INTRODUCTION TO HIGH-PERFORMANCE COMPUTING (HPC)

11 March 2025 - Guest lecture for HOWEST (Campus Bruges Station)

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whoami

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`@boegel` *(GitHub, Slack)*

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`@boegel.bsky.social` *(BlueSky)*

- Masters (2005) & PhD (2010) in Computer Science from Ghent University
- PhD topic: machine learning applied to software performance, compilers, ...
- Joined HPC-UGent team in October 2010
- **Main tasks: user support & training, software installations, EuroHPC projects**
- Likes family, beer, loud music, FOSS, helping people, dad jokes, stickers, ...
- Doesn't like CMake, SCons, Bazel, TensorFlow, OpenFOAM, ...

LIVE POLL

- A couple of poll questions will be raised during the presentation
- Please join in (anonymously), no login required
- Use your smartphone or browser
- Visit menti.com + use 3706 7451, or scan this QR code:

menti.com (3706 7451)

OUTLINE

- What are supercomputers? What are they used for?
- HPC infrastructure in Flanders
- Important concepts in HPC: multi-core, MPI, Amdahl's law, …
- **Hands-on exercises** on the HPC-UGent infrastructure
- Trends in HPC: GPUs, AI, cloud computing, Intel vs AMD vs Arm vs ...
- Quantum computing in a nutshell

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TERMINOLOGY

- Supercomputer, nodes, processors, cores, interconnect, FLOPS
- High-Performance Computing (HPC), scientific computing
- Parallel computing, shared memory vs distributed memory computing
- OpenMP, threads, MPI, processes, CPUs, GPUs, ...
- Accelerated computing, cloud computing
- Quantum computer, qubits

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POLL

How familiar are you with supercomputing?

- I have no idea what it is, or why I should care.
- I have a vague idea of what a supercomputer is.
- I know what a supercomputer is, but never used one.
- I have used a supercomputer already.
- I frequently use a supercomputer.
- I am an HPC system administrator
- I have my own supercomputer.

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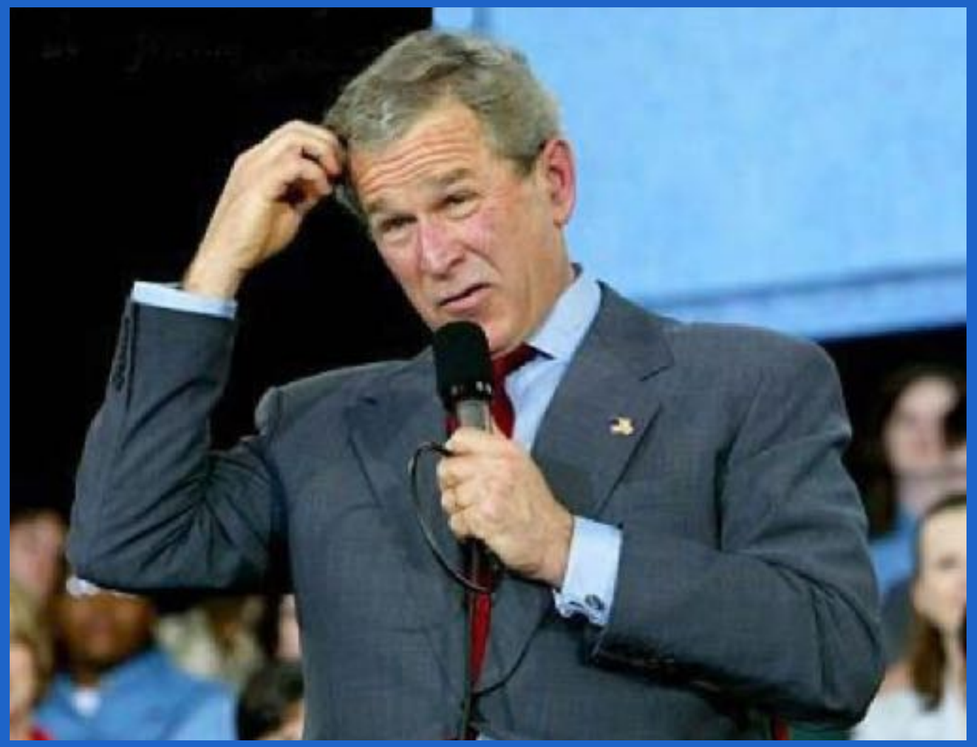

WHAT IS A SUPERCOMPUTER?

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WHAT IS HIGH-PERFORMANCE COMPUTING (HPC)?

Harnessing the power of multiple interconnected cores/nodes/processing units.

"Rack" with desktop PCs in a basement

HPC-UGent Tier-2 infrastructure

LUMI, pre-exascale EuroHPC supercomputer

Finland (2022)

Over 450,000 CPU cores + 12,000 AMD MI250X GPUs

~531 PFLOPS

~145 million Euro

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WHAT IS A SUPERCOMPUTER?

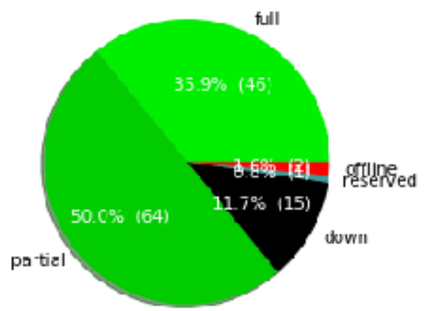
- A bunch of "normal" computers (a.k.a. servers, (worker)nodes, ...)
- **Fast local network** to link them together ("interconnect")
- Large amount of **shared storage**, various types (tape, disks, SSDs, ...)
- Can be considered one big system (in some sense)
- Used for **resource-intensive workloads** (compute, memory, storage, ...)
- Sometimes with special-purpose accelerator hardware (like GPUs)
- Usually in a dedicated (part of a) datacenter

TERMINOLOGY: NODES

- Example cluster from the HPC-UGent

  Tier-2 infrastructure: doduo (default cluster)

- 128 **nodes**, also referred to as “servers”
- 1 node is the equivalent of 1 computer (but with more cores, memory, …)
- Also: compute nodes, worker nodes, …



TERMINOLOGY: CORES, CPUS, PROCESSORS

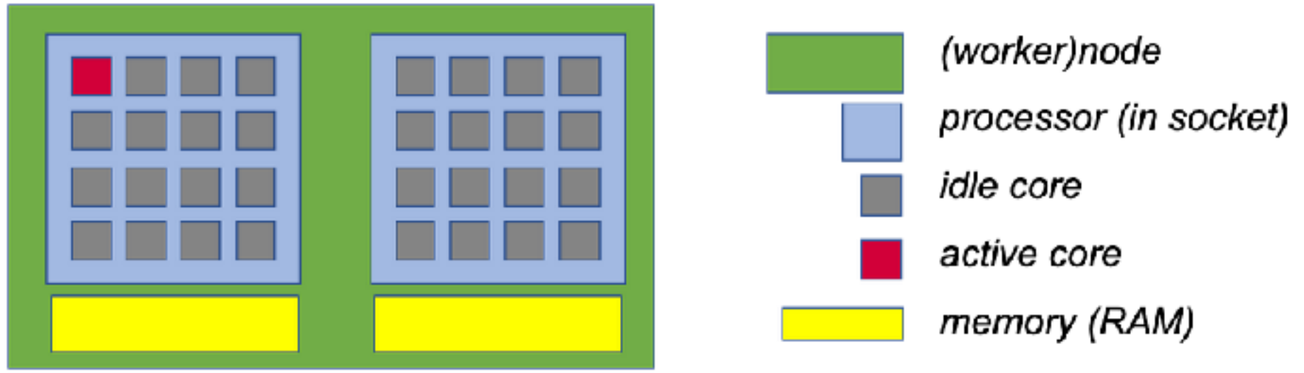
Modern servers, also referred to as **(worker)nodes** in the context of HPC,

include one or more *sockets*, each housing a **multi-core processor**

(next to memory, disk(s), network cards, GPUs, …).

A modern (micro)processor consists of **multiple cores** that are used to perform calculations.

Example:
a single workernode
with two 16-core processors
running a single core job



Not shown here: local disk, network cards, GPUs, …

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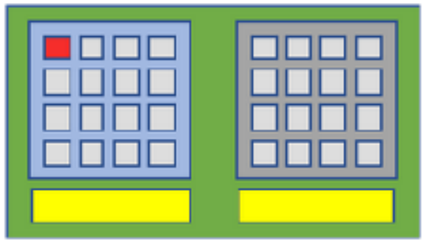
TERMINOLOGY: PARALLEL VS SEQUENTIAL SOFTWARE

Sequential (a.k.a. serial) software does not do calculations in parallel,

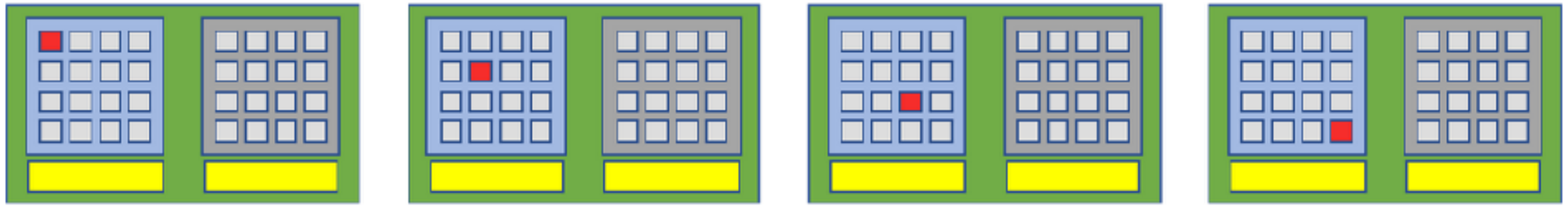
it only uses one **single core** of a single workernode.



This type of software does not run faster by just throwing cores (or nodes) at it...

But, you can run multiple instances of the same program at the same time!

Example: running a Python script 100 times, each on 1 core, to quickly analyse 100 datasets



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TERMINOLOGY: PARALLEL VS SEQUENTIAL SOFTWARE

In **parallel** software, many calculations are carried out simultaneously.

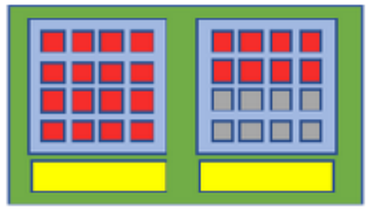
This is based on the principle that large problems can often be divided into smaller tasks,which are then solved concurrently (“in parallel”).

Example: OpenFOAM can easily use 160 cores at the same time to solve a CFD problem.

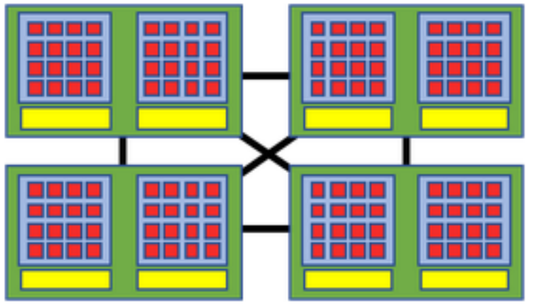
There are two common parallel programming paradigms (among others):

- **OpenMP** for shared memory systems (multi-threading) → using cores of a single node
- **MPI** for distributed memory systems (multi-processing) → using cores of multiple nodes

*OpenMP software can use **multiple cores** in a **single node** by running **threads** that share memory*



*MPI software can use (all) cores in **multiple nodes** by running **processes** that communicate*



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TERMINOLOGY: PERFORMANCE IN FLOPS

- Performance of supercomputers are usually measured in FLOPS:
  (64-bit) floating-point operations per second
  - Example of one FLOP: 1.34 x 54.97 = 73.6598
- Used to create Top 500 list of supercomputers since 1993
- 1 megaFLOPS (MFLOPS): 1 million FLOPS (10^6)
- x1000 each generation: gigaFLOPS, teraFLOPS, petaFLOPS, exaFLOPS
- Current generation of (largrst) supercomputers: in order of **exaFLOPS** (10^{18})

  1 EFLOP = 1,000,000,000,000,000,000 floating-point operations per second

  For comparison: there are about 7.5 x 10^{18} grains of sand on Earth

POLL

Where is the current fastest supercomputer in the Top 500 located?

- Europe
- Russia
- United States
- Japan
- China
- Somewhere else…

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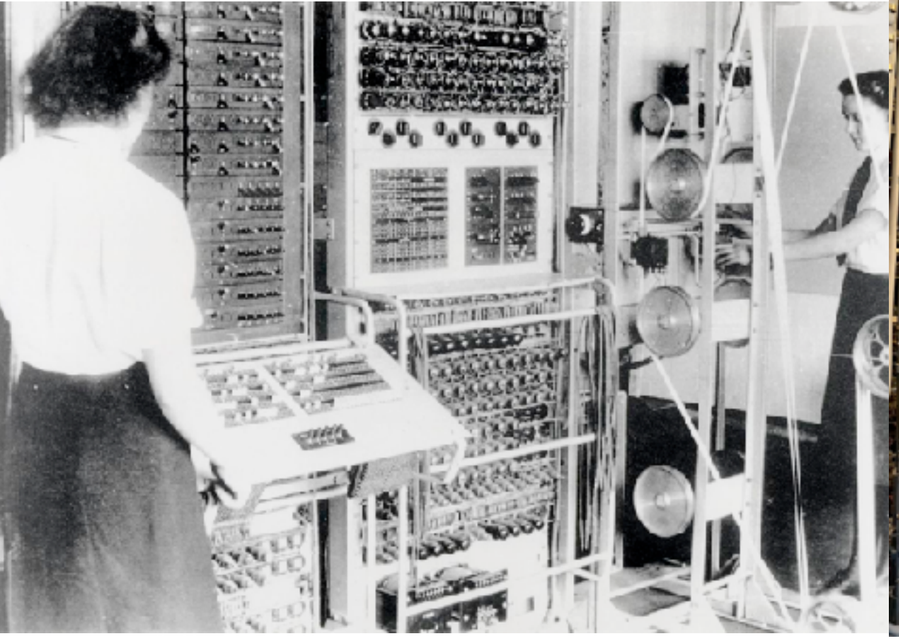
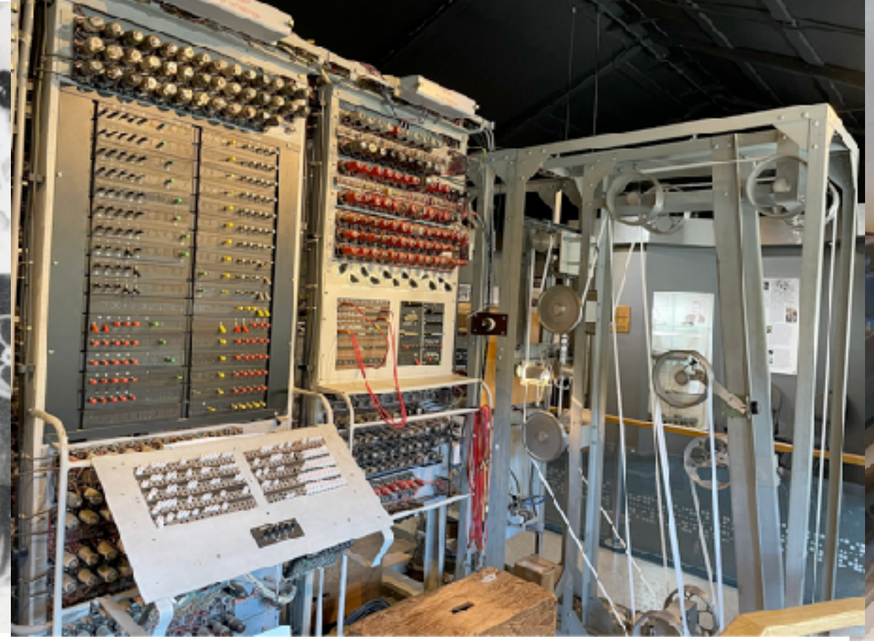
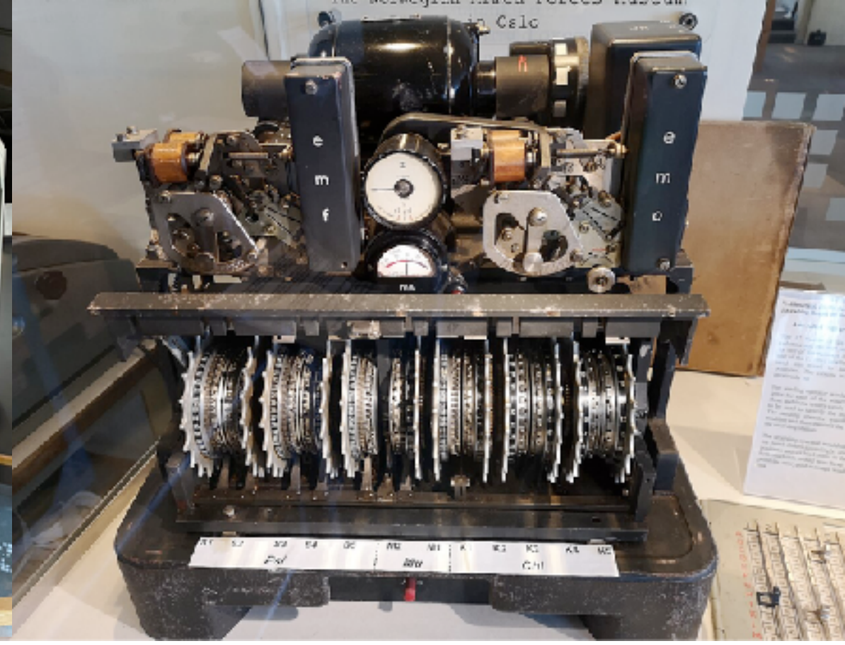

