High-Performance Computing & Data Analytics

MeluXina, a Competitive Advantage for Luxembourg

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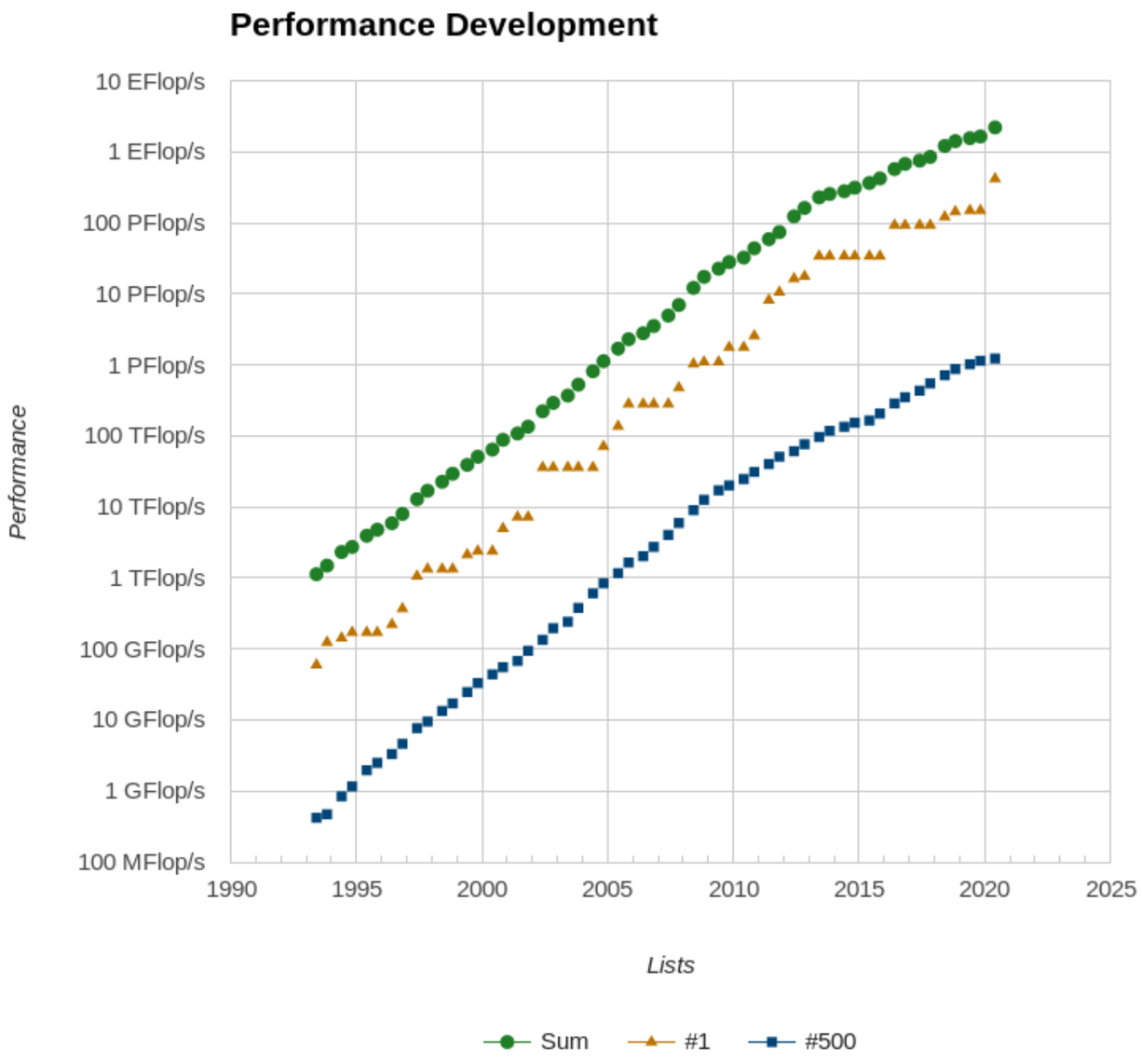
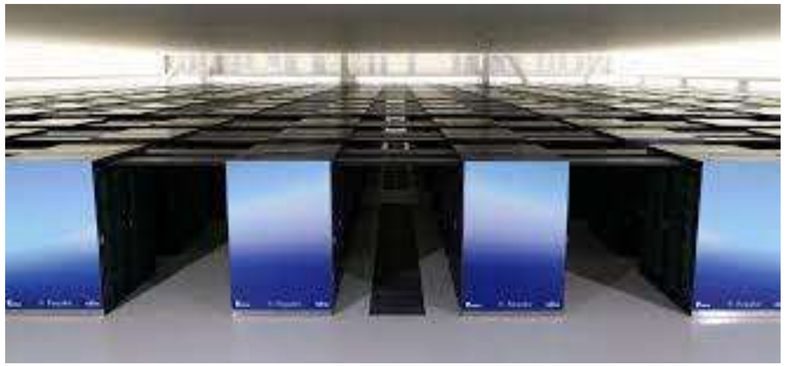

Performance Development
10 EFlop/s
1 EFlop/s
100 PFlop/s
10 PFlop/s
1 PFlop/s
100 TFlop/s
10 TFlop/s
1 TFlop/s
100 GFlop/s
10 GFlop/s
1 GFlop/s
100 MFlop/s
Performance
1990
1995
2000
2005
2010
2015
2020
2025
Lists
Sum
#1
#500

1. Frontier (Oak Ridge, USA) 1,1 Exaflops

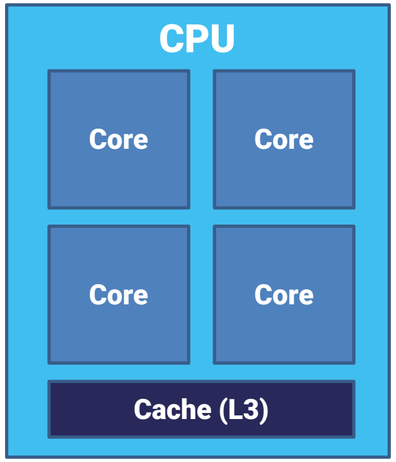


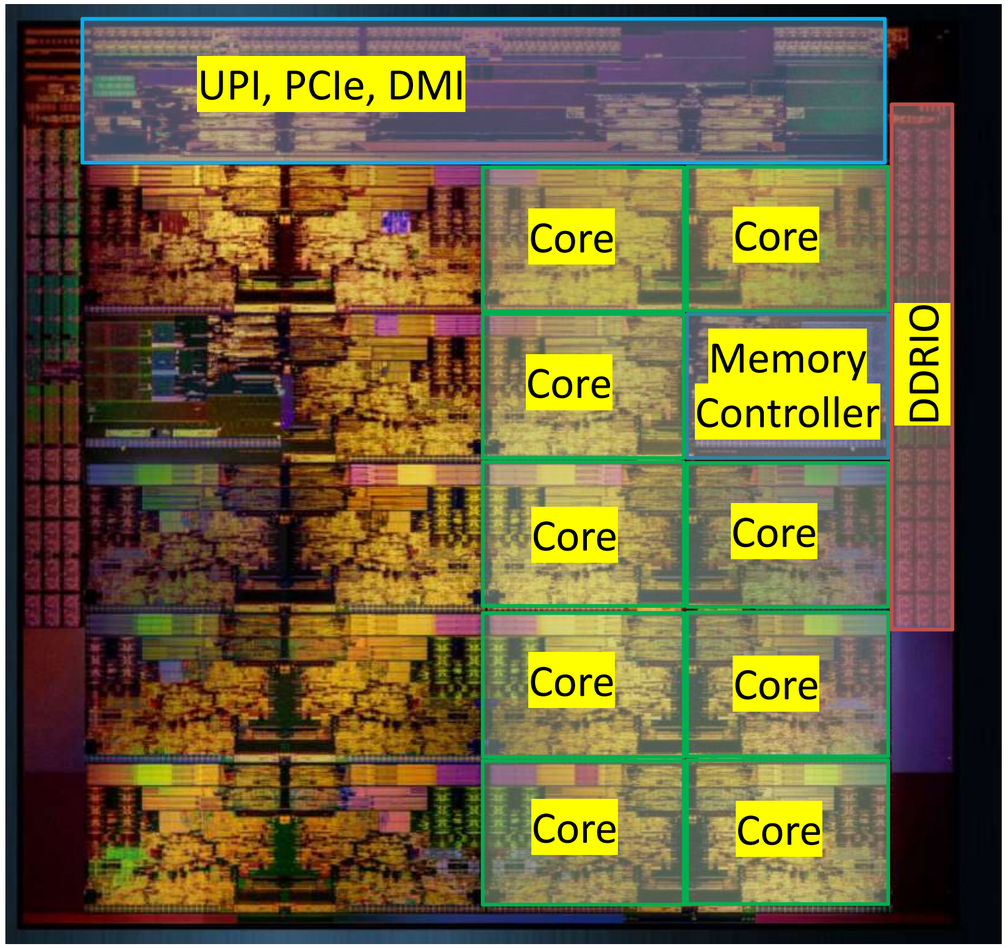
2. Fugaku (Riken, Japan) 442 PFlops

48.MeluXina (Bissen, Luxembourg) 10 PFlops

Ranking Top500 June 2022

CENTRAL PROCESSING UNIT (CPU)

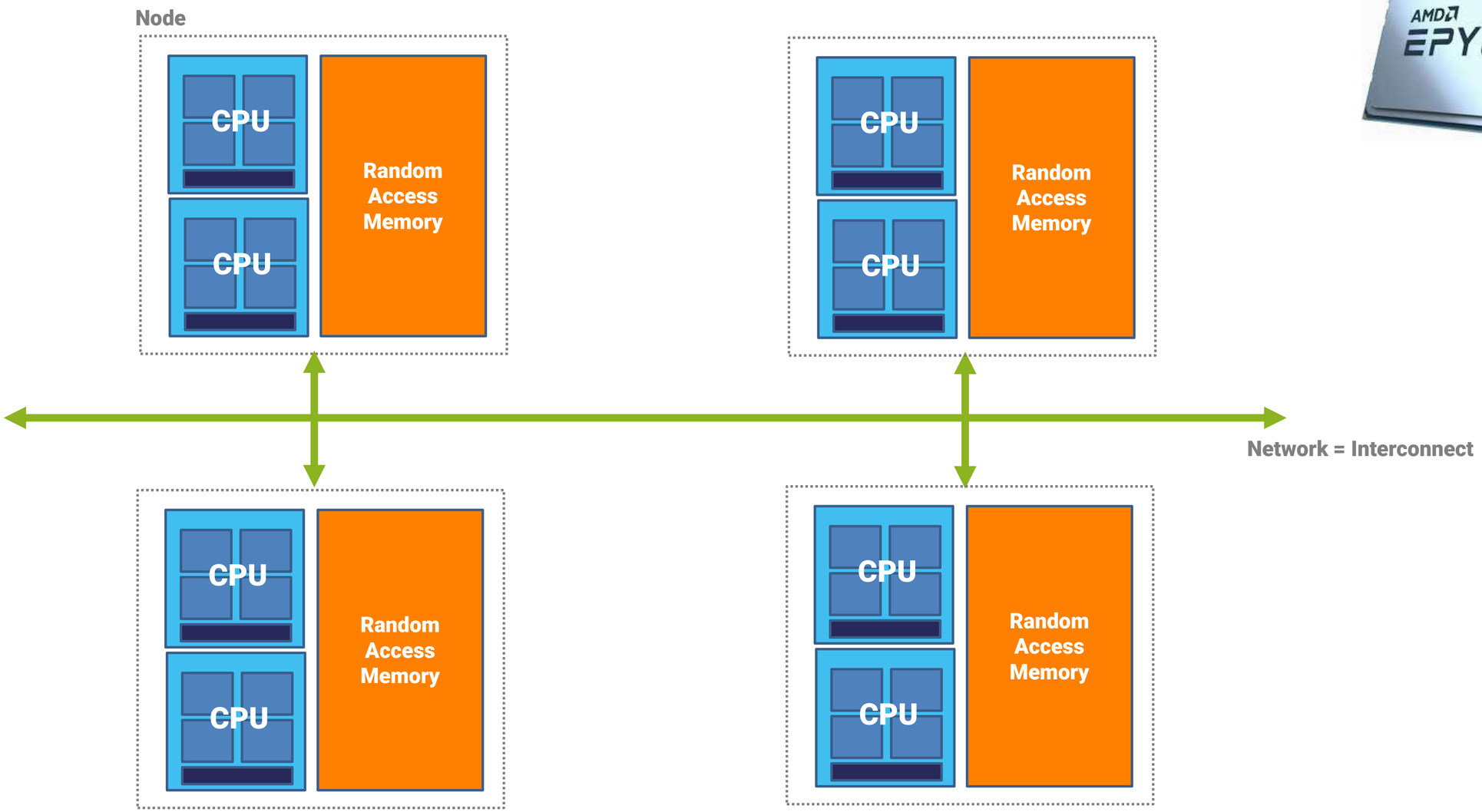




Intel Skylake (Courtesy of Intel)

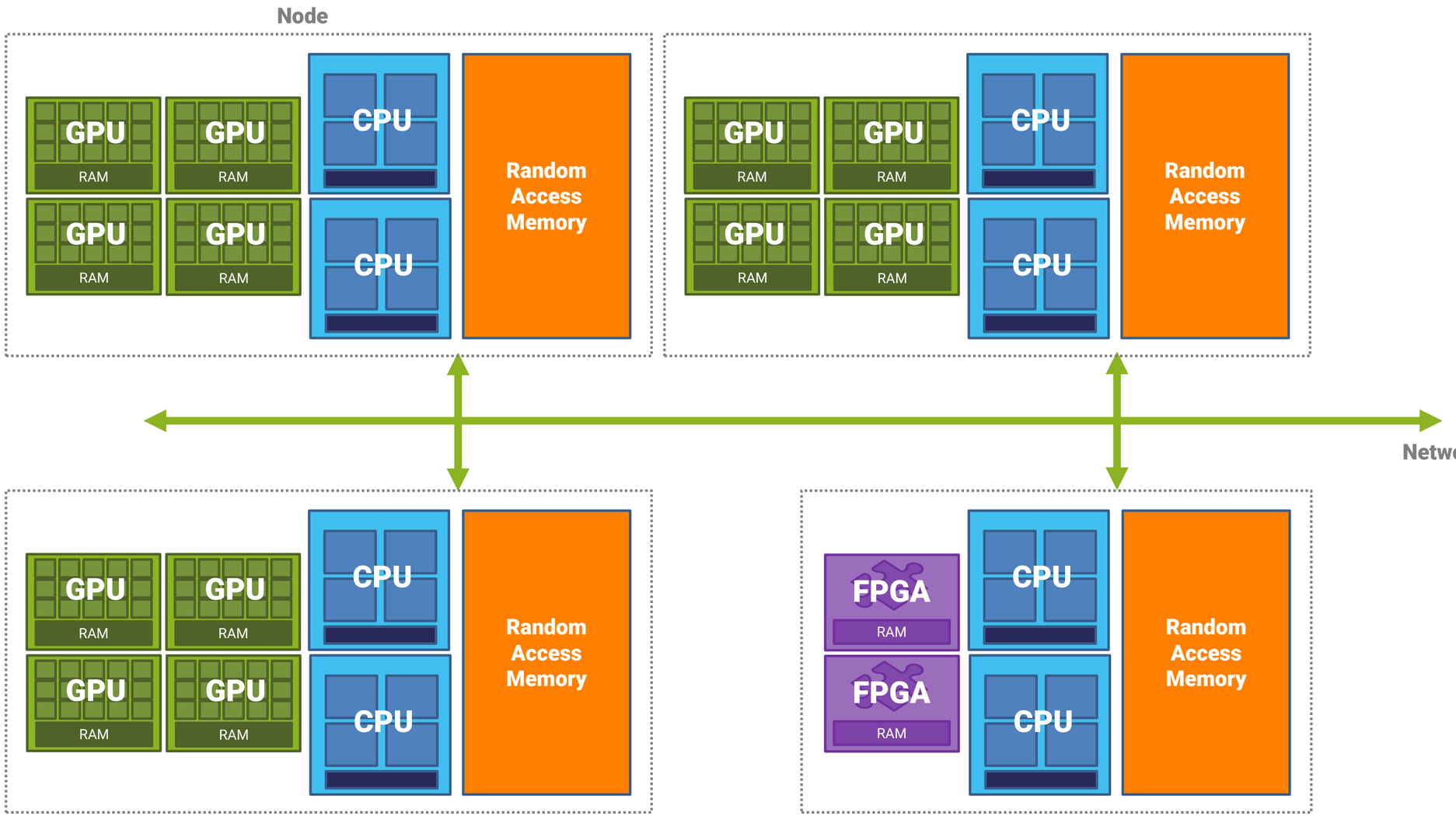
Core Definition (Jarp):
"A complete ensemble of execution logic, and cache storage as well as register files plus instruction counter (IC) for executing a software process or thread."

