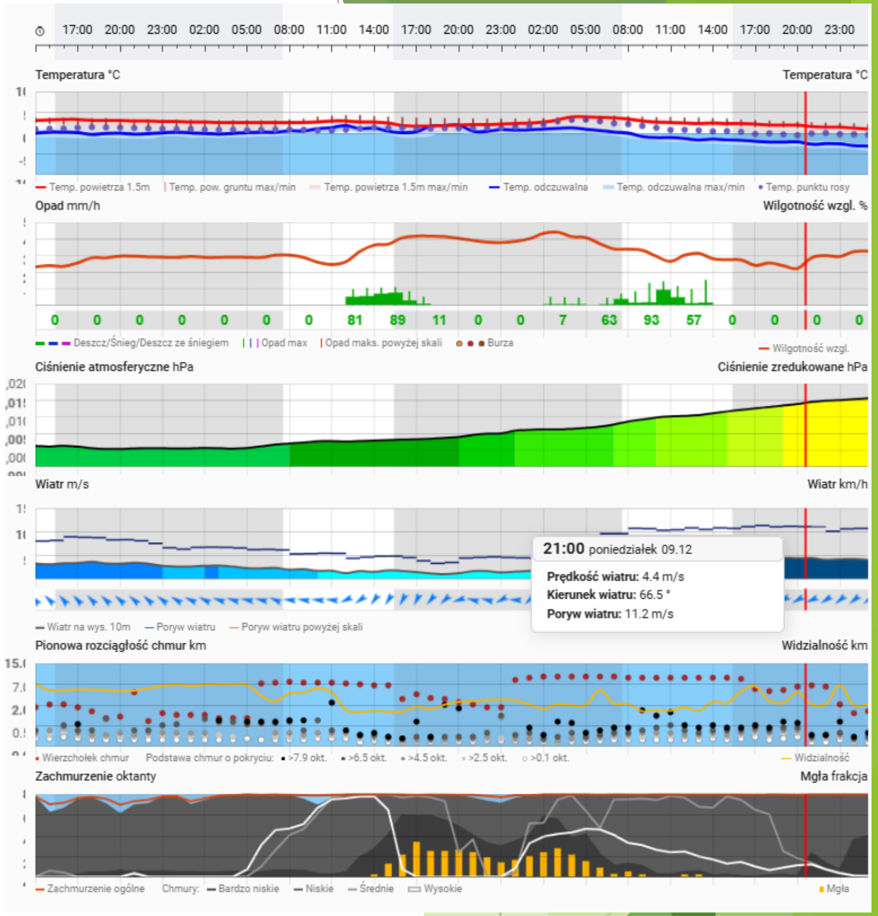
Cosmology



Li, Yin & Ni, Yueying & Croft, Rupert & Matteo, Tiziana & Bird, Simeon & Feng, Yu. (2021). AI-assisted superresolution cosmological simulations. Proceedings of the National Academy of Sciences of the United States of America. 118. 10.1073/pnas.2022038118.

Numerical weather forecast





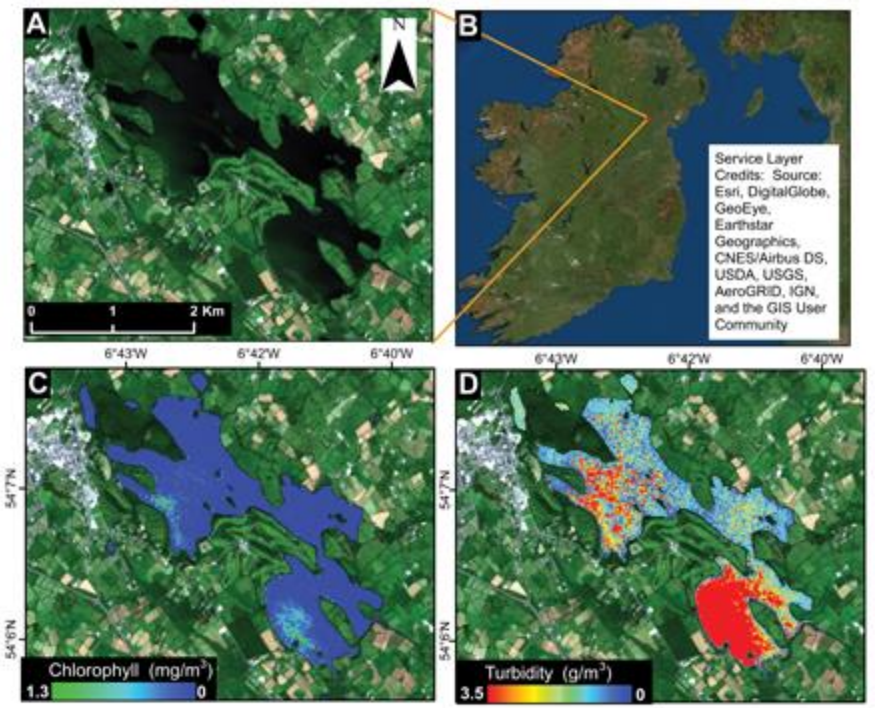
Numerical Weather Prediction (NWP) is the process of forecasting weather conditions using mathematical models that simulate the atmosphere's physical and dynamic processes. These models rely on equations that describe the behavior of atmospheric variables such as temperature, pressure, wind speed, and humidity.

https://www.meteo.pl/meteogramy

HPC in search for natural resources

HPC is indispensable in natural resource exploration and management due to its ability to handle the scale, complexity, and speed required for analyzing geological phenomena. It not only enhances efficiency and accuracy but also reduces costs and environmental impacts, making it a cornerstone of modern resource discovery.

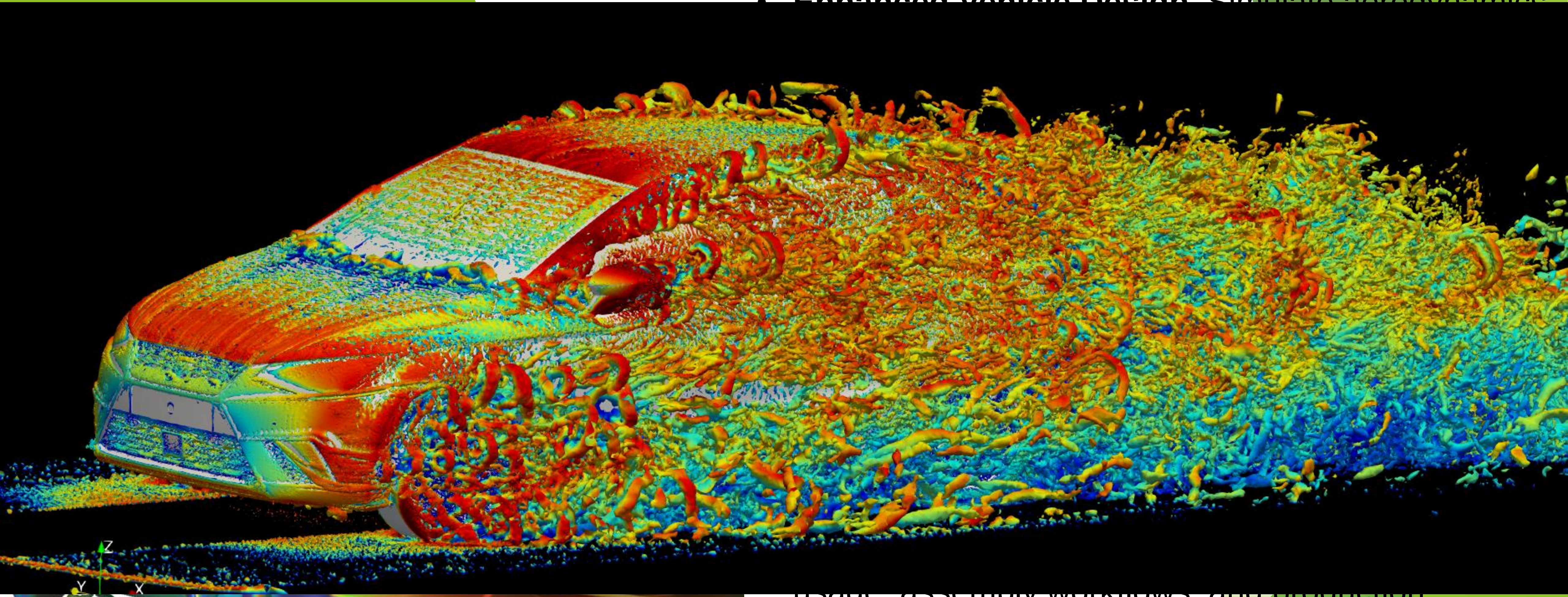
- Seismic Data Analysis
- Reservoir Simulations
- Environmental Impact Analysis



https://www.eolasmagazine.ie/high-performance-computing-accelerating-earth-observation-and-inland-water-quality-research/

https://www.ansys.com/blog/empowering-innovation-through-hpc-ai-enabled-simulation

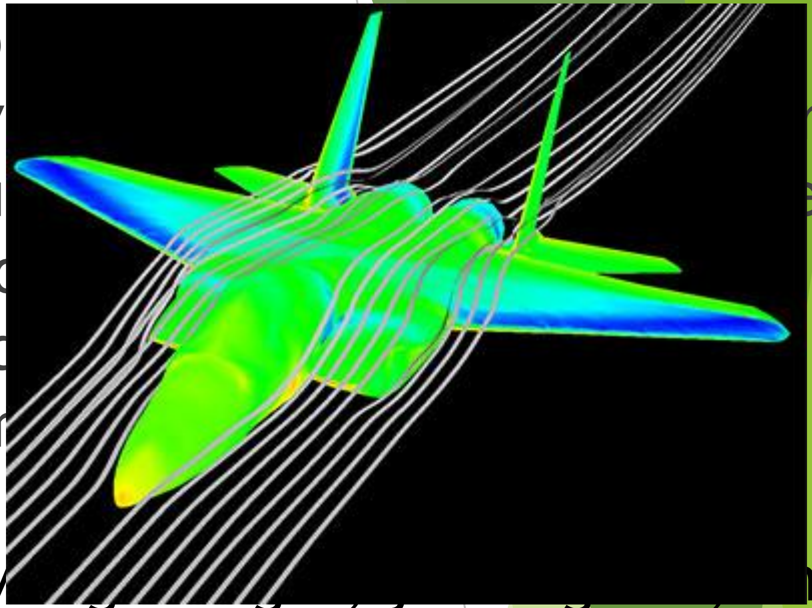
- **Enhanced Vehicle Design**: Simulate aerodynamics