Colossus (1943)

First “digital programmable computer”

Processed ~25,000 characters of input per second (5-way parallel),

no concept of memory or storage yet

Used during WWII in codebreaking (Lorenz cipher)

Existence was secret until mid-1970s

See it at National Museum of Computing @ Bletchley Park

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CDC 6600 (1964)

"first supercomputer"

3 MFLOPS, up to 982 kilobytes of memory

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Cray-2 (1985)

1.9 GFLOPS (first gigascale system)

4 vector processors, 256 MWords of memory

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ASCI Red, US (1997)

1.6 TFLOPS (first terascale system)

9,298 processors (76 nodes)

1,212 GB of RAM memory

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Jaguar, US (2009)

1.75 PFLOPS (first petascale system)

18,688 AMD Opteron nodes (224,256 cores)

360TB of memory, 10PB of storage

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Titan, US (2013)

17.58 PFLOPS - 18,688 nodes (~300,000 CPU cores)

Each node: 16-core AMD Opteron CPU + 1 NVIDIA Tesla GPU

~700TB of memory (CPU+GPU), 40PB of storage

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Piz Daint, Lugano - Switzerland (2016)

~25 PFLOPS

~7,500 Intel Xeon nodes, ~133,000 cores + 5,704 NVIDIA P100 GPUs

8.8 PB shared storage, Cray Aries interconnect

#3 in Top500 (June 2017)

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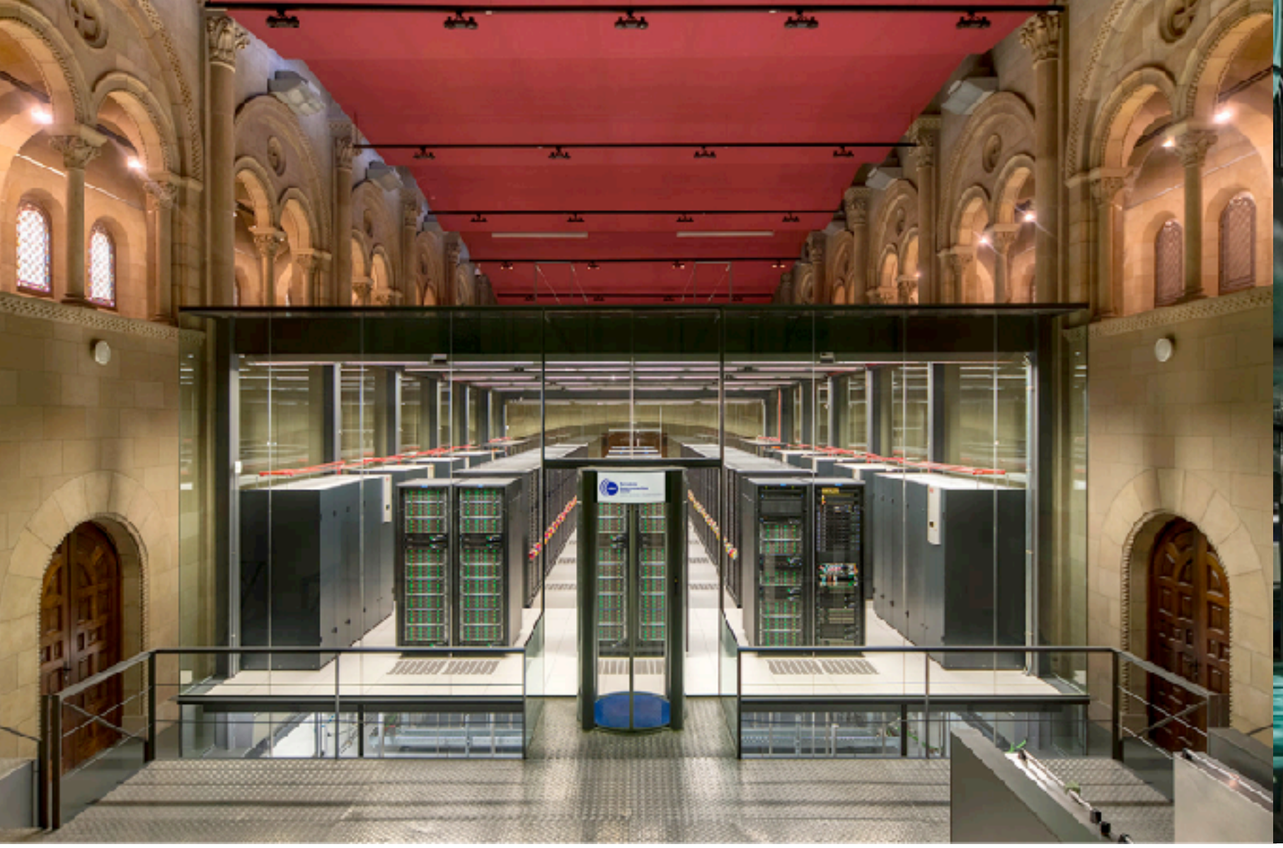

MareNostrum 4, Barcelona (2017)

11.15 PFLOPS , 1.3 MW power

3,456 Intel Xeon nodes (165,888 cores)

14 PB shared storage, Omnipath interconnect

#13 in Top500 (June 2017)

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Fugaku, Japan (2020)

#1 in Top500 in June 2020

158,976 nodes (7.6 million cores), **442 PFLOPS**

Fujitsu A64FX CPUs (Arm 64-bit)

Torus fusion interconnect, 150 PB of shared storage

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El Capitan, US (2024)

Current #1 in Top 500 of supercomputers (Nov'24)

~1 million CPU cores (AMD Genoa) + ~43,800 AMD MI300A GPUs

Slingshot interconnect (12.8 Tbits/sec)

2.75 exaFLOPS (peak)

First exascale system (but actually, not really…)

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NVIDIA V100 GPU (2018)

~$10,000

7.8 TFLOPS

Equivalent with #1 supercomputer in 2000!

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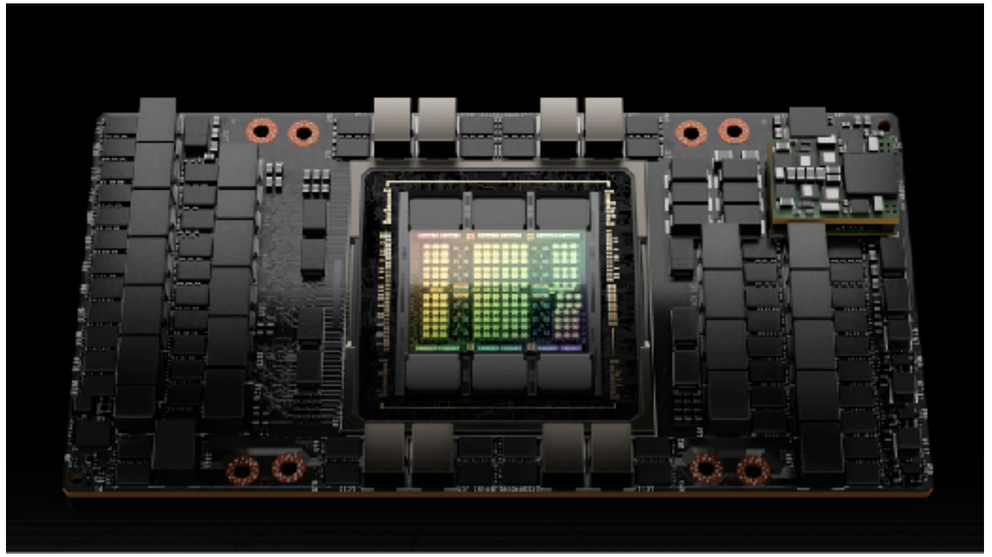

NVIDIA H100 GPU (2023)

~$25,000

34 TFLOPS

Equivalent with #1 supercomputer in June 2004!

iPhone X (2017)

~500 EUR

Includes NPU (Neural Processing Unit) of ~600 GFLOPS

Equivalent with #1 supercomputer in 1996!

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POLL

Where is the fastest supercomputer in Flanders?

- There is none
- Antwerp
- Bruges
- Brussels
- Ghent
- Leuven
- Somewhere else

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EUROPEAN TIERS OF SCIENTIFIC COMPUTING

Tier-0
Europe

Tier-1
Regional / National

Tier-2
University

Tier-3
Personal workstation (desktop, laptop)

EURO

EuroHPC
Joint Undertaking

VLAAMS SUPERCOMPUTER CENTRUM

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HPC-UGent (since 2008)

Current Tier-2 infrastructure:

- 3 CPU clusters, 2 (+1) GPU clusters, 1 debug/interactive cluster
- ~22,000 CPU cores in total, 3 different generations of AMD CPUs
- 76 (+16) GPUs - NVIDIA V100, A100 (+ H100)
- All clusters with Infiniband interconnect
- ~4PB of shared storage in total

https://docs.hpc.ugent.be/infrastructure

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INTERACTIVE DEBUG CLUSTER “DONPHAN”

- 16 nodes, each with 36 CPU cores (Intel Cascade Lake) + ~738GB of memory
  1 shared NVIDIA Ampere A2 GPU (16GB of GPU memory)
- Incl. high-speed network, fast access to shared storage, local disk (NVMe)
- **Heavily oversubscribed!** More running jobs => All jobs run slower (due to CPU sharing)
- **Strict user limits:**
  - Max. 3 jobs running, 5 jobs in queue
  - Max. 8 cores + 27GB of memory in use (in total)
- ⇒ **No waiting time for jobs to start!** Perfect for debug jobs, or interactive use (web portal)

- See also dedicated section in HPC-UGent documentation:
  docs.hpc.ugent.be/interactive_debug

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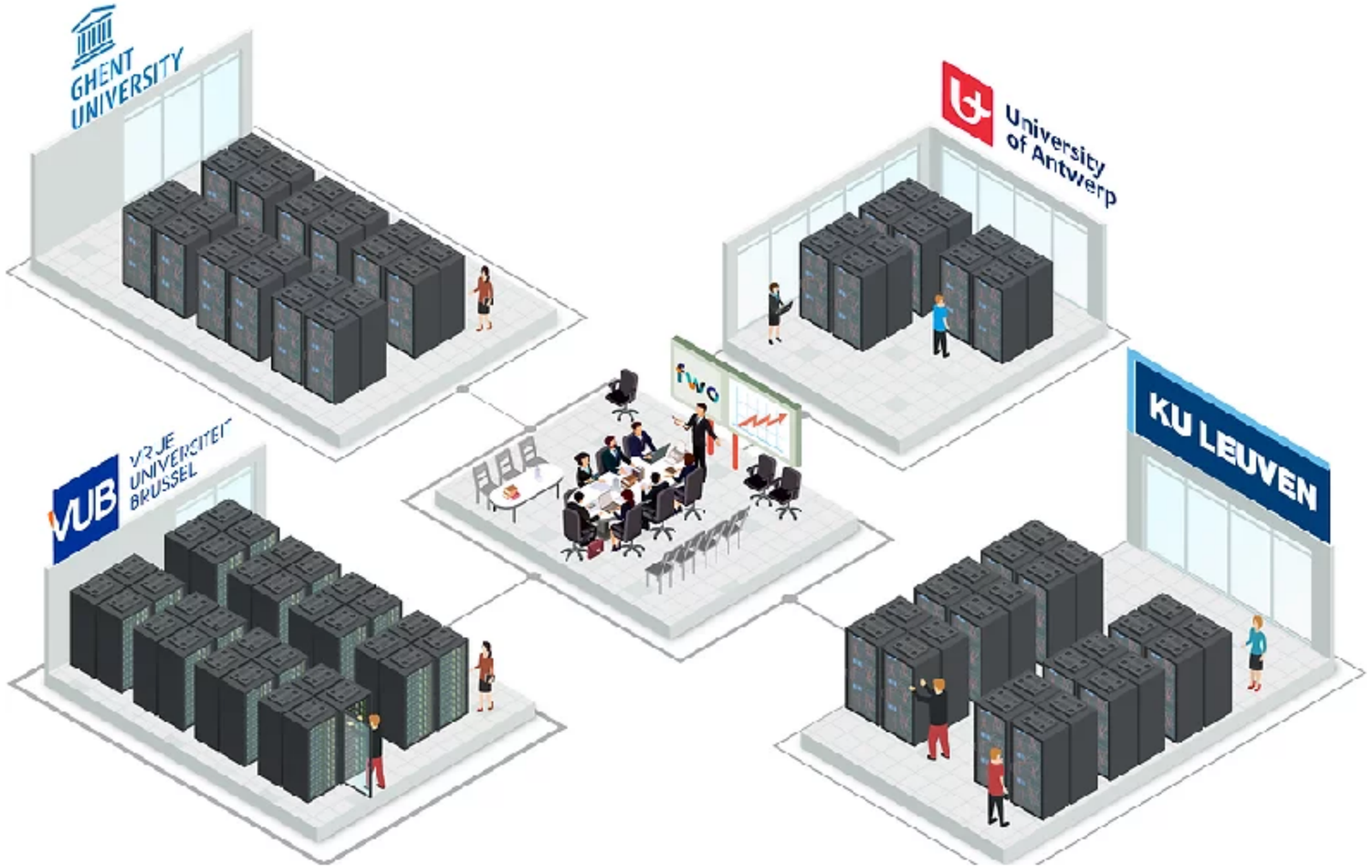
FLEMISH SUPERCOMPUTER CENTRE (VSC)

- Partnership between different Flemish universities
- Virtual centre with hubs in Ghent, Leuven, Brussels, Antwerp
- Shared infrastructure: account management, cloud, Tier-1, ...
- Funded by Flemish governement + universities
- More info: https://www.vscentrum.be

VSC TIER-2 INFRASTRUCTURE



More info: docs.vscentrum.be/compute.html

VSC TIER-1 COMPUTE “HORTENSE”

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- Hosted, operated, and supported by HPC team at Ghent University since 2021
- 2x 384 CPU-only nodes (128-core AMD Rome or Milan CPUs) + 40 GPU nodes (4x NVIDIA A100)
- **Over 100,000 CPU cores + 160 GPUs in total!**
- High-speed Infiniband network (HDR-100) + 6PB of dedicated scratch storage

- Project-based access (free of charge, funded by FWO)
- 3 cut-off dates per year for submitting project proposals
- Project duration is typically 8 months
- 500k - 5M core hours (CPU-only) or 1k - 25k GPU hours

