
BSC
Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Computació, dades i IA: quin rol hi pot jugar Barcelona?

Sopars Claris
Amics UAB / Fundació Cat Eu

Dr. Josep M. Martorell

BSC Associate Director

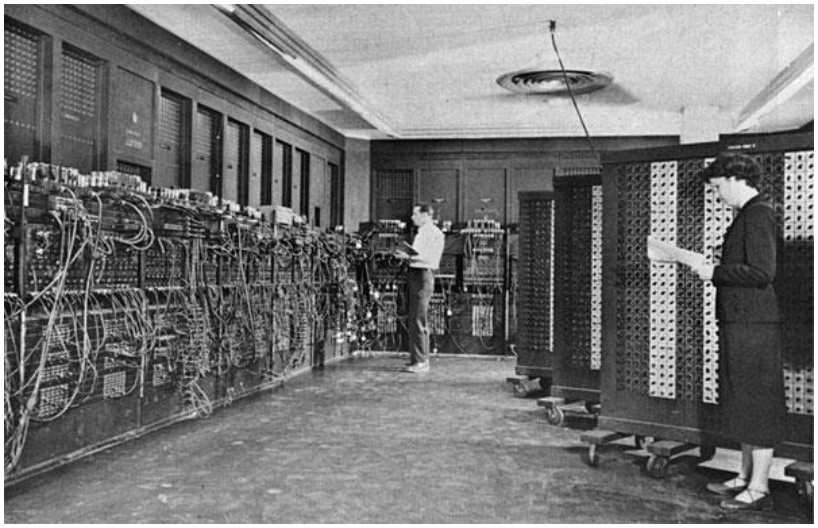
06/2019

Today's menu

- **Let's understand the role of HPC & AI in the current and future European Challenges**
  - Evolution of computing power
  - Evolution of AI technologies
  - Impact on Research (and the role of the BSC)
  - Impact on Health, Industry, Environment,…

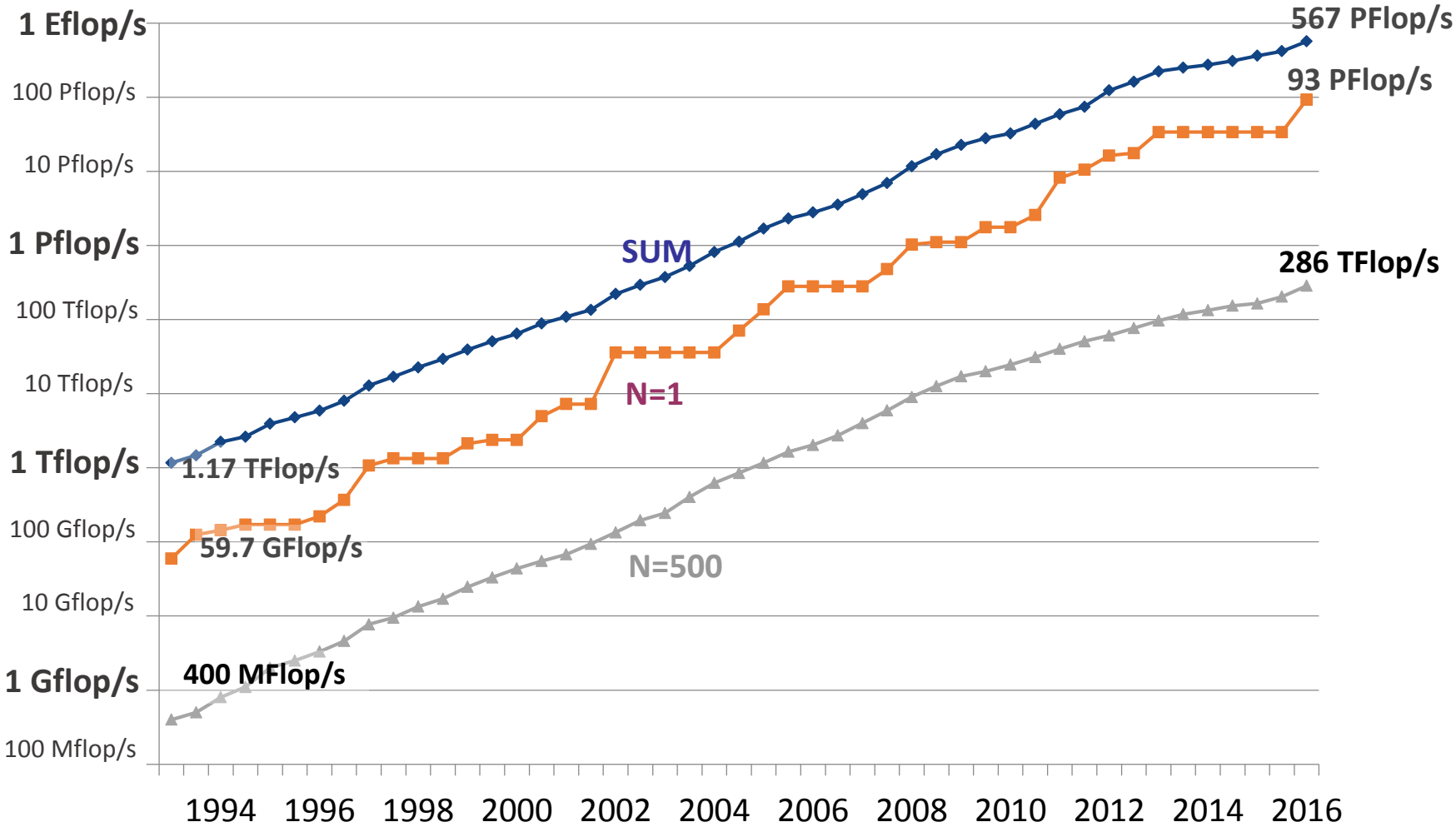
- **Let's discuss the role of Europe (&BCN) in the future revolutions**
  - In HPC
  - In AI
  - In Quantum