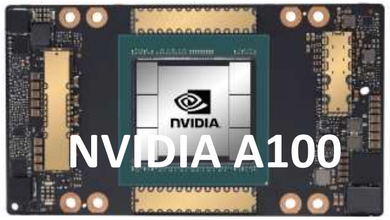
CPU “CLUSTER”


Node
CPU
CPU
Random Access Memory
CPU
CPU
Random Access Memory
CPU
CPU
Random Access Memory
CPU
CPU
Random Access Memory
Network = Interconnect

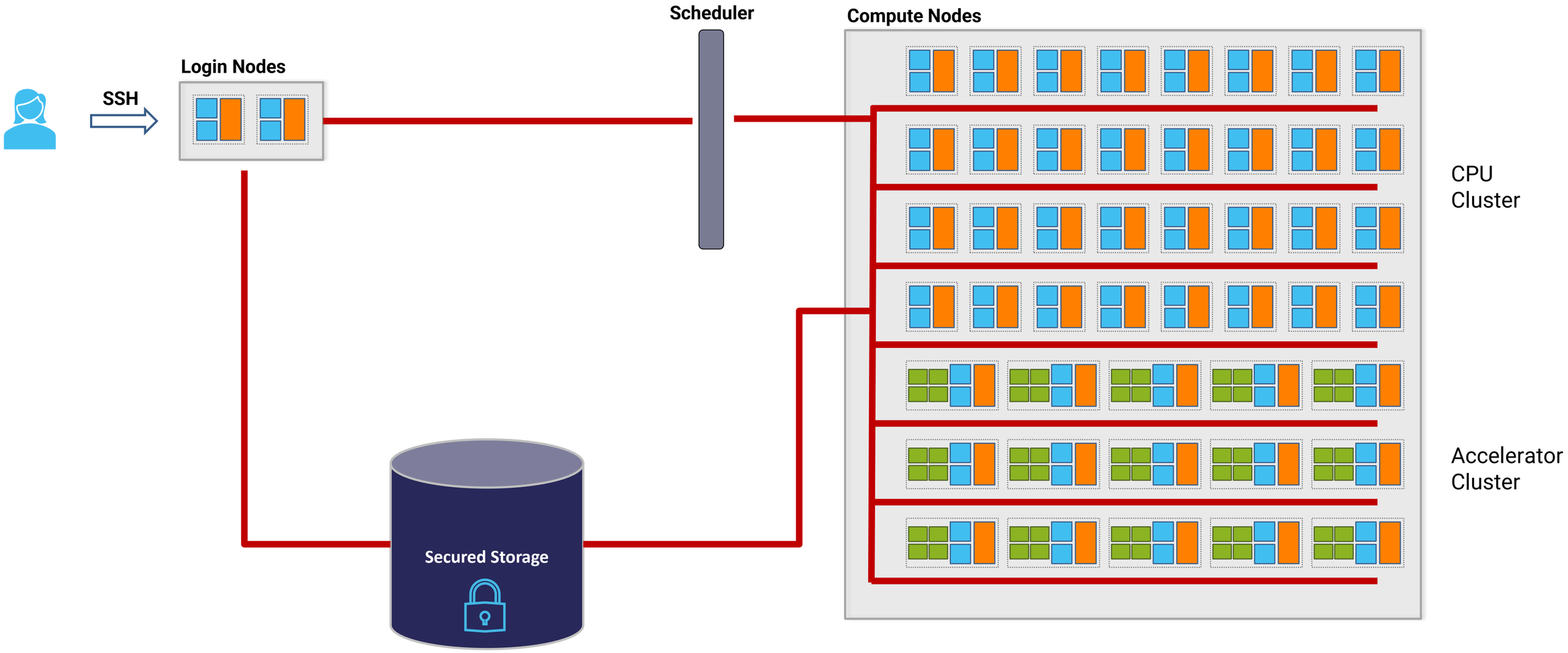

AMD
EPYC

ACCELERATOR “CLUSTER”

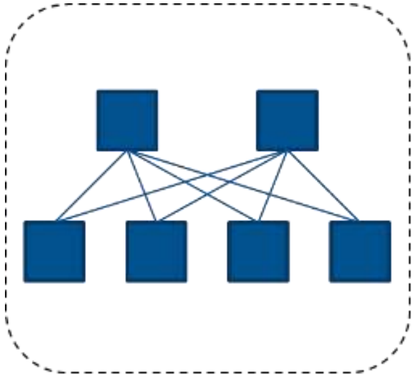




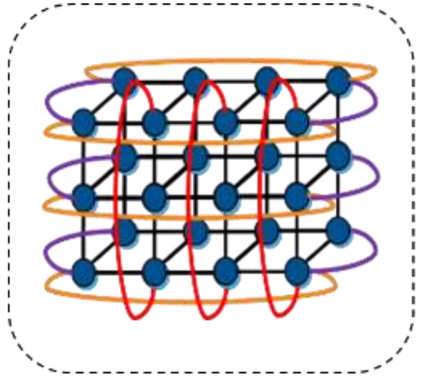
BASIC CLUSTER ACCESS LAYOUT



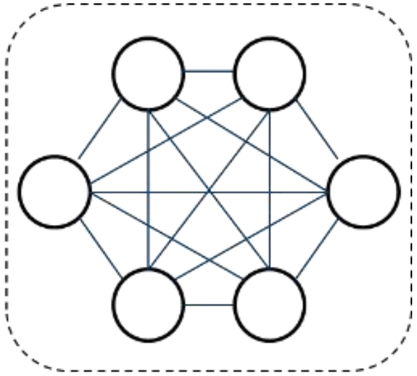
Network Topologies



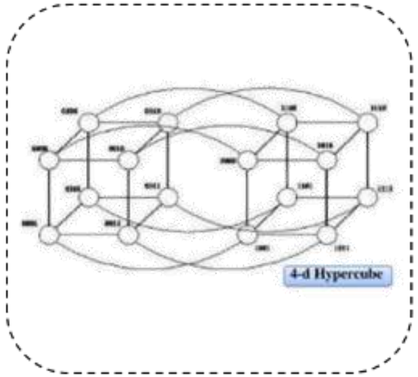
Fat Tree



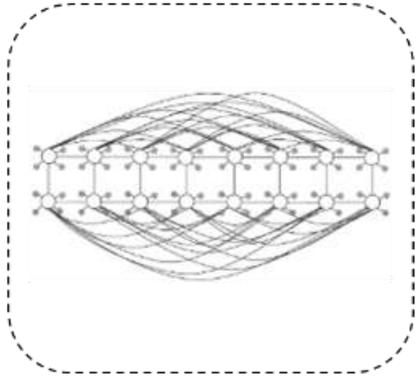
Torus



Dragonfly

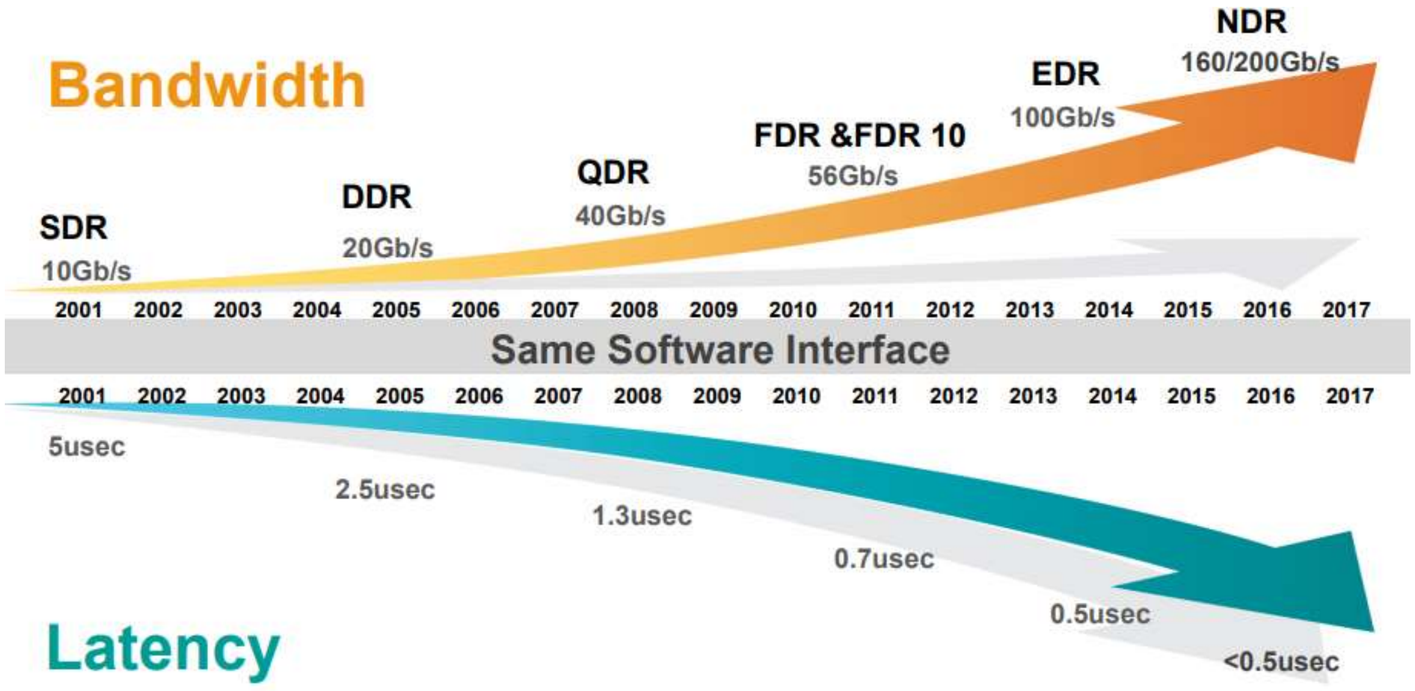


Hypercube

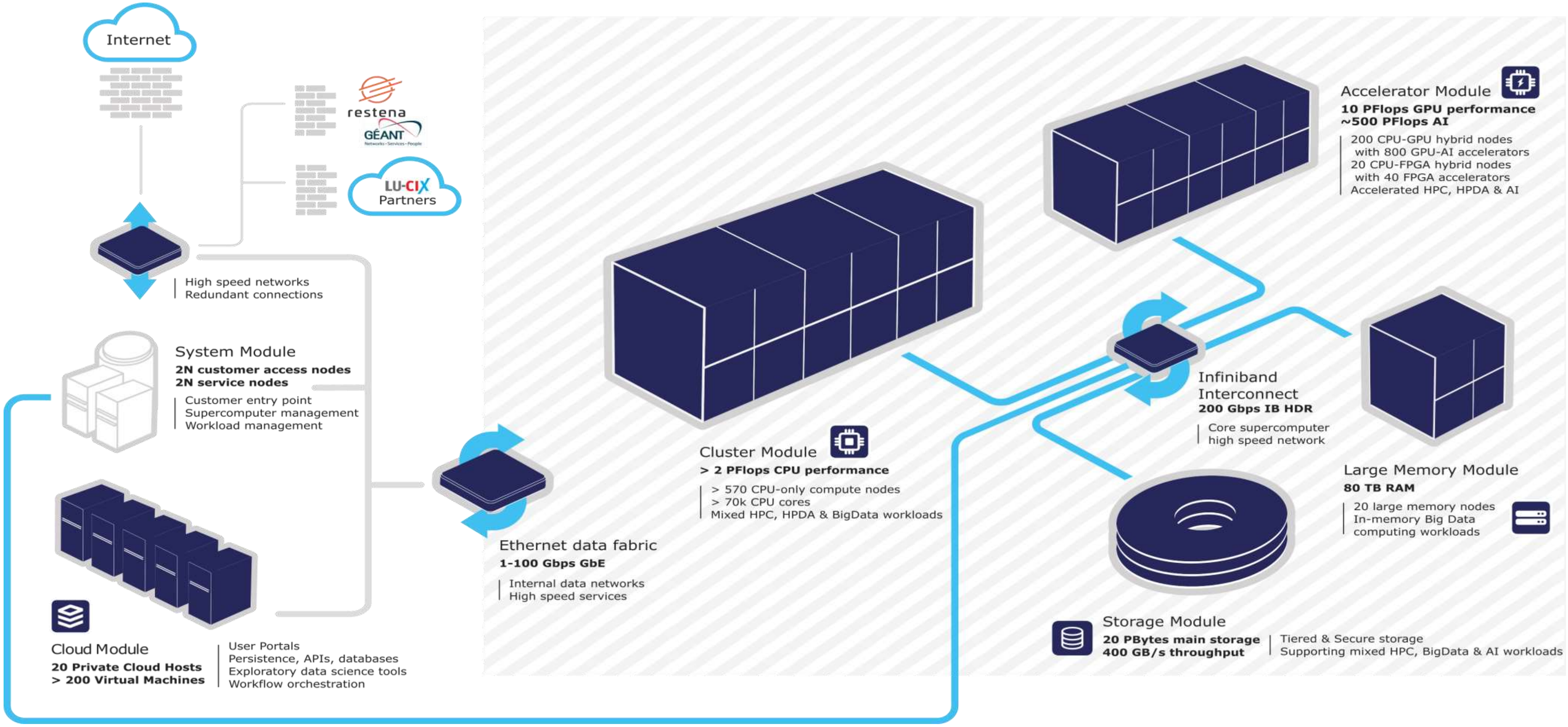


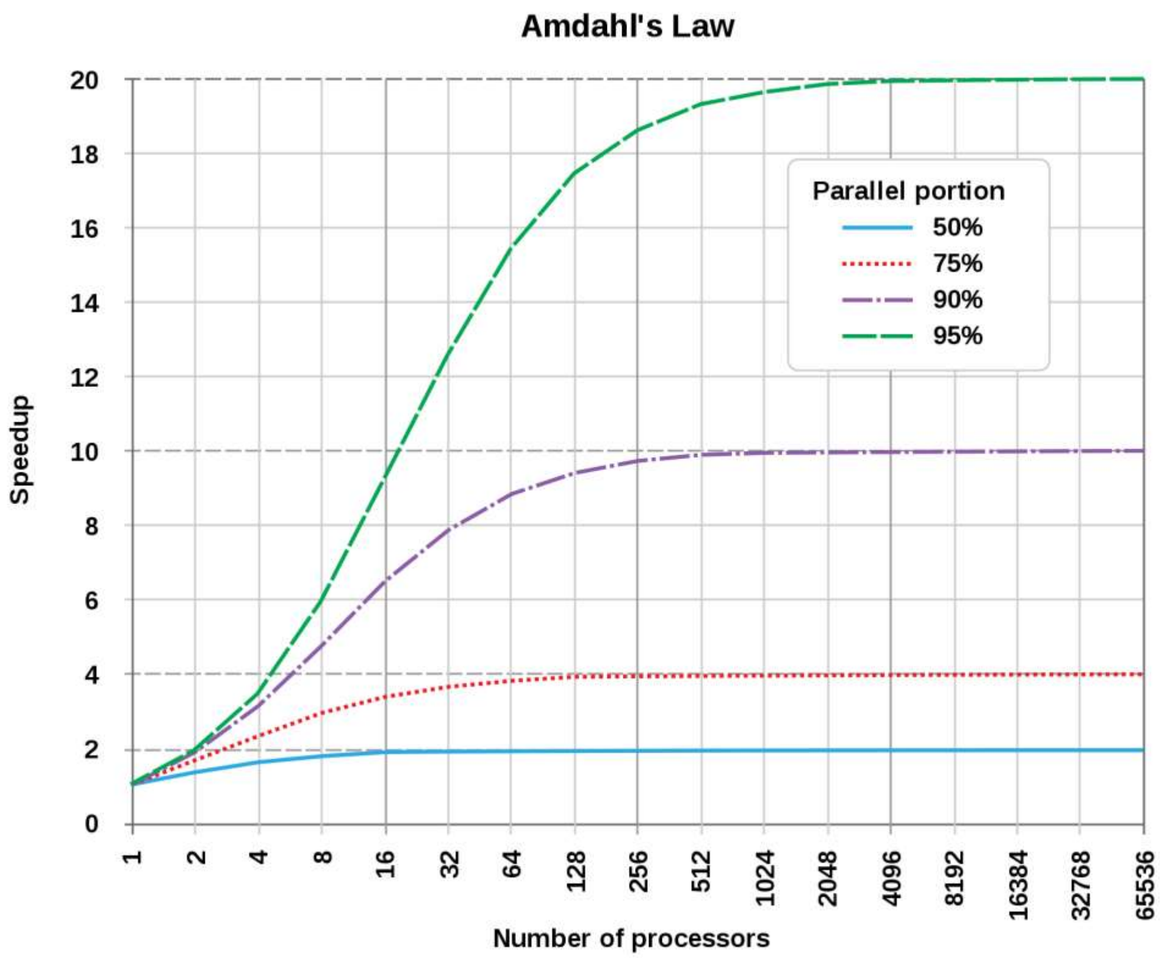
HyperX

Infiniband


Bandwidth
SDR
10Gb/s
DDR
20Gb/s
QDR
40Gb/s
FDR &FDR 10
56Gb/s
EDR
100Gb/s
NDR
160/200Gb/s
2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017
Same Software Interface
2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017
5usec
2.5usec
1.3usec
0.7usec
0.5usec
<0.5usec
Latency