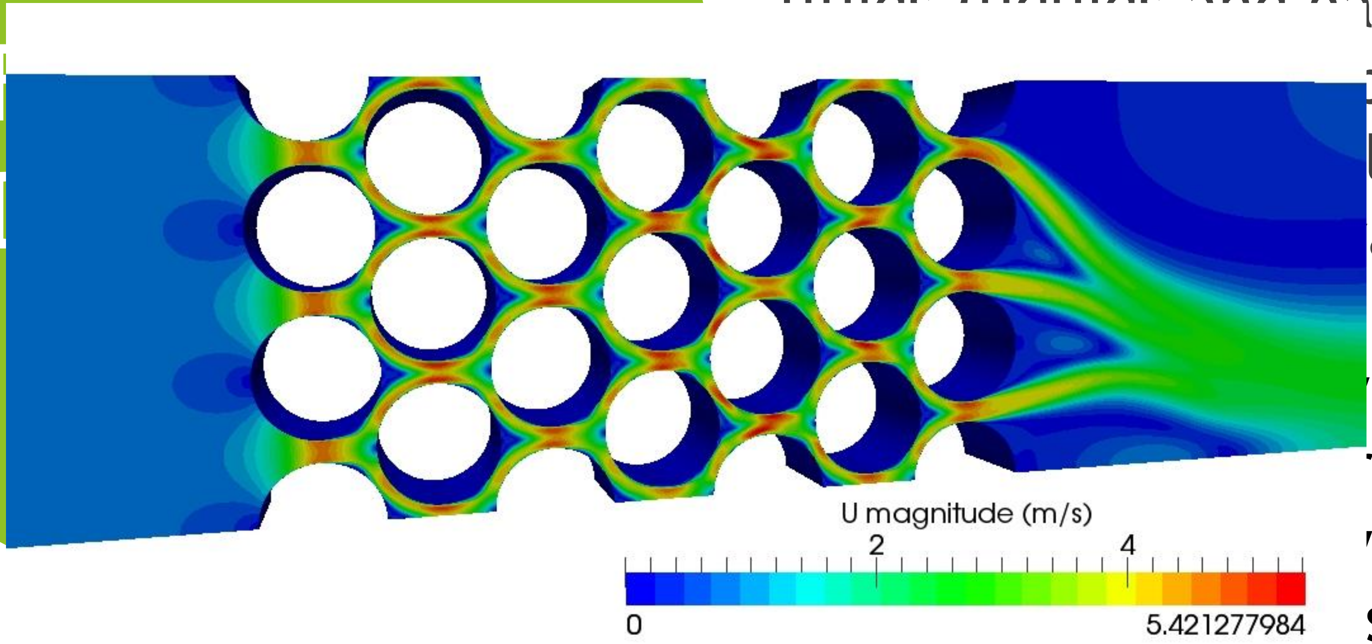


usage, assembly workflows, and production processes to save costs and reduce defects.

https://www.bsc.es/discover-bsc/organisation/research-departments/large-scale-computational-fluid-dynamics https://www.uab.edu/engineering/mme/?view=category&id=85

HPC helps in solving **Comp**... **(CFD)** problems, which inv... of fluids (liquids and gases) u...ese ...putatio... ...low eq... ...ast am...

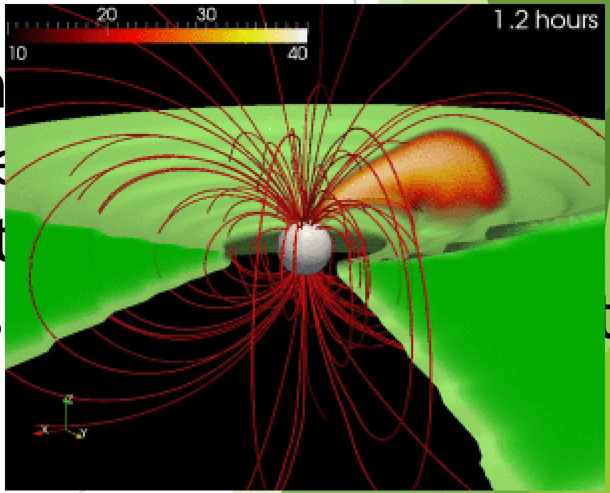




...s for v...nd ...y.

...namics an...

...s and unde...

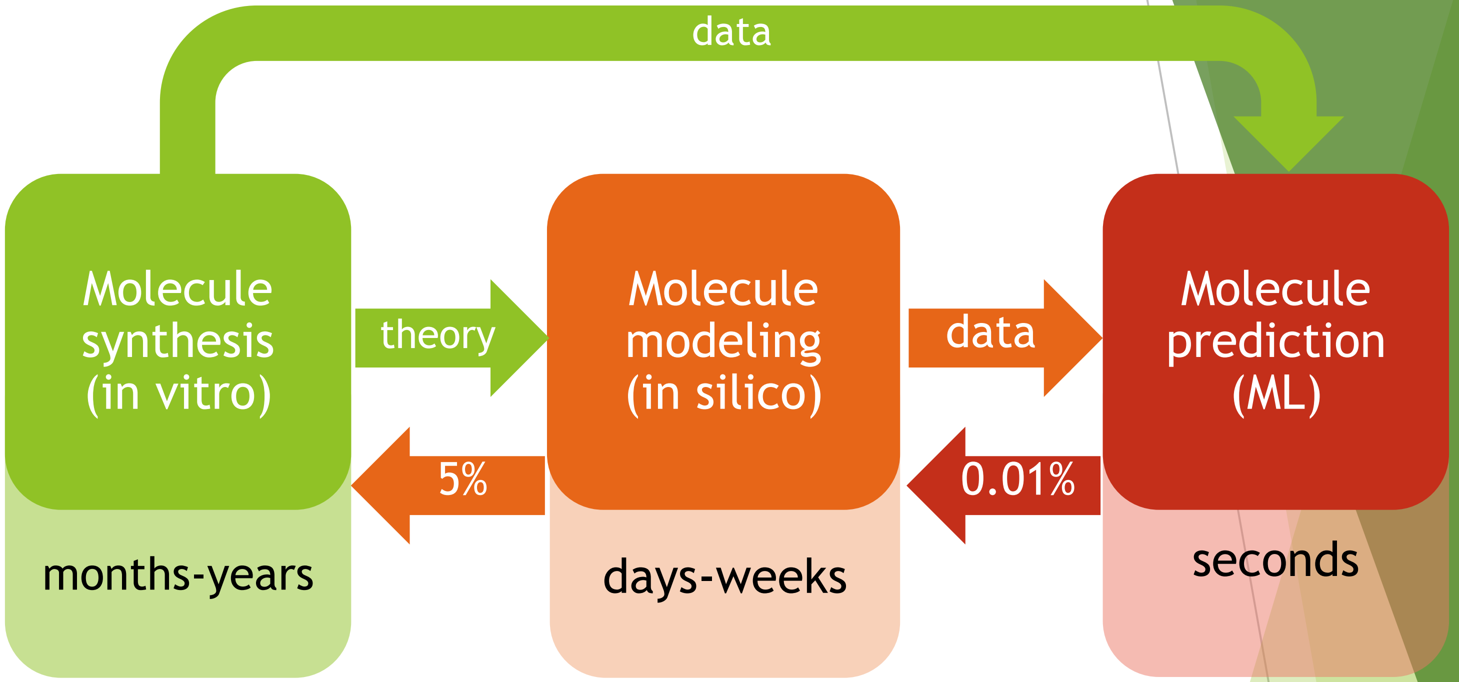


- Studying fluid flow in infrast... dams
- Predicting weather patterns ...tion dispersion.