7 decades of Computing

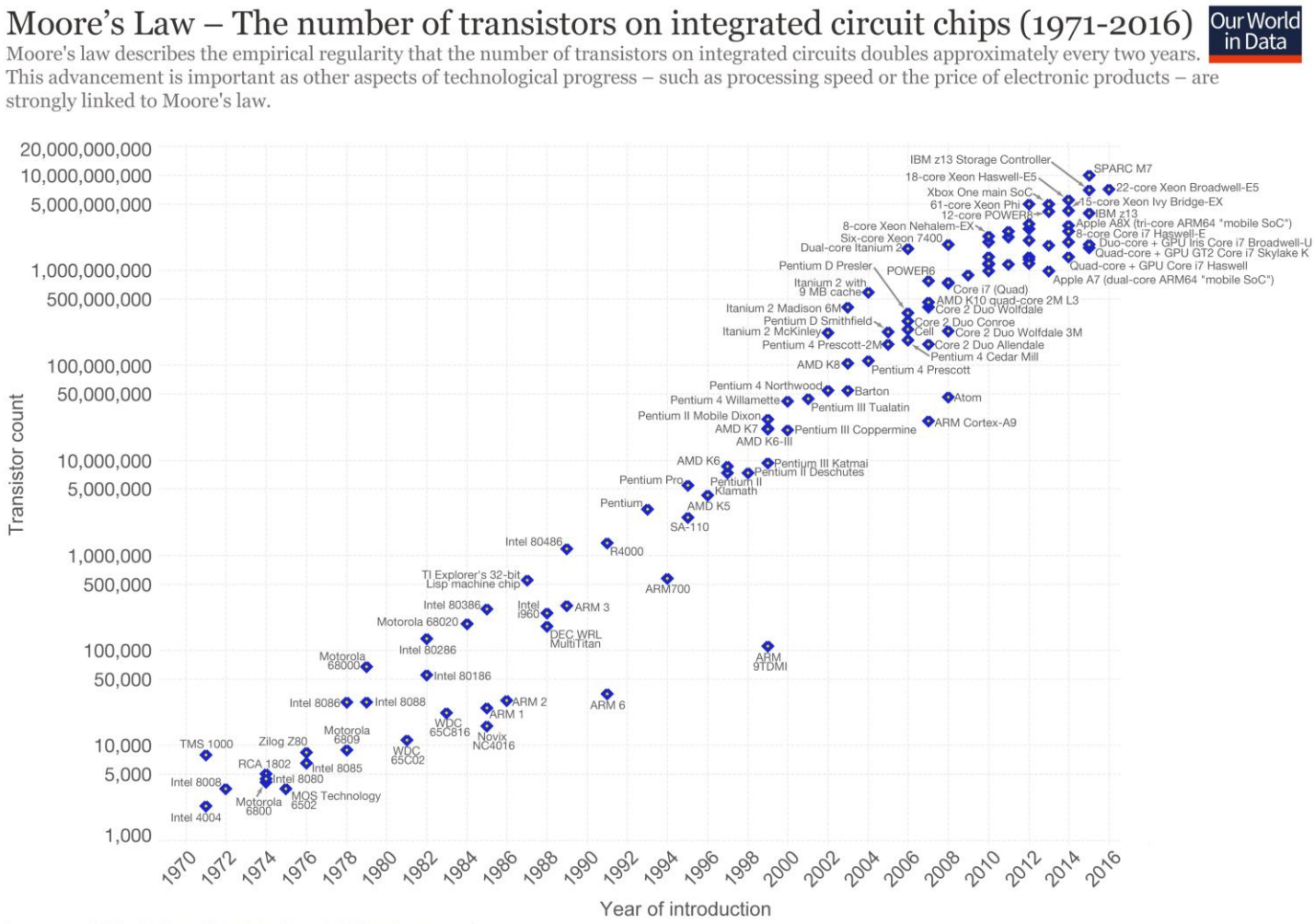


About 10^{17} times most powerful = 100.000.000.000.000.000

Performance Development of HPC over the Last 23 Years from the Top500



Is winter coming?