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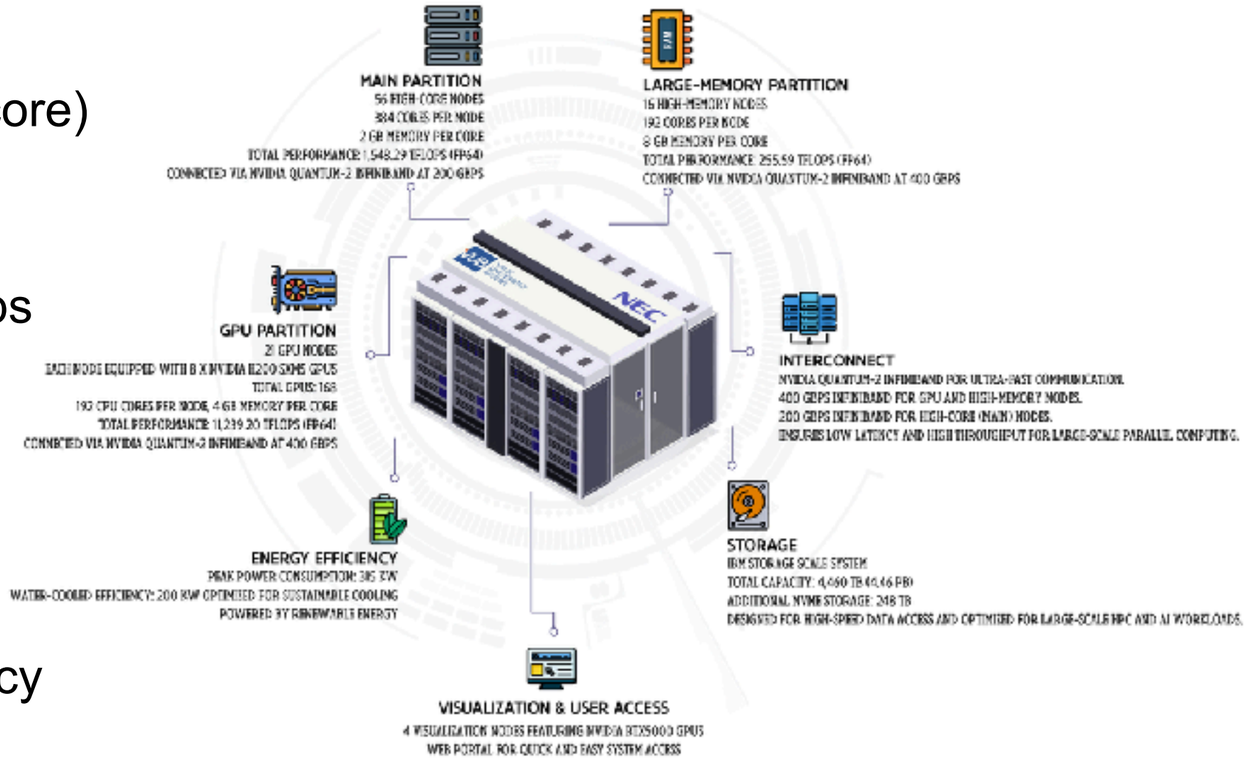
More info: https://www.vscentrum.be/tier-1

NEXT VSC TIER-1 COMPUTE

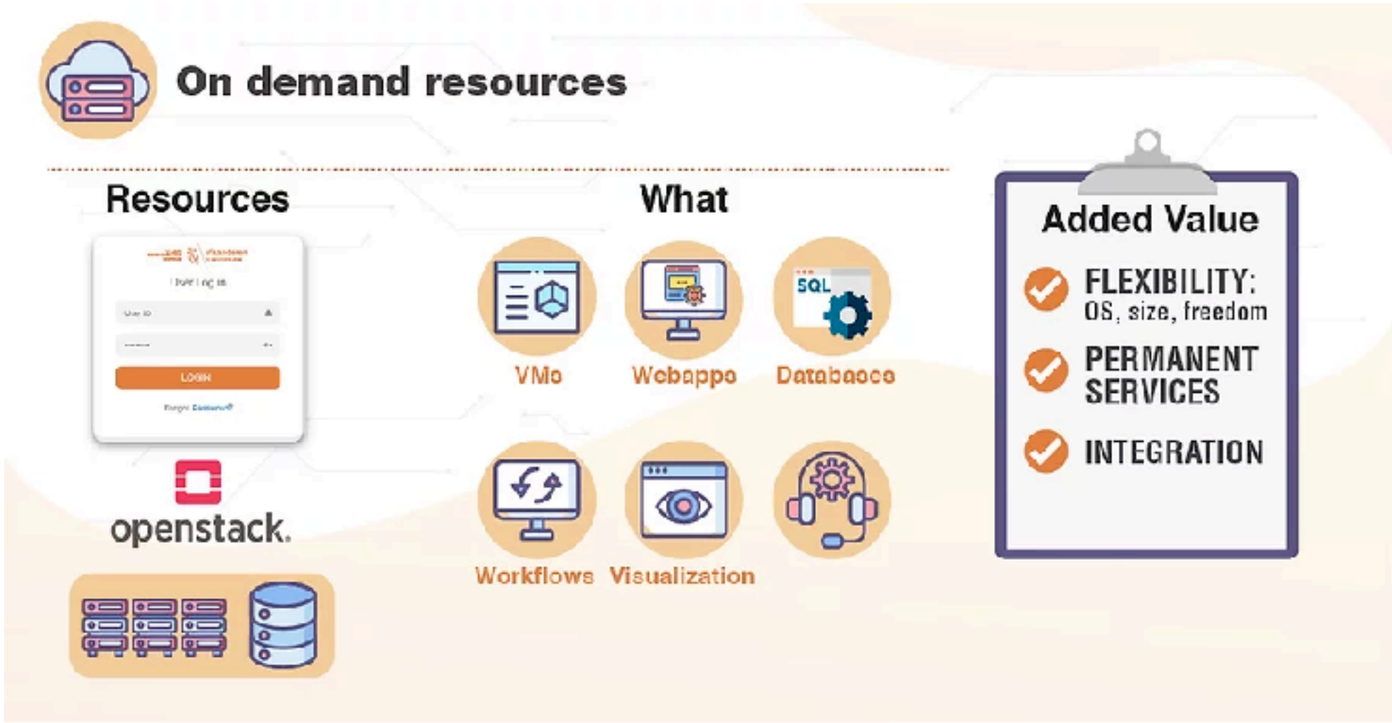
vscentrum.be/post/flanders-invests-in-a-new-supercomputer-to-accelerate-research-and-innovation

- Coming soon (fall 2025) at Green Energy Park in Zellik, operated by VUB
- Investment of 8.6 million Euro
- ~25,000 CPU cores (with 2GB or 8 GB RAM per core)
- 168 NVIDIA H200 GPUs
- NVIDIA Quantum-2 InfiniBand network at 200 Gbps
- 4 visualisation nodes
- 4460 TB of scratch storage + 24 TB NVME
- Peak power consumption of 315 kW,
  200 kW water-cooled for improved energy efficiency



VSC TIER-1 CLOUD

- Private cloud setup for VSC
- Project-based access
- Free of charge
- Self-managed virtual machines
- For use cases that are not a good fit for compute clusters
- More info: vscentrum.be/cloud
- Contact: cloud@vscentrum.be



HIGH-PERFORMANCE COMPUTING (HPC)

- Running **large scale** calculations (on a supercomputer)
- Example: running a physics simulation on 100,000 cores
- Typically heavily relying on fast interconnect, shared storage, ...
- Related:
    - High-Throughput Computing (HTC):

      running **a lot** of (small & short) calculations
    - Scientific computing: simulations, data analysis, machine learning, ...

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EVOLUTION IN SCIENTIFIC COMPUTING: BIGGER, FASTER

Margaret Hamilton (1969)

Standing next to source code she developed for the Apollo moon mission

Katie Bouman (2019)

Showing hard drives that store the data collected to make the first image of a black hole (5PBs = 5000 TBs)

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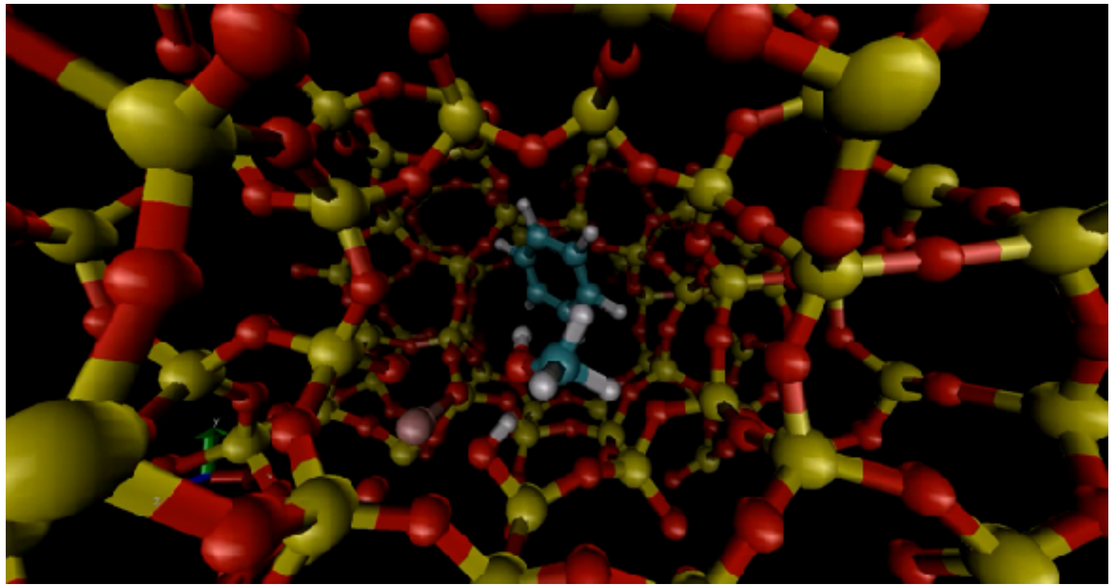
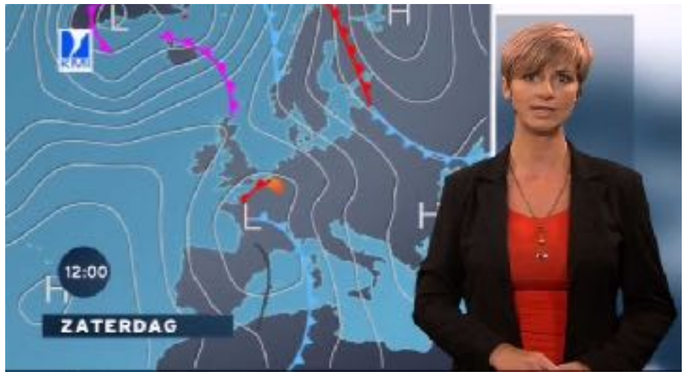
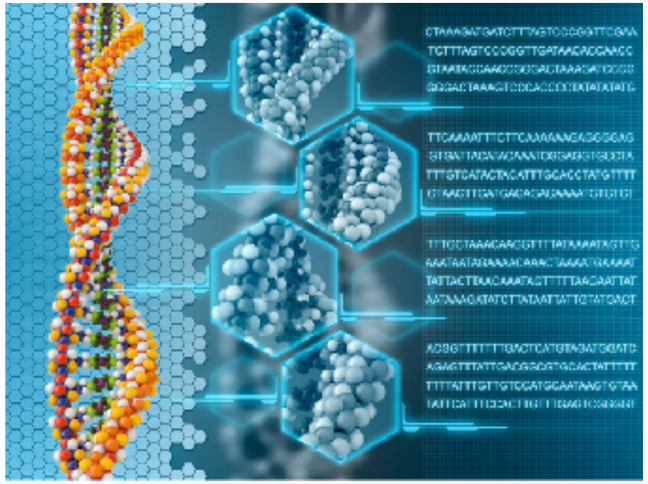
APPLICATIONS ACROSS ALL SCIENTIFIC DOMAINS



Material research (CMM @ UGent)



Weather predictions & climate simulations (RMI)



DNA analysis, for example
in cancer research (CRIG @ UGent)

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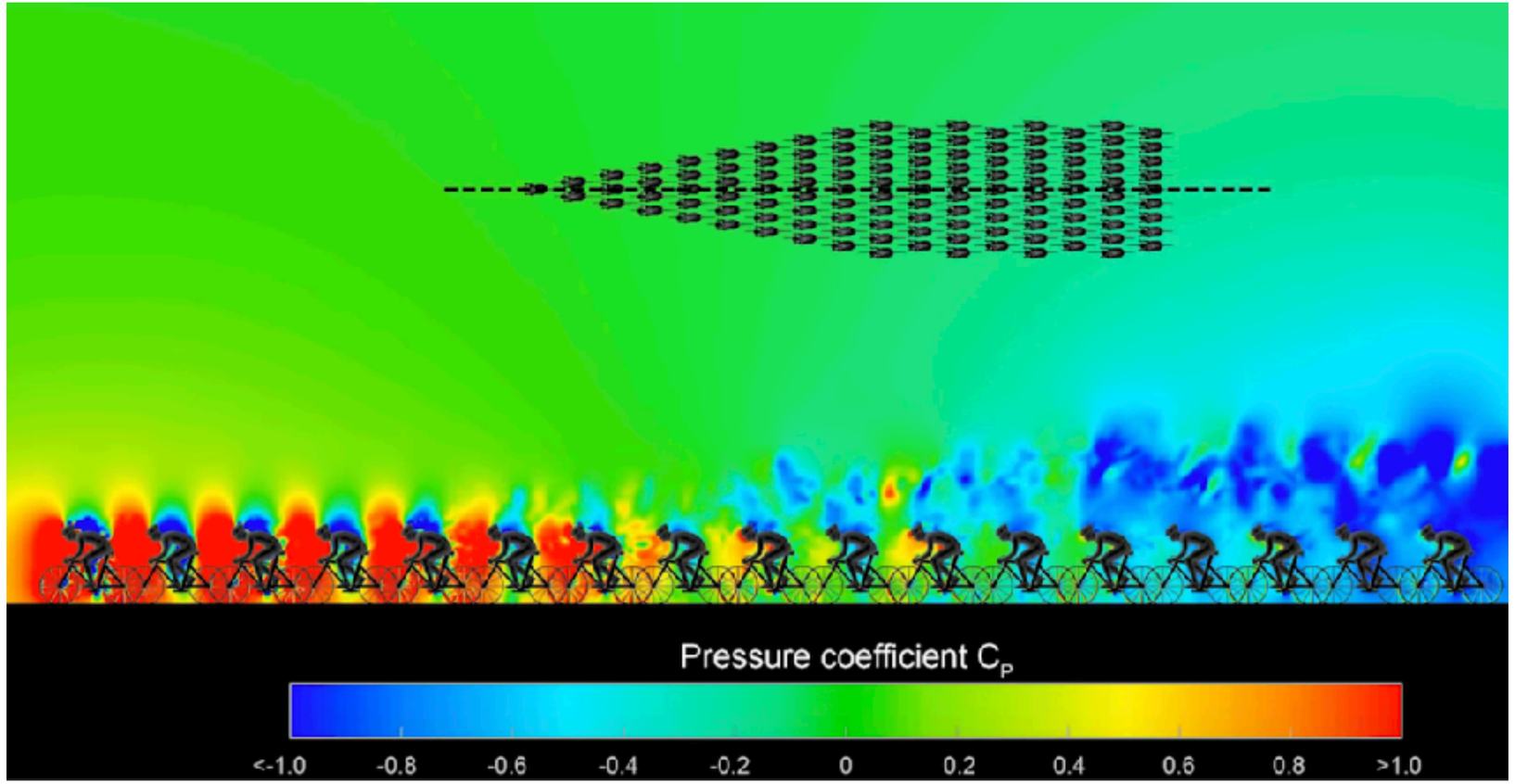
COMPUTATIONAL FLUID DYNAMICS

- Example: determine reduce of drag on riders well embedded in peloton (only ~5-10% compared to drag of isolated rider!)
- "Largest sports simulation to date" (July 2018)



https://www.youtube.com/watch?v=kZBh-fpv2sY

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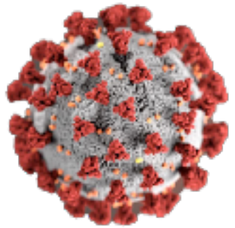
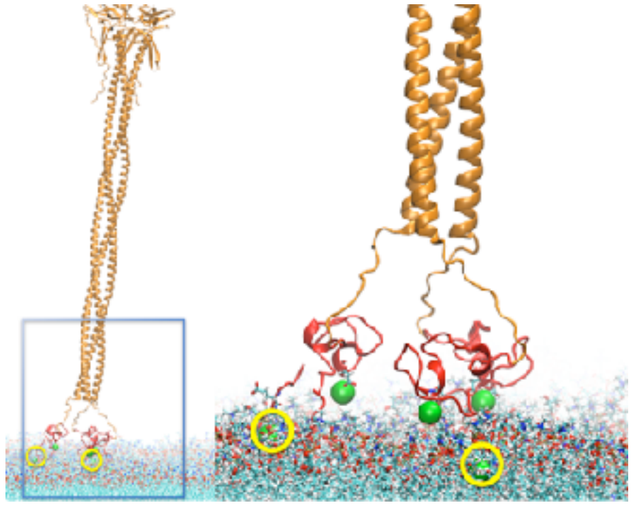
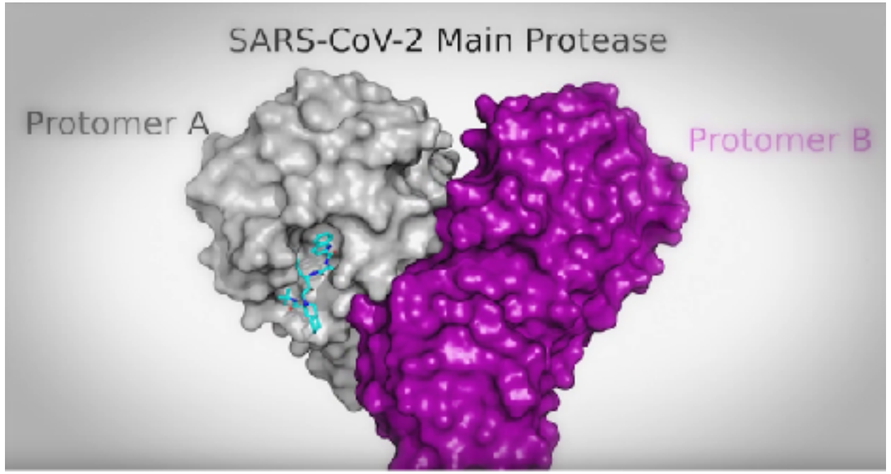
FIGHTING COVID-19 WITH HPC



- **COVID-19 High Performance Computing Consortium** (industry + academia)
- Free access for researchers to some of the largest supercomputers in the world
- ~600 PFLOPS of available compute resources in total
- CFD simulations of airflow in rooms & airplanes to evaluate distribution of particles
- Analysis of virus RNA to trace back how virus was spread, identify variants, ...
- No doubt had positive impact on time-to-market for effective vaccines, drugs, etc.





