An approach to architectural design for exascale systems

19th Workshop on high performance computing in meteorology

20 September 2021

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Atos
#1 HPC provider in Europe

ECMWF new data center in Bologna

ECMWF new supercomputer
Bull Sequana XH2000

Growing Application Requirements

From Petascale to Exascale

Exascale

- Larger Power Consumption
- New Computing Elements
- More Parallelism
- Much more computing
- Live Data
- More Data Input/Output
- More parameters
- Larger Datasets

- 10-30MW
- GPUs, FPGAs, AI, Quantum
- Millions threads
- ExaFlops
- Data Streaming
- Exabytes
- Realistic models
- x1000

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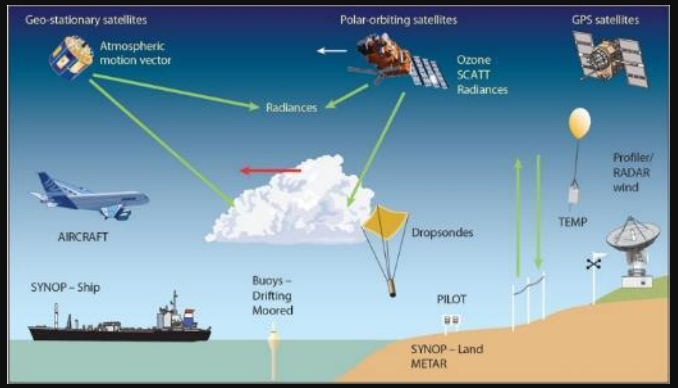
Weather Forecast HPC and (big) data

courtesy ECMWF



40 Million observations/day, from 85 satellites (50 instruments) + many ground-based and airborne measurement systems.

- weather forecast is the typical HPC application
- large computing resources
- + large datasets assimilation

} best forecast

"When it comes to events like Hurricane Dorian, accurately predicting the weather can save lives. But the US' system has lagged behind Europe's for years"

… "**data assimilation** is the crucial reason why ECMWF has better forecasts."

https://www.wired.co.uk/article/hurricane-dorian-weather-predictions-us-europe

"Drop in aircraft observations could have impact on weather forecasts"

https://www.ecmwf.int/en/about/media-centre/news/2020/drop-aircraft-observations-could-have-impact-weather-forecasts

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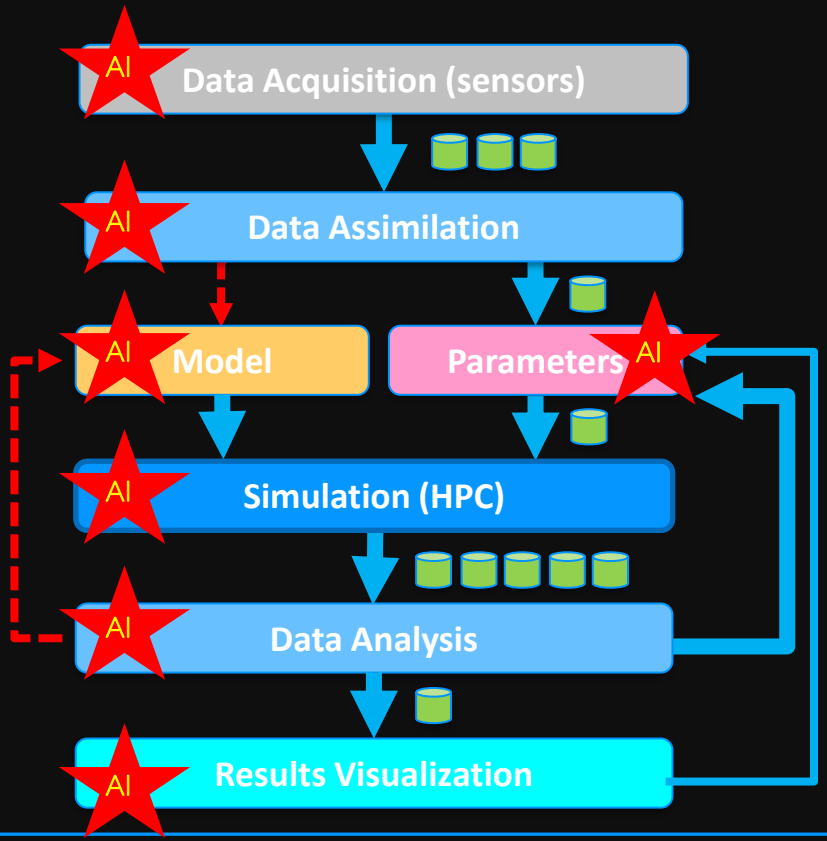
HPC Exascale workflows