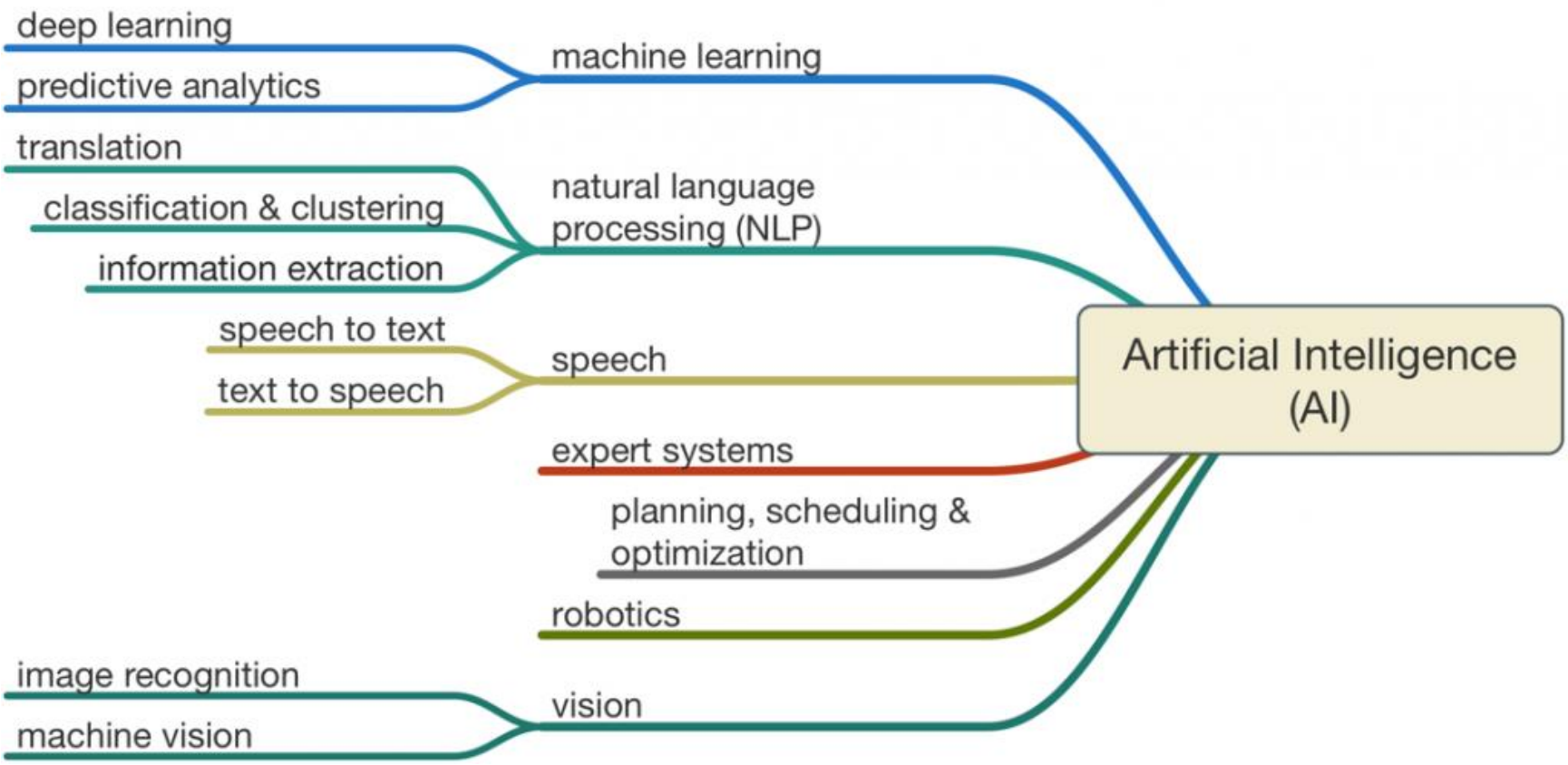


Data source: Wikipedia (https://en.wikipedia.org/wiki/Transistor_count)
The data visualization is available at OurWorldinData.org. There you find more visualizations and research on this topic.

Top25, Nov 2018

Rank	Name	Site	Manufacturer	Country	Rmax [TFlop/s]	Rpeak [TFlop/s]	GFlops/Watts
1	Summit	DOE/SC/Oak Ridge National Laboratory	IBM	US	143,500	200,794.88	14.67
2	Sierra	DOE/NNSA/Lawrence Livermore National Lab.	IBM/NVIDIA	US	94,640	125,712	12.72
3	Sunway TaihuLight	National Supercomputing Center in Wuxi	NRCPC	China	93,014.59	125,435.90	6.05
4	Tianhe-2ª	National Super Computer Center in Guangzhou	NUDT	China	61,444.50	100,678.66	3.33
5	Piz Daint	Swiss National Supercomputing Centre	Cray Inc.	Switz	21230	27.154.3	8.90
6	Trinity	DOE/NNSA/LANL/SNL	Cray Inc.	US	20,158,7	41,461.15	2.66
7	AI Bridging Cloud Inf.	National Inst. of Adv Industrial Science & Tech.	Fujitsu	Japan	19,880.00	32,576.63	12.05
8	SuperMUC-NG	Leibniz Rechenzentrum	Lenovo	Germany	19,476.6	28,872,86	
9	Titan	DOE/SC/Oak Ridge National Laboratory	Cray Inc.	US	17,590.00	27,112.55	2.14
10	Sequoia	DOE/NNSA/Lawrence Livermore National Lab.	IBM	US	17,173.22	20,132.66	2.18
11	Lassen	DOE/NNSA/Lawrence Livermore National Lab.	IBM	US	15,430	19,904.4	
12	Cori	DOE/SC/LBNL/NERSC	Cray Inc	US	14,014	27,880.65	3.56
13	Nurion	Korea Inst. of Science and Tech Information	Cray Inc.	Sth Korea	13,929.30	25,705.90	
14	Oakforest-PACS	Joint Center for Advanced HPC	Fujitsu	Japan	13,554.60	24,913.46	4.99
15	HPC4	Eni S.p.A.	HPE	Italy	12,210.00	18,621.14	9.25
16	Tera-1000-2	Commissariat a l'Energie Atomique (CEA)	Bull	France	11,965.50	23,396.35	3.77
17	Stampede2	Texas Adv. Computing Center/Univ. of Texas	Dell EMC	US	10,680.70	18,309.22	
18		RIKEN Advanced Institute for Computational Science	Fujitsu	Japan	10,510.00	11,280.38	0.83
19	Marconi Intel Xeon Phi	CINECA	Lenovo	Italy	10,384.9	18,816	
20	Taiwania 2	National Center for High Performance Computing	Quanta Comp	Taiwan	9,000	15,208.23	11.28
21	Mira	DOE/SC/Argonne National Laboratory	IBM	US	8,586.61	10,066.33	2.18
22	TSUBAME3.0	GSIC Center, Tokyo Institute of Technology	HPE	Japan	8,125.00	12,127.07	10.26
23		United Kingdom Meteorological Office	Cray Inc.	UK	7,038.93	8,128.51	
25	Theta	DOE/SC/Argonne National Laboratory	Cray Inc.	US	6,920.90	11,661.31	
25	MareNostrum	Barcelona Supercomputing Center	Lenovo	Spain	6,470.80	10,296.12	3.97

What does AI mean?