MELUXINA


Internet
restena
GÉANT
LU-CIX
Partners
High speed networks
Redundant connections
System Module
2N customer access nodes
2N service nodes
Customer entry point
Supercomputer management
Workload management
Cloud Module
20 Private Cloud Hosts
> 200 Virtual Machines
User Portals
Persistence, APIs, databases
Exploratory data science tools
Workflow orchestration
Ethernet data fabric
1-100 Gbps GbE
Internal data networks
High speed services
Cluster Module
> 2 PFlops CPU performance
> 570 CPU-only compute nodes
> 70k CPU cores
Mixed HPC, HPDA & BigData workloads
Accelerator Module
10 PFlops GPU performance
~500 PFlops AI
200 CPU-GPU hybrid nodes
with 800 GPU-AI accelerators
20 CPU-FPGA hybrid nodes
with 40 FPGA accelerators
Accelerated HPC, HPDA & AI
Infiniband
Interconnect
200 Gbps IB HDR
Core supercomputer
high speed network
Large Memory Module
80 TB RAM
20 large memory nodes
In-memory Big Data
computing workloads
Storage Module
20 PBytes main storage
400 GB/s throughput
Tiered & Secure storage
Supporting mixed HPC, BigData & AI workloads


Amdahl's Law
Speedup
20
18
16
14
12
10
8
6
4
2
0
1
2
4
8
16
32
64
128
256
512
1024
2048
4096
8192
16384
32768
65536
Number of processors
Parallel portion
50%
75%
90%
95%

- Federation of national and regional HPC centers (see also PRACE/PRACE2) EU HPC strategy initiated in 2012 implementation within H2020 program
- EU Member States sign the **EuroHPC initiative** and prepare its implementation (Mar. 2017)
- Creation of EuroHPC JU (Jan. 2019) based in Luxembourg with 1 Billion Euros funding for Peta, Pre-Exa and Exascale solutions
- A common effort to create and grow the European supercomputing ecosystem

EuroHPC JU

EuroHPC
Joint Undertaking

2019-2020: PUTTING EUROPE IN THE LEAD

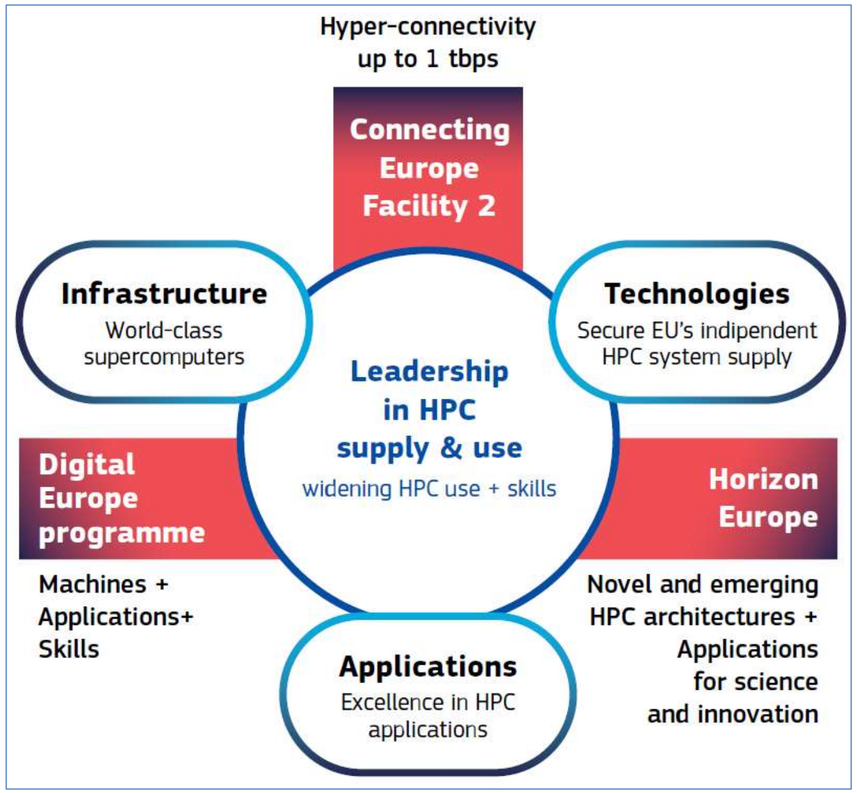
The EuroHPC Joint Undertaking

EuroHPC
Joint Undertaking

Legal and funding body created by the Council in September 2018

- 29 Participating States + EU
- Site: Luxembourg
- Budget (2019-2020): €1.5 Billion
- Operational: 11/2018 to 2026

Mission: Pool European resources to establish an integrated world-class supercomputing & data infrastructure and support a highly competitive and innovative HPC and Big Data ecosystem.



ec.europa.eu/digital-single-market/en/policies/high-performance-computing

2021

DIGIBYTE | Publication 28 May 2021

Commission welcomes Council's support for a €7 billion investment in Europe’s supercomputing infrastructure

The European Commission welcomes today's General Approach in the COMPET Council by Research Ministers on the European High Performance Computing Joint Undertaking Regulation.

EuroCC & CASTIEL Projects

MORE THAN INFRASTRUCTURE…

- EuroCC project about kickstarting **National (HPC, HPDA & AI) Competence Centers**
- 1 NCC per country, 33 participating countries
- **Luxembourg NCC**: LuxInnovation, the University of Luxembourg and LuxProvide

… ALL ABOUT EXPERTISE

- NCCs will provide **broad service portfolio** tailored to national needs
- … of industry, academia & public administration
- LuxProvide leading work on **Technology Transfer**, Business Development & **Collaboration with Industry**
- … will also organize trainings, workshops

… AND COORDINATION

- CASTIEL project will promote interaction & exchanges across NCCs

Find out more about EuroCC Luxembourg: **eurocc-luxembourg.lu**

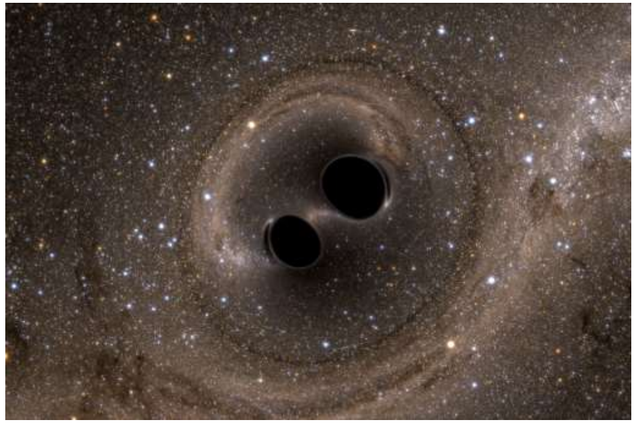
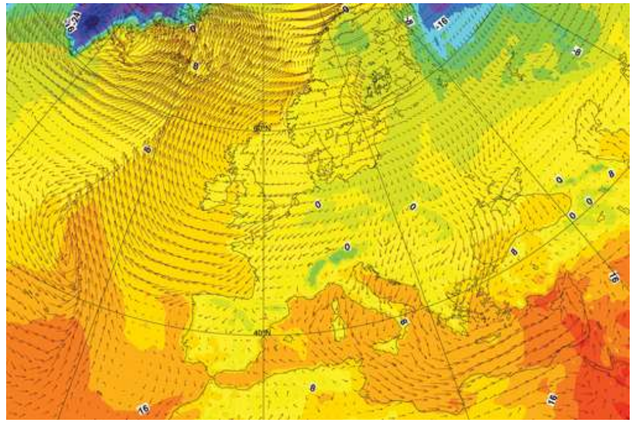
linkedin.com/company/eurocc-luxembourg twitter.com/EuroCC_Lux

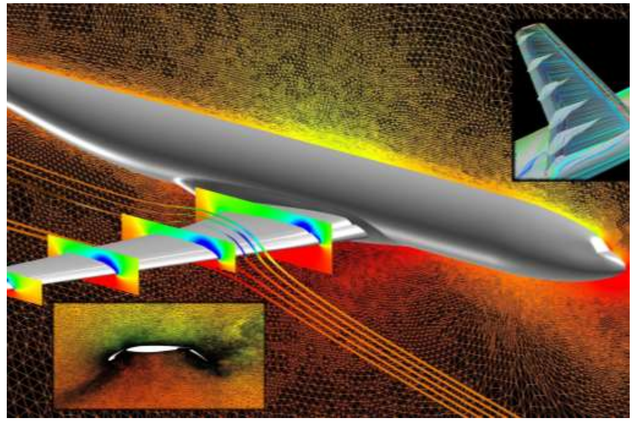
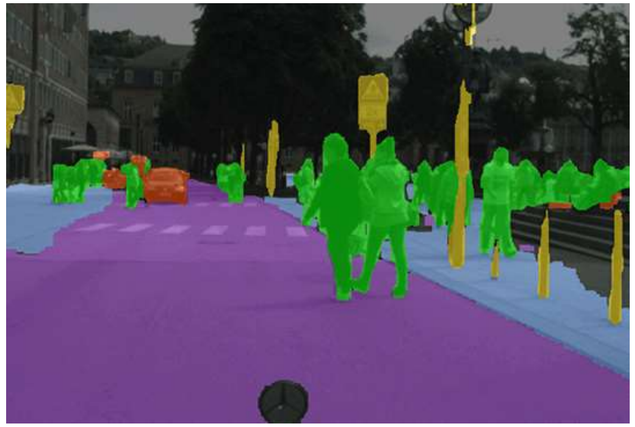
The Scientific Case for Computing in Europe 2018-2026

The PRACE Scientific Steering Committee

Erik Lindahl & Sinéad Ryan

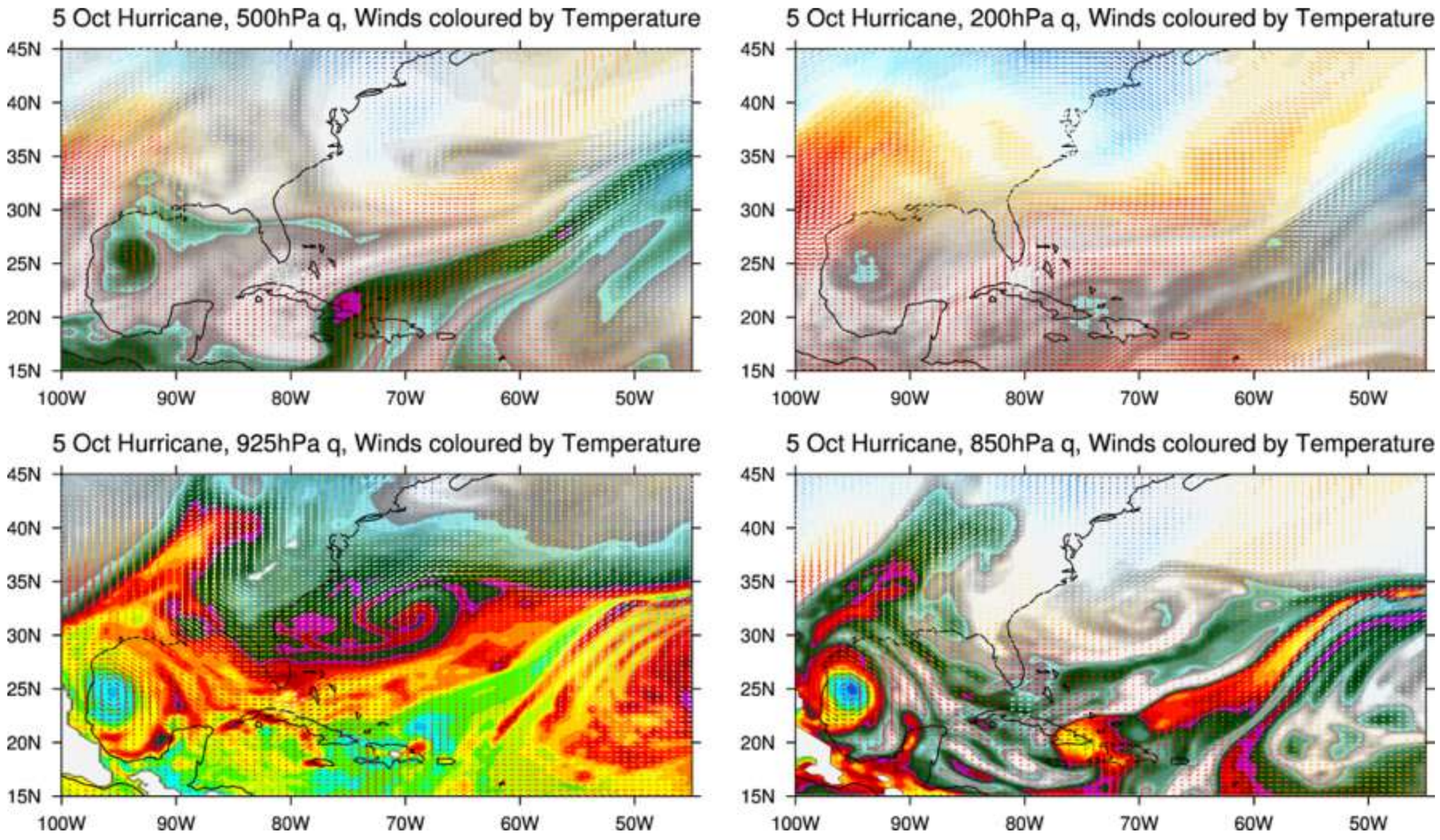
European Computing Solves Societal Challenges

PRACE's goal is to help solve these challenges. The days when scientists did not have to care about the hardware are over, and so are the days when compute centers did not have to worry about the scientific application!