- Accelerated Computing
- Accelerated data analysis / assimilation
- Optimized Applications for new computing elements
- Converged architecture
  - High Performance Computing
  - Data Analytics
  - Artificial Intelligence
- Optimized SW stack
  - Smart Data Management
  - Smart Computing…

… and **AI everywhere**



The Ultimate Hardware specialization

Smartphones use more than 20 specialized HW acceleration chips

- Many different applications:
  - Phone, Visio-conferencing
  - Camera, Video
  - Web, TV, Newspaper,
  - Email, Social networks
  - Game console
  - Shopping, Credit card,
  - Health assistant …

- Dedicated HW for different tasks

  5G, Bluetooth, Wi-Fi, GPS, camera, video, display, fingerprint, security …
  + general purpose multi-core CPU

- Performance & Energy efficiency are the main drivers for HW specialization

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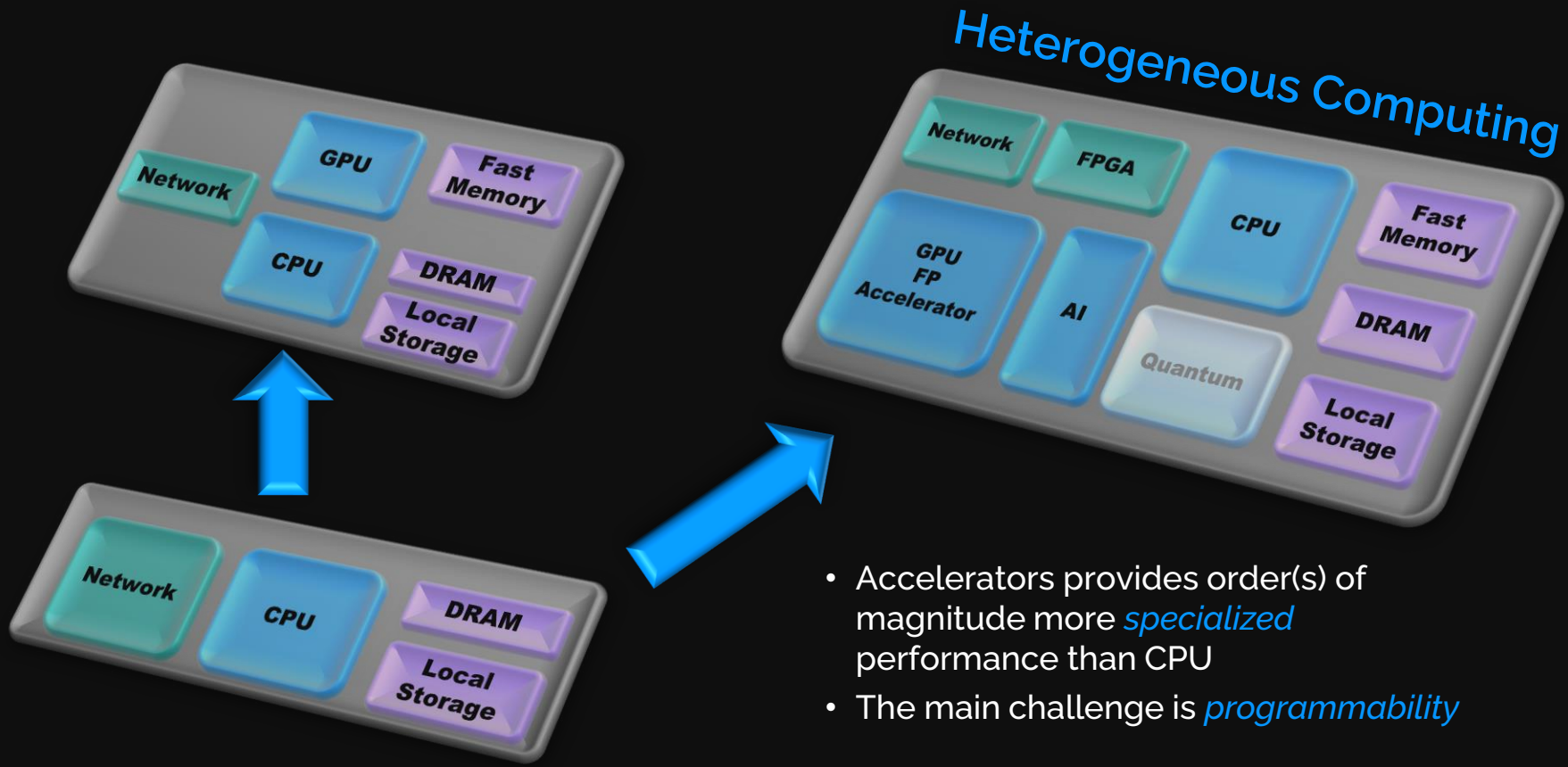
HW acceleration for HPC