Deep Learning

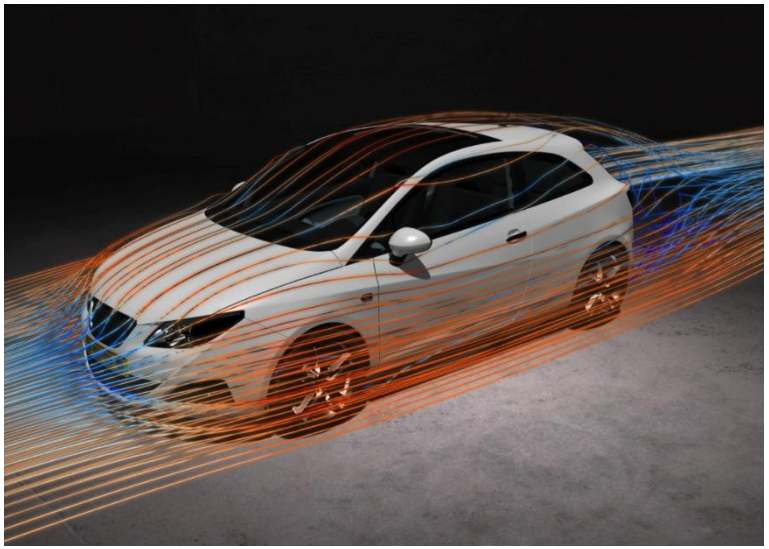
Deep Learning

AlphaZero AI beats champion chess program after teaching itself in four hours

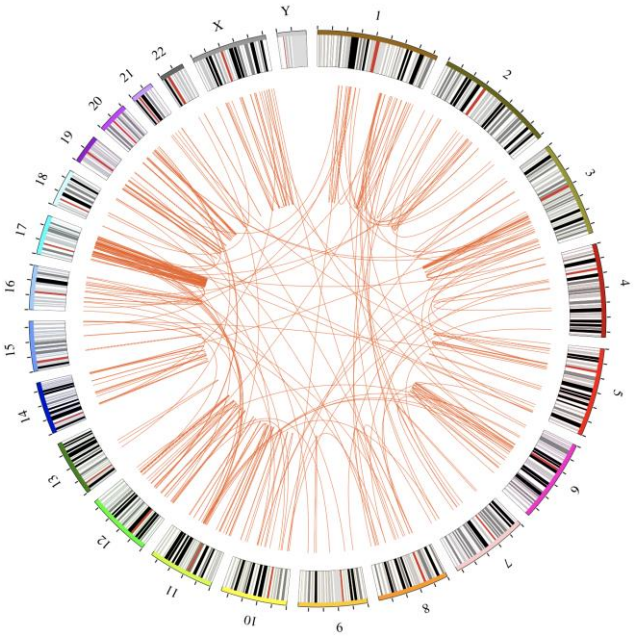
Google's artificial intelligence sibling DeepMind repurposes Go-playing AI to conquer chess and shogi without aid of human knowledge

Two different problems

“Model known”



“Model Unknown”