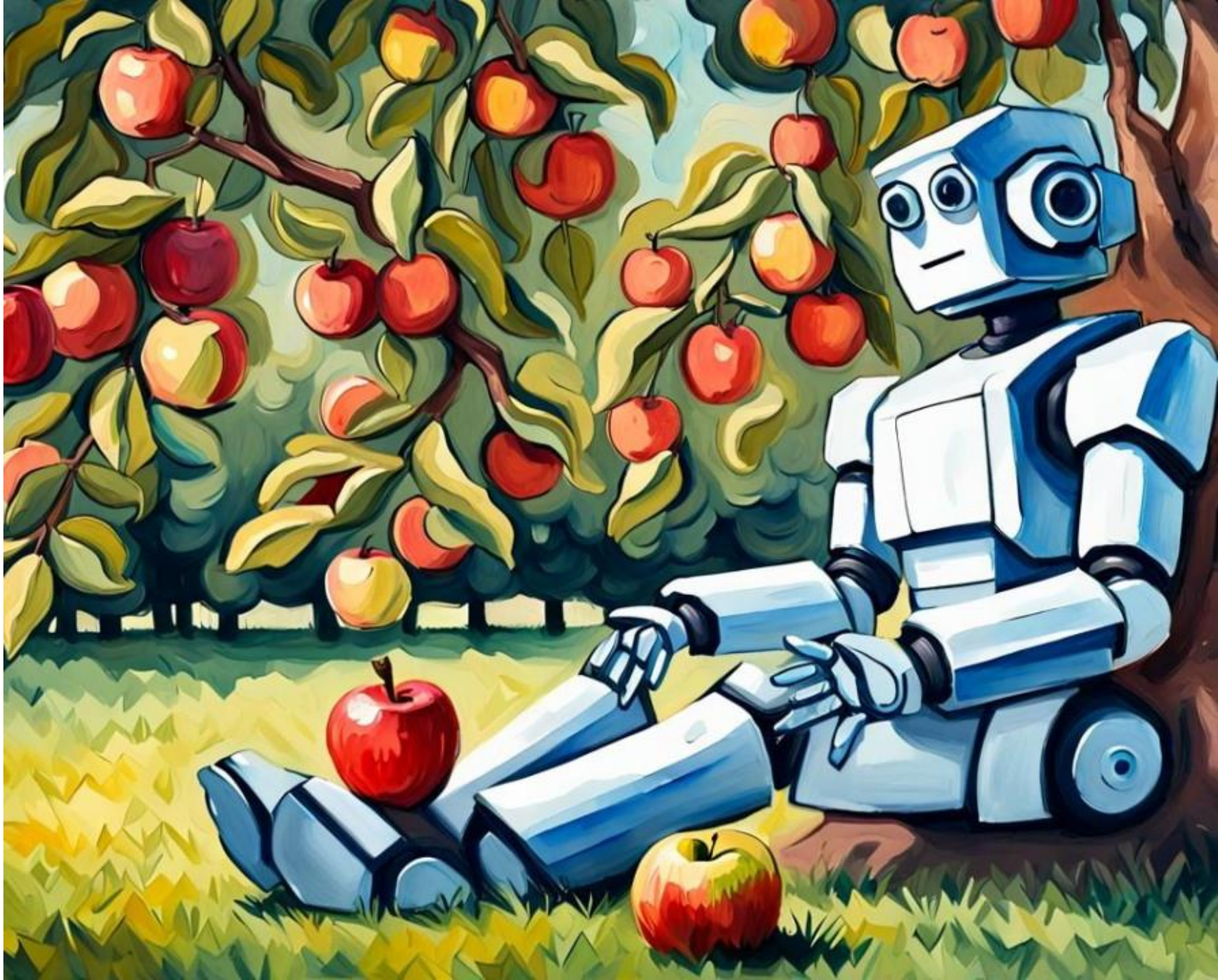
https://www.astropa.inaf.it/scientific-and-technological-activities-in-brief/computational-fluid-dynamics-for-astrophysical-plasma-and-high-performance-computing/

https://hpc.rtu.lv/hpc/hpc-services/cfd-eng/?lang=en

HPC in science



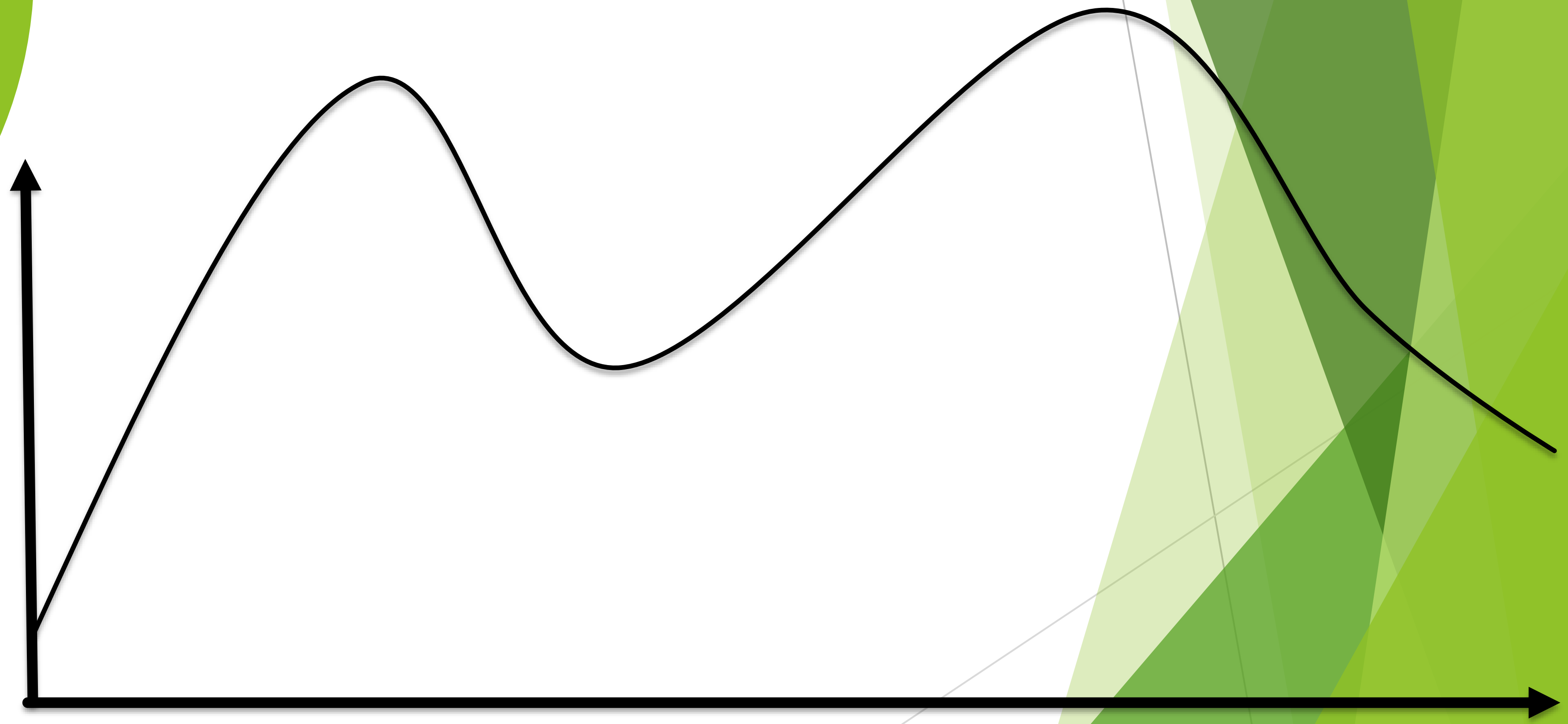
HPC definitions



Parallel computing

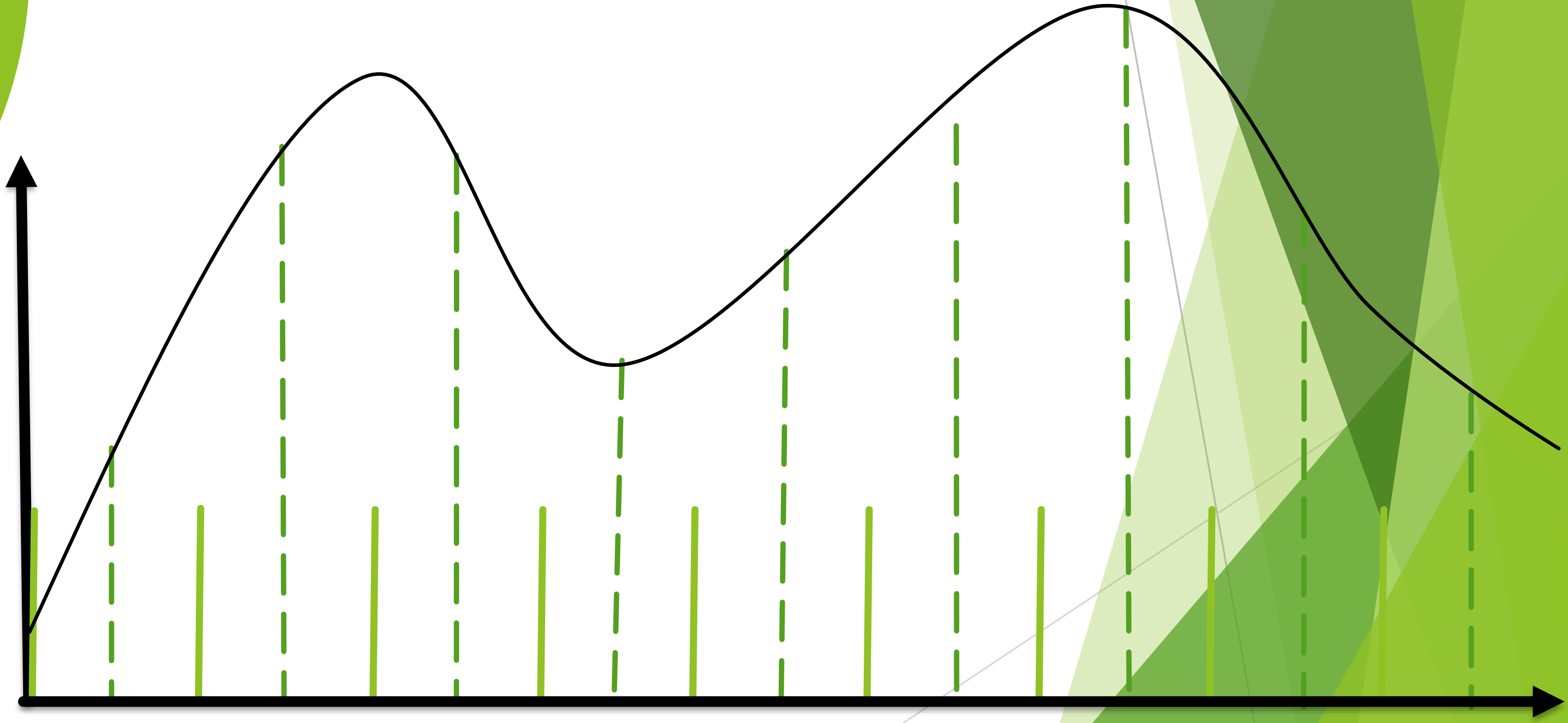
- **Parallel computing** - a type of computation in which many calculations or processes are carried out **simultaneously**. **Large** problems can often be **divided** into smaller ones, which can then be solved at the **same time**.
- Parallel computing allows for significant **improvements** in computational **speed** and **efficiency** by leveraging **multiple** processors or cores to work on a task concurrently.