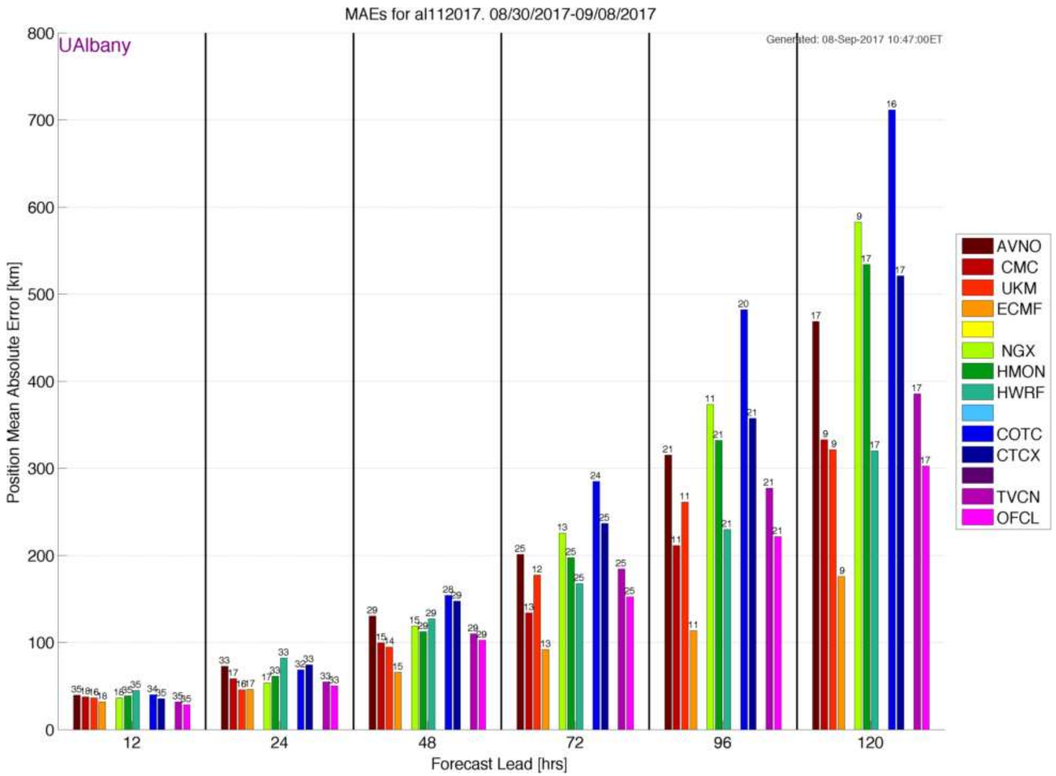
Climate, Weather & Earth Ecosystems



Europe leads international code development

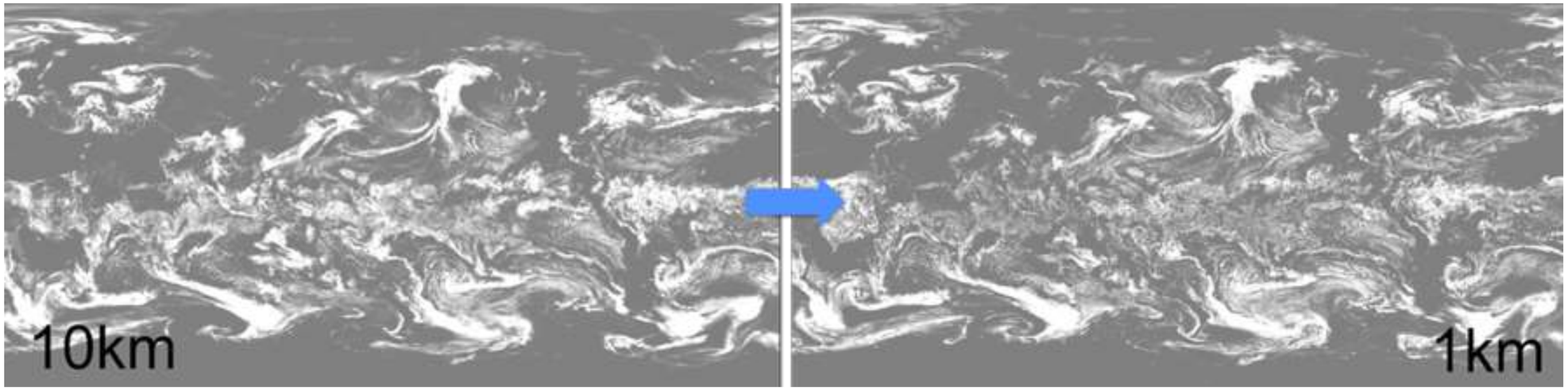
Predicting evacuation needs is a life/death matter – but avoiding it saves €250M

The best forecast codes are European
Arguably, the US would have done better by investing less in machines and more in software



Maintaining our European lead on software should be one of our investment priorities

The Centers of Excellence are Working

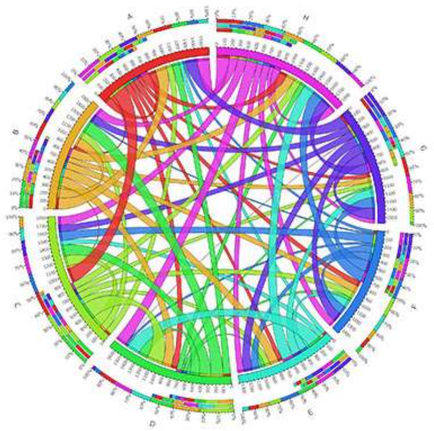


The Centers of Excellence are Working

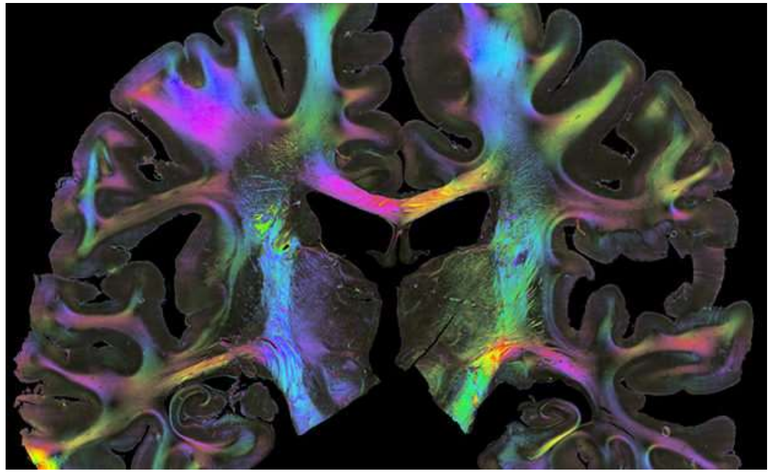
Accurate 20 day weather forecasts would translate to higher revenues in agriculture, tourism and production

- Excellent to outstanding impact in a number of research & code areas
- Important not to be short-sighted: Changing codes is a *longer* process than building an Exascale machine, but with greater long-term European impact. Give them room to focus on the real goal.
- Substantial impact on European competitiveness through workforce education & degrees
- But: Beware that the present CoEs do not cover all areas of science!

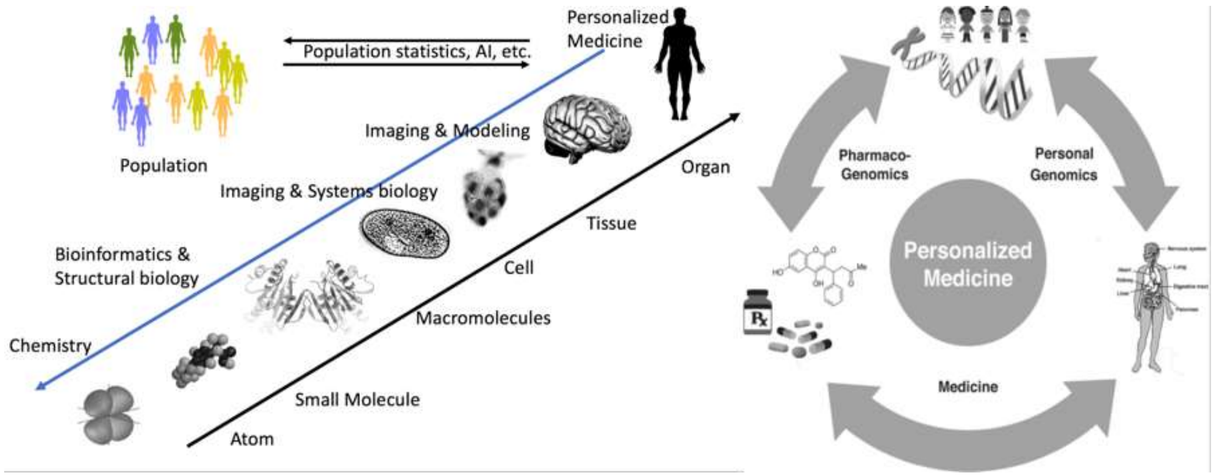
Improving Human Health



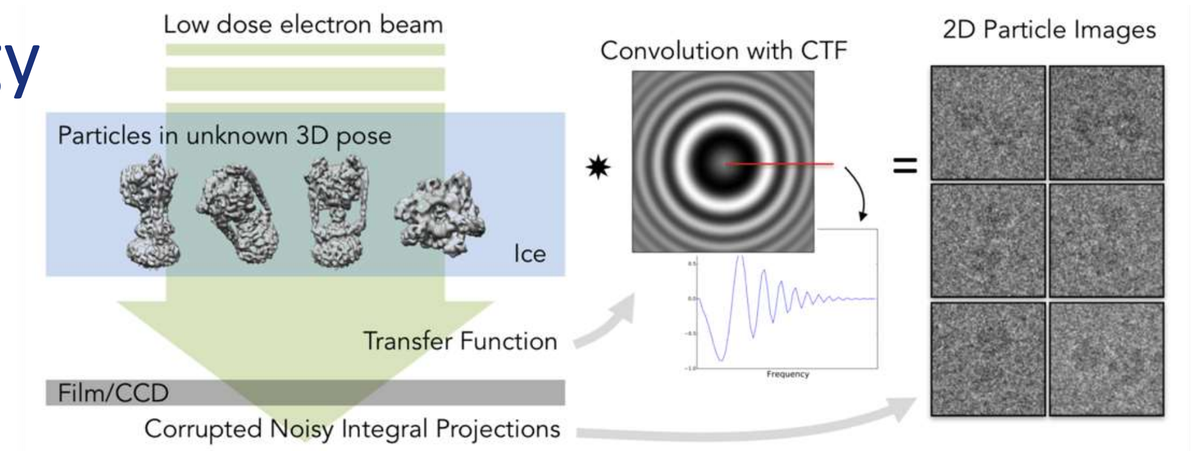
Genomics data grows even faster than computer speed. Future computational resources will enable real-time diagnostics, and predict disease before it happens – preventive care based on broad range of data.



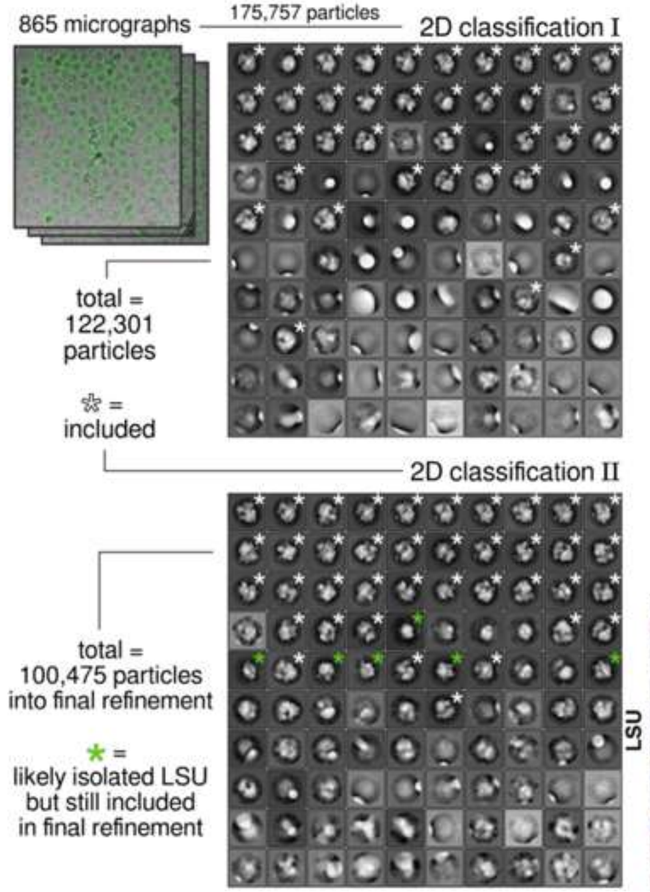
The Human Brain EU Flagship project

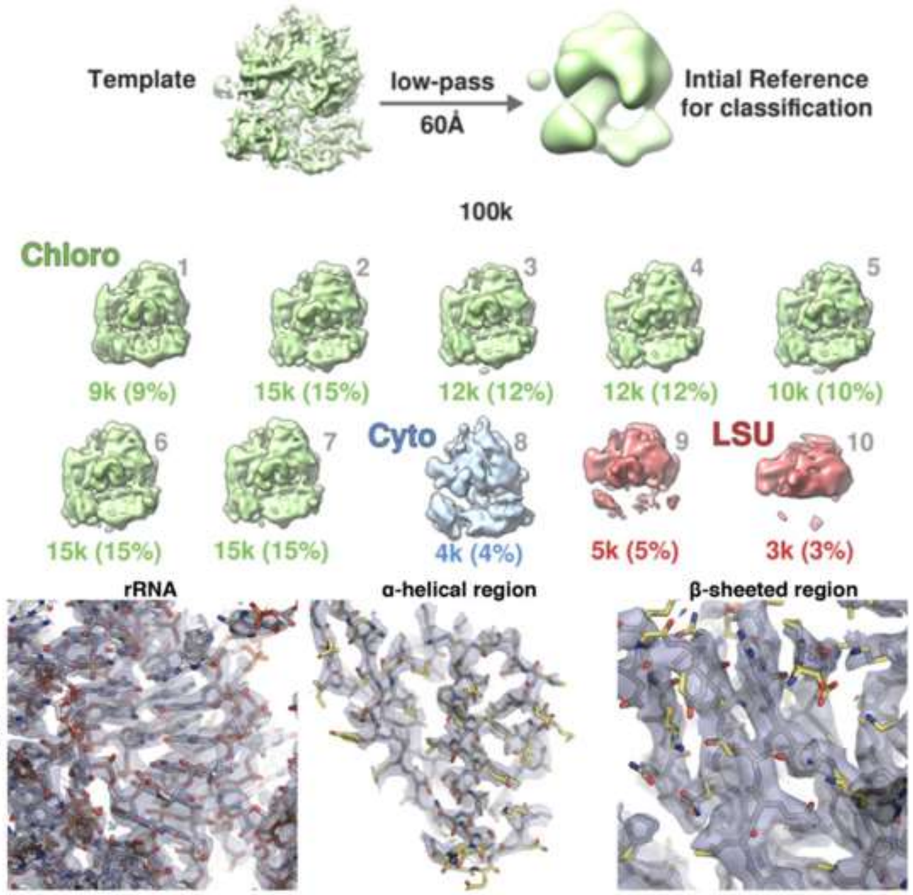


Future Structural Biology is Computational

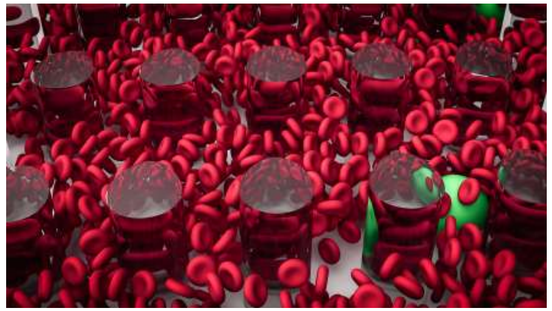


Cryo-electron microscopy (Nobel 2017):
Better computers & algorithms make it possible to understand how molecules move, and design new types of drugs