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https://covid19-hpc-consortium.org - https://www.youtube.com/watch?v=6GQs9M_O95A

TRAINING LARGE LANGUAGE MODELS

- Example HPC workload: training Large Language Models

  For GPT-4o (one of the ChatGPT models):

  - 25,000 NVIDIA A100 GPUs
  - Took 90-100 days
  - Estimated cost: $100 million
  - Energy consumption: ~50 GWh

- Training LLMs requires lots of GPUs *in a single system* (fast interconnect)
- In some sense, LLM training is “just another HPC workload”
- Dedicated “AI Factories” are currently being set up at various EuroHPC sites
  - Supercomputers with specific features (lots of GPUs) + dedicated support for AI workloads

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source: https://chat.deepseek.com - https://seifeur.com/gpt-4-gpu-usage

POP QUIZ

Most popular programming languages in scientific computing?

- Assembly
- C
- C++
- C#
- COBOL
- Delphi
- FORTRAN
- Go
- Java
- Javascript
- MATLAB
- Perl
- PHP
- Python
- R
- SQL
- Swift
- Ruby
- Visual Basic
- ...

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GETTING ACCESS

https://www.ugent.be/hpc/en/access/policy/access

Logging in

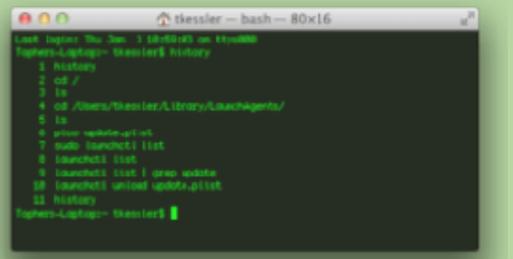
https://login.hpc.ugent.be

Web portal (no SSH key required)

or

ssh login.hpc.ugent.be

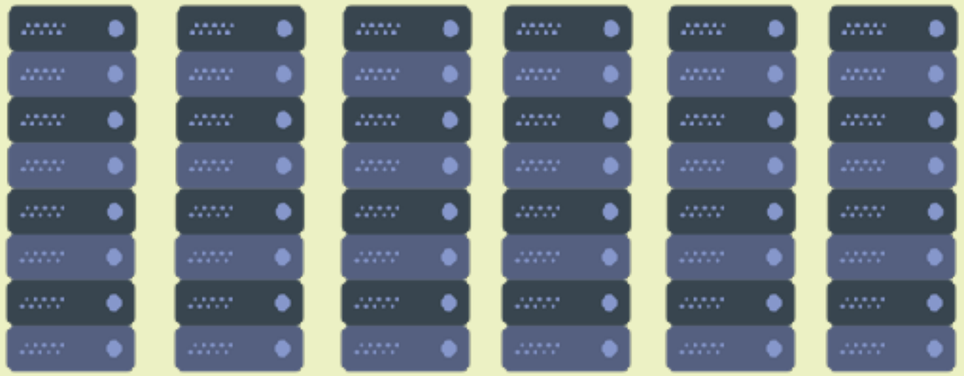
Terminal (requires SSH key)



Login nodes

gligar09 or gligar10

Cluster (worker) nodes



Shared filesystems

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HANDS-ON: LOGGING IN + UP/DOWNLOADING DATA

- VSC accountpage: https://account.vscentrum.be
- Login via HPC-UGent web portal: https://login.hpc.ugent.be
- Login via SSH: `ssh vsc40000@login.hpc.ugent.be`
- Uploading/downloading data via WinSCP, scp, rsync
- Uploading/downloading data via web portal
- Editing files directly on the system (editor in terminal, editor in web portal)

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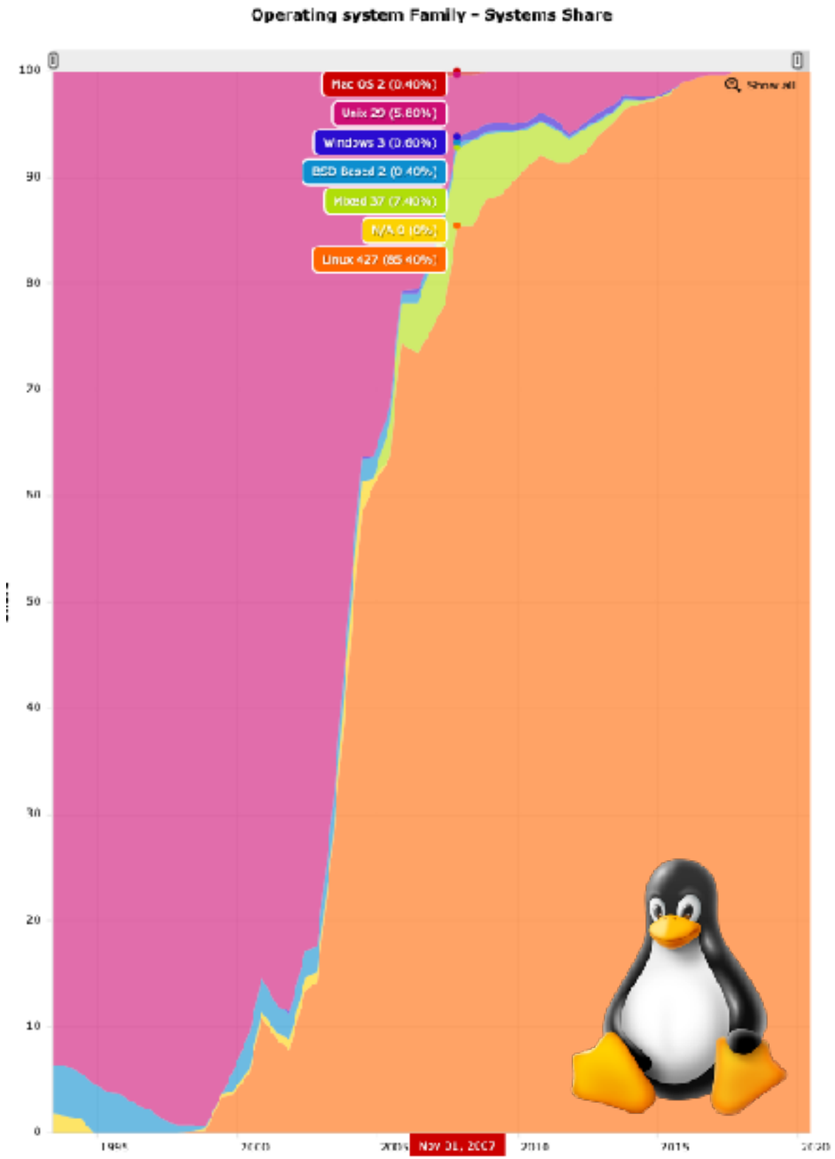
SYSTEM SOFTWARE ON HPC SYSTEMS

https://top500.org/statistics/overtime

- 100% of supercomputers in Top 500 list runs Linux!
- Mix of commercial and open source software on top
- Specific tools & services
  - Shared filesystems (GPFS, Lustre, ..)
  - Job scheduling (Slurm, ...)
  - Environment modules (Lmod)
  - Testing (ReFrame)
  - Custom scripting (Python, ...)
  - Monitoring of systems and services (nagios, Kibana, ...)



SOFTWARE ENVIRONMENT ON TIER-2 + TIER-1 HORTENSE

- HPC-UGent Tier-2 clusters all run **Red Hat Enterprise Linux 9** (RHEL9)
  - Tier-1 Hortense is (for now) still running RHEL8
- Shared filesystems accessible from all login nodes + worker nodes:
  - On Tier-2: IBM Storage Scale (a.k.a. GPFS) for home/data/scratch
  - On Tier-1: Lustre + NFS export of Tier-2 home/data
- Slurm as resource manager (with Torque/PBS frontend)
- Scientific software via environment modules system (via Lmod modules tool)
- Apptainer to run container images

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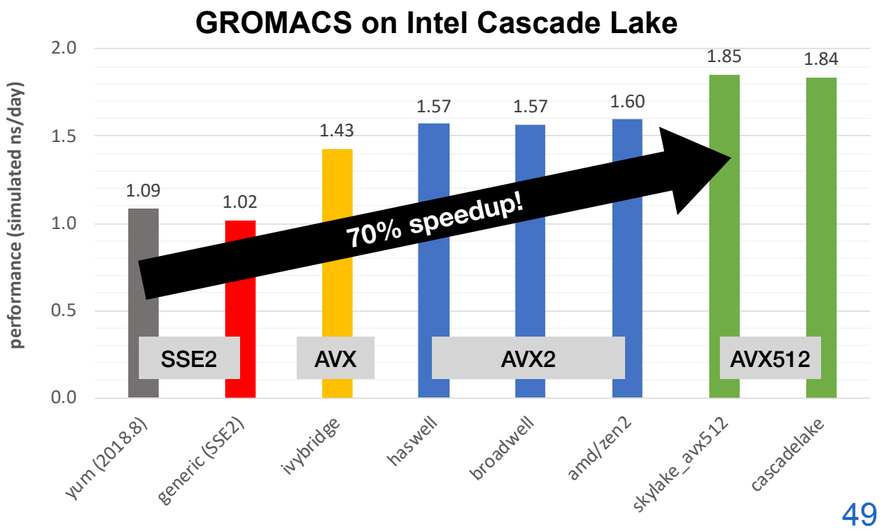
GETTING SCIENTIFIC SOFTWARE INSTALLED

- Scientific software can be difficult to install
  (scientists are often not trained software developers...)
- Ideally built from source code (results in better performance)
- Used to be a very time-consuming, tedious and manual task...
- EasyBuild was created by the HPC-UGent team to **automate** this
- Open source software: github.com/easybuilders
- Implemented in Python
- Now used by hundreds of HPC sites worldwide!

https://easybuild.io



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SCIENTIFIC SOFTWARE MADE EESSI

https://eessi.io

- Getting scientific software installed can be a challenge…
- More and more software is used by researchers
- Diversity in hardware is increasing (Intel/AMD/Arm/RISC-V CPUs, …)
- “Mobily of compute”: from laptop to cloud to HPC systems
- **European Environment for Scientific Software Installations (EESSI)**
  - Stack of optimized installations of scientific software
  - Works on any Linux system (incl. WSL in Windows, Linux VM on macOS, …)
  - “Streaming software”: what’s needed is downloaded on demand (like Netflix, Spotify)

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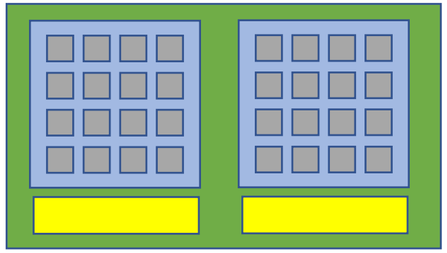
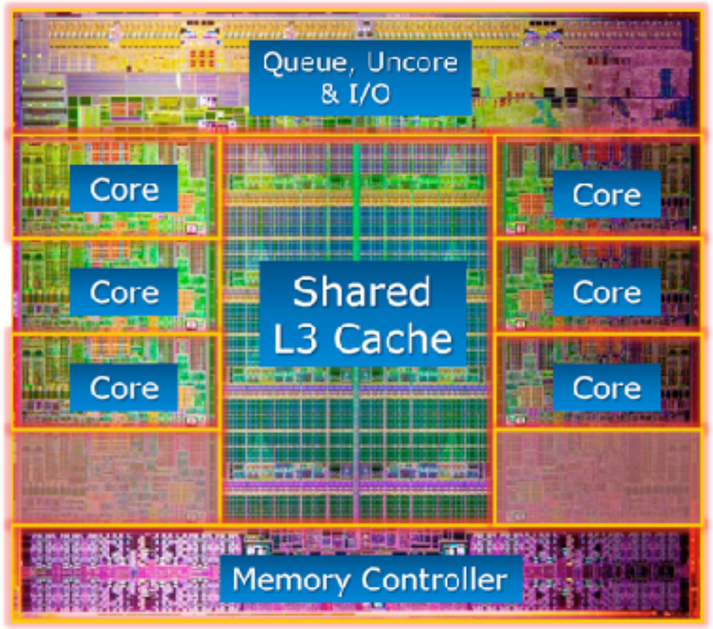
MODERN MULTI-CORE PROCESSORS

- CPU (central processing unit) a.k.a. (micro)processor
- **Multiple cores** to run multiple computations in parallel
- Hierarchy of small (~MBs) but (very) fast on-chip *cache* memory
- Channels to access memory & co
- Typically 2 multi-core processors per node
  (each housed in a *socket*)
- Simplified view (2x 16 cores):





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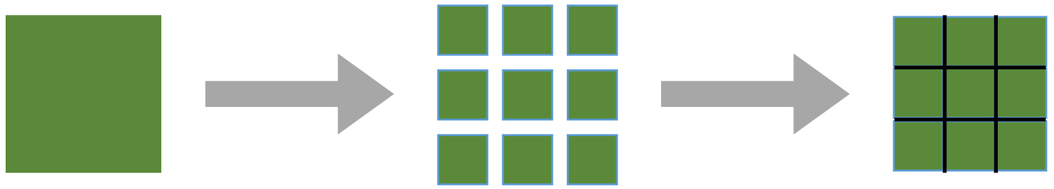
PARALLEL COMPUTING



- Long-running calculations can be done faster through **parallelization**
- Split up large problem into smaller problems, divide and conquer
- Challenge is to **keep all cores busy** (doing useful work)
  - Avoid *bottlenecks*: slow memory/disk, network latency, limited bandwidth
  - Avoid *load imbalance:* waiting for longest running part to be done
  - Avoid *overhead* (extra work) in breaking up problem + composing final result

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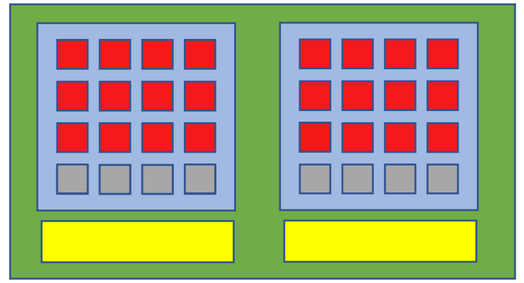
SHARED MEMORY PROGRAMMING

- **Intra-node** parallel computing: using multiple *threads* **on a single node**
- Each thread runs calculations on 1 core
- Communication between threads via shared data structures in memory
- Limited to resources available in a single node (cores, memory, ...)
- Care must be taken when writing to shared data structures (use of locks)
- Typical programming paradigm: OpenMP

```
#pragma omp parallel for
for(int x=0; x < width; x++){
    ...
}
```