Parallel integral

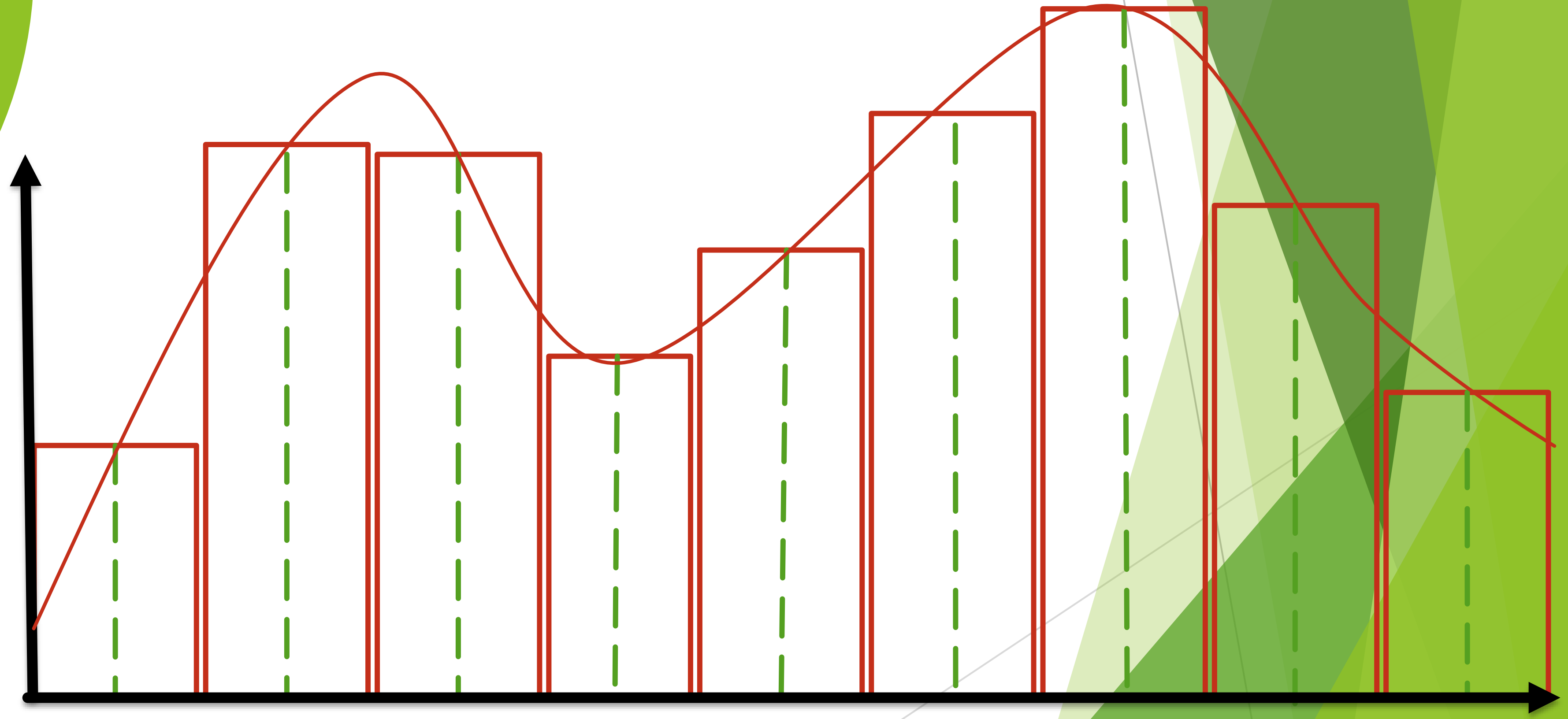


Parallel integral

$t = T$



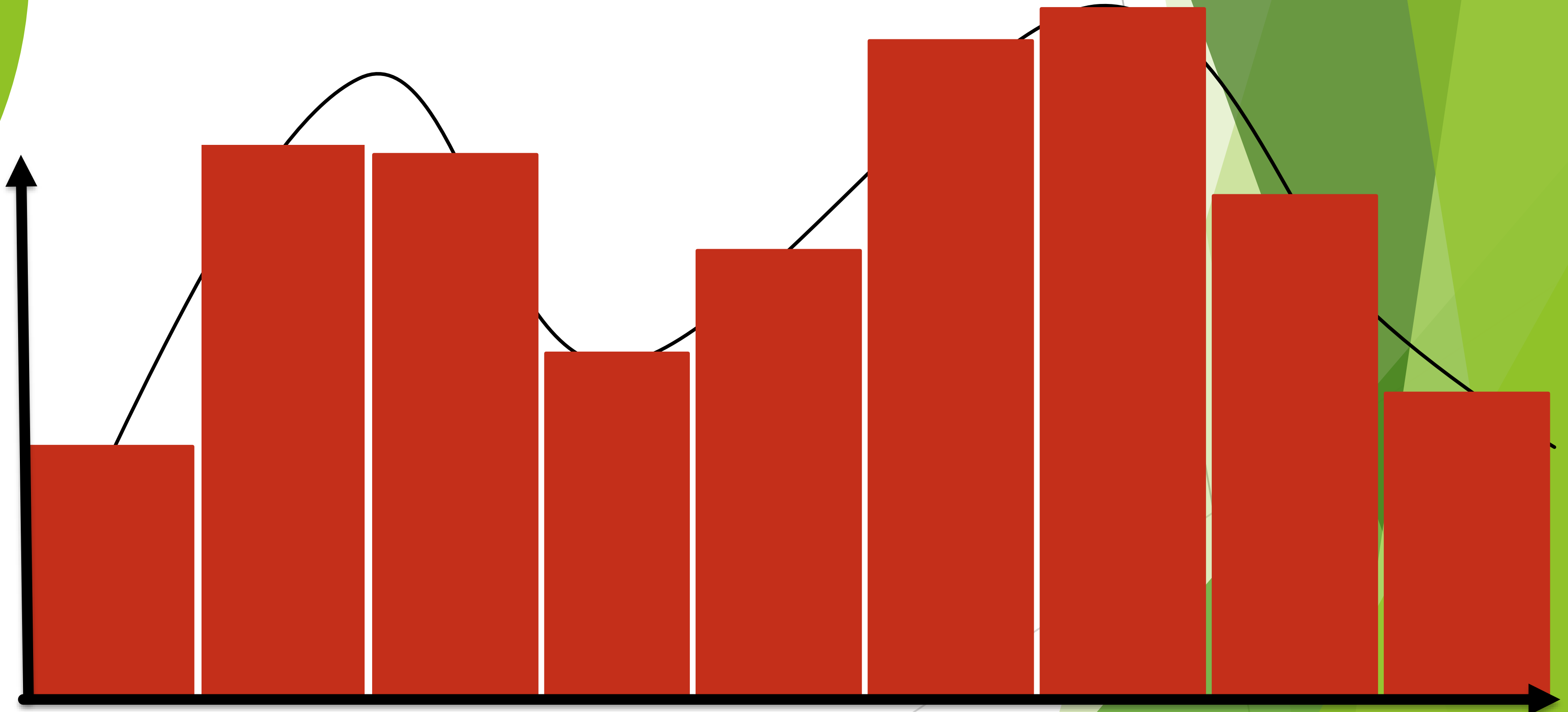
Parallel integral



t =T

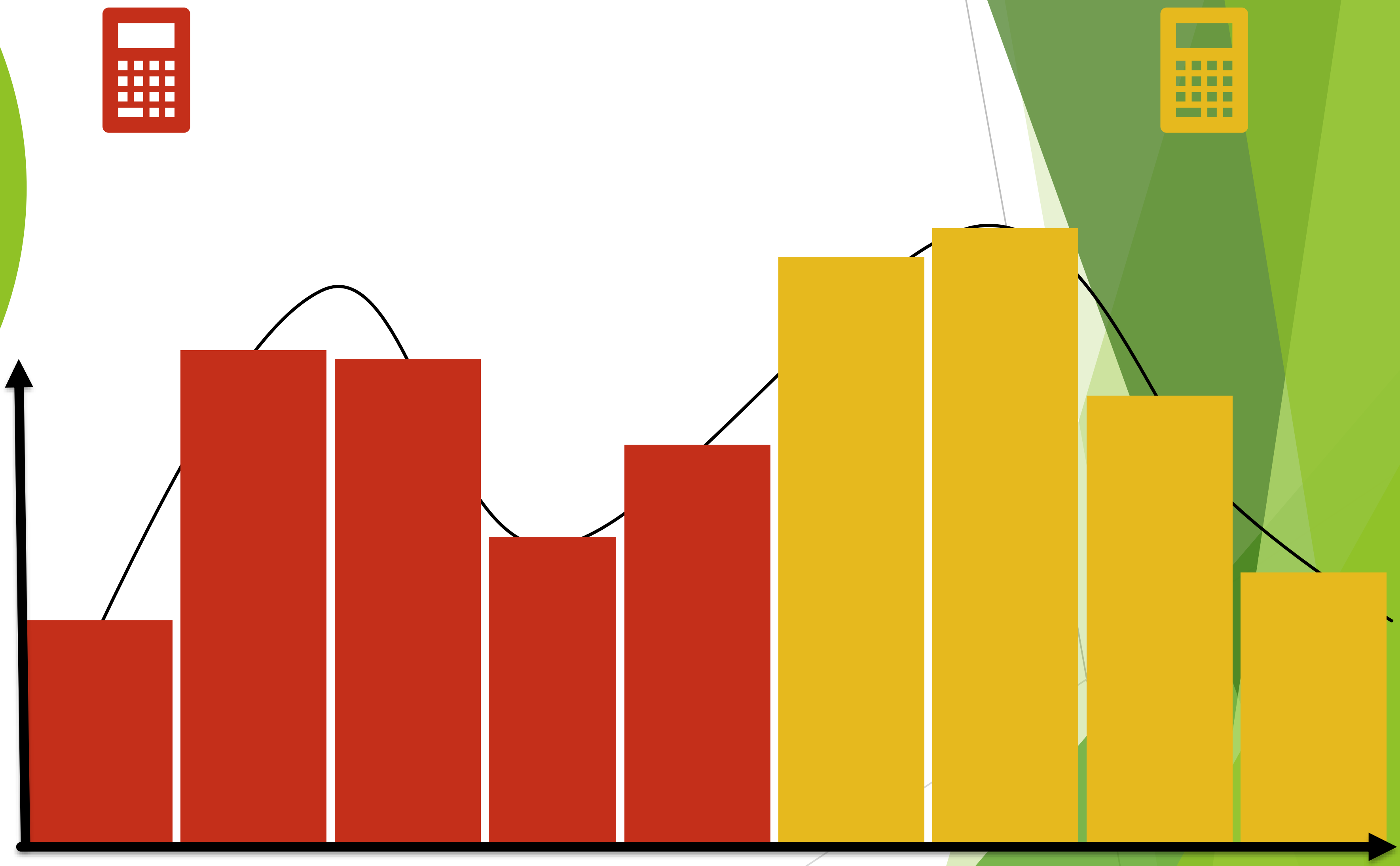
Parallel integral

t =T



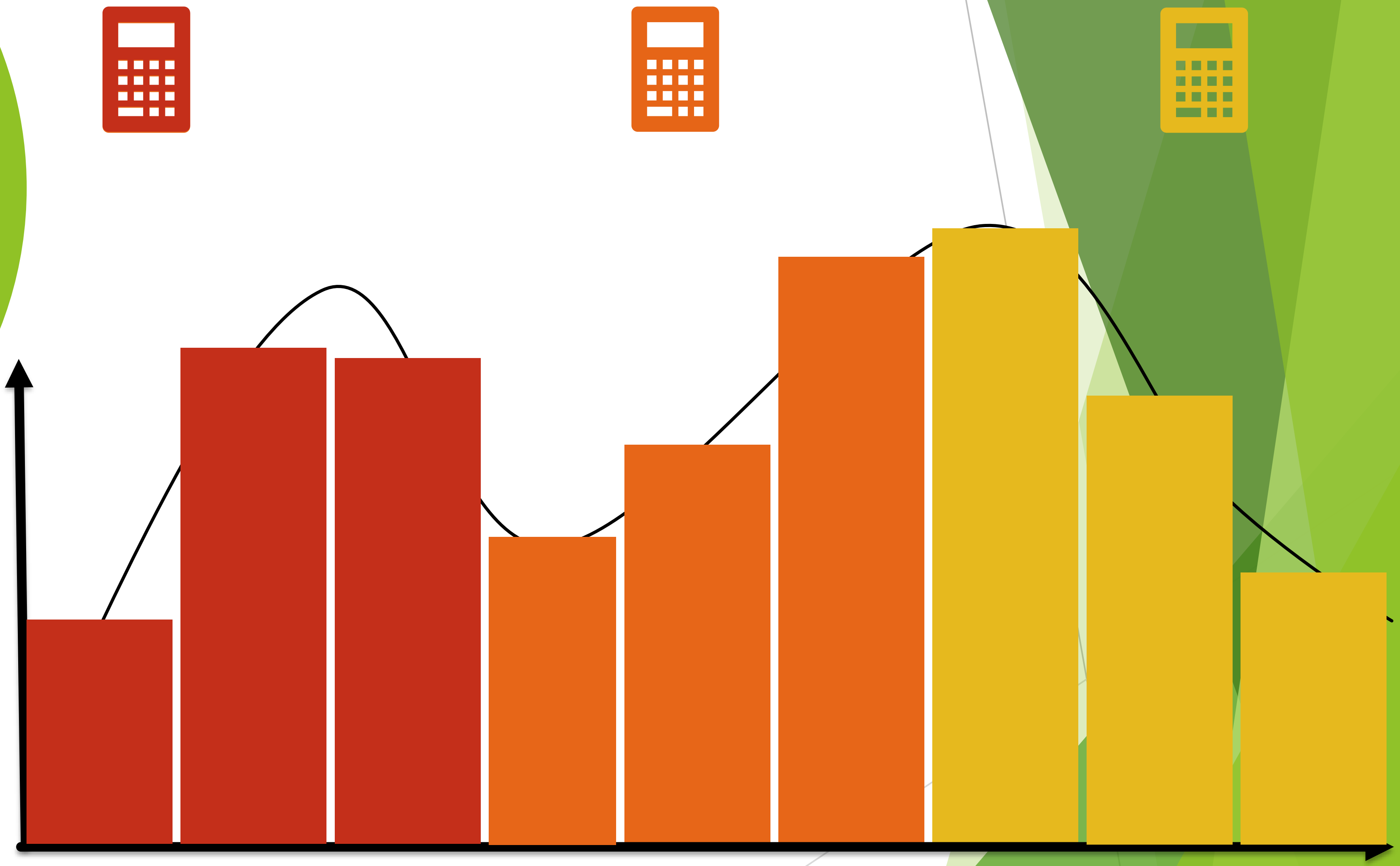
Parallel integral

t =T/2