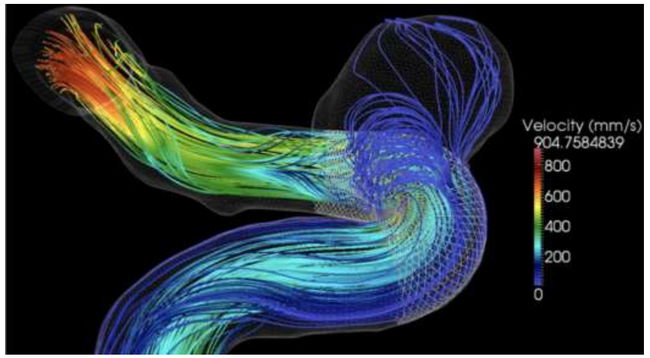




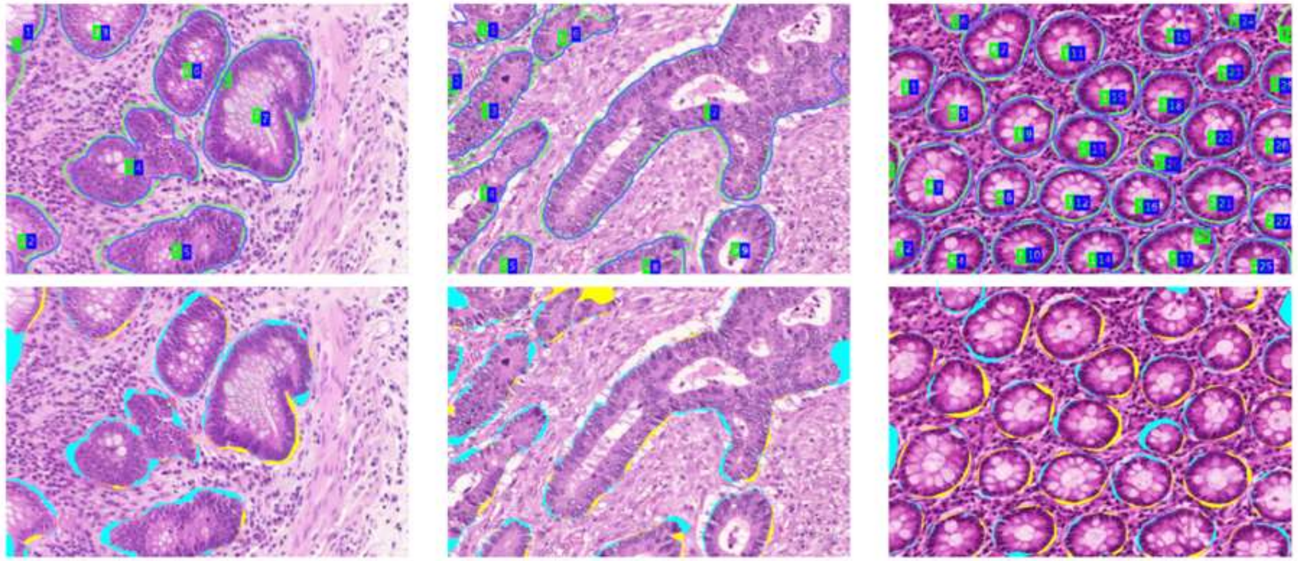
Human Health Computing is Translational



It will become possible to design microfluidics & nanobiotechnology devices to target e.g. specific cancer cells by modeling flow/interactions



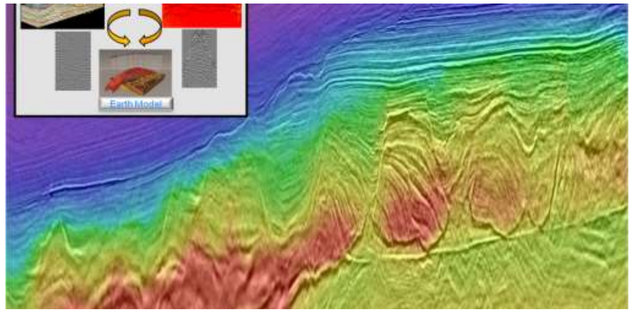
Lattice-Boltzmann enable simultations of blood flow, e.g. effects of using a stent to treat brain aneurysm. On-demand computing!



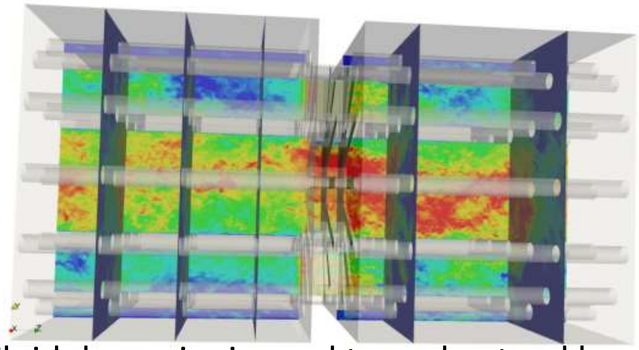
(a) benign (b) malignant (c) benign

Tumor classification with deep learning neural networks now beats the best pathologists

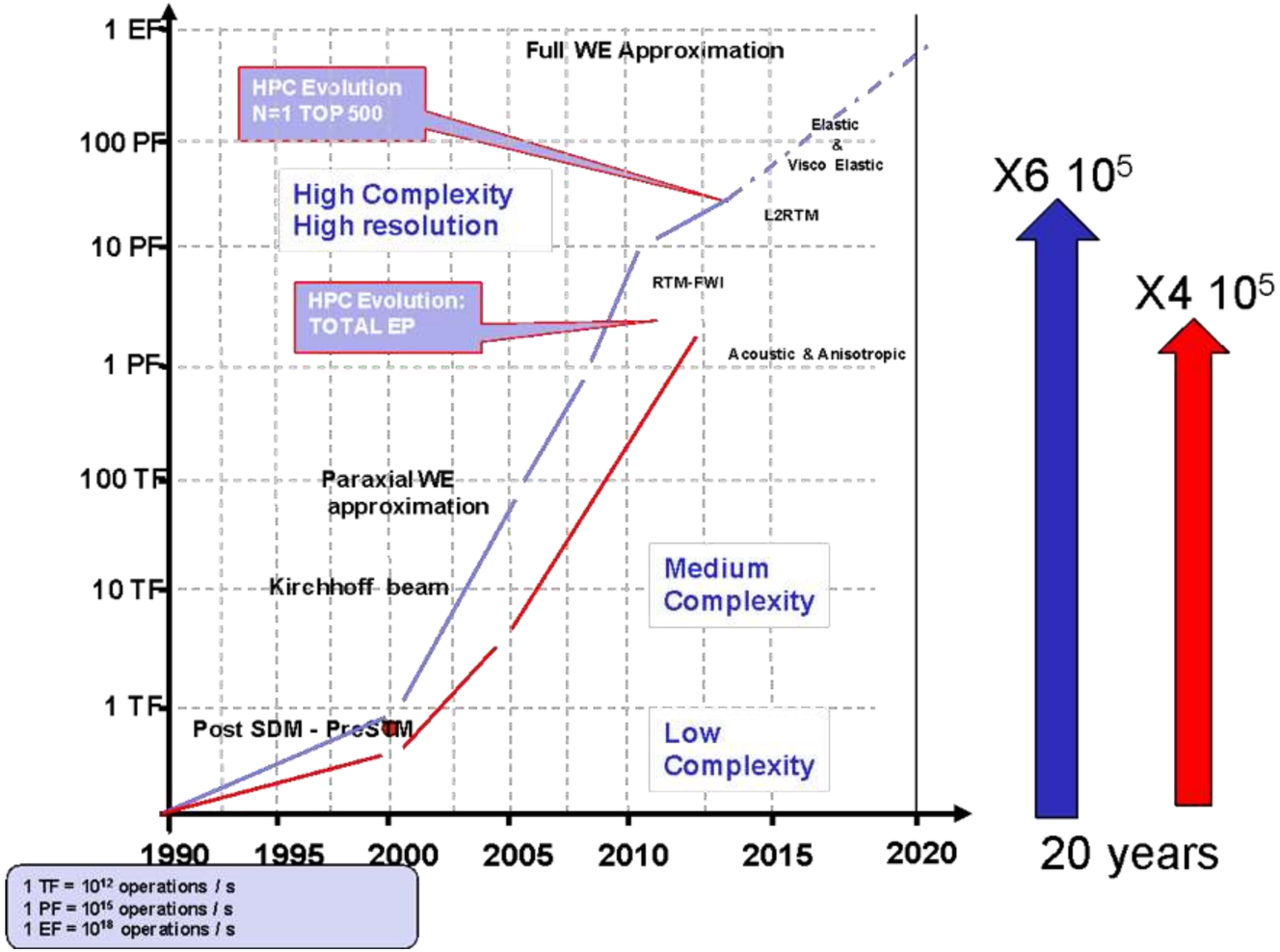
Energy applications need Exascale



Oil & gas is one of the world's largest users of HPC – because computing saves time & money

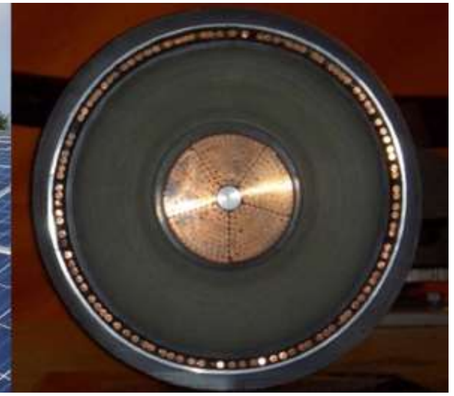


Fluid dynamics is used to understand heat & flow in nuclear reactors



Computing is Driving Renewable Energy

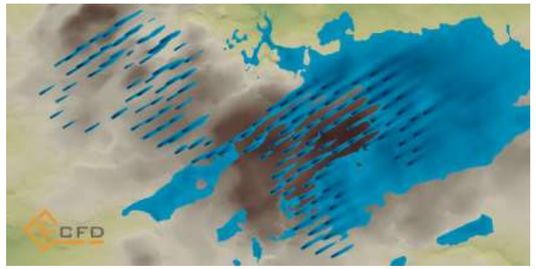


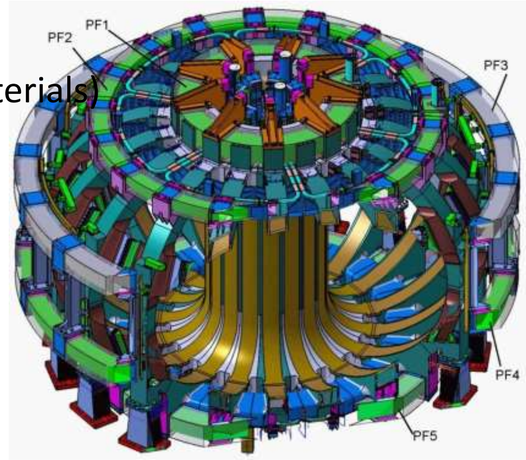



HPC is creating new generations of insulators that enable higher voltage cables, which reduces losses

Optimisation of wing shapes placement of wind farms

New generations of solar cells (materials)

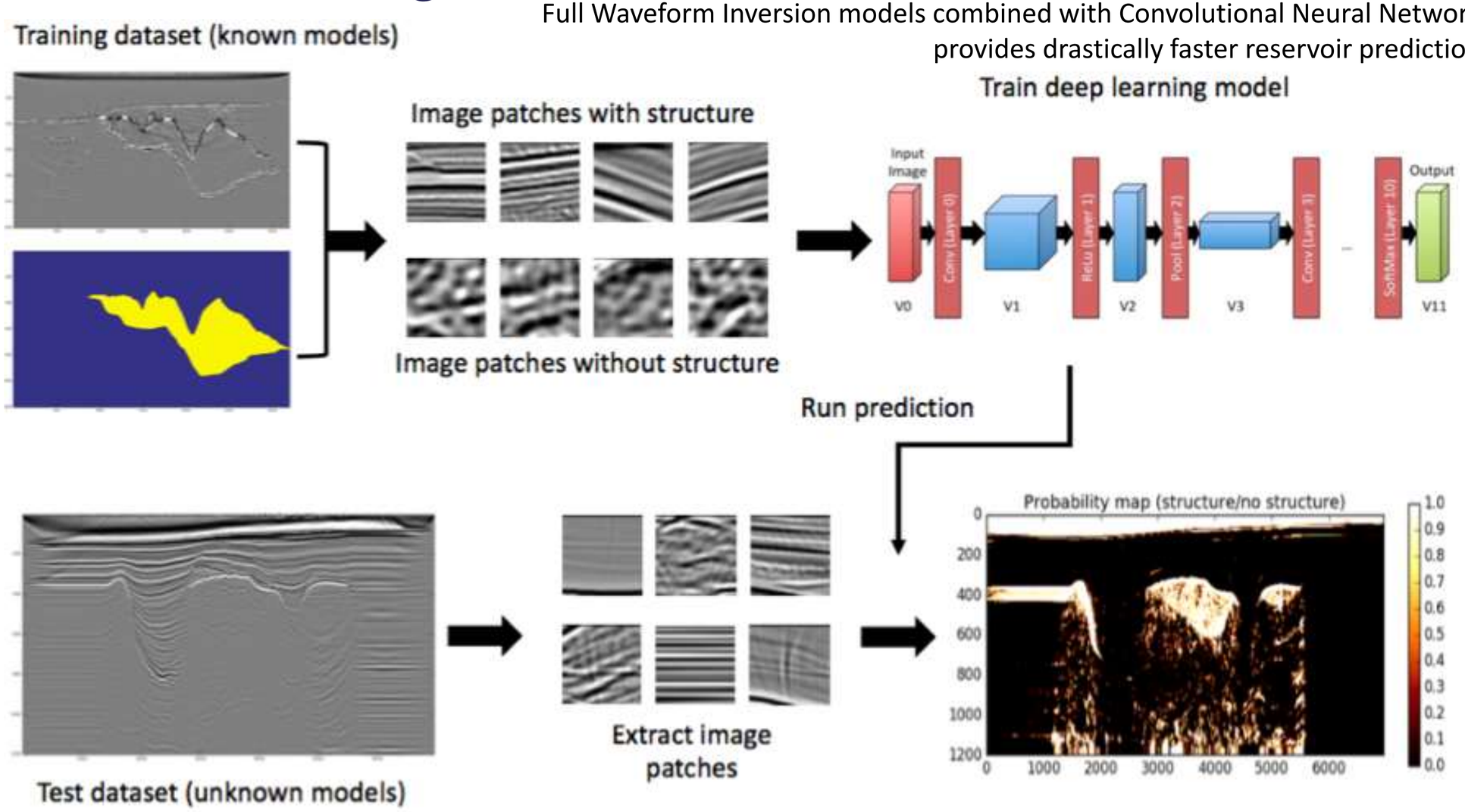





Advanced MHD simulations are critical to make the plasma stable enough to make Tokamaks like ITER useful for energy production through fusion

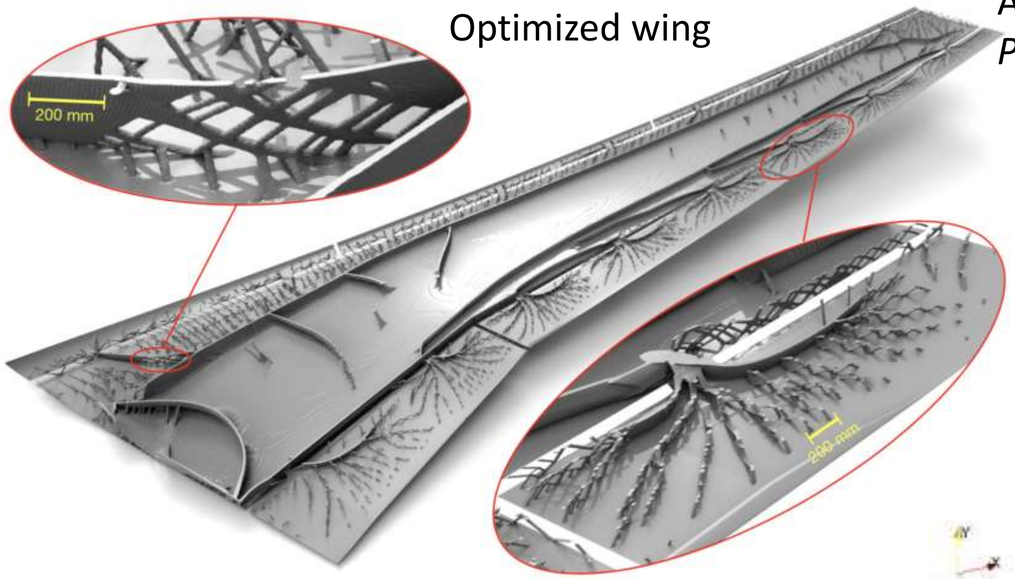
Exascale is causing even traditional fields to turn to AI

Full Waveform Inversion models combined with Convolutional Neural Networks provides drastically faster reservoir predictions