- Accelerators provides order(s) of magnitude more *specialized* performance than CPU
- The main challenge is *programmability*

providing performance: CPU → GPU (Accelerators)

GPU vs CPU

x4 Flops

x5 Memory BW

But non-coherent

More difficult to program

GPU memory / CPU

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AI for HPC

2020 ACM Gordon Bell Prize Awarded to Team for Machine Learning Method that Achieves Record Molecular Dynamics Simulation

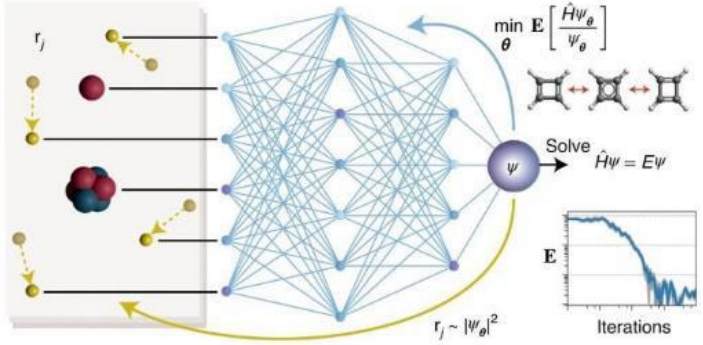
New Tool Simulates Interactions of 100 Million Atoms

Association for Computing Machinery

New York, NY, November 19, 2020 – ACM, the Association for Computing Machinery, named a nine-member team, drawn from Chinese and American institutions, recipients of the 2020 ACM Gordon Bell Prize for their project, "Pushing the limit of molecular dynamics with *ab initio* accuracy to 100 million atoms with machine learning."

Artificial Intelligence Solves Schrödinger's Equation

Scientists at Freie Universität Berlin develop a deep learning method to solve a fundamental problem in quantum chemistry



AlphaFold: a solution to a 50-year-old grand challenge in biology

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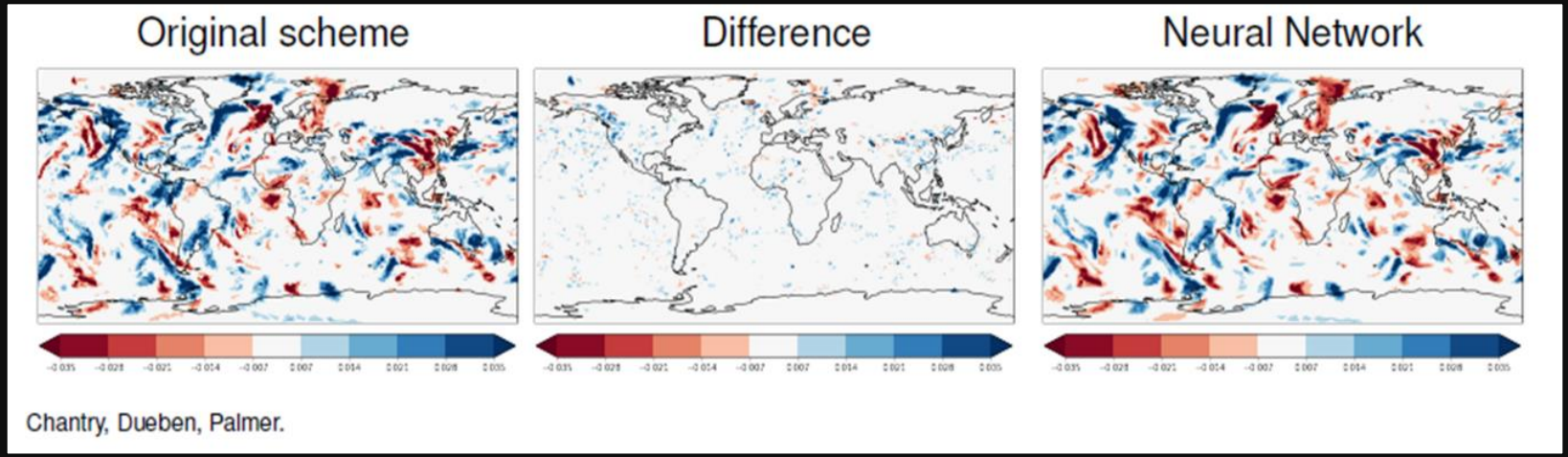
AI applications to Weather forecast simulations