Parallel integral

$t = T/3$



Parallel integral

t =T/9

Parallel integral

t =T/9

Speed up

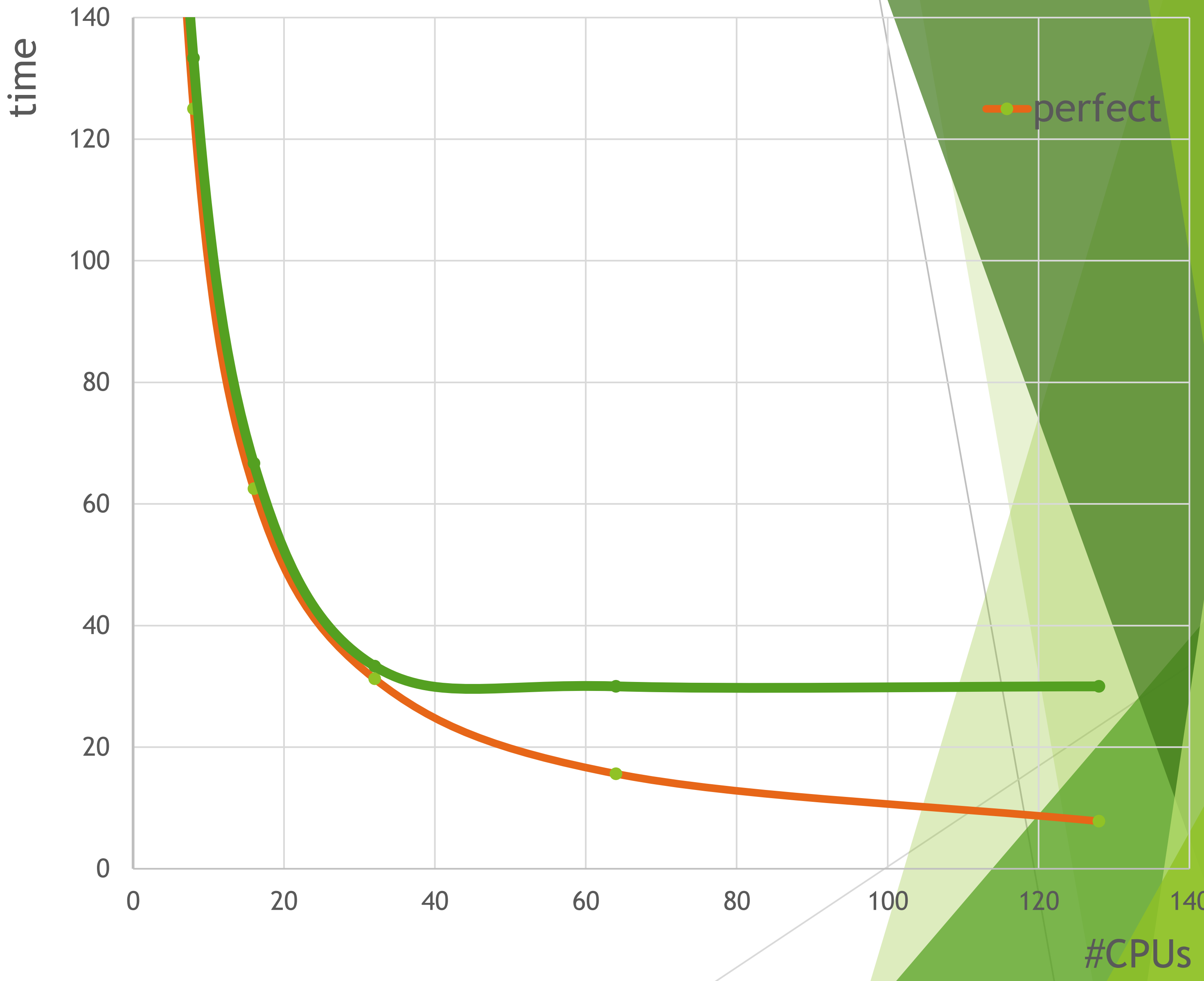
Speed up - the measure of the performance improvement achieved by executing a task on a parallel computing system compared to a sequential or single-processor system.