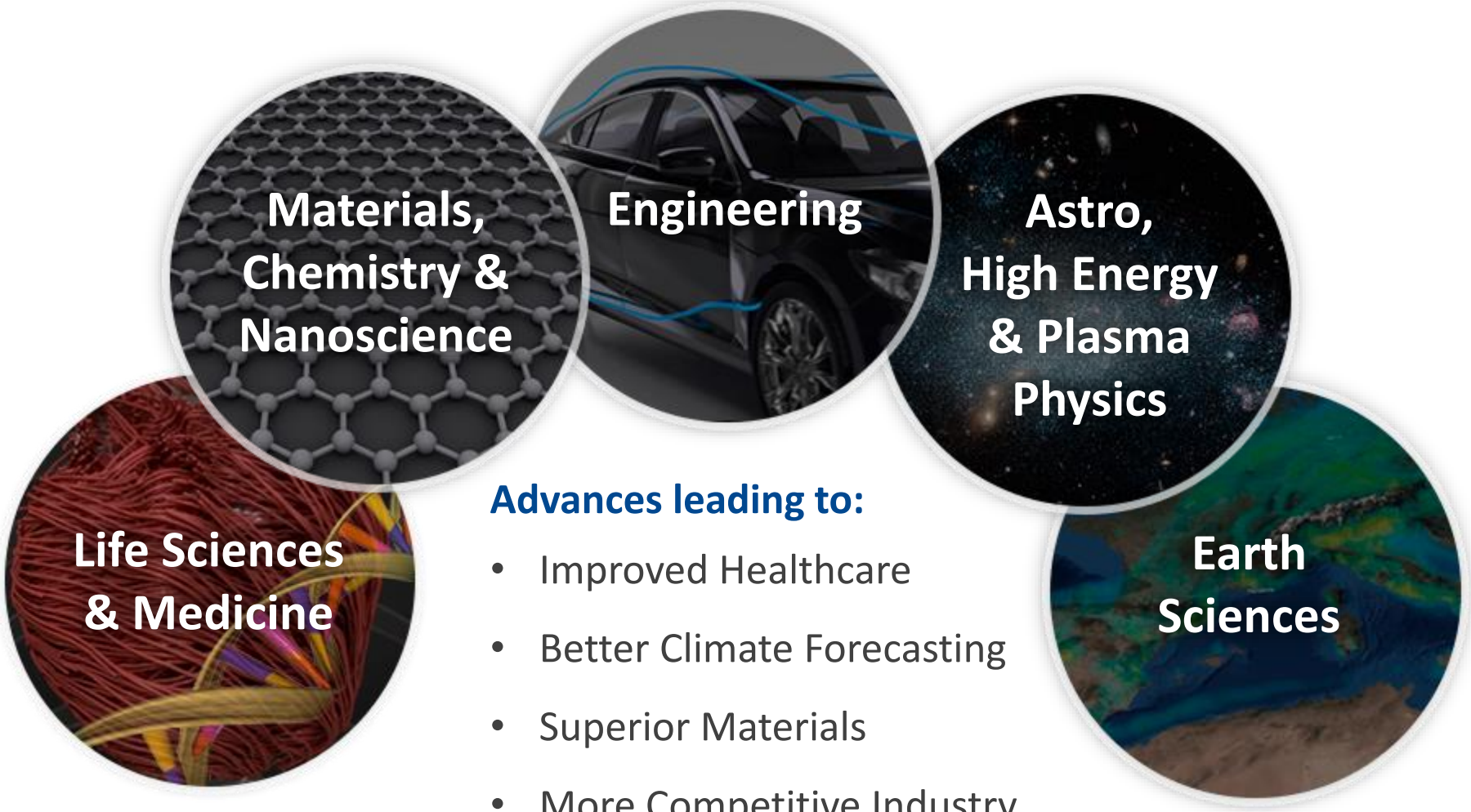


The Evolution of the Research Paradigm

Numerical Simulation and Big Data Analysis

- Reduce expense
- Avoid suffering
- Help to build knowledge where experiments are impossible or not affordable

HPC: An enabler for all scientific fields



Advances leading to:

- Improved Healthcare
- Better Climate Forecasting
- Superior Materials
- More Competitive Industry

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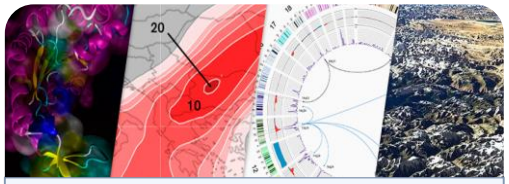
Supercomputing services to Spanish and EU researchers



R&D in Computer, Life, Earth and Engineering Sciences

PhD programme, technology transfer, public engagement

BSC-CNS is a consortium that includes

- **Spanish Government**
- **Catalonian Government**
- **Univ. Politècnica de Catalunya (UPC)**

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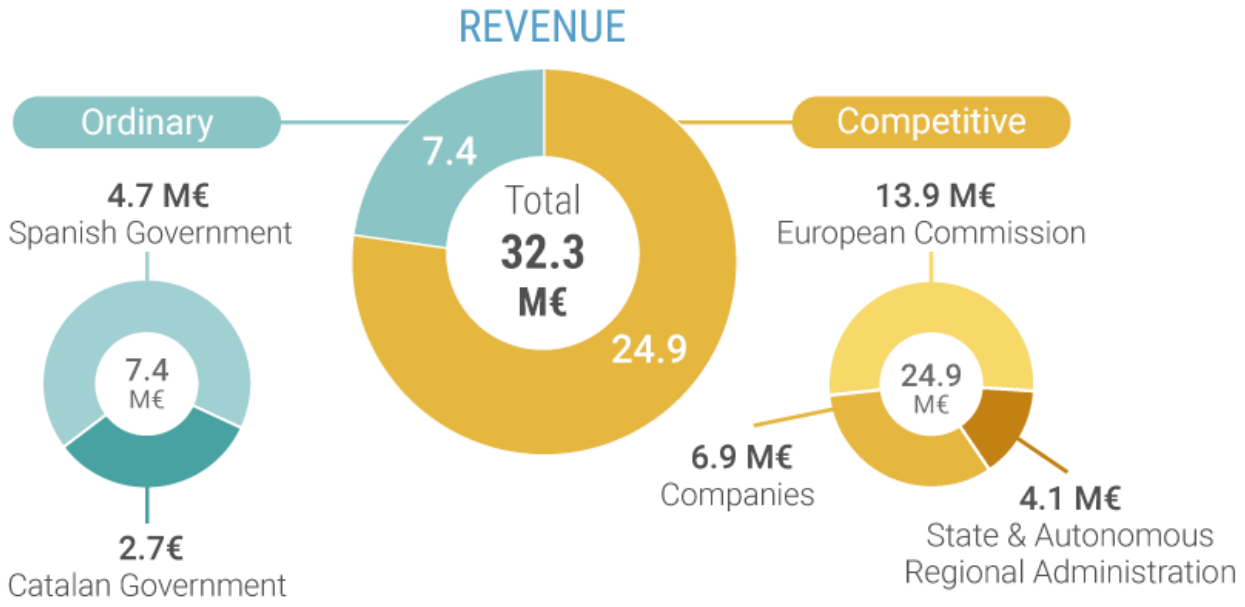
BSC Resources