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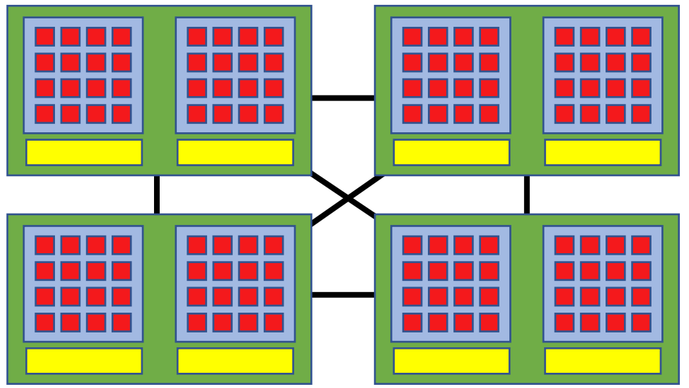
DISTRIBUTED MEMORY PROGRAMMING

- **Inter-node** parallel programming: using cores in **multiple nodes**
- Multiple instances of same software are started (*processes, ranks*)
- Coordination by exchanging messages (who does what, partial results, ...)
- Fast interconnect is *crucial* if a lot of *communication* is needed to coordinate
- Typical programming paradigm: Message Passing Interface (MPI)

```
MPI_Send(...)
MPI_Recv(...)
```

- *Hybrid* parallel programming (OpenMPI + MPI): multiple processes, each with multiple threads



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AMDAHL'S LAW

$$speedup(c) = \frac{1}{(1-p) + \frac{p}{c}}$$

c: number of cores

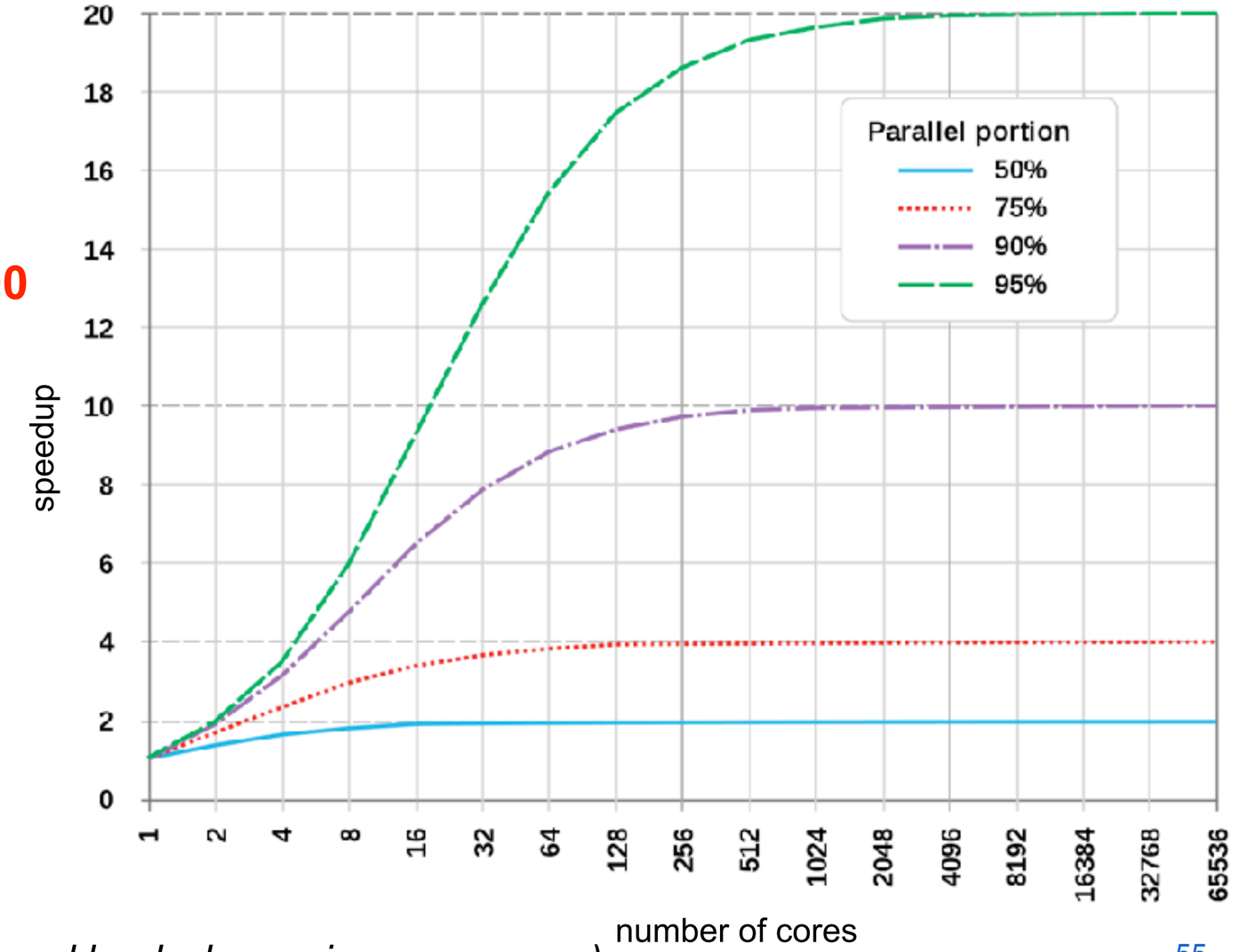
p: parallel portion ([0, 1])

Examples:

- p = 0.5, 2 cores → speedup = 1.33
- p = 0.5, 64 cores → speedup = 2
- **p = 0.99, 1 million cores → speedup = 100**

Assumptions:

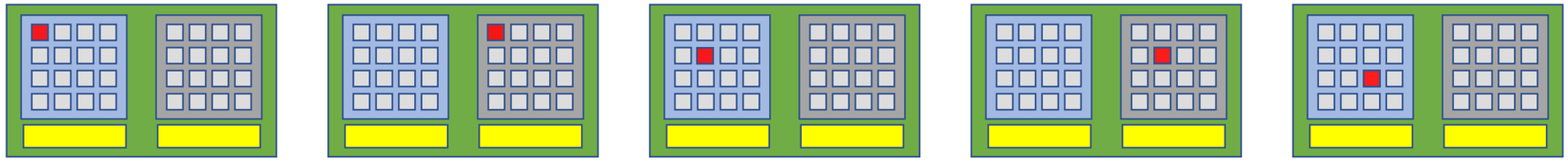
- Fixed workload (strong scaling*)
- Parallel portion is *perfectly* scalable
- No bottlenecks, overhead, etc.



(weak scaling: increase workload when using more cores)*

EMBARASSINGLY PARALLEL TASKS

- What if you need to run a lot of very small (single-core) calculations?
- a.k.a. High-Throughput Computing (HTC)
- Only uses part of available resources (no need for fast interconnect or shared storage)
- Same software can be started multiple times within a single job
- Each instance is running independent of the others (no communication between them)
- Tools: worker, GNU parallel, dask, ...



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PROGRAMMING LANGUAGES IN SCIENTIFIC COMPUTING

(back in top 20 of programming languages, currently #11)

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ACCELERATED COMPUTING

- Some type of calculations can benefit from special-purpose hardware
- Prime example of these ***accelerators*** are GPUs
- Originally created for detailed video game rendering

- Now also GPGPU: General Purpose Graphics Processing Unit
- Programming paradigm: CUDA, OpenCL, OpenACC, ...
- Difficult to use efficiently: separate GPU memory, lots of tiny cores, ...
- Potentially spectacular speedup: ~10-100x (but not for everything...)

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SUBMITTING AND MANAGING JOBS

- HPC-UGent clusters run **Slurm** as resource manager + job scheduler
- **Torque (PBS) frontend is (still) available and recommended** (via *jobcli* project)
  - `qsub` command to submit jobs, `qdel` command to delete jobs
  - `qstat` command to list queued + running jobs
  - `qalter` command to change jobs (before they start running)
  - `qhold` command to put jobs on hold, `qrls` to release them again
- Use `--help` option to get list of available options for each command
- Use `--debug` option to get more information about what's going on behind the scenes
- Use `--dryrun` option to inspect what will be done (without actually doing it)

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HANDS-ON: INTERACTIVE JOB

- Start an interactive job via **`qsub -I`** `# dash capital I`
- Make sure you are targetting the debug/interactive cluster!

  First run: **`module swap cluster/donphan`**
- Try running a small Python script (Hello World) in the interactive job
- What do you notice in terms of environment in which you're working?
- To stop the session, run the `exit` command

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WHAT IS A JOB SCRIPT?

```
#!/bin/bash
echo "I am a minimal job script"
```

A job script is (bash) shell script, a text file that includes shell commands, that specifies:

- The **resources** that are required by the calculation
  (number of nodes & cores, amount of memory, how much time is required, …)
- The **software** that is used for the calculation (usually via `module load` commands)
- The steps that should be done to execute the calculation (starting from home dir.),
  specified as **shell commands**, typically:
  - 1) Staging in of input files
  - 2) Running the calculation
  - 3) Staging out of results

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REQUIRED RESOURCES VIA #PBS DIRECTIVES

```
#!/bin/bash
#PBS -N solving_42              # job name
#PBS -l nodes=1:ppn=4           # single-node job, 4 cores
#PBS -l walltime=10:00:00       # max. 10h of wall time
#PBS -l vmem=50gb               # 50GB of (virtual) memory required
# rest of job script goes here ...
```

- Required resources can be specified via `#PBS` lines in job script
- Or via options to job submission command (`qsub -l ...`)
- **Maximum walltime of jobs on HPC-UGent clusters: 72 hours (3 days)**
- For longer calculations: break it up in shorter jobs, use a different (faster) cluster, use more cores (if software scales), use some form of “checkpointing”, …

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CENTRAL SOFTWARE STACK VIA MODULES [1/2]

- **Scientific software is made available via *environment modules***
- An environment module prepares the environment for using a particular software application
- Module naming scheme: `<name>/<version>-<toolchain>[-<suffix>]`
- Interacting with module files is done via the `module` command (Lmod)
- Load a module to prepare the session or job environment for using the software:

```
module load SciPy-bundle/2023.07-gfbf-2023a
```

- Modules that are required as dependencies will be loaded automatically
- To see list of currently loaded modules, run `module list` (or `ml`)

CENTRAL SOFTWARE STACK VIA MODULES [2/2]

- To get an overview of *all* available modules, run `module avail` (or `ml av`)
- To see available versions for specific software, run `module avail soft_name/`
- To unload all currently loaded modules, run `module purge`
- Modules are installed using a particular toolchain (`foss`, `intel`, ...),
  which includes C/C++/Fortran compilers, MPI library, BLAS/LAPACK/FFT libraries
- **You should only combine modules that were installed with the same toolchain**,
  or a subtoolchain thereof (for example `foss/2023a` + `GCC/12.3.0`)
- See also HPC-UGent documentation: docs.hpc.ugent.be/running_batch_jobs/#modules
  docs.hpc.ugent.be/available_software

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CENTRAL SOFTWARE STACK VIA MODULES (EXAMPLE)

```
$ python -V; which python
Python 3.6.8
/usr/bin/python
```

```
$ python -c 'import numpy; print(numpy.__version__)'
Traceback (most recent call last):
  File "<string>", line 1, in <module>
ModuleNotFoundError: No module named 'numpy'
```

```
$ module load SciPy-bundle/2023.07-gfbf-2023a
$ python -V; which python
Python 3.11.3
/apps/gent/RHEL8/zen2-ib/software/Python/3.11.3-GCCcore-12.3.0/bin/python
$ python -c 'import numpy; print(numpy.__version__)'
1.25.1
```

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USEFUL ENVIRONMENT VARIABLES FOR JOB SCRIPTS

(most of these are only defined in the context of a running job!)

- **`$PBS_JOBID`**: job id of running job
- **`$PBS_O_WORKDIR`**: directory from which job was submitted on login node
  - It is common to use `cd $PBS_O_WORKDIR` at beginning of a job script
- **`$PBS_ARRAYID`**: array id of running job
  - Only relevant when submitting array jobs (`qsub -t`)
- **`$TMPDIR`**: unique *local* directory specific to running job
  - Cleaned up automatically when job is done, so make sure to copy result files!
- **`$EBROOTXYZ`, `$EBVERSIONXYZ`**: root directory/version for software package XYZ
  - Only available when module for XYZ is loaded

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INPUT/OUTPUT DATA AND SHARED FILESYSTEMS

- See HPC-UGent docs: docs.hpc.ugent.be/running_jobs_with_input_output_data
- Think about input/output:
  - How and where will you *stage in* your data and input files?
  - How and where will you *stage out* your output and result files?

- Manually (on login nodes) vs automatically (as a part of job script)
- **Home filesystem** (`$VSC_HOME`): only for limited number of small files & scripts
- **Data filesystem** (`$VSC_DATA*`): 'long-term' storage, large files
- **Scratch filesystems** (`$VSC_SCRATCH*`): for 'live' input/output data in jobs

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STORAGE QUOTA (DISK SPACE)

- Home directory (`$VSC_HOME`): 3GB (fixed!)
- Personal data directory (`$VSC_DATA`): 25GB (fixed!)
- Personal scratch directory (`$VSC_SCRATCH`): 25GB (fixed!)
- Current quota usage can be consulted on VSC accountpage
- **More storage quota (100s of GBs, even TBs) available for *virtual organisations (VOs)***; see dedicated section on VOs in HPC-UGent documentation
- Additional quota can be requested via VSC accountpage (“Edit” tab)
- Shared directories with VO members: `$VSC_DATA_VO`, `$VSC_SCRATCH_VO`
- Personal VO subdirectories: `$VSC_DATA_VO_USER`, `$VSC_SCRATCH_VO_USER`

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FULL EXAMPLE JOB SCRIPT (SINGLE-CORE JOB)

```
#!/bin/bash
#PBS -N count_example      # job name
#PBS -l nodes=1:ppn=1      # single-node job, single core
#PBS -l walltime=2:00:00    # max. 2h of wall time

# load Python 3.11, with batteries included (extra PyPI packages)
module load Python-bundle-PyPI/2023.06-GCCcore-12.3.0
# copy input data from location where job was submitted from
cp $PBS_O_WORKDIR/input.txt $TMPDIR
# go to temporary working directory (on local disk) & run Python code
cd $TMPDIR
python -c "print(len(open('input.txt').read()))" > output.txt
# copy back output data, ensure unique filename using $PBS_JOBID
cp output.txt $VSC_DATA/output_${PBS_JOBID}.txt
```

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FULL EXAMPLE JOB SCRIPT (MULTI-NODE MPI JOB)

```
#!/bin/bash
#PBS -N mpi_hello              # job name
#PBS -l nodes=2:ppn=4          # 2 nodes, 4 cores per node
#PBS -l walltime=2:00:00       # max. 2h of wall time

module load foss/2023a
module load vsc-mympirun

# go to working directory, compile and run MPI hello world program
cd $PBS_O_WORKDIR
# C code for MPI Hello: https://mpitutorial.com/tutorials/mpi-hello-world
mpicc mpi_hello.c -o mpi_hello
mympirun ./mpi_hello
```

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JOB OUTPUT FILES

- **Your job script may produce informative, warning, and/or error messages.**
  - Two output files are created for each job: stdout (`*.o*`) + stderr (`*.e*`)
  - Located in directory where job was submitted from (by default)
  - Messages produced by a particular command in the job script can be "caught" and redirected to a particular file instead:

```
example > out.log 2> err.log
```

  (see dedicated section of our Linux tutorial for more details)
- In addition, the software used for the calculation may have generated additional output or result files (which is very software-specific).