$$s = \frac{T_1}{T_N}$$

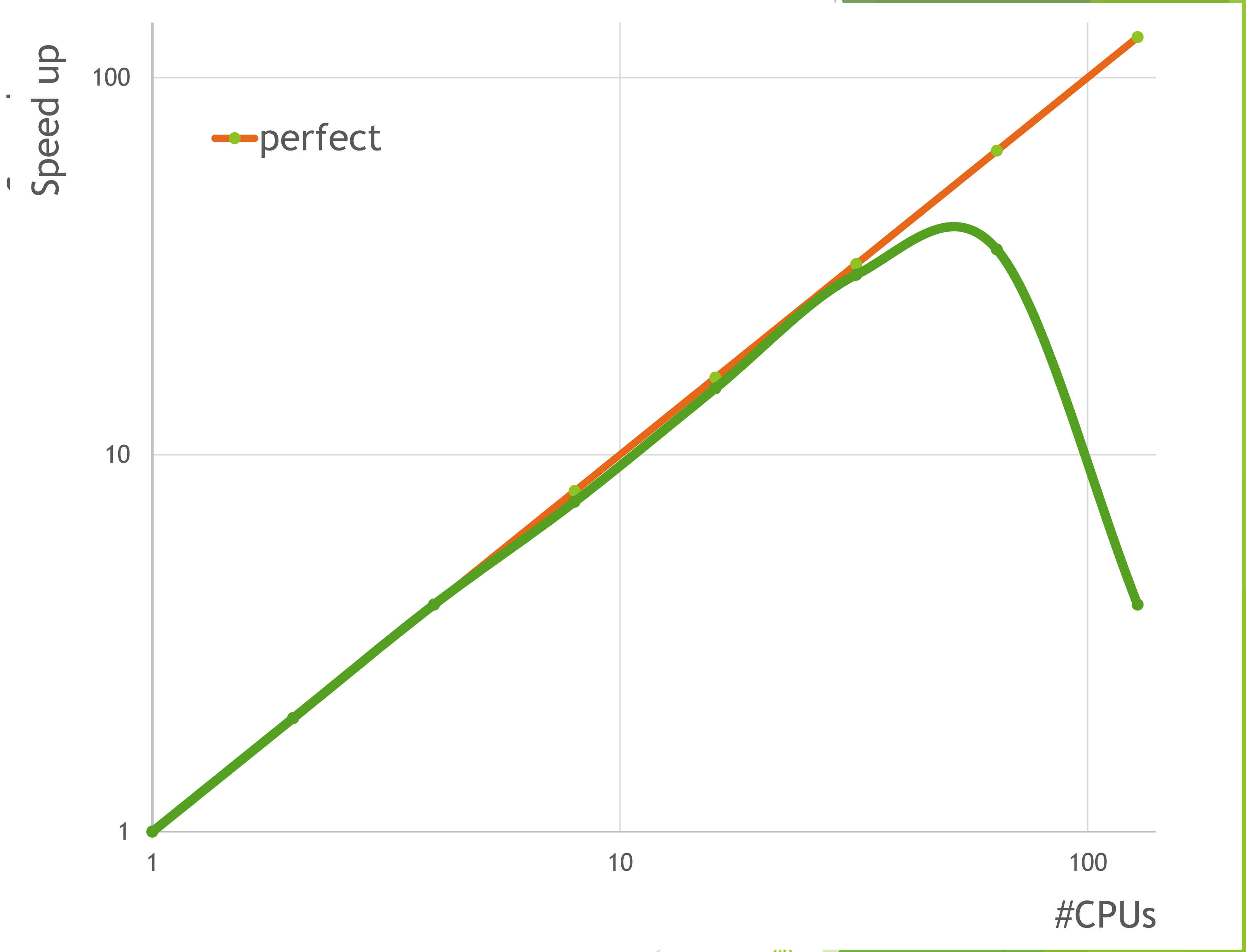
Weak vs strong scaling

- **Weak scaling** is the ability of a parallel algorithm or application to maintain a **fixed** problem **size per processor** as the number of processors increases (as more resources are added, the workload per resource remains constant).
- **Strong scaling** is the ability of a parallel algorithm or application to solve a **fixed-size problem** in less time as the number of processors increases (as more resources are added, the total computation time decreases proportionally).

Scalability time

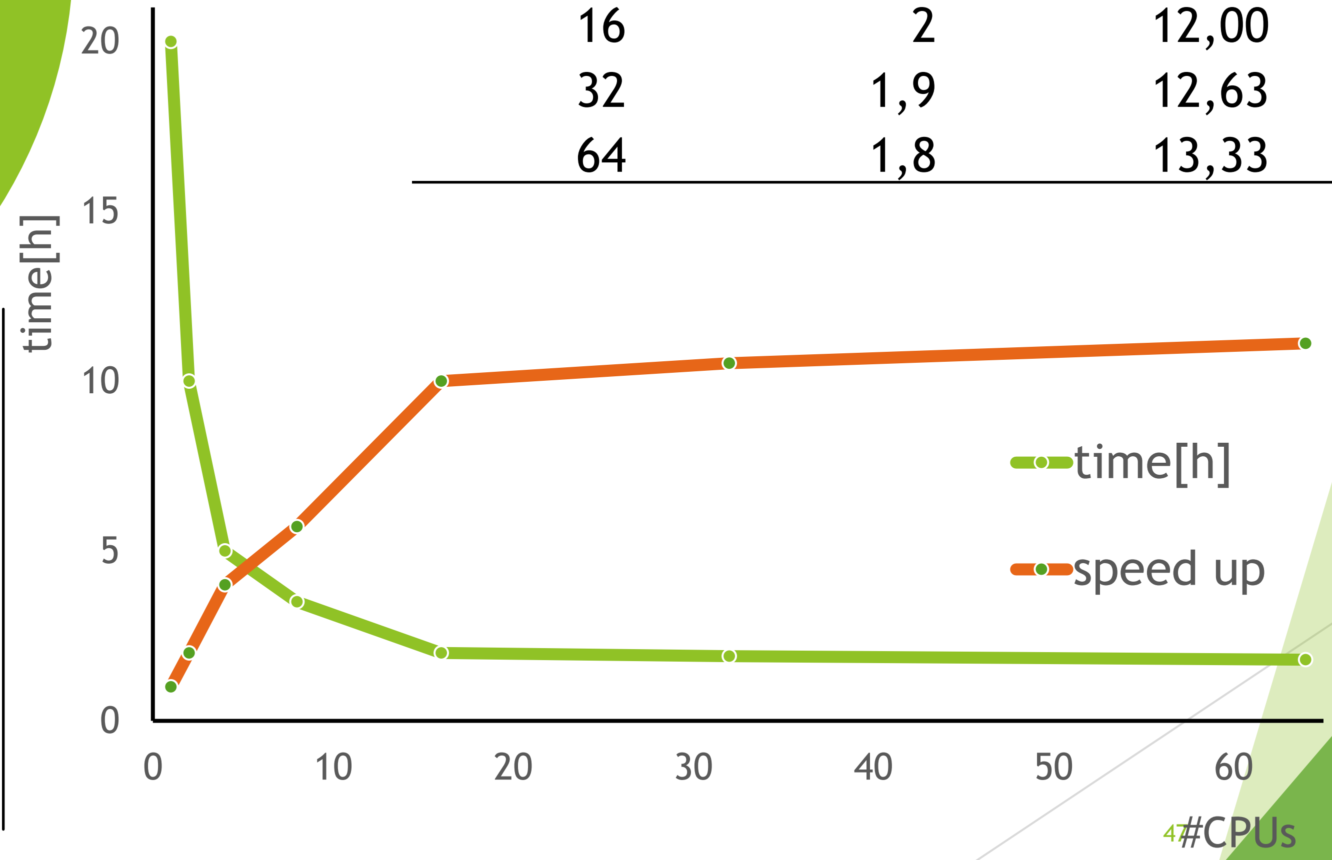


Scalability speed up



Scalability time

#CPUs	time[h]	#jobs per day	#jobs per day on 64 CPUs
1	20	1,20	76,80
2	10	2,40	76,80
4	5	4,80	76,80
8	3,5	6,86	54,86
16	2	12,00	48,00
32	1,9	12,63	25,26
64	1,8	13,33	13,33