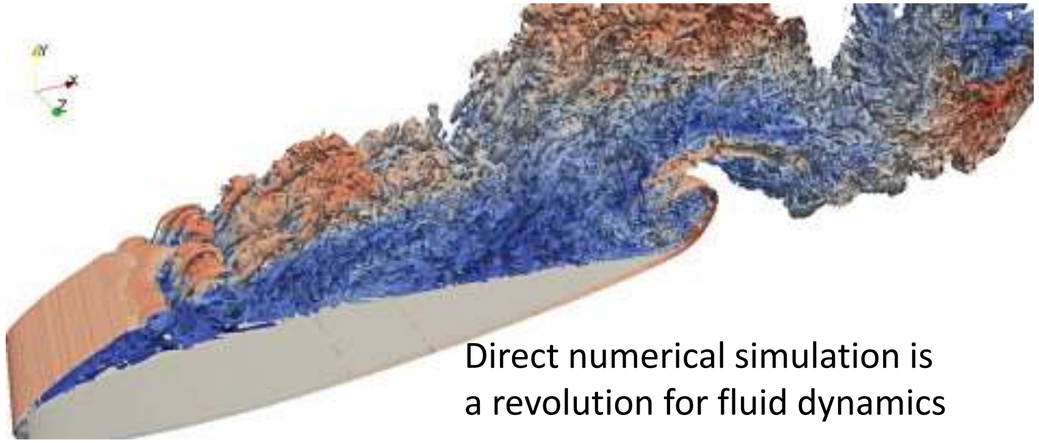
Infrastructure & Manufacturing for Humankind

Optimized wing



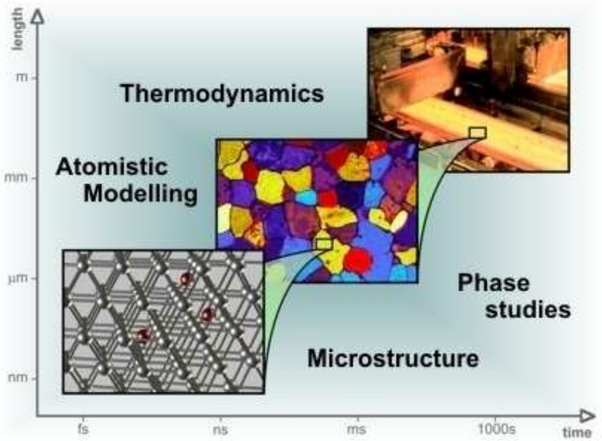
Aage et al., Nature 550, 84 (2017)
PRACE industrial project

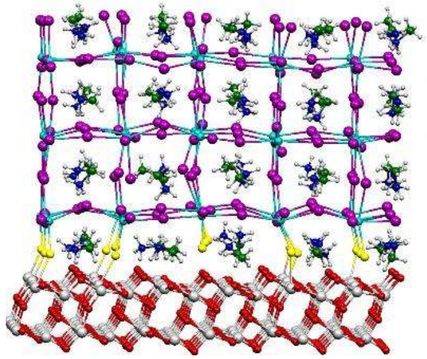
Reach design goals such as:
Stronger, Lighter, Faster
Use less raw material
Cheaper, Safer
Reduce time-to-market



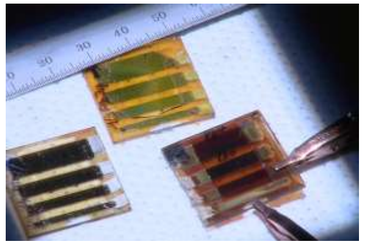
Direct numerical simulation is
a revolution for fluid dynamics

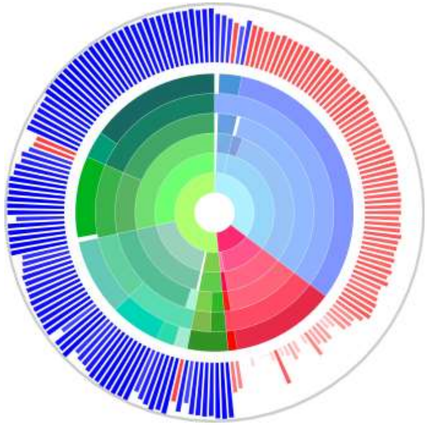
Future Materials: From Molecules to Machines



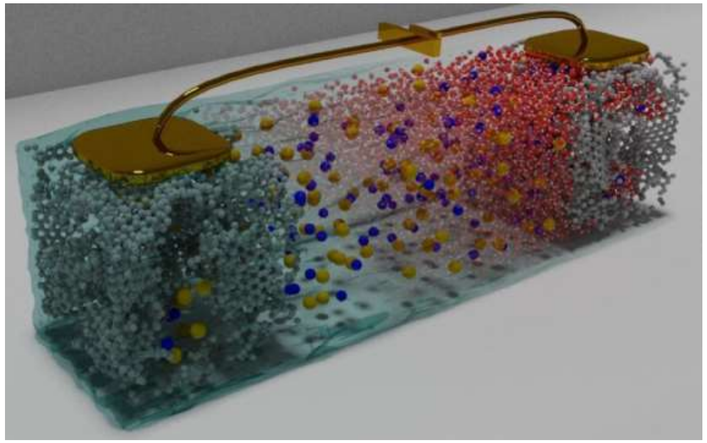


Perovskite solar cells have outstanding efficiency, but contain lead. Simulations used to develop lead-free versions



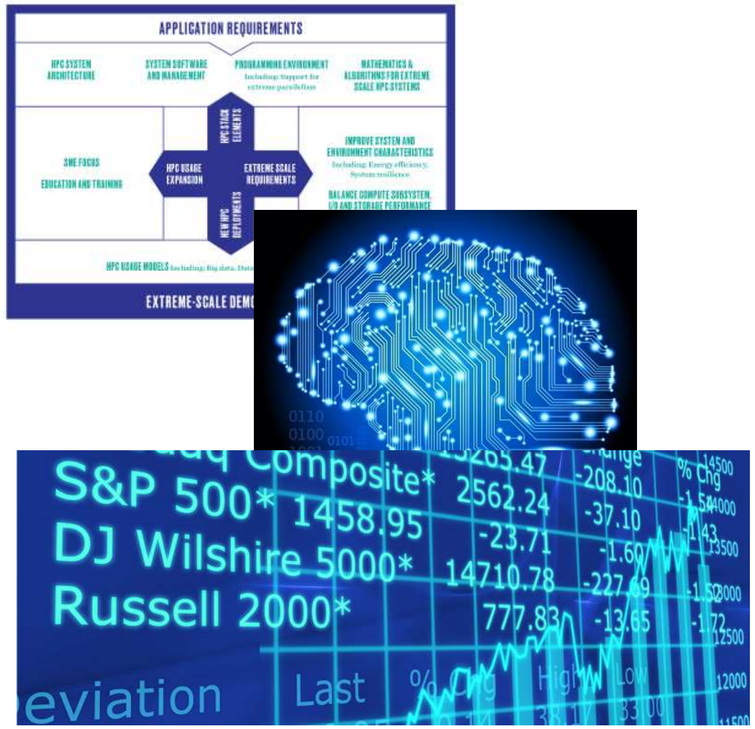


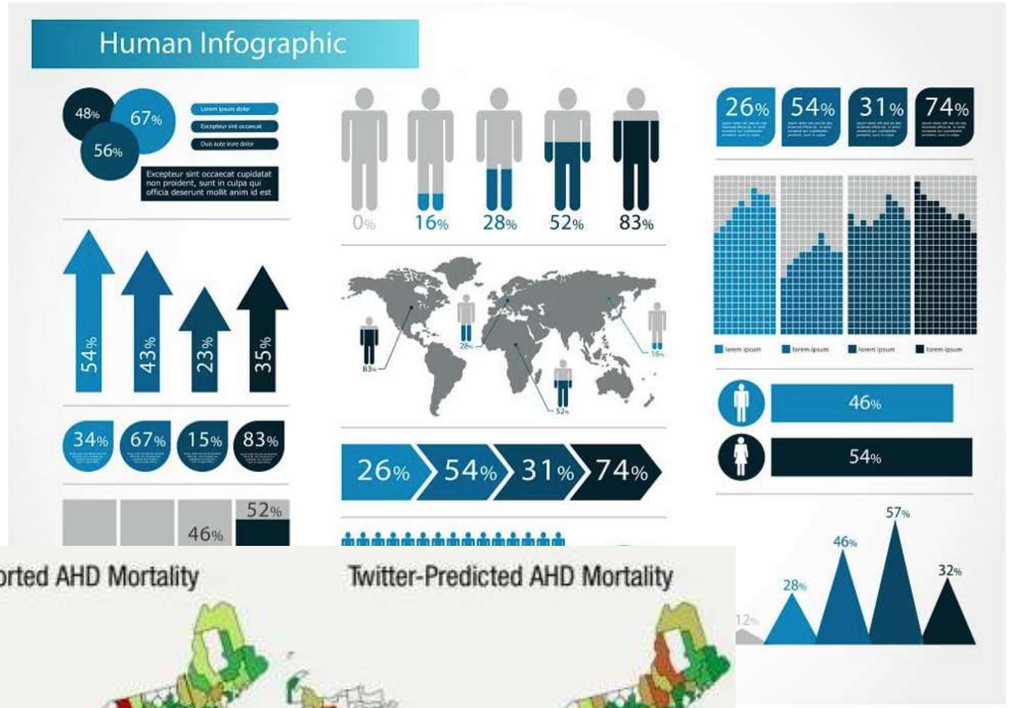
Modern materials design is increasingly data-driven, using AI/deep learning methods to rapidly predict properties without full DFT calculations

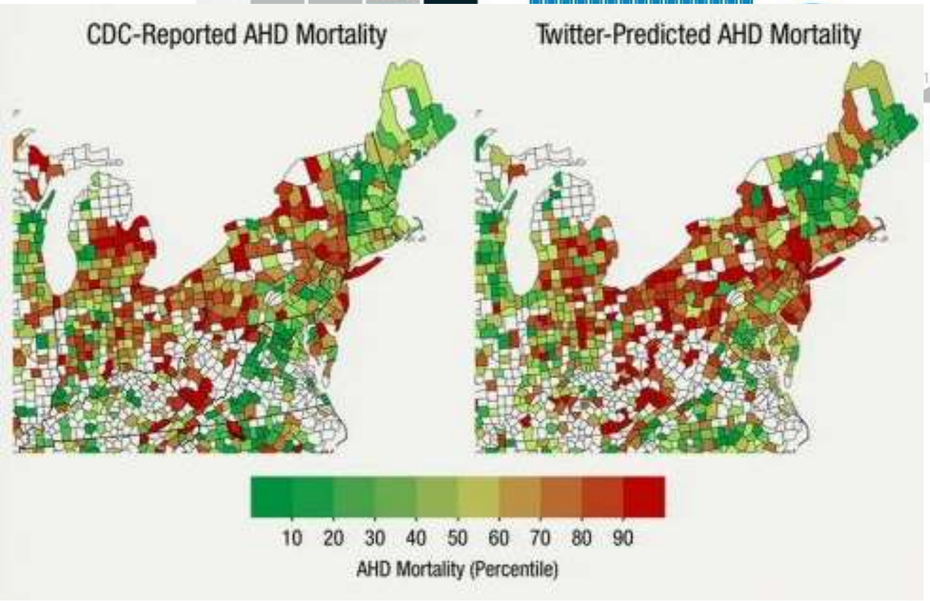


Supercapacitors are used to store energy e.g. in braking kinetic-energy recovery systems in cars/buses. Molecular simulations are used to understand the charge build-up to improve their capacity and efficiency

Complexity & Data







Centres of Excellence in HPC

bioexcel
Centre of Excellence for Computational Biomolecular Research

ChEESE
Center of Excellence for Exascale in Solid Earth

FocusCoE

CompBioMed

EoCoE

esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

HiDALGO

LUX PROVIDE

EXCELLERAT

POP

MAX DRIVING THE EXASCALE TRANSITION

Key Infrastructure Requirements

- Urgent need for more compute cycles - but also high demands for memory bandwidth & I/O
- Scientific Applications are not only ready to use Exascale, but have specific high-impact research goals that can only be realized with access to next-generation resources
- However: Exascale will require new approaches to scaling by using ensembles, deep learning, and statistical models. High-end computing will dominate, but tomorrow's solutions will be different than yesterday's
- Exascale systems will need to be able to handle tens of thousands of active jobs and large I/O requests
- Software & algorithms take longer to change than hardware - first-generation systems must be based on present concrete needs, rather than hopes about being able to co-design
- Linux rules the modern computing world: All systems will need to support a full Linux stack of development tools
- Centers & their staff need to engage directly in software development together with scientific communities

Aside from the HPC efforts, the European Commission is increasing its annual investments in AI by 70% under the research and innovation programme Horizon 2020. It will reach EUR 1.5 billion for the period 2018-2020.

Now How to Transfer Knowledge to SMEs?

National HPC Competence Centres
Education and Training
Next generation portals and domain workflows
Easier access to Computing cycles

MELUXINA: A WORLD CLASS HPC SYSTEM

Compute

18 Petaflops (10^{15})

Peak aggregated performance
Heterogeneous supercomputing

Compute intensive workloads Excellent for simulation, data analytics & AI

Faster than
17,000 x

Storage

25 Petabytes (10^{15})

Tiered HPC storage, excellent for HPDA & AI
+ Long Term Archival capabilities

Massive data sets
Perfect for innovative data exploration

More than
20,000 x

Networking

400 Gigabits/s (10^{9})

Infiniband HDR links on every MeluXina node +
High speed external connectivity

Large scale workloads
Lightning-fast data processing

Better than
768,000 x

It is like running a full marathon in 0.4 seconds or flying from Paris to London in 0.1 seconds.

The *MUSE*: MeluXina User Software Environment

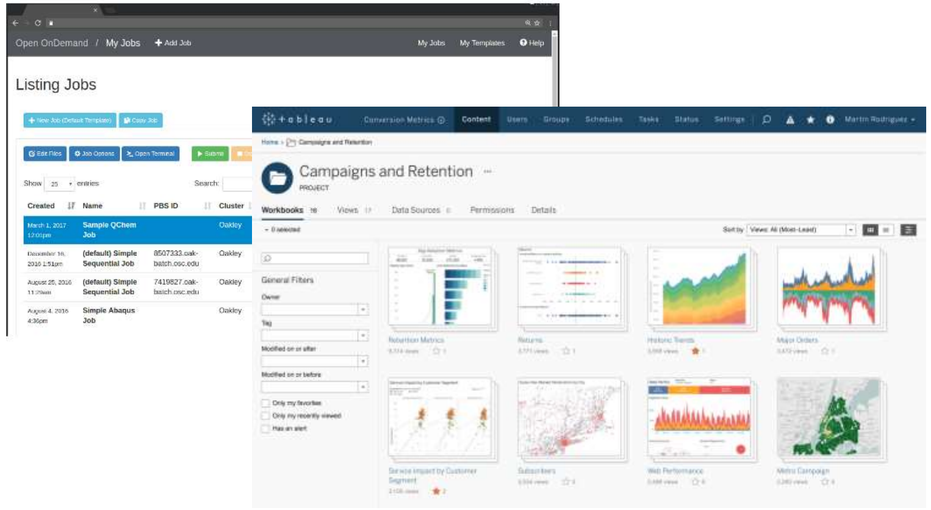
- Operating System: **Linux**
- Rich software environment with Open Source & commercial tools
- Ease of provisioning and use of provided software
- User can install their own software
- … or use containers

Compilers, Languages & Performance Eng.	Parallelization tools, MPI suites & acceleration libraries	Numerical & data libraries	Frameworks, runtime & platform tools	End user applications
• AOCC • GCC • Intel • NVIDIA HPC SDK ✓ incl. PGI • Support for various programming languages ✓Python ✓R ✓Julia ✓Go ✓Rust • Performance and debugging tools ✓Intel ✓NVIDIA ✓ARM (Forge) ✓Scalasca ✓SCORE-P ✓Extrae ✓PAPI ✓Valgrind ✓GDB ✓AMD-uProf ✓ Nsight-Systems ✓ Nsight-Compute ✓ Vtune ✓ gperf ✓ extrap ✓ Inspector • Many build & support tools (Autotools, CMake, …)	• OpenMPI • Intel MPI • ParaStationMPI • NVHPC • TBB • PETSc • KOKKOS • cuBLAS • cuFFT • cuDNN • NCCL • TensorRT	• BLIS • Intel MKL • FFTW • OpenBLAS • ScalaPACK • Boost • Eigen • ARPACK • HDF5 • netCDF • OpenCV • CDO	• PyTorch • Torch Text+Vision • TensorFlow + Hub • Horovod • Keras • Theano • Jupyter Lab • Apache Spark • Matlab Runtime • dotNET Core + SDK • Dakota • Quantum Computing/AI • Cirq • QsimCirq	• GROMACS • OpenFOAM • FOAM-Extend • CP2K • QuantumESPRESSO • NAMD • QMCPACK • NWChem • HOOMD-blue • Freud-analysis • DualSPHysics • POV-Ray • Blender • MDAnalysis • BioPython • QUDA • Visualisation ✓ParaView ✓VMD ✓OVITO ✓NCO ✓ NCView