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JOB SUBMISSION AND MANAGEMENT

- Submit job scripts from a login node to a cluster for execution using `qsub` command:

```
$ module swap cluster/donphan
$ qsub example.sh
12345
```

- An overview of the active jobs is available via the `qstat` command:

```
$ qstat
Job ID   Name         User              Time Use S Queue
-------  -----------  ---------------  --------- - -------
12345    example      vsc40000          1:32:57  R donphan
```

- To remove a job that is no longer necessary, use the `qdel` command: `qdel 12345`

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JOB SCHEDULING

- All HPC-UGent clusters use a **fair-share scheduling** policy.
- No guarantees on when job will start (and impossible to predict), so **plan ahead**!
- Job priority is determined by various factors:
  - *Historical usage*
    - Aim is to balance usage over users
    - Infrequent/frequent users => higher/lower priority
  - *Requested resources* (# nodes/cores, walltime, memory, ...)
    - Larger resource request => lower priority
  - *Time waiting in queue*
    - Queued jobs get higher priority over time

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PYTHON VIRTUAL ENVIRONMENTS (VENV'S)

- Isolates project dependencies from the system-wide Python installation
- Makes local installation of Python packages (which are not available via modules) easier
- Recommendations & caveats on HPC clusters:
  - Prefer using **Python software installed as module** (if available): better performance
  - **Activate** the Python virtual environment with the **same modules loaded**
  - Virtual environment built on one cluster **will likely not work** on another cluster (diff. OS / CPU)
- Making a virtual environment (manually):

```
$ module load SciPy-bundle/2023.11-gfbf-2023b
$ python -m venv example-venv
$ source example-venv/bin/activate   # activate virtual environment (similar to 'module load')
$ pip install example                # install package not available as module
$ python script.py                   # use virtual environment to run Python script
$ deactivate                         # deactivate virtual environment (like 'module unload')
```

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docs.hpc.ugent.be/setting_up_python_virtual_environments

VSC-VENV: PYTHON VIRTUAL ENVIRONMENT WRAPPER SCRIPT

- Encapsulates the creation and management of Python virtual environments
- Facilitates working with Python virtual environments across HPC-UGent clusters
- It makes sure that:
  - The same modules are loaded on each activation
  - A new virtual environment is created for each cluster OS & CPU microarchitecture
- Arguments for the `vsc-venv` tool:
  - ***modules.txt*** (optional): file with list of names of environment modules to load
  - ***requirements.txt*** (required): file with list of Python packages to install

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docs.hpc.ugent.be/setting_up_python_virtual_environments

VSC-VENV: EXAMPLE + DEMO

modules.txt:

```
SciPy-bundle/2023.11-gfbf-2023b
Pillow/10.2.0-GCCcore-13.2.0
```

requirements.txt:

```
beautifulsoup4==4.12.3
```

```
$ module load vsc-venv
$ source vsc-venv --activate --requirements requirements.txt --modules modules.txt
$ python --version          # Python provided by dependency of SciPy-bundle module
Python 3.11.5
$ python -c "import PIL”      # import PIL from Pillow module
$ python -c "import numpy”    # import numpy from SciPy bundle
$ python -c "import bs4”      # import bs4 from beautifulsoup4 package
```

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docs.hpc.ugent.be/setting_up_python_virtual_environments

HANDS-ON: SUBMITTING JOBS

- Single-core “Hello World” job
- Running a Python or R script in a job
- Multithreaded “Hello World” jobs (OpenMPI)
- Multiprocess “Hello World” job (MPI)

Tip: use donphan cluster to avoid waiting in the queue

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HANDS-ON: OPENMP HELLO WORLD

```c
#include <stdio.h>
#include <omp.h>

int main() {
    // Parallel region
    #pragma omp parallel
    {
        int thread_id = omp_get_thread_num();  // Get the thread ID
        int n_threads = omp_get_num_threads(); // Get total # threads
        printf("Hello, World! from thread %d of %d\n", thread_id, n_threads);
    }
    return 0;
}
```

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Compile with:

```
gcc example_openmp.c -fopenmp -o example_openmp
```

HANDS-ON: MPI HELLO WORLD

```
#include <mpi.h>
#include <stdio.h>

int main(int argc, char** argv) {
    MPI_Init(&argc, &argv);  // Initialize MPI

    int world_rank, world_size;
    MPI_Comm_rank(MPI_COMM_WORLD, &world_rank); // Get process rank
    MPI_Comm_size(MPI_COMM_WORLD, &world_size); // Get # processes

    printf("Hello, World! from process %d of %d\n", world_rank, world_size);
    MPI_Finalize(); // Finalize MPI
    return 0;
}
```

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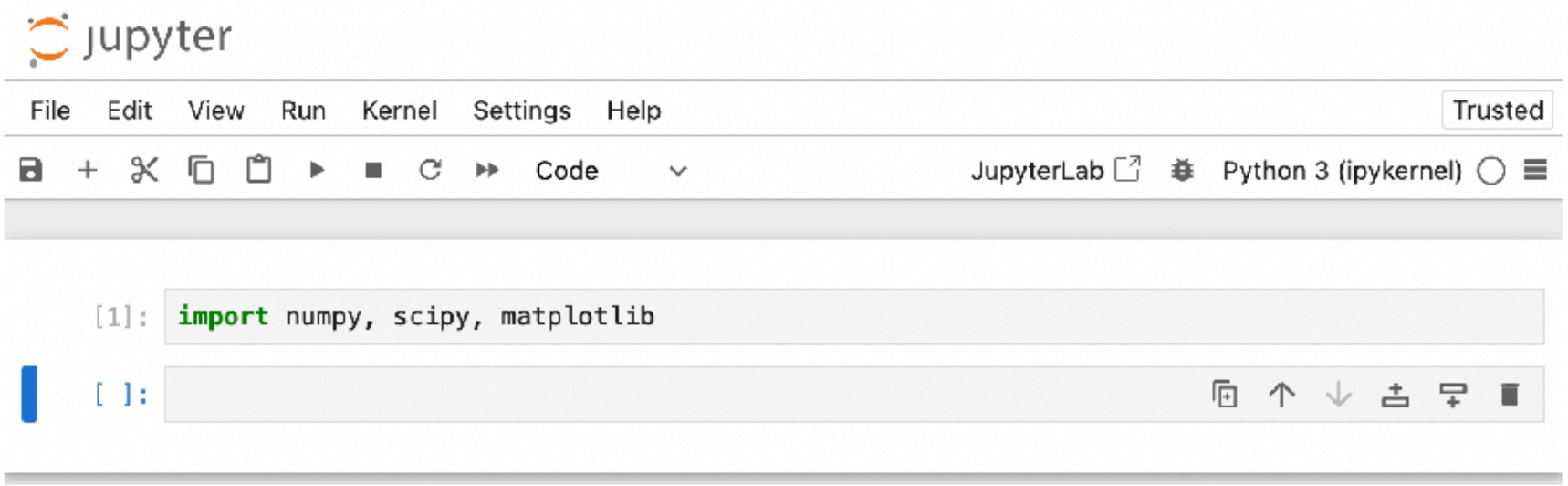
Compile with: `mpicc example_mpi.c -o example_mpi`

Run with: `mpirun -np 4 ./example_mpi # or use mympirun`

HANDS-ON: JUPYTER NOTEBOOK

- Start a Jupyter notebook via “Interactive apps” on HPC-UGent web portal
- Use “donphan” cluster to avoid waiting in the queue
- Make sure that numpy, scipy, matplotlib Python packages can be used



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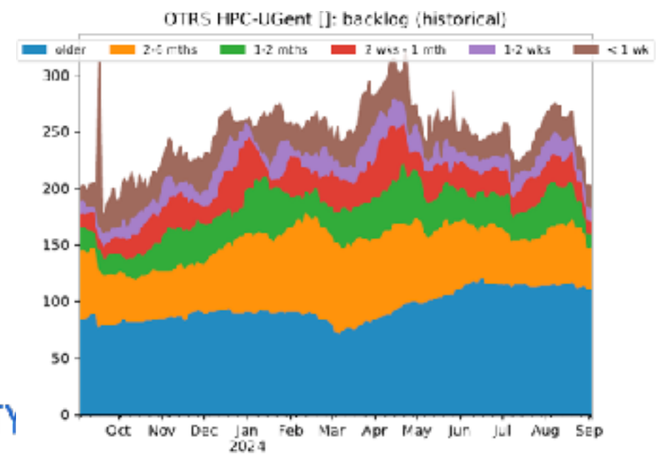
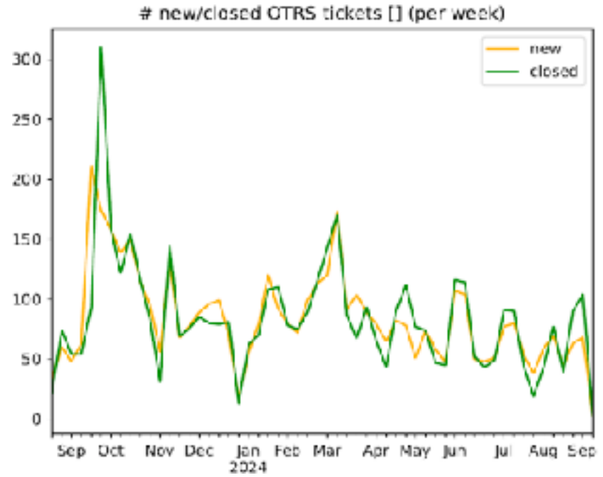
docs.hpc.ugent.be/jupyter

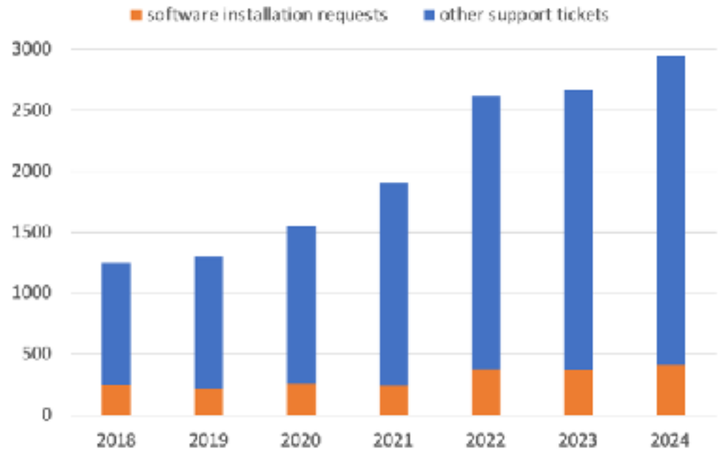
QUESTIONS, PROBLEMS, GETTING HELP (BE PATIENT…)

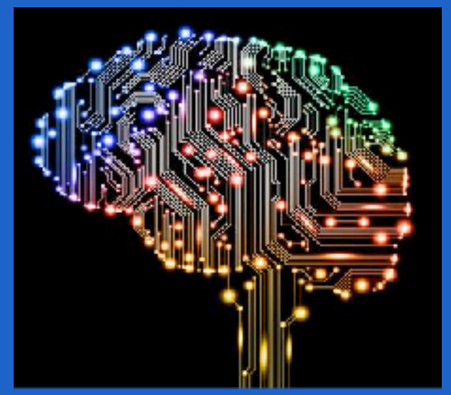
Don't hesitate to contact the HPC-UGent support team via hpc@ugent.be,
but be patient…

- We're doing what we can to keep up with incoming support questions + software installation req.
- We have been getting **50-100 new tickets per week** recently, and have usually have a backlog
- **Help us help you**: read the docs, provide sufficient details (like job IDs, output files, etc.), …
- Feel free to send a reminder in the same ticket or mail thread, especially if your work is blocked









artificial intelligence

cloud computing

TRENDS IN HPC

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RETURN OF THE PROCESSOR WARS!

- In the last decade, Intel was king (w.r.t. microprocessors in servers)
- AMD is back in the game since ~2017 (AMD EPYC processor generation)
- Interest in ARM CPUs is booming (see Fugaku, Apple M1, NVIDIA Grace)
- IBM POWER is still around (sort of)
- In the (near?) future: "open source" high-performance RISC-V processors?

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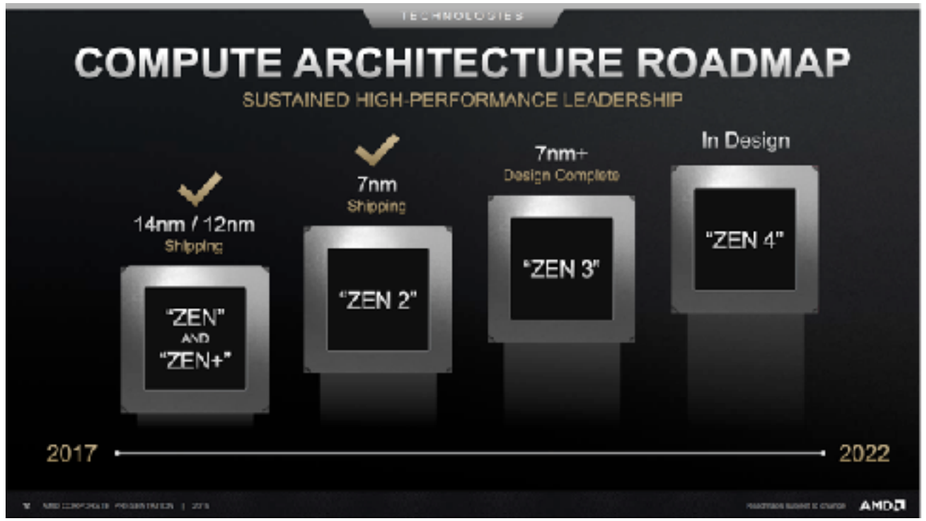
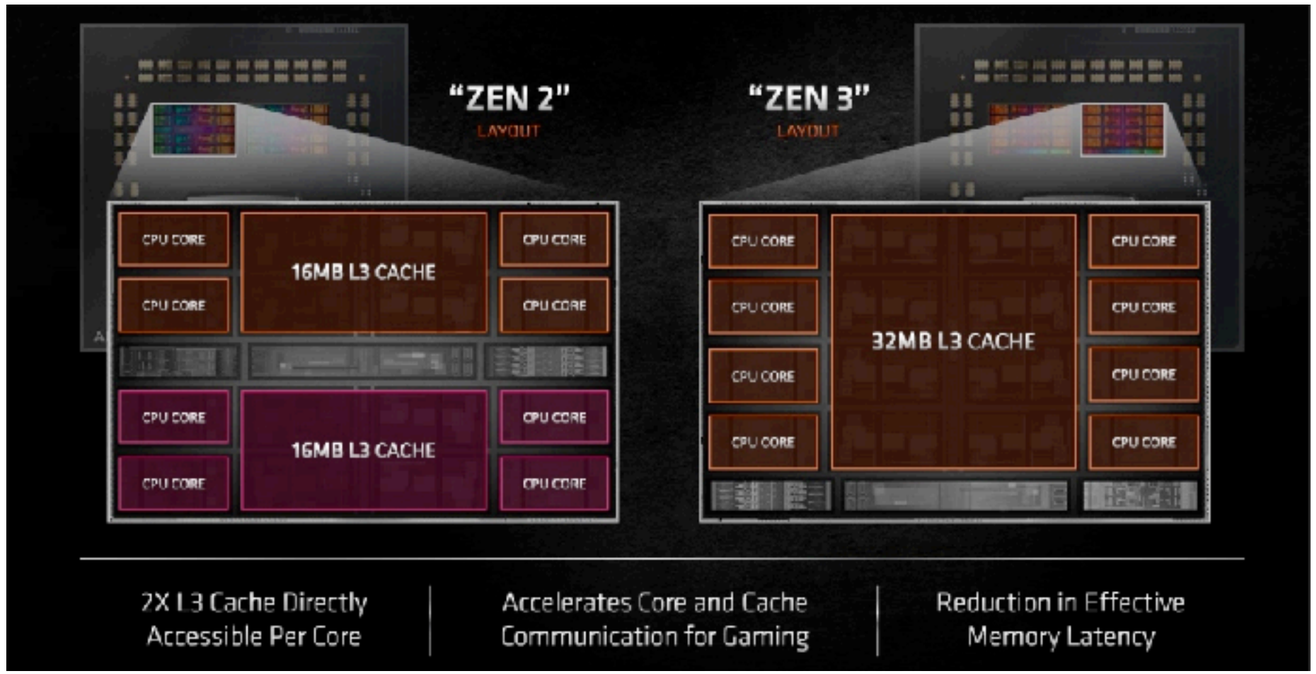
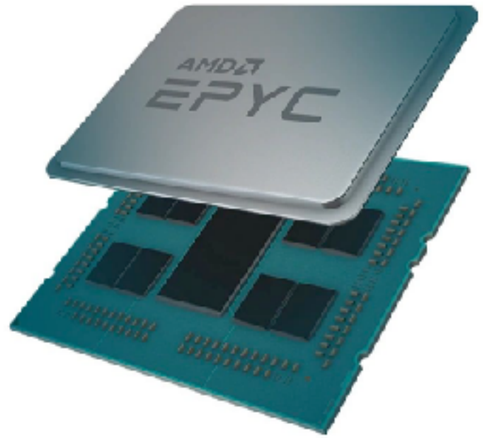
AMD EPYC PROCESSORS (ZEN* MICROARCHITECTURE)

- **AMD is competitive again with Intel**
- Different microarchitecture ("chiplet" design), same instruction set architecture (x86_64)



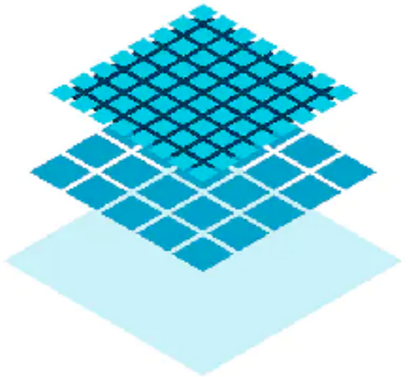




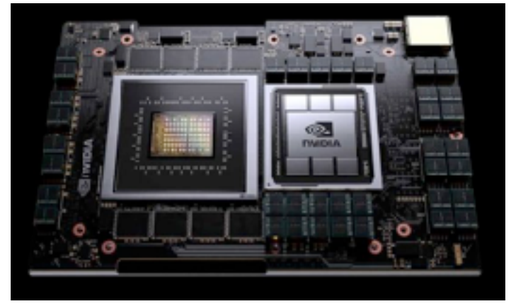
INTEREST IN ARM CPUS IS PICKING UP SPEED

- ARM is a different processor Instruction Set Architecture (ISA)
- ARM processors are the most common in the world
  - > 1 billion units per year, used in smartphones, tablets, wearables, ...
- License from Arm Ltd. is required to use ARM CPU designs
- ARM CPUs are now also used in recent large supercomputers:

  Fugaku (Japan), Isambard (UK), Astra (US), Deucalion (Portugal), …



- NVIDIA has announced its first ARM-based server CPU "Grace"
  - Will be used in first European exascale supercomputer: JUPITER



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RISC-V OPEN STANDARD ISA

- RISC-V is the 5th generation of RISC (Reduced Instruction Set Computer) ISA
- **Open source licensed**: free to use by anyone (no license fees)
- Several companies are designing RISC-V processors (some general purpose)
- Long term goal of European Processor Initiative (EPI) project is to design and produce a RISC-V processor for supercomputers & co, manufactured in Europe
- “Digital Autonomy with RISC-V in Europe” (DARE) project
  led by Barcelona Supercomputing Centre: 38 partners, 240 million Euro
- Will we see a (European?) RISC-V based supercomputer soon?
- Lots of work to be done on software side: libraries, applications, etc.