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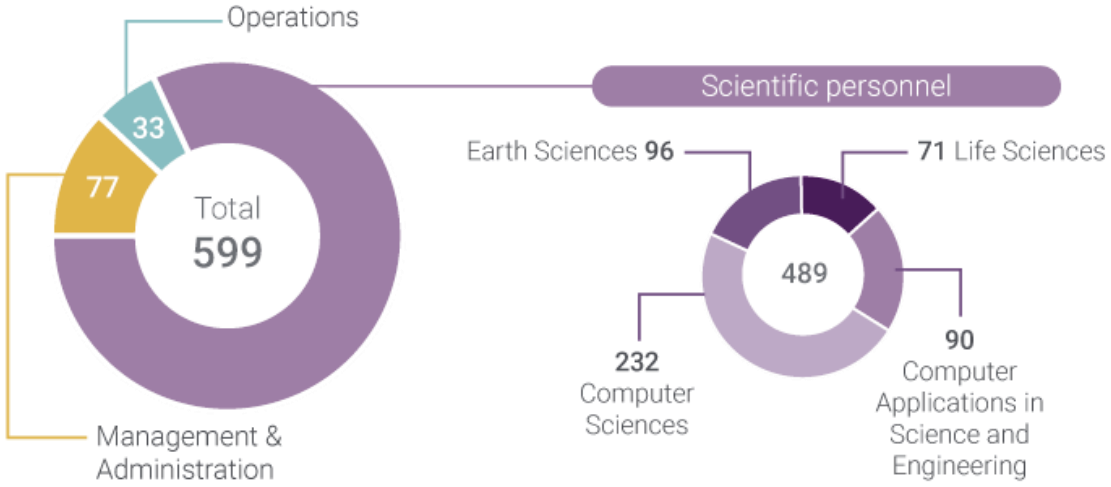
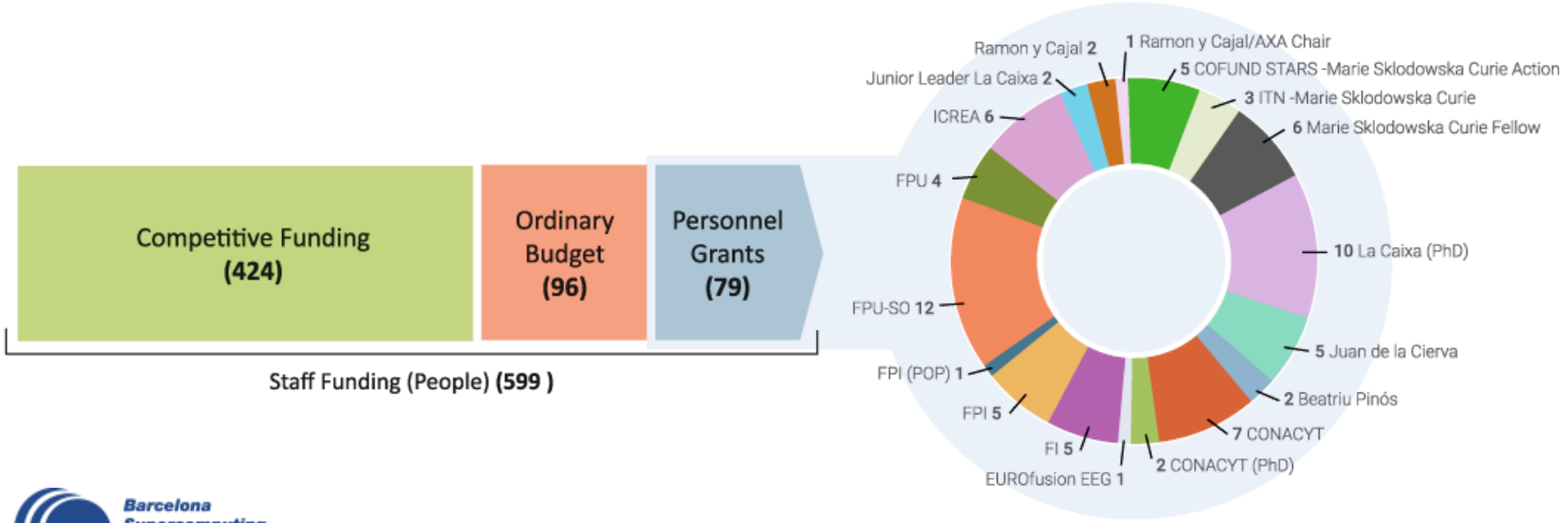
Estimated executed budget at December 31, 2018