Over **300** tools pre-installed on MeluXina *today*

MELUXINA: DEMOCRATIZING HPC & HPDA

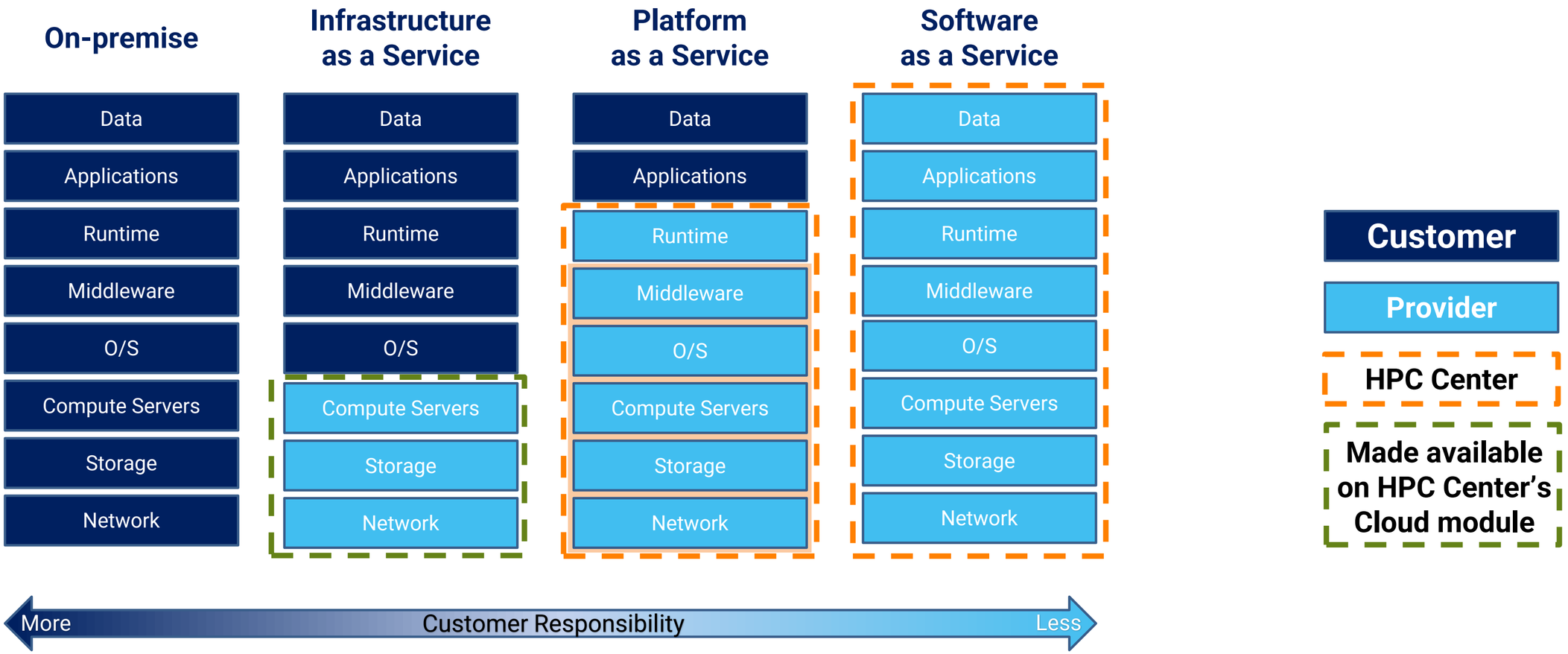
```
Welcome the Luxembourg - EuroHPC supercomputer

MeluXina

You are on a MeluXina login node

                    System information: Compute

| Nodes | CPU                      | RAM     | Accelerator              | Disk  |
|-------|--------------------------|---------|--------------------------|-------|
| 573N  | 2x AMD 7H12: 128c @2.6G  | 512GB   | -                        | -     |
| 200N  | 2x AMD 7452:  64c @2.3G  | 512GB   | 4x NVIDIA A100-40        | 1.92G |
| 20N   | 2x AMD 7452:  64c @2.3G  | 512GB   | 2x Intel Stratix 10MX-16 | 1.92G |
| 20N   | 2x AMD 7H12: 128c @2.6G  | 4096GB  | -                        | 1.92G |

                    System information: Data

| Tier           | Capacity | Speed    | Type | Location on compute/login |
|----------------|----------|----------|------|---------------------------|
| Scratch        | 0.5PB    | 400GB/s  | NVMe | /project/scratch          |
| Home/Project   | 12.5PB   | 180GB/s  | HDD  | /home/users, /project/home |
| Backup         | 7.5PB    | 30GB/s   | HDD  | -                         |

                    System information: Interconnect

Fabric: Infiniband HDR, 200Gbps, DragonFly+ topology
Links : 1x on CPU nodes, 2x on GPU, FPGA & LargeMemory nodes

                    System information: Software

Production software stack: 2021.2
Modules system: LMod, use `module av` to discover the environment

                         Center information

News & Events      : luxprovide.lu
Documentation      : docs.lxp.lu
Support            : servicedesk.lxp.lu, servicedesk@lxp.lu

LinkedIn & Twitter : @luxprovide #meluxina @EuroHPC_JU
```



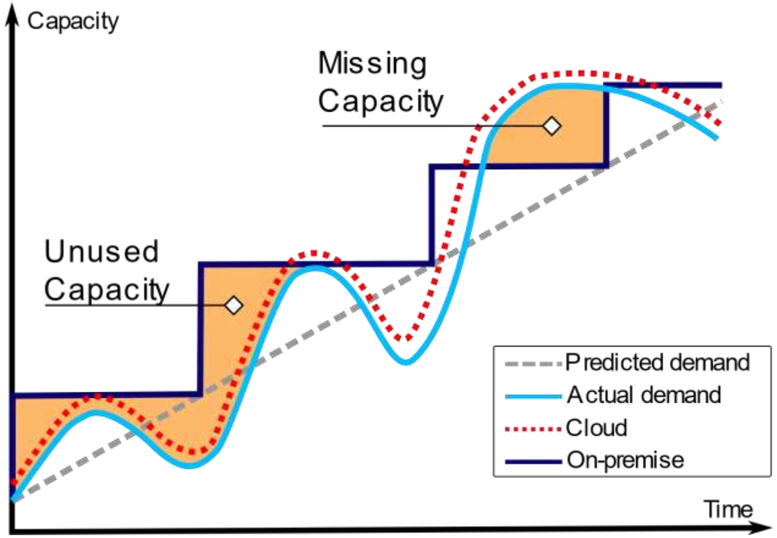
MeluXina's Cloud Module:

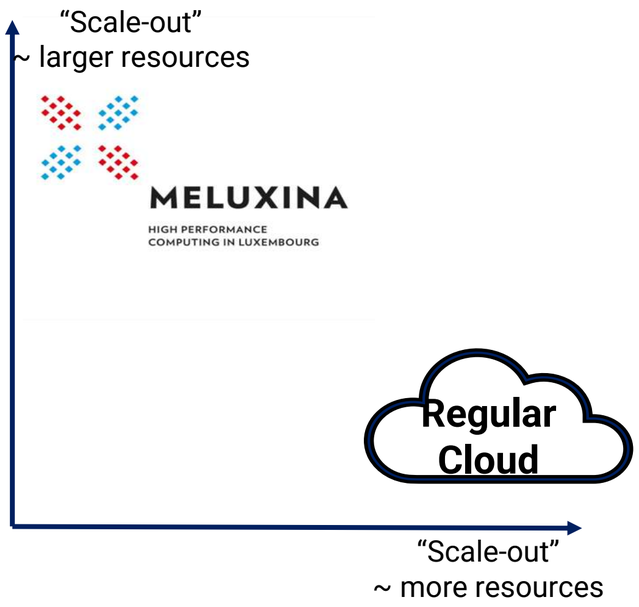
- User Portals
- Dedicated VMs for special workloads
- Data-Scientist friendly AI & ML platforms
- Data streaming for IoT
- Persistent databases
- …

CLOUD RESPONSIBILITY MODES & HPC



CLOUD & HPC





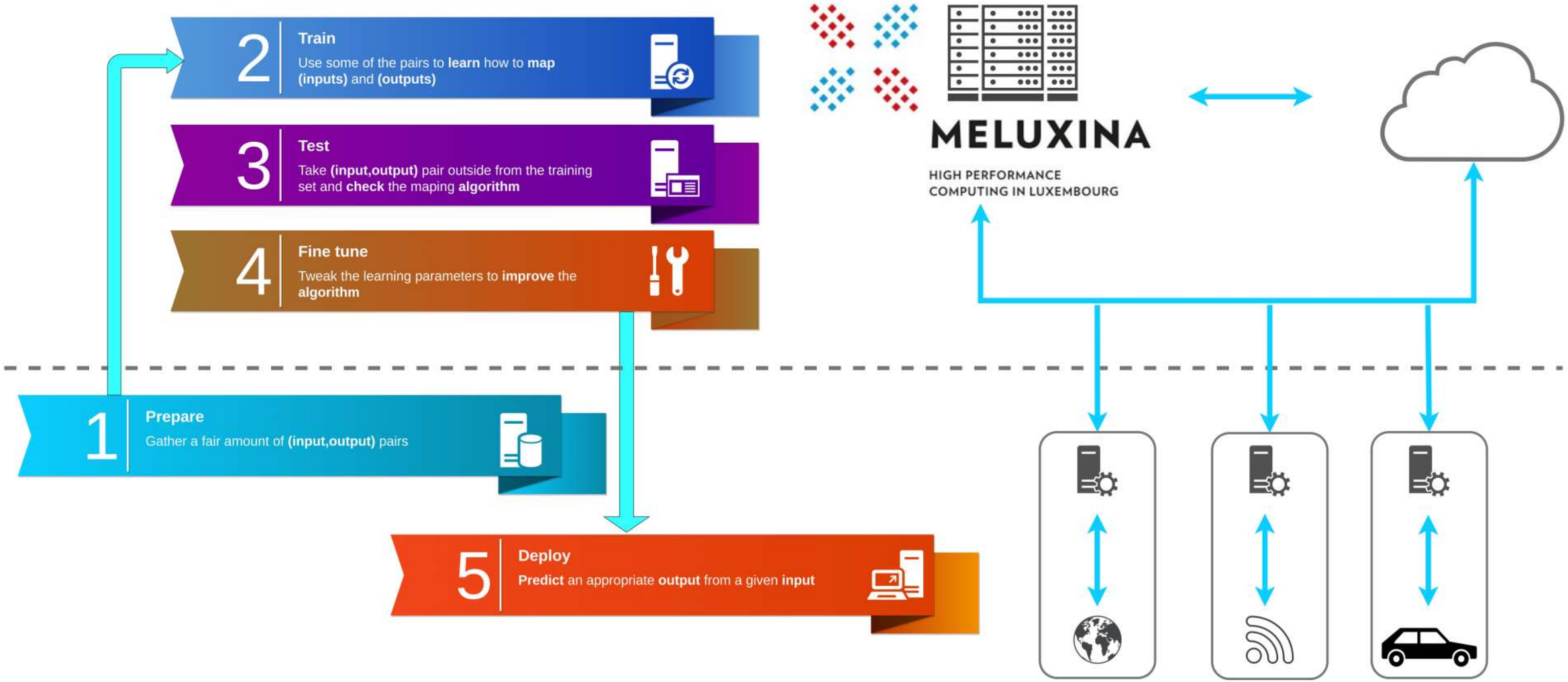
Similarities with "regular" cloud

- On-demand compute and storage
- Pay-per-use model
- Operated by a third party
- Huge but limited resources

Differences with "regular" cloud

- Mostly "batch" based (i.e., not real-time)
- Unified machine
- Located in a well identified place