- AI frameworks hold big promises to speed up

Atos AI in HPC, AI for HPC and AI enhanced HPC

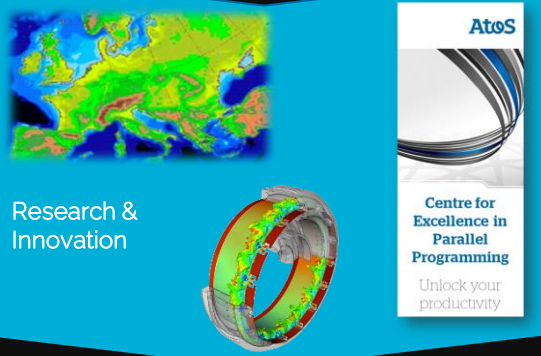
HPC/AI Converged Infrastructure

- ✓ Reduce TCO for HPC and AI
- ✓ Data science platform for HPC & Large-Scale AI

AI-driven optimization tool

- ✓ Boost performance with AI
- ✓ Learn from your production

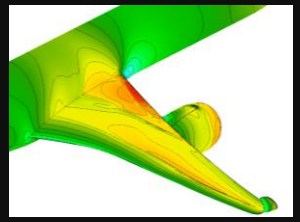
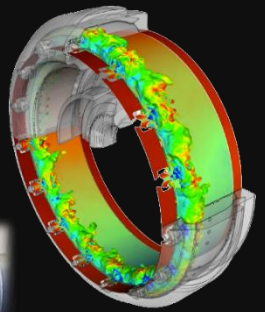
Integrating ML in Science application

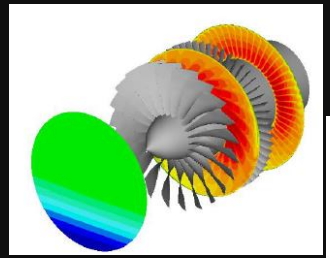
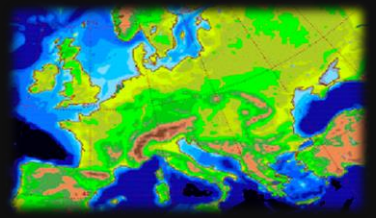


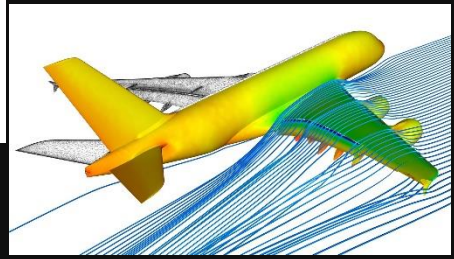
- ✓ Improve simulation with data-driven approach
- ✓ Atos data science teams