People





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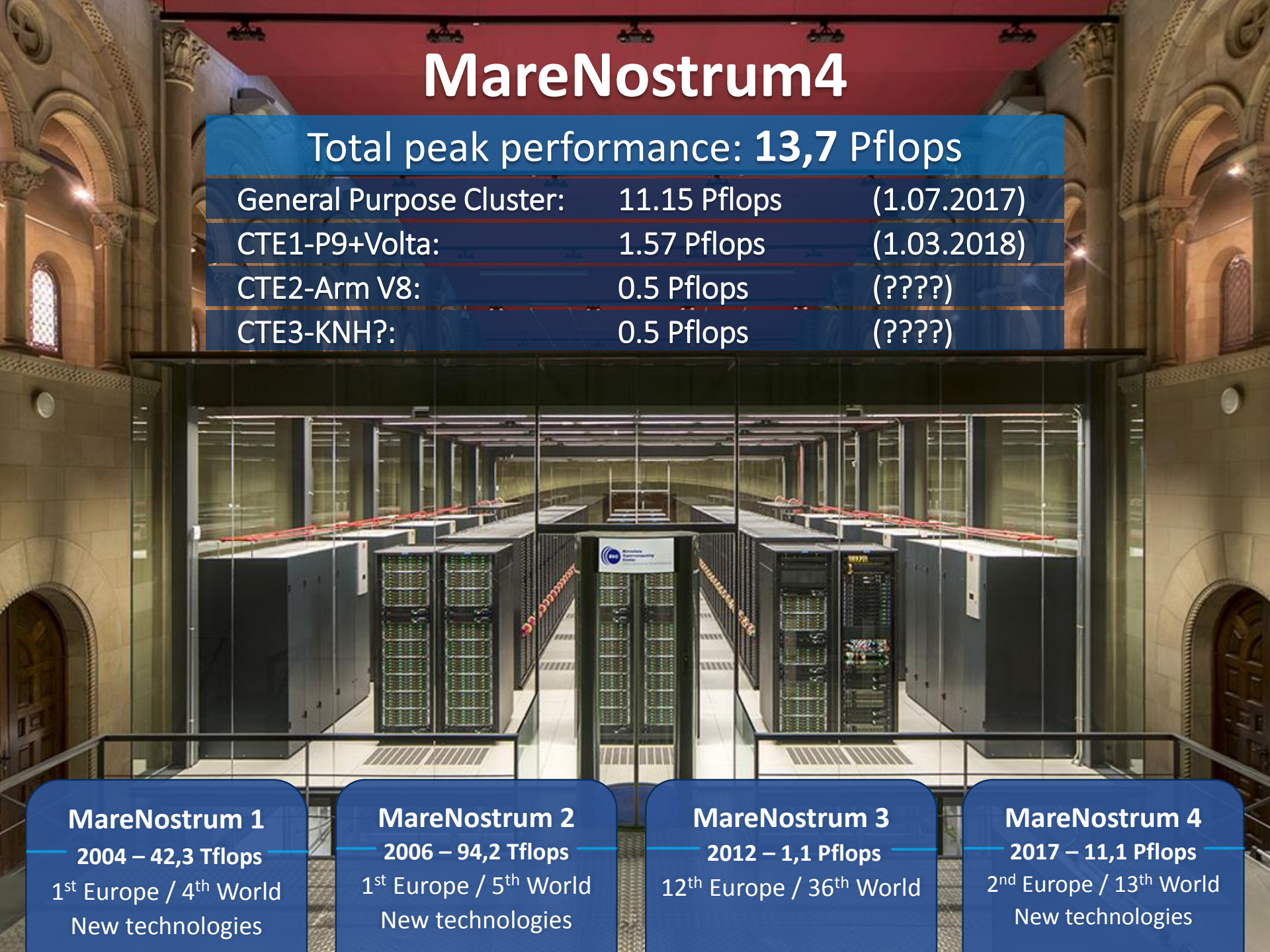
Data as December 31, 2018

MareNostrum4

Total peak performance: **13,7** Pflops		
General Purpose Cluster:	11.15 Pflops	(1.07.2017)
CTE1-P9+Volta:	1.57 Pflops	(1.03.2018)
CTE2-Arm V8:	0.5 Pflops	(????)
CTE3-KNH?:	0.5 Pflops	(????)



MareNostrum 1
2004 – 42,3 Tflops
1st Europe / 4th World
New technologies

MareNostrum 2
2006 – 94,2 Tflops
1st Europe / 5th World
New technologies

MareNostrum 3
2012 – 1,1 Pflops
12th Europe / 36th World

MareNostrum 4
2017 – 11,1 Pflops
2nd Europe / 13th World
New technologies

Distributed Supercomputing Infrastructure

26 members, including

5 Hosting Members

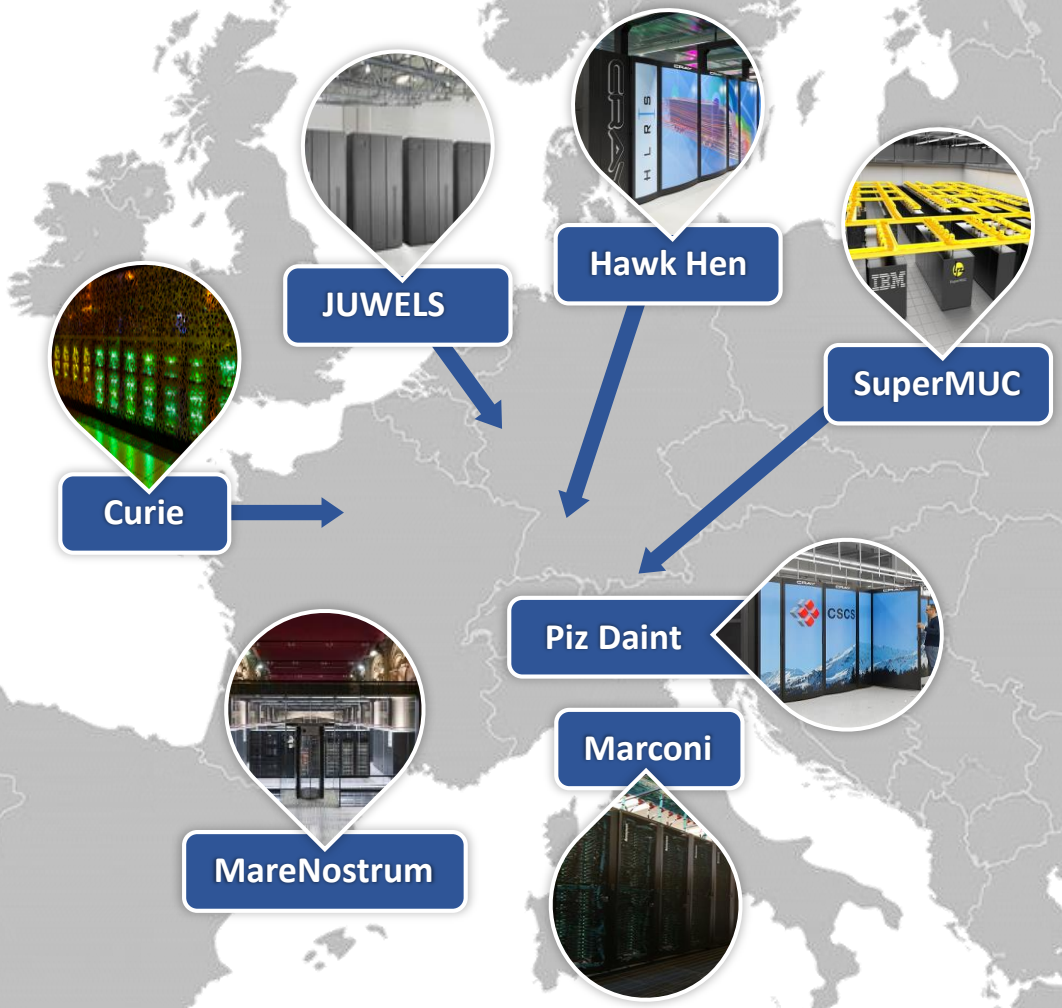
(Switzerland, France, Germany, Italy and Spain)