CLOUD, EDGE, IoT & HPC



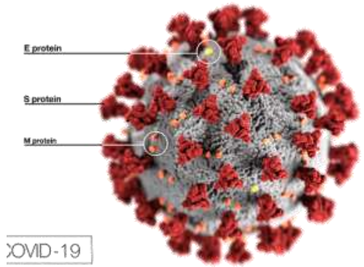
CREATING COMPETITIVE ADVANTAGES

Through High-Performance Computing

Improve time to market

Beat competition with new and better products

Race to find COVID-19 medication



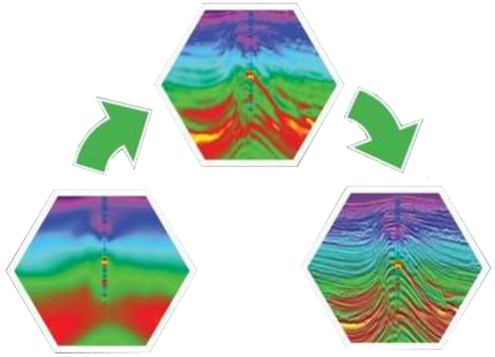
Source: Elsevier

Tackle larger problems

Assimilate more data

Improve physics & algorithms

Increase resolution



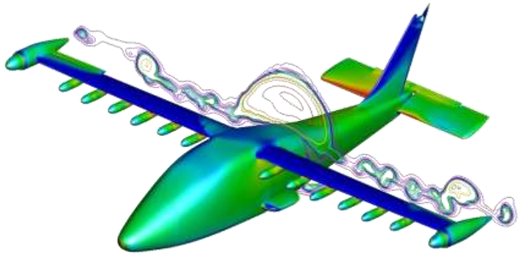
Source: The Leading Edge

Save costs

Reduce needs for costly tests

Safe test environments

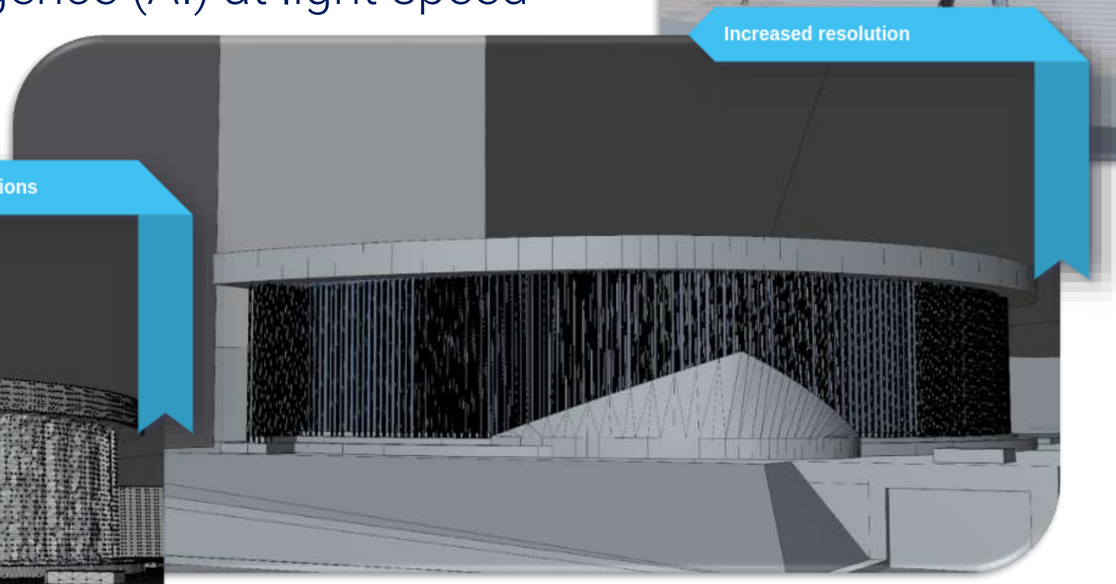
Test more configurations

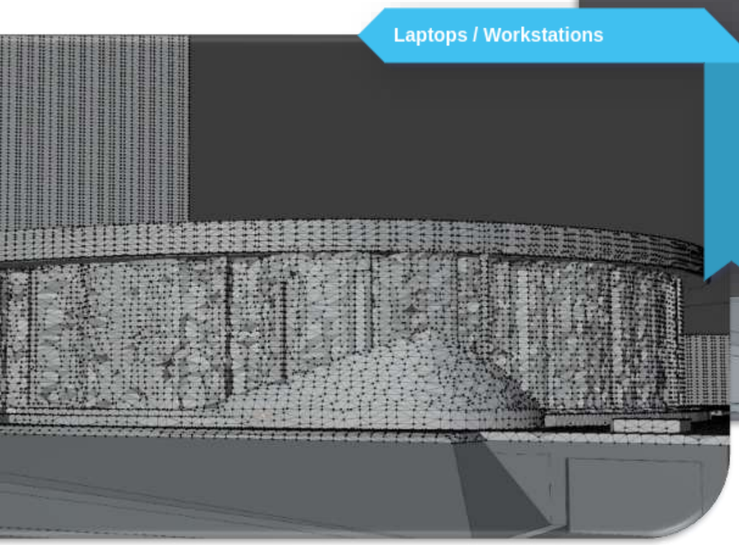


Source: NASA

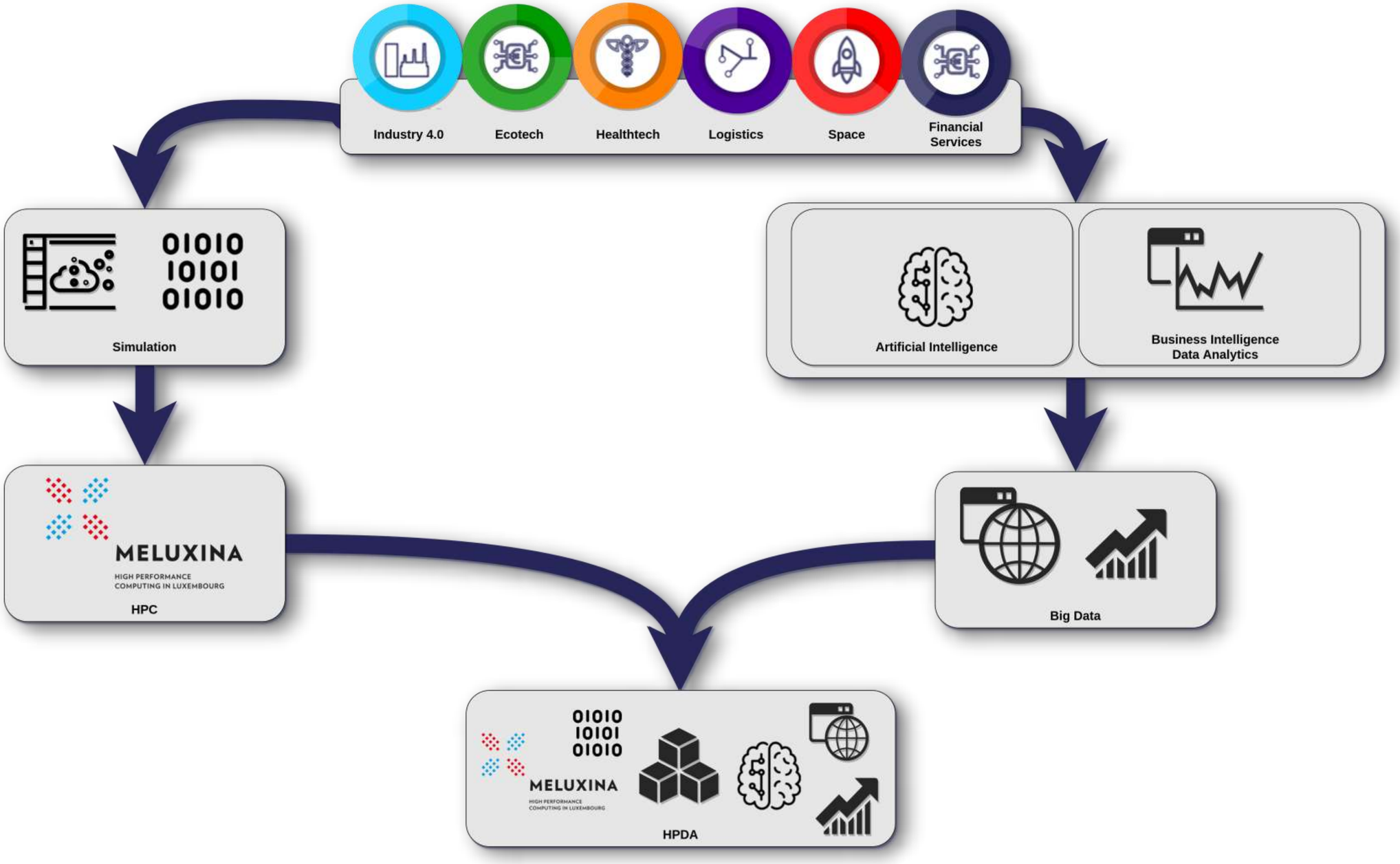
BEYOND LIMITATIONS WITH MELUXINA

- **Increase** resolution, granularity, problem's size
- **Explore multiple meteorological conditions**
- **Parallel** execution to **reduce time to solution**
- **Post-process** huge amount of data
- **Train** Artificial intelligence (AI) at light speed





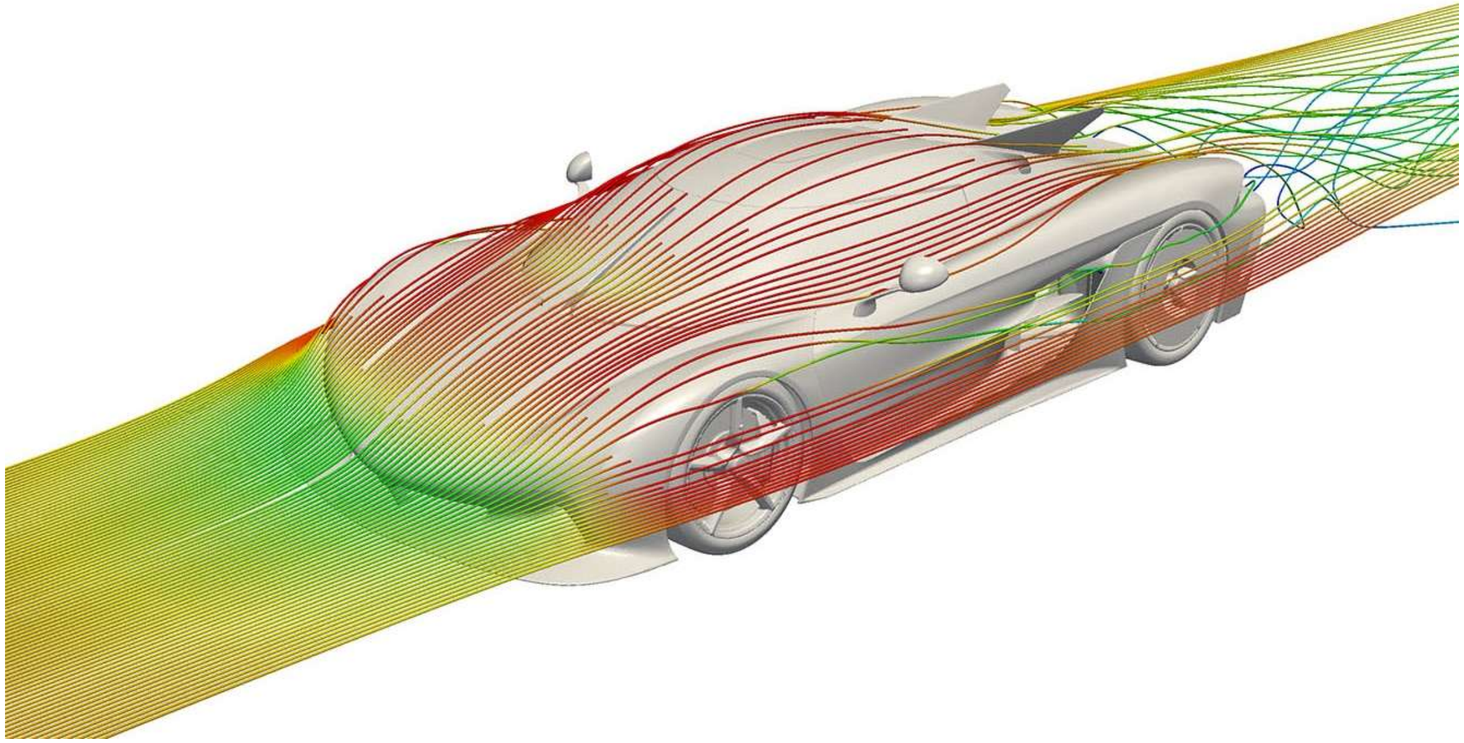
MELUXINA
HIGH PERFORMANCE
COMPUTING IN LUXEMBOURG


Industry 4.0
Ecotech
Healthtech
Logistics
Space
Financial Services
01010
10101
01010
Simulation
Artificial Intelligence
Business Intelligence
Data Analytics
MELUXINA
HIGH PERFORMANCE
COMPUTING IN LUXEMBOURG
HPC
Big Data
01010
10101
01010
MELUXINA
HIGH PERFORMANCE
COMPUTING IN LUXEMBOURG
HPDA

KOENIGSEGG

Sports-car aerodynamics

HPC-based **computational fluid dynamics** (CFD) simulations **help to build** First “megacar” with one-megawatt power and power-to-weight ratio of 1:1



Benefits

30%
in design costs

50%
less wind tunnel testing

60%
in prototyping costs

30%
shorter time to market

Return on investment in
3 month

FORTISSIMO

COPERNICUS & PROVIDERS

Europe's eyes on Earth

Huge EU program to collect **large satellite/in-situ database** and provide **free and open information services**.

Several **Start-ups and SMEs** exploit Copernicus data using **HPC, HPDA or IA** to provide **real business**: Agriculture, Ocean Monitoring, Air Quality, Oil&Gas, Urban Monitoring, Renewable Energies, ...etc

Benefits

Beyond 2020 Copernicus related project are set to generate €1 BILLION of revenue and create 4,000 jobs/year

20 Start-ups incubations / year ~ €1 million / year

(Copernicus Incubation – A boost to your business journey (copernicus-incubation.eu)

TEXA

Diagnostic Instruments for Motor Vehicles

On-board diagnostics system of sensors
Data gathered and processed by **HPC provider**
Predictive maintenance from how the vehicle is driven, failure patterns, and overall health of the vehicle.

Benefits

Better prediction of failures

New services to produce €1.2M revenue over the next 3 years

FORTISSIMO

KALEIDO IDEAS & LOGISTICS

Worldwide Logistics and Intermodal Transport

Logistics represent up to a 20% of manufacturing costs and **marine freight** up to 90% of transport costs

Estimation of marine freight costs using **deep learning**

Benefits

Ability to predict freight costs

Faster quotations, improve performance

by 5%

Quick access to prediction produces a return of €75K during a two-year amortization period

FORTISSIMO

HPC & HPDA: GO / NO GO CRITERIA

Go

- Dataset size larger than several GB
- Long running, compute intensive workloads
- Necessity to scale to stay ahead of competitors

Later

- Limited but growing dataset
- Algorithms with low processing intensity (time and resources)
- Design a growth strategy with HPC in mind

No Go

- Interactive applications (web apps, gaming, …)
- Purely database-driven applications
- In general, deploying real-time applications

ESTIMATING COSTS

Extras

- Login nodes
- Firewall
- …
- …

Software environment

- Proprietary performance tools
- Proprietary parallel debuggers
- Proprietary compilers
- Full module based env.
- Licensed software
- Open-Source Software
- …

Compute

- Cores / vCPUs
- Accelerators (GPU/FPGA)
- Memory (RAM)
- Local SSD

Data

- Data transfers
- Parallel filesystem
- Encryption
- …

Network

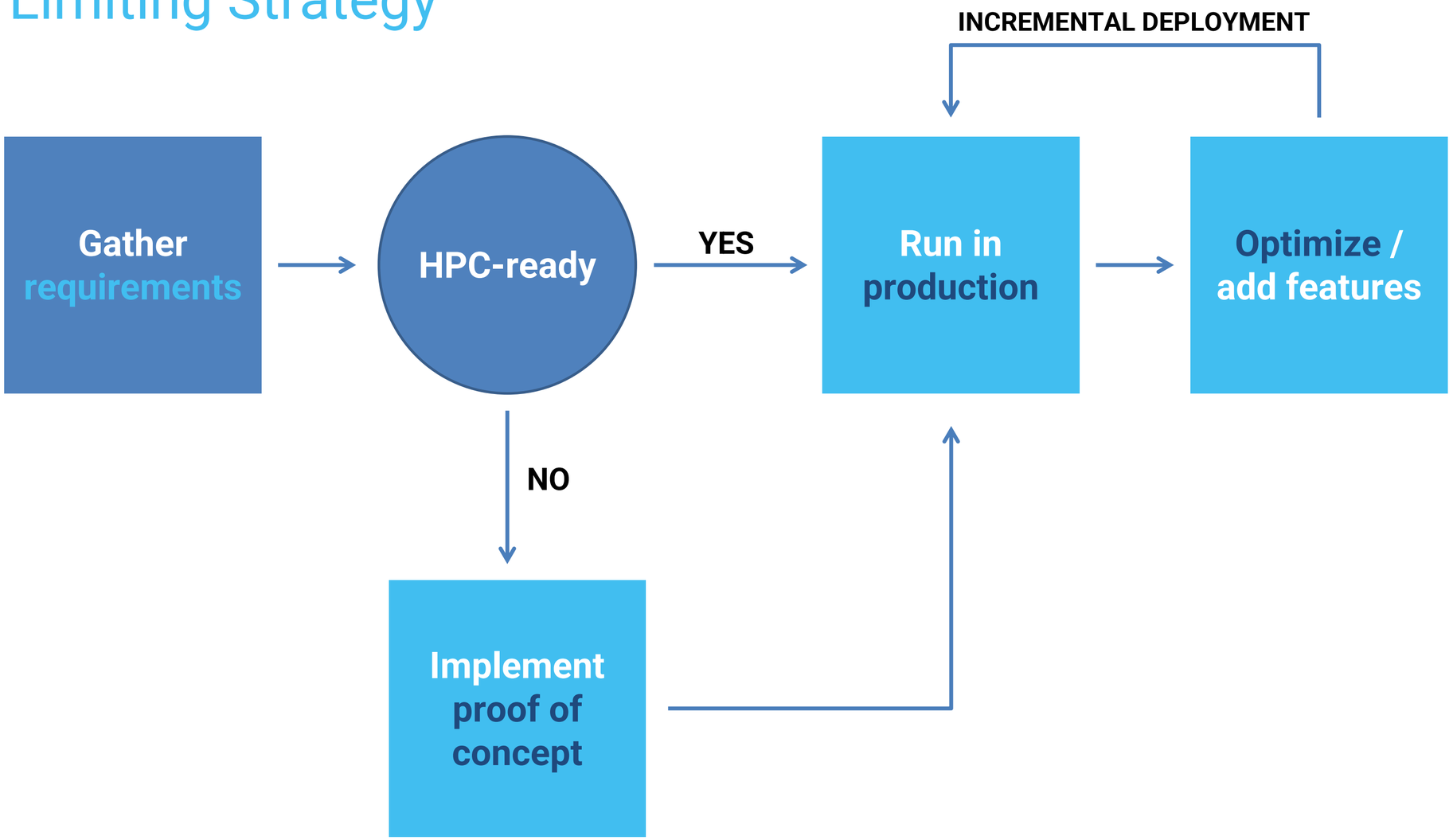
- Ethernet
- Low latency network
- Black fiber access
- …

Expertise

- Solution Engineering
- Software Engineering
- L1/L2 Support
- Project Management

AGILE IMPLEMENTATION AND DEPLOYMENT

A Risk Limiting Strategy



LUX PROVIDE

Thank you!