AI4Simulation: an R&D collaboration program

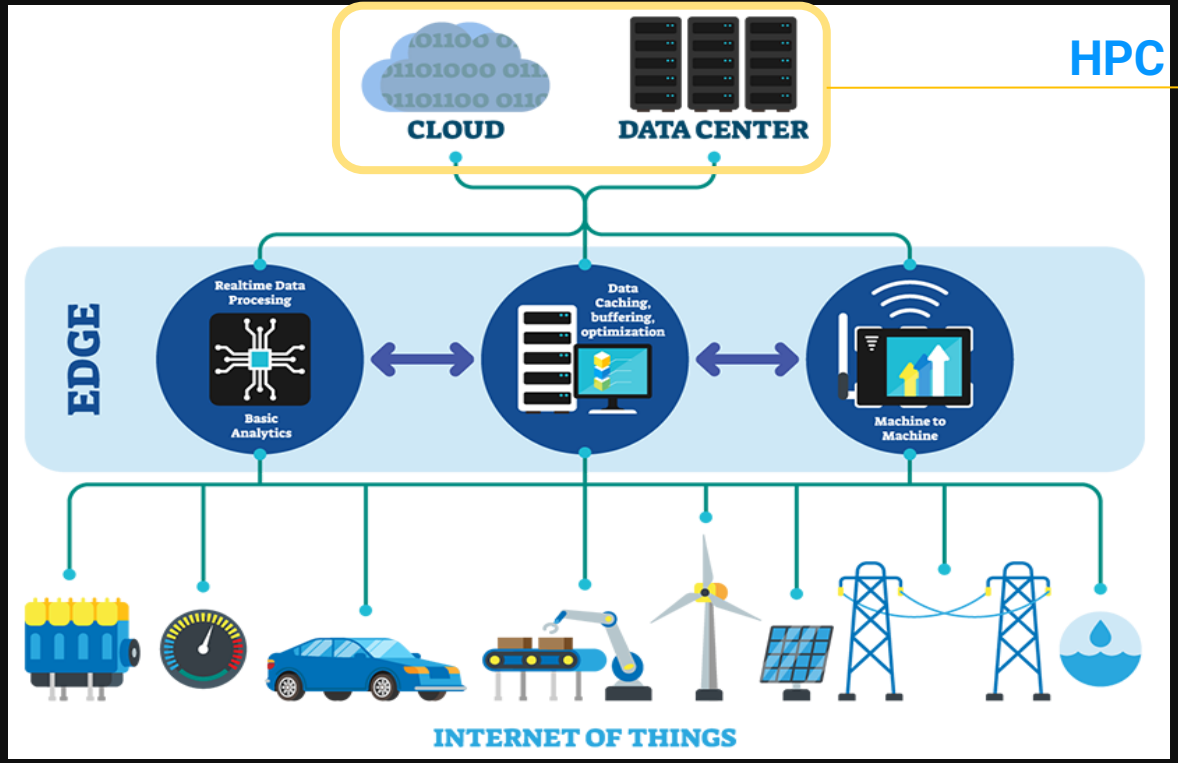
The AI4Sim program aims at **co-designing and co-developing simulation solutions** with industrial and academic partners to demonstrate how **artificial intelligence** can make physical modeling **more accurate and efficient** and how they enable addressing new simulation challenges.