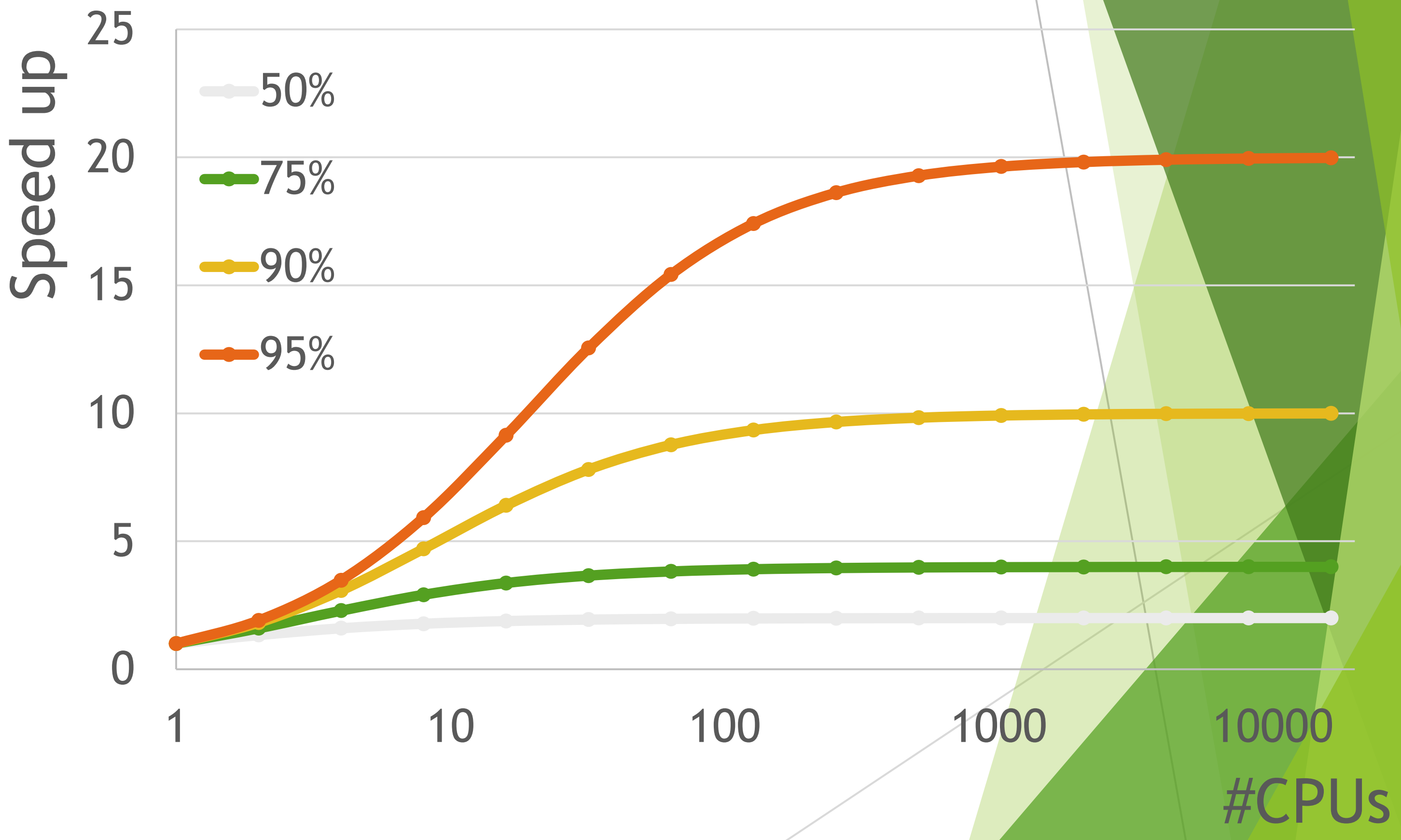
Amdahl's law

$$S_{MAX} = \frac{1}{(1-P)+\frac{P}{N}}$$

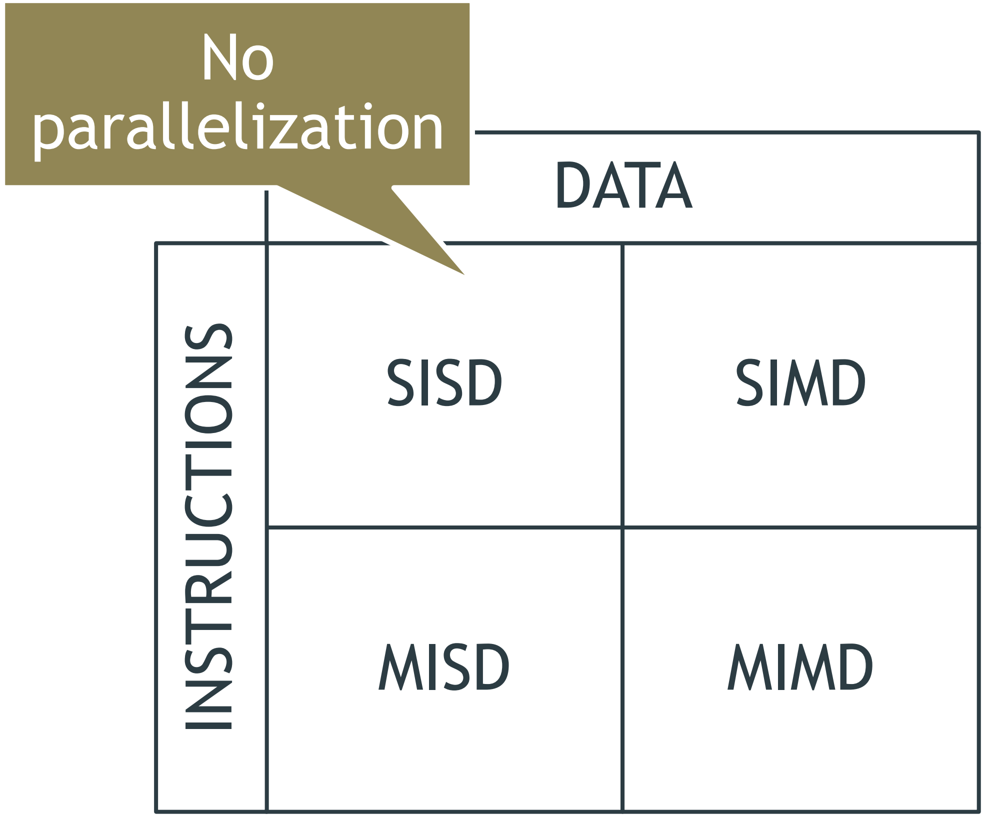
P - Part of the code that can be parallelized