RISE OF CLOUD COMPUTING

- Several companies provide "cloud computing" services
- "Rent" computing time & co, pay only for what you use
- Easy (?) to **create your own (throwaway) supercomputer!**
- Including shared storage, GPUs, fast interconnect, ...
- Very flexible, but also expensive (or is it?)
- "There is no cloud, just somebody else's computer."

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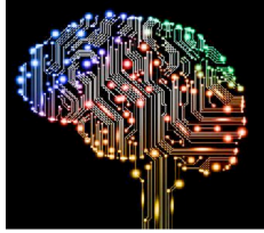
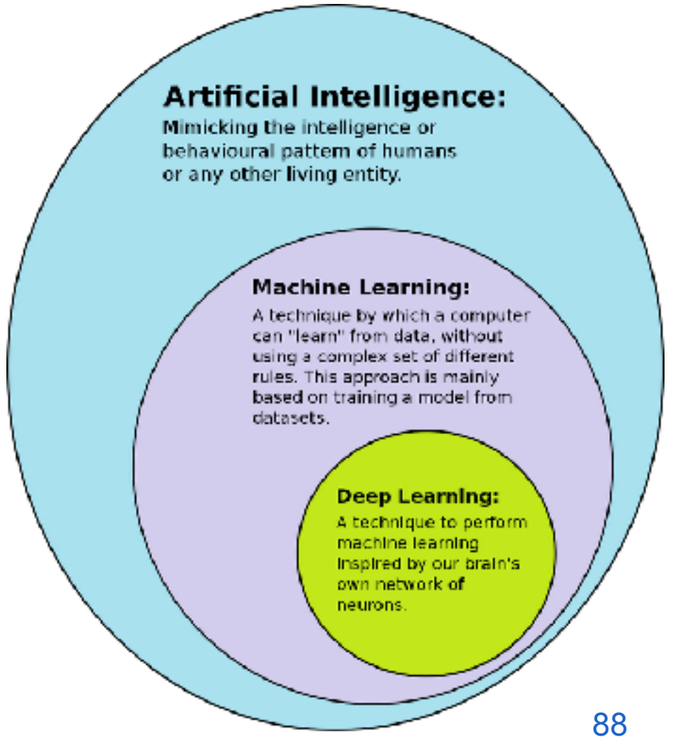
ARTIFICIAL INTELLIGENCE: A NEW HOPE



- Increased interest and adoption of machine learning techniques
- Fueled by capabilities of high-end computers (incl. supercomputers, GPUs)
- Typically requires large amounts of data ("big data")
- Lots of applications: digital imaging, self-driving cars, ...
- Deep learning "big bang" in 2009 fed by GPU boom
- **Large Language Models (LLMs) fueling the hype!**



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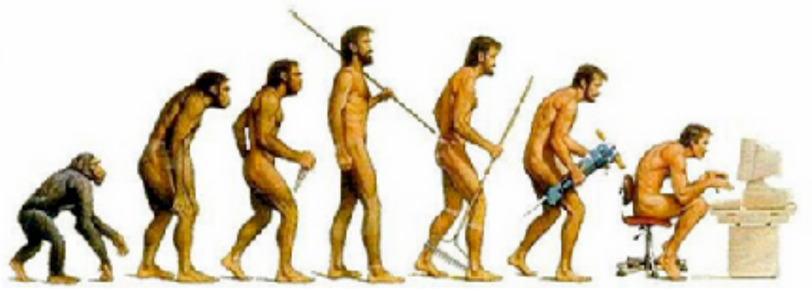
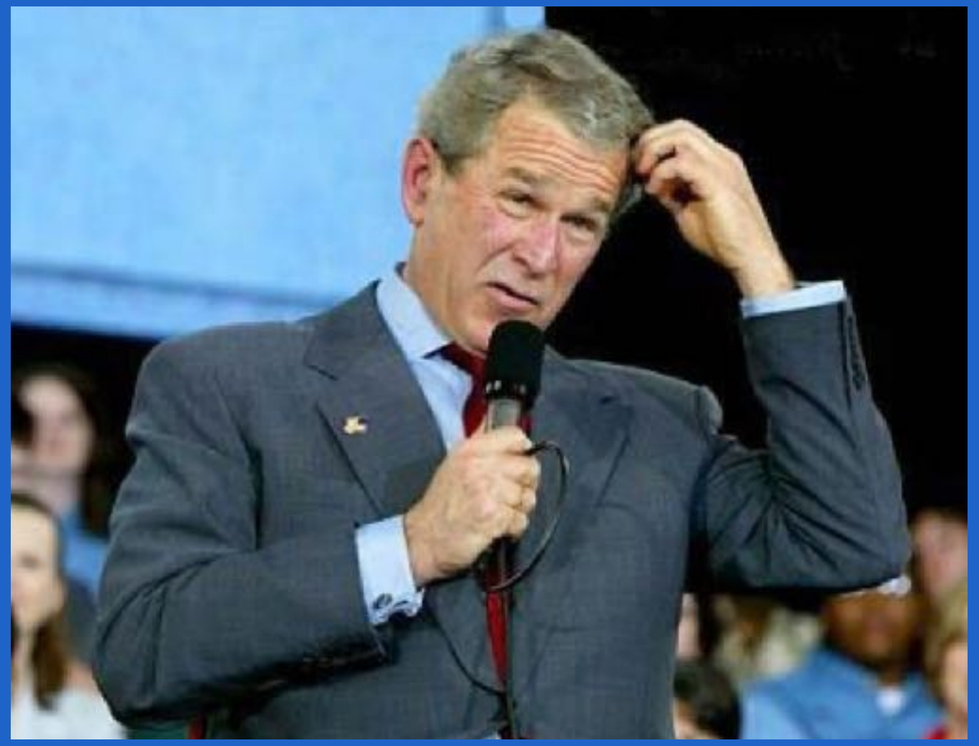
POLL

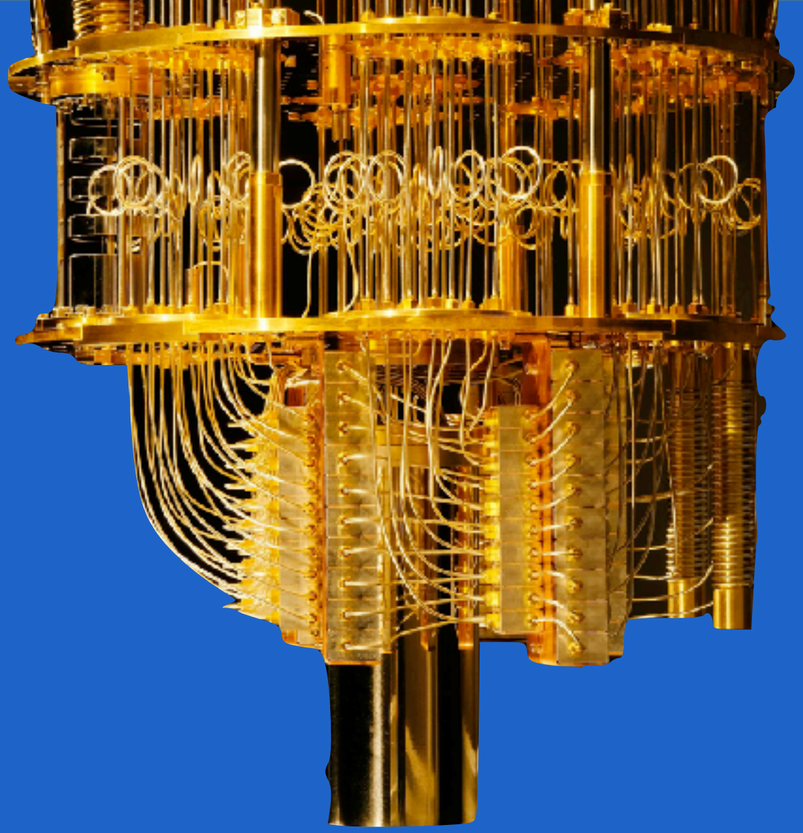
What will be the next big (r)evolution in scientific computing?

- Exascale supercomputers
- End of Intel/AMD processors as most prominent CPUs, switch to Arm
- High-performance RISC-V microprocessors
- HPC in the cloud
- Quantum computing
- Something else



menti.com (3706 7451)





QUANTUM COMPUTING (IN A NUTSHELL)

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DISCLAIMER

- **I am *not* an expert in quantum computing.**
- I have been trying to follow progress in quantum computing for a couple of years.
- Statements I make may be oversimplying things too much
  (or may even be incorrect).
- I am *totally* skipping the math behind all this (complex numbers, probability, etc.)
- Some of this is likely outdated already.
- Wikipedia & ~~Google~~ ChatGPT was my friend when puzzling this together...
- Please don't invest money based on what I say (unless you don't need it).

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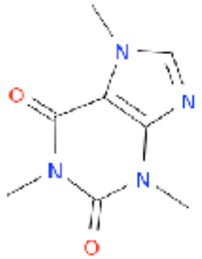
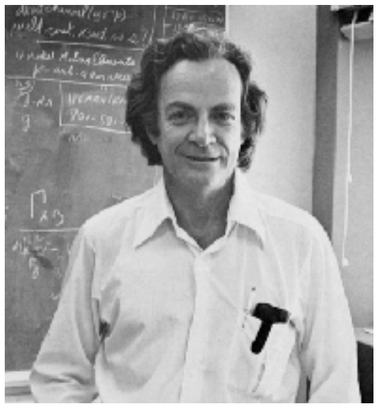
QUANTUM COMPUTING: HYPE OR REVOLUTION?

- Some problems are just **too big**, even for the largest (future) supercomputers!
    - Would takeway too long to solve, require too much memory, etc.
- Example: exact simulation of a caffeine molecule



    - ~95 electrons, would require ~10^{48} classical bits (1 terabyte = ~2^{40} = ~10^{12} bytes)
- **Quantum computers** could be the answer...
- We're getting close to "*quantum supremacy*"

  (or maybe we are there already...)



Richard Feynman (1918-1988)

"father" of quantum computing

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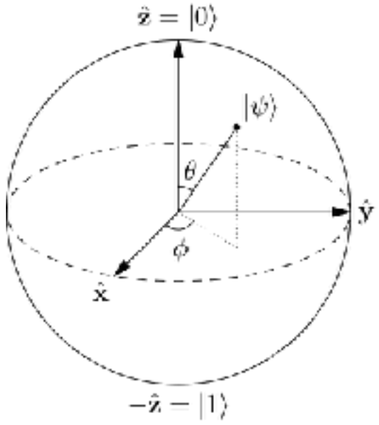
CLASSICAL BITS VS QUBITS

- Classical bits are either 0 or 1 (like flipping a coin: heads or tails)

- **Quantum bits ("qubits")** can be in a state somewhere in between 0 and 1...
  - Like a *spinning* coin, in some sense they can be "both 0 and 1 at the same time"

- Measuring (observing) a qubit collapses the state to either 0 or 1 (with a certain probability)
- Geometrical representation of a single qubit: *Bloch sphere*

$$|\psi\rangle - \alpha\,|0\rangle + \beta\,|1\rangle$$



  - North pole : $|0\rangle$ (equivalent with 0 in classical bit)
  - South pole: $|1\rangle$ (equivalent with 1 in classical bit)
  - Equator: 50% probability of observing 0 or 1 when measuring
  - Somewhere else on surface of the sphere: leaning towards either $|0\rangle$ or $|1\rangle$ ...

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LEVERAGING QUANTUM PHYSICS

- **Superposition**
  - A qubit can be put in a state between $|0\rangle$ and $|1\rangle$
  - A collection of qubits can be manipulated to **favor** the "optimal" state
- **Entanglement**
  - Two qubits can be "entangled": measuring one impacts the other
  - The distance between the entangled qubits doesn't matter!
  - Can used for *teleportation* of information (faster-than-light communication!)
  - Einstein called this "spooky action at a distance"
- **Interference**
  - The state of a qubit can be changed via constructive or destructive interference

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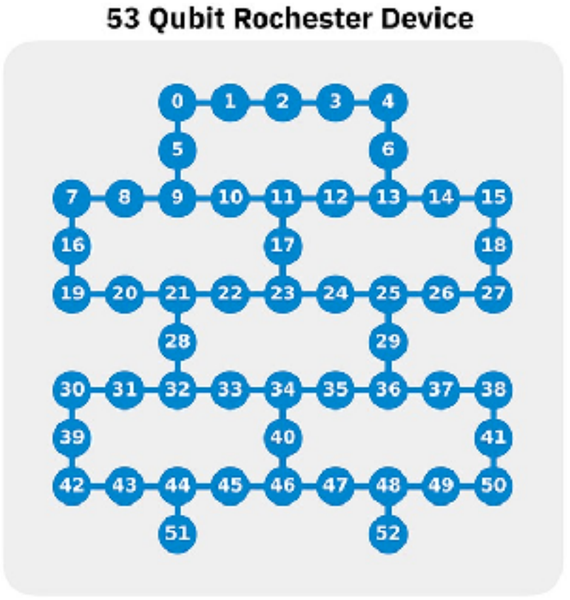
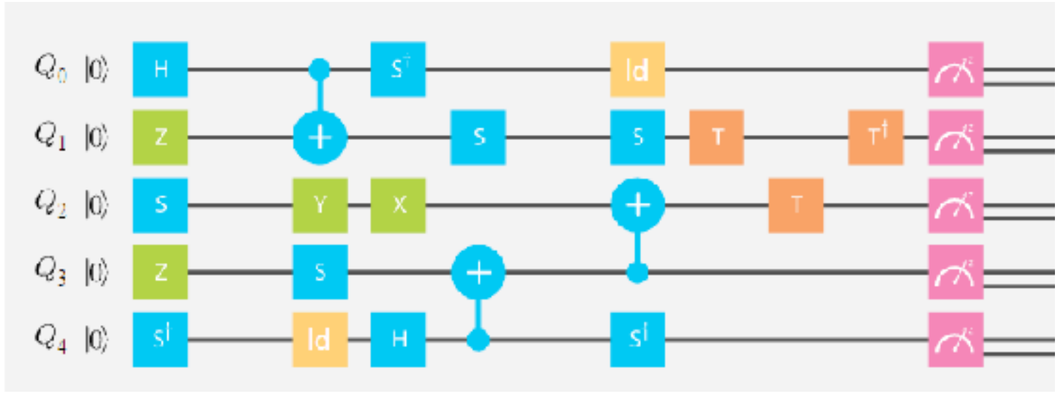
QUBITS AND QUANTUM CIRCUITS

- Combining multiple qubits makes things interesting...
- In some sense, every qubits *doubles* the compute power
  - Assuming each qubit is connected to all others *(which it won't be)*
- *Quantum circuits* can be used to manipulate a set of qubits
  - Gate-model quantum computing: a circuit is a series of *gates*
  - Equivalent to a computer program in classical computers



Operator	Gate(s)
Pauli-X (X)	X
Pauli-Y (Y)	Y
Pauli-Z (Z)	Z
Hadamard (H)	H
Controlled Not (CNOT, CX)	
Controlled Z (CZ)	Z



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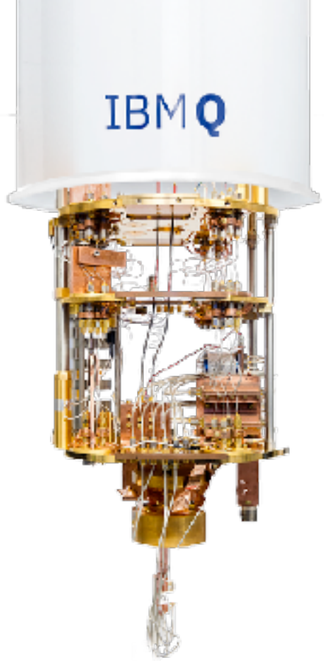
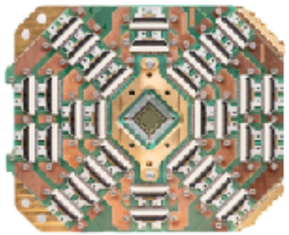
TYPES OF QUANTUM COMPUTERS



- **Circuit-based quantum processors**
  - IBM, Google, Intel, Rigetti, Xanadu Quantum Technologies, …
  - Different technologies: superconducting, trapped ions, quantum dot, …

- **Quantum annealers**
  - Can only be used for certain type of problems (optimization)
  - D-Wave One (2011): 128 qubits
  - D-Wave 2000Q (2017): 2048 qubits
  - D-Wave Advantage (2020): 5760 qubits

    Recently <u>purchased</u> by Jülich Supercomputing Centre!