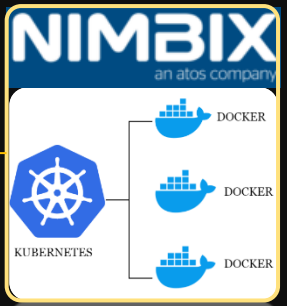



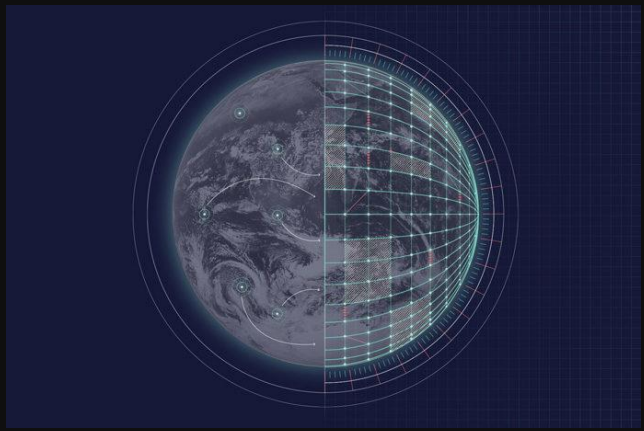


Digital Continuum
Hybrid SuperComputing



HPC anywhere





Top European HPC system 2010-2020 – Green, Greener

2010: 0.23 GF/W

2020: 25 GF/W

x110 greener

- Electronics technology evolution
- Accelerators (GPUs) use
- Free Cooling

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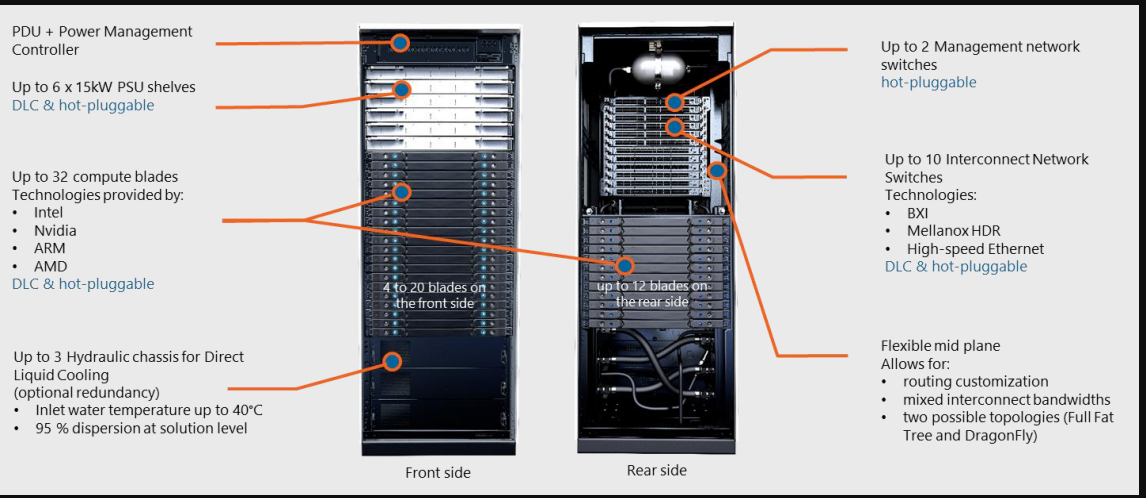
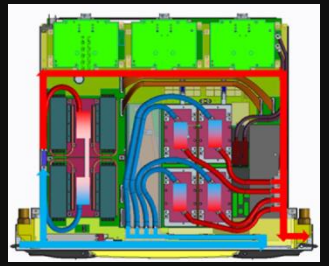
Bull Sequana XH2000
the most energy efficient HPC platform



BullSequana XH2000



Fan-less design
Direct Liquid Cooling
using warm water up to 40°C
→ Free Cooling

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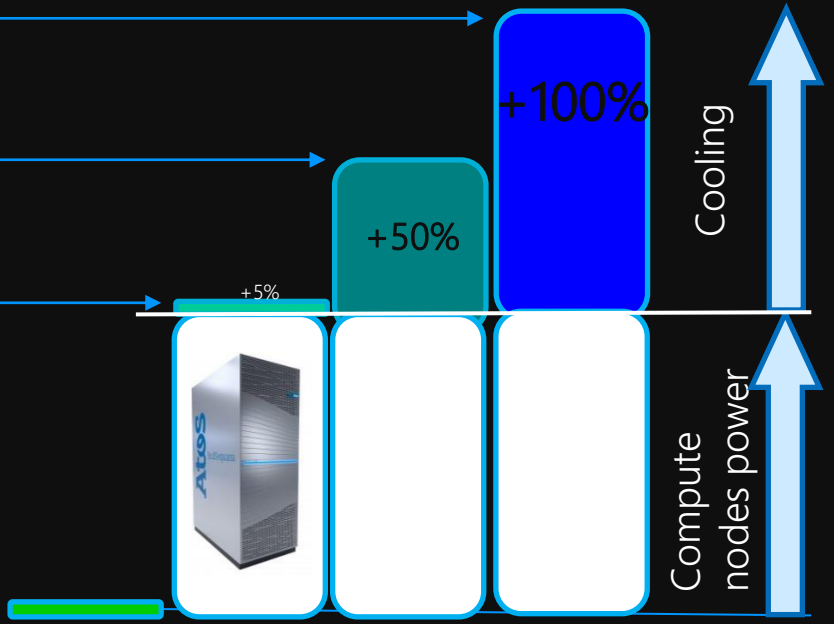
Meeting the Energy Challenge towards Full decarbonization