N - Number of CPUs

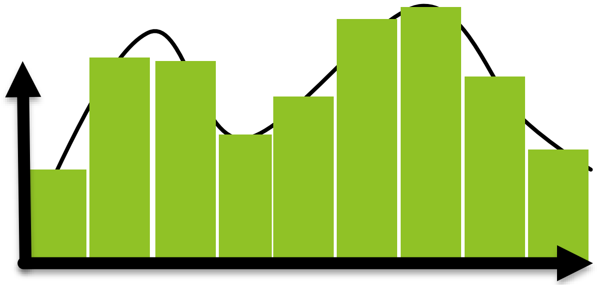
$$s = \frac{T_1}{T_N}$$



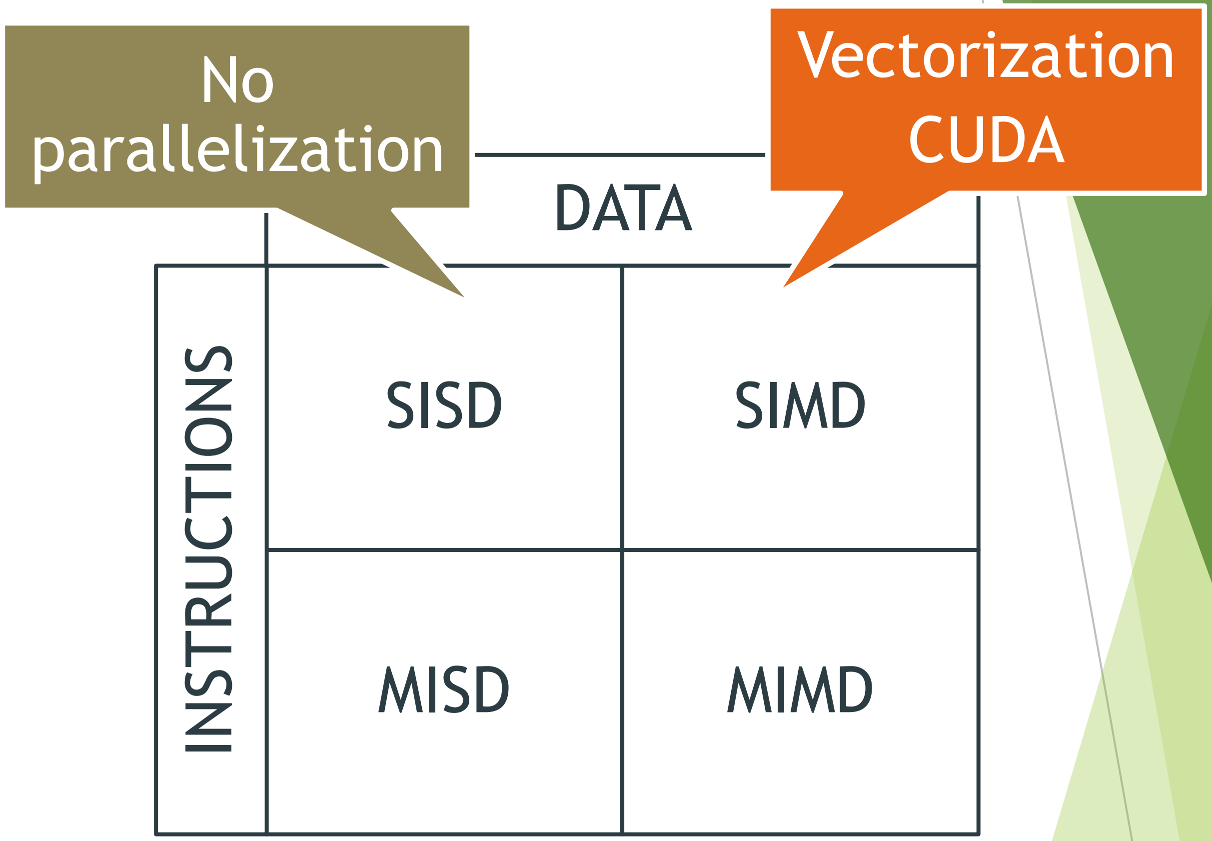
Parallelism models



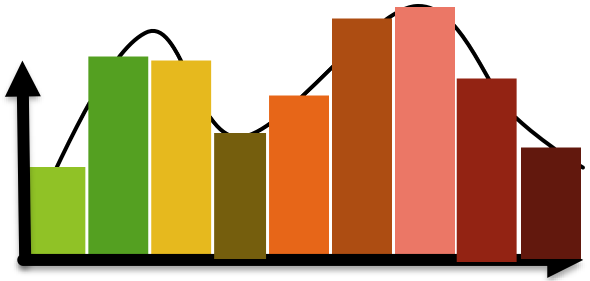
Computing in parallel



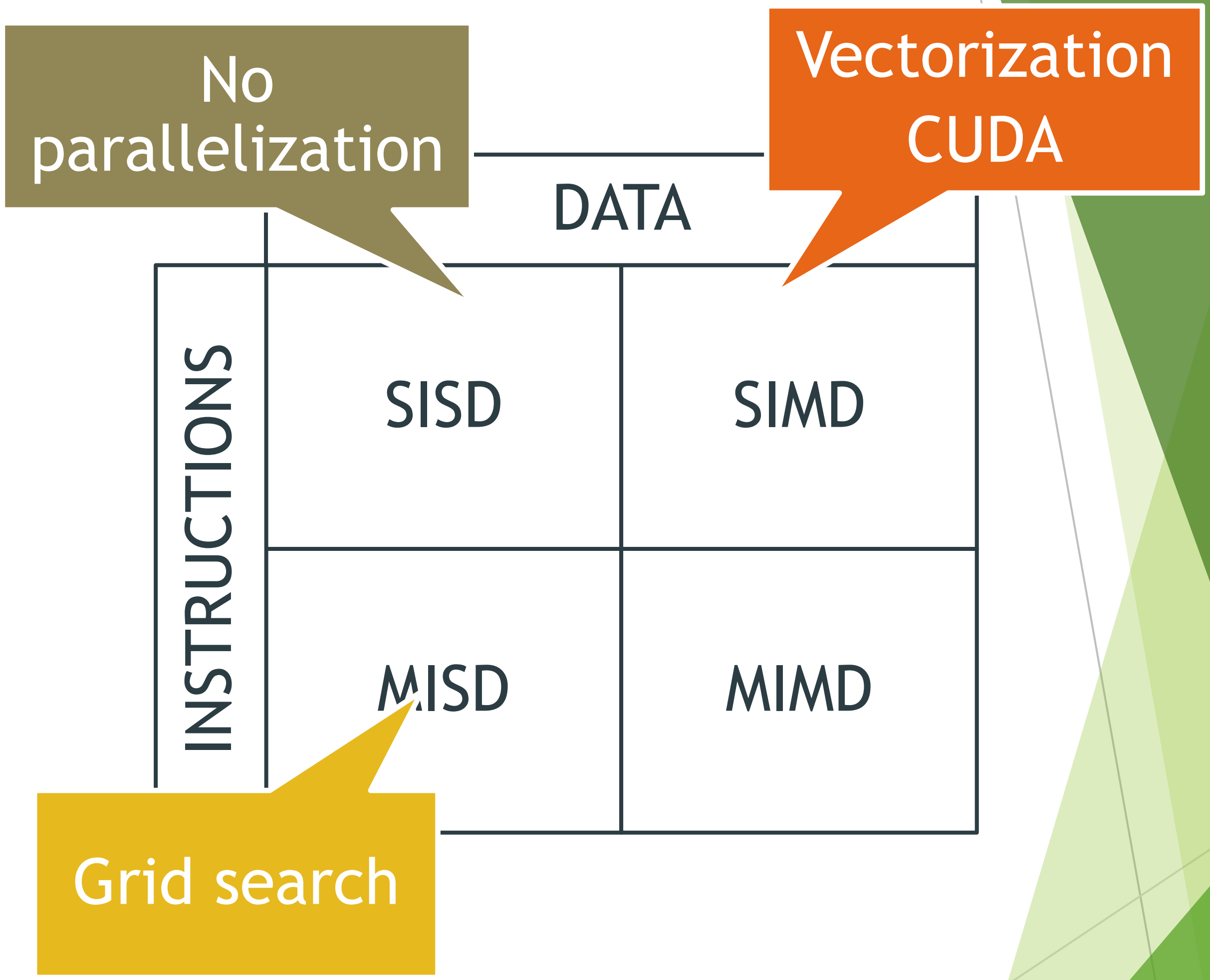
Parallelism models



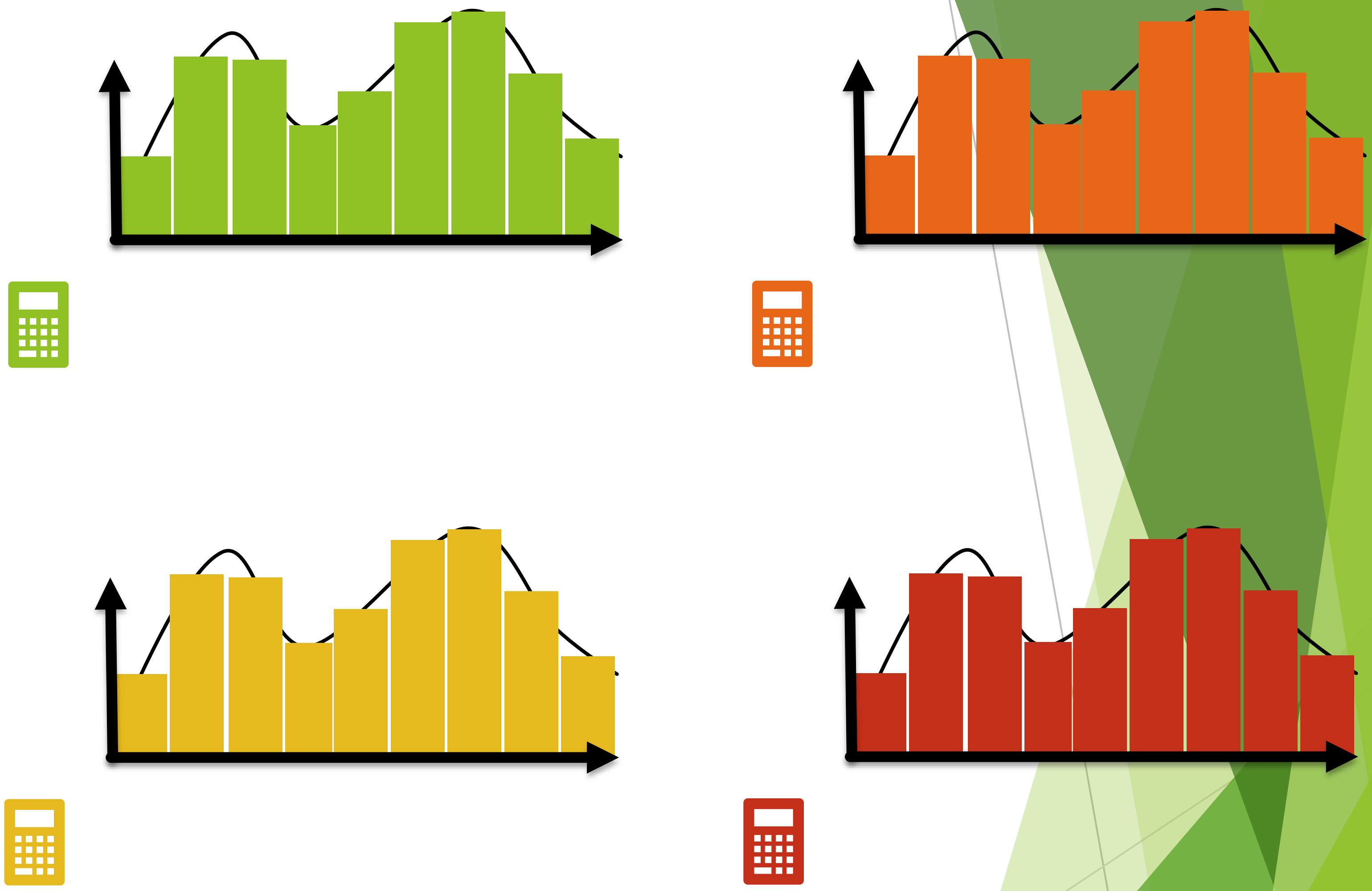
Computing in parallel



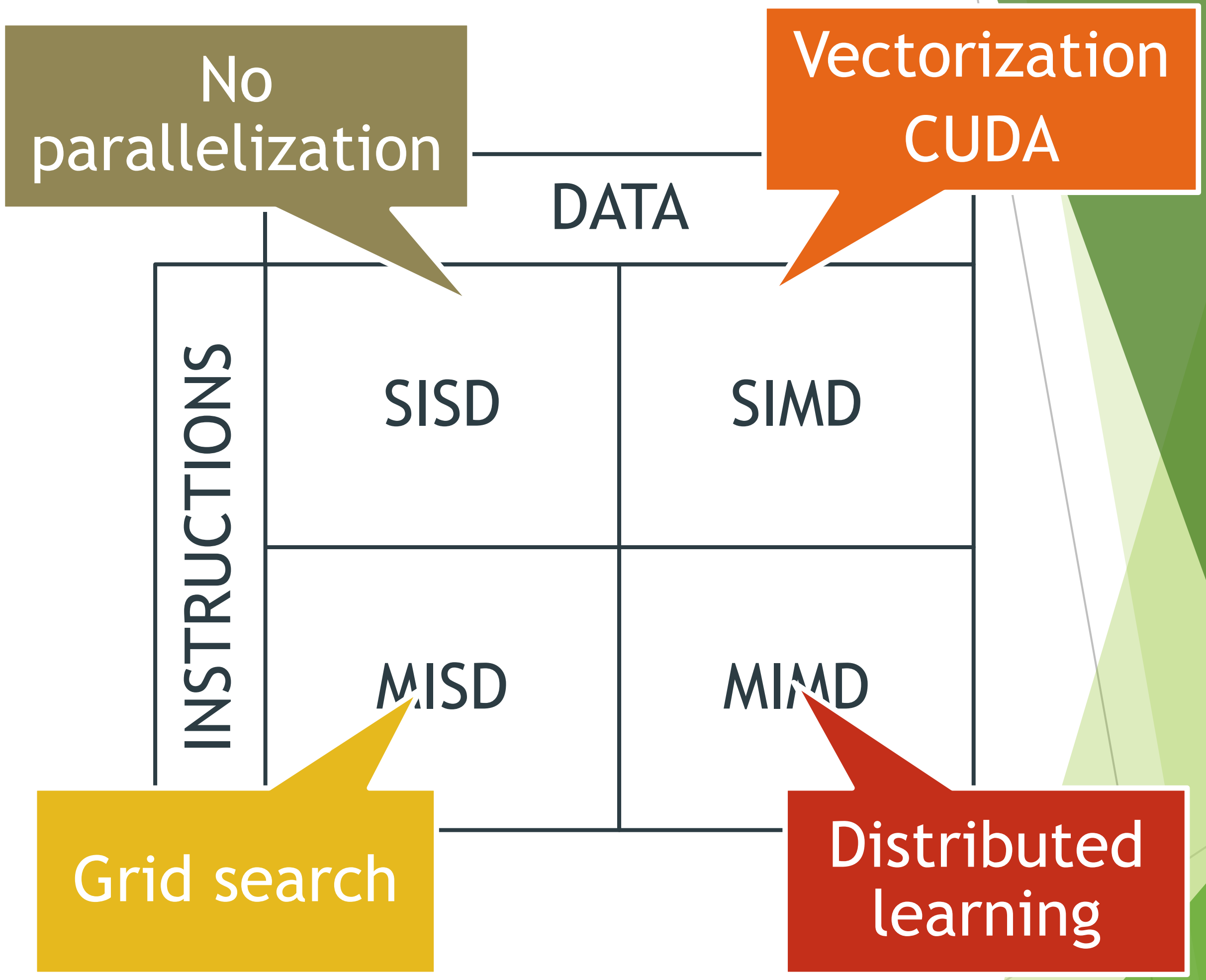
Parallelism models



Computing in parallel



Parallelism models



Computing in parallel