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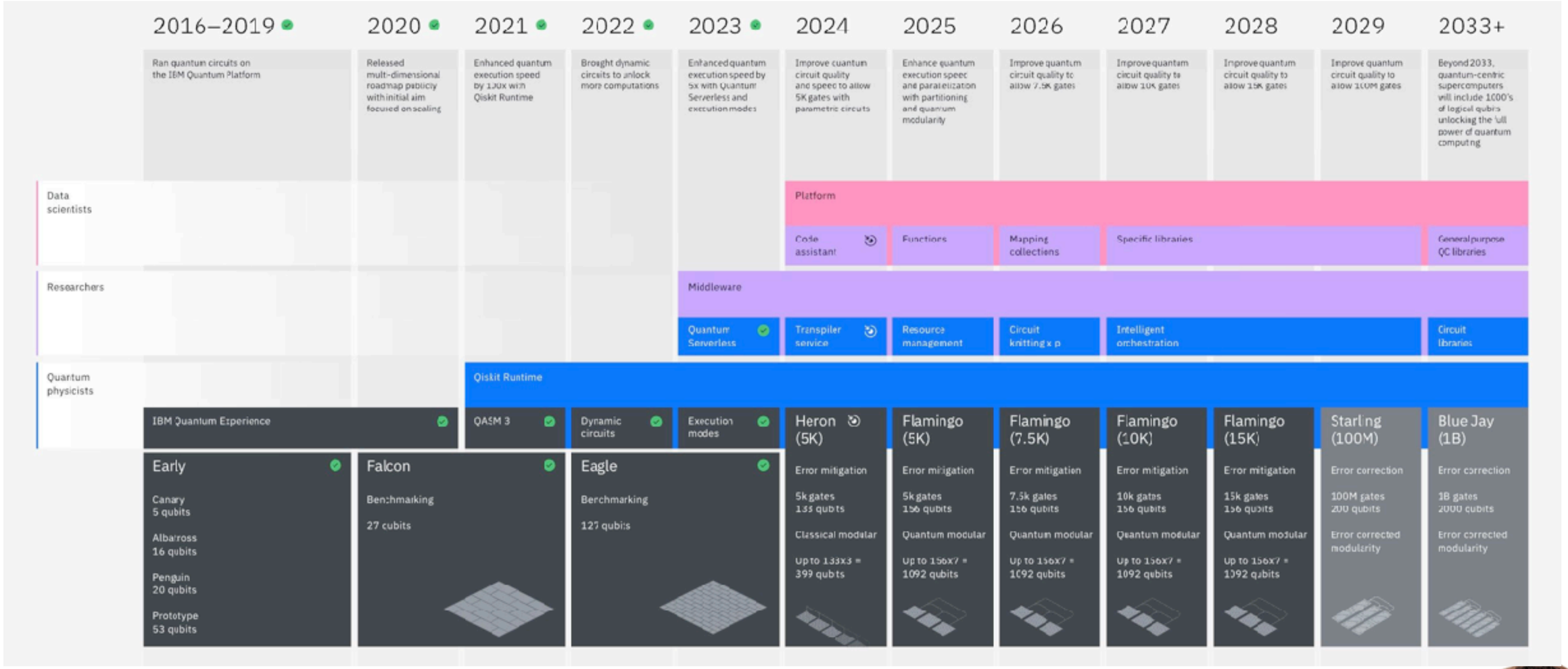
IBM QUANTUM ROADMAP



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https://www.ibm.com/quantum/blog/ibm-quantum-roadmap-2025

APPLICATIONS FOR QUANTUM COMPUTING

Cryptography

- Break popular encryption algorithms (RSA)
- Would be *very* distruptive (quantum computing as a "weapon")
- Post-quantum cryptography (who wins the race?)

Machine learning

- Quantum Machine learning algorithms already exist today
- Artificial Intelligence (AI) more popular than ever
- Could be the way to AGI / the "Singularity"

Simulation of quantum physics

- Molecular simulations, drug development, etc.
- Very popular application in supercomputers today
- Some problems are impossible to solve today, even on supercomputers

Search & optimization

- Searching for "best" item in unstructured space
- Can be proved Grover's is the *optimal* way of searching

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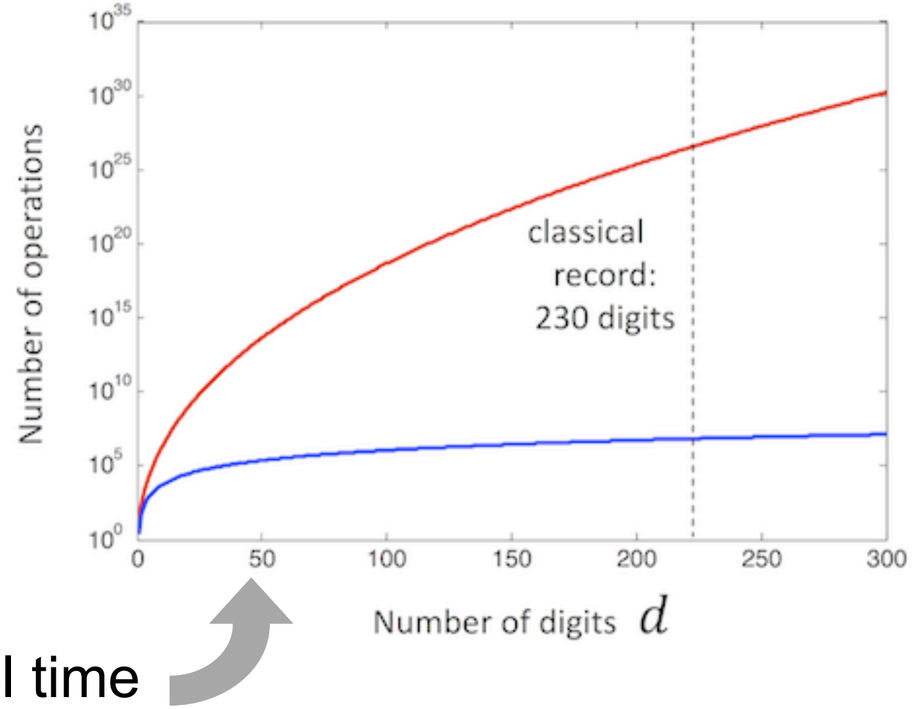
QUANTUM ALGORITHMS

- **Grover's search algorithm**
  - Unstructured search problem: find best out of N
  - On average: $\frac{N}{2}$ classically, $\sqrt{N}$ with Grover's



- **Shor's algorithm**
  - Factoring integer numbers into primes in polynomial time
  - Can be used to break RSA encryption (uses 2,048 bit integers, or larger)
  - Shor requires ~2N *logical* qubits (N: number of bits to represent integer to factor)

- **Quantum phase estimation**
  - Central building block for many quantum algorithms

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CHALLENGES IN QUANTUM COMPUTING

- **Physics**
  - Creating and controlling qubits: superconducting, photonics, ...
  - Keeping out the noise, temperatures close to 0K (colder than outer space!)
- **Decoherence**
  - Qubits "collapse" due to outside influence: noise, vibrations, radiation, ...
  - Quantum "programs" must finish before decoherence happens (< 1 ms currently)
- **Connectivity**
  - Multiple qubits must be as connected as possible so they can be entangled, etc.
  - Quantum "compilers" are used to map quantum circuits on physical qubit layout
- New generation of **programmers** needs to be trained to use quantum computers...

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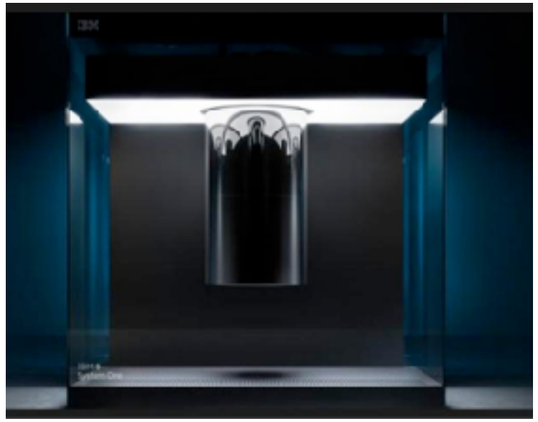
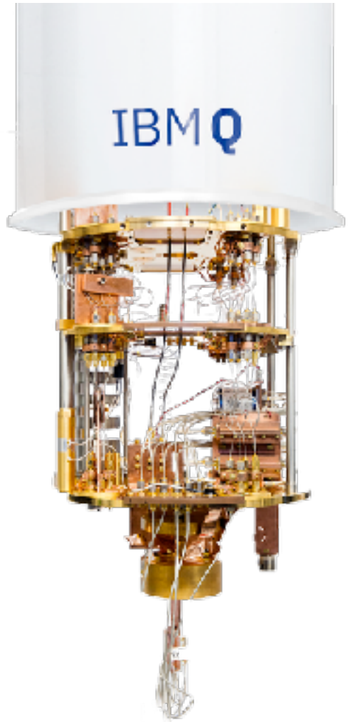
CURRENT QUANTUM COMPUTERS

- Currently in **Noisy Intermediate Scale Quantum** (NISQ) era
- Small number of qubits, very short coherence time (~0.1 ms)
- Examples: Google Willow (105 qubits), IBM Heron (156 qubits)
- Procurement of quantum computers @ EuroHPC sites ongoing…



IBM Q System One
Commercial quantum computer (20 qubits)

"Naked" quantum computer



IBM Q System Two (2023)
3x IBM Heron (each with 156 qubits)

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IBM QUANTUM PLATFORM

IBM Q™

- You can play with a **real quantum computer** yourself (or simulate one).
- In the cloud! For free! Using Python code!

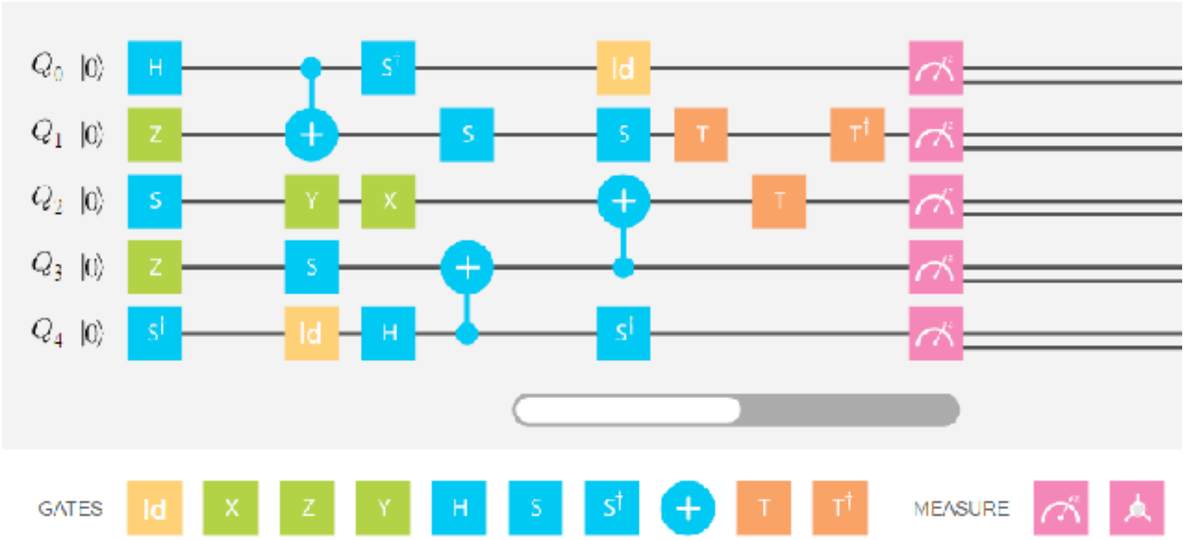
```
from qiskit import QuantumCircuit

# Create a Quantum Circuit (2 qubits, 2 classical bits)
circuit = QuantumCircuit(2, 2)

# Add a H gate on qubit 0
circuit.h(0)

# Add a CX (CNOT) gate on control qubit 0 and target qubit 1
circuit.cx(0, 1)

# Map the quantum measurement to the classical bits
circuit.measure([0,1], [0,1])
```



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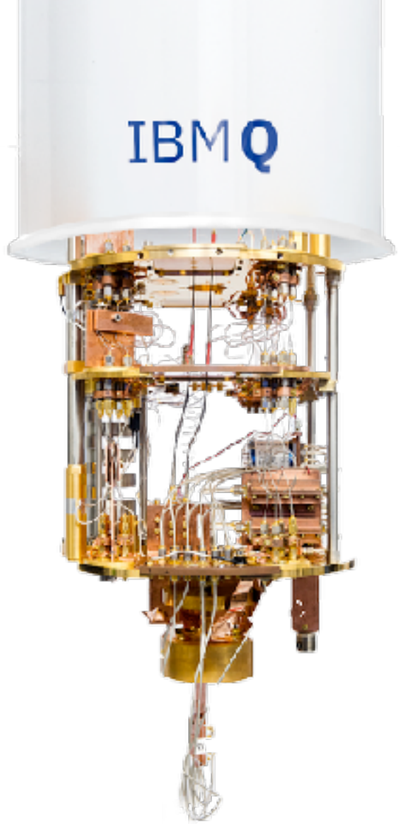
See https://quantum.ibm.com, https://qiskit.org

WOULD YOU LIKE TO KNOW MORE?



- Quantum Open Source Foundation: https://www.qosf.org
- https://learning.quantum.ibm.com/catalog/tutorials
- https://fosdem.org/2025/schedule/track/quantum
- https://www.youtube.com/playlist?list=PLqxhJj6bcnY92IuCrMt78ThcBOJ5Nb5_O
- https://www.thequantumdaily.com/2020/05/15/7-quantum-computing-books-for-the-uninitiated

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MOVIES + TV SERIES TO WATCH

The Imitation Game (2014)

Biography of Alan Turing, father of theoretical computer science and artificifial intelligence, invented the "bombe" to decode Enigma machine of Nazi Germany during World War II.

Hidden Figures (2016)

Story about the African-American female mathematicains who served as "human computers" at NASA in 1961, who taught themselves FORTRAN in order to operate the IBM computer which was set to replace them.

Devs (2020)

“A computer engineer investigates the secretive development division in her company, which she believes is behind the disappearance of her boyfriend.”

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Questions?

Kenneth Hoste

HPC system administrator

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