Traditional Datacenter

Water Cooled doors 2009

Direct Liquid Cooling 2014

Fully decarbonized HPC 2028



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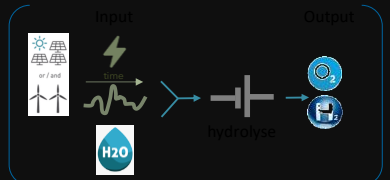
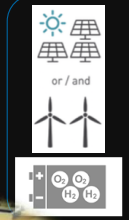
Research on Hydrogen (HPC)

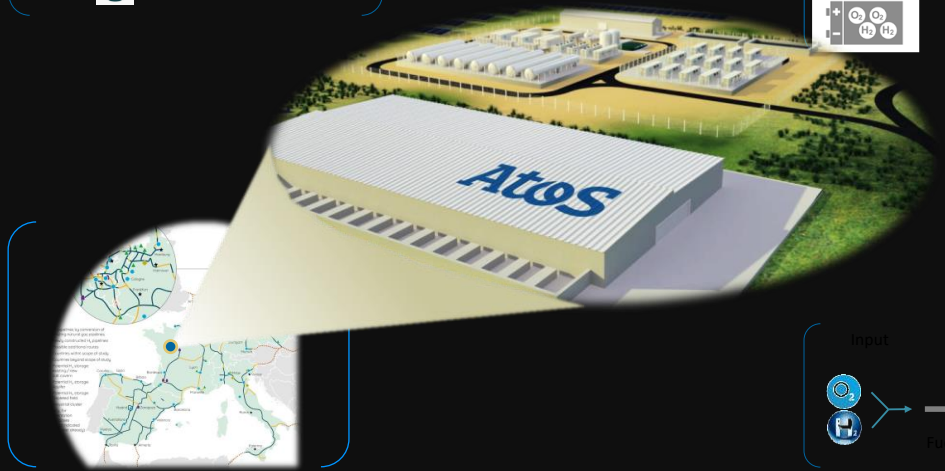
Produce H_2



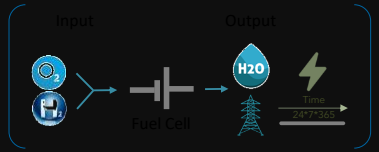
Smart Consumption



Smart powering of DCs with Green energies



Transport H_2



Local H_2 Energy

CONSIDERATIONS

Atos and its partner Hydrogène de France (HDF) to develop an **end-to-end solution based on green H_2** (target: zero carbon footprint for electricity) :

1. **PRODUCE**… H_2 in regions where it is possible to leverage raw green electricity (solar, wind)
2. **TRANSPORT**… H_2 with a EU green H2 pipeline network from where it is produced to where it is required
3. **LOCAL ENERGY** … build H_2 powered DC in urban area (how to)? Technical, Logistical, Security requirements.
   a. Pilot project in Angers to leverage HDF RenewStable® concept
   b. Co-Dev with HDF of H_2 cell designed for HPC
4. **SMART CONSUMPTION**… Green AI to predictively optimize energy consumption

Exascale Motivations Trends and Challenges

- Classical HPC (hard science, engineering) ever exploding computing requirements
- New societal priorities
  - Life science (Pandemics), Emergency computing (Extreme Weather Forecast)
- New workloads
  - Data centric computing → Data Analytics
  - Computing Continuum from Edge to Datacentre (Digital Twins, Smart Cities)
- Hybrid Computing
  - On-Premises + Cloud → Application containerization
- New technologies
  - Hardware Acceleration (GPUs, AI …), Quantum Computing
  - Software Acceleration (AI frameworks, …)
- Formidable Challenges
  - Porting/tuning applications
  - Green Computing – Decarbonization

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For further information → Friday, 24 September

10:10 → 10:30 Overview of the Heterogeneous Computing Project in the Weather & Climate Center of Excellence
Erwan Raffin (Atos)

13:40 → 14:00 Machine learning models to emulate gravity wave drag by Atos Center of Excellence
Alexis Giorkallos (Atos), Christophe Bovalo (Atos)

https://atos.net/en/solutions/high-performance-computing-hpc

Thank you!

Atos