652 scientific projects **enabled**

110 PFlops/s of peak performance on **7 world-class systems**

>12.000 people trained by **6 PRACE Advanced Training Centers** and others events

Access prace-ri.eu/hpc-acces



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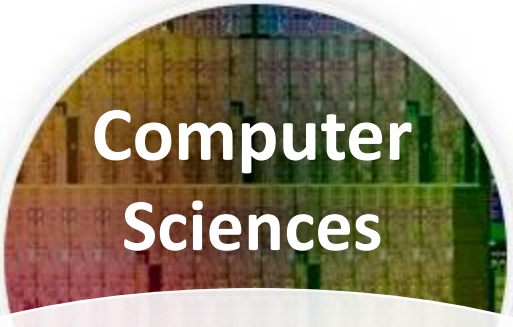
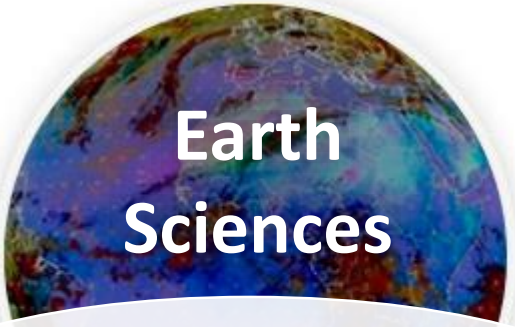
Mission of BSC Scientific Departments

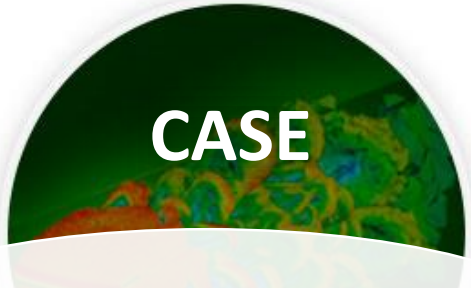


To influence the way machines are built, programmed and used: programming models, performance tools, Big Data, computer architecture, energy efficiency



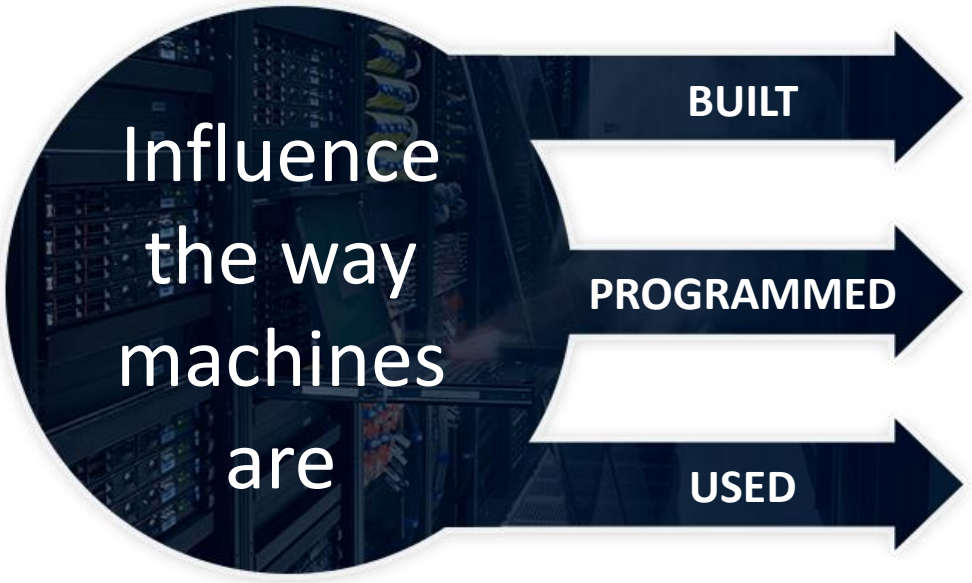
To develop and implement global and regional state-of-the-art models for short-term air quality forecast and long-term climate applications

To understand living organisms by means of theoretical and computational methods (molecular modeling, genomics, proteomics)



To develop scientific and engineering software to efficiently exploit super-computing capabilities (biomedical, geophysics, atmospheric, energy, social and economic simulations)

Computer Sciences



Holistic Computer Architecture Research

20 years innovating in Programming Models

Performance Analytics Tools: From Data to Insight

In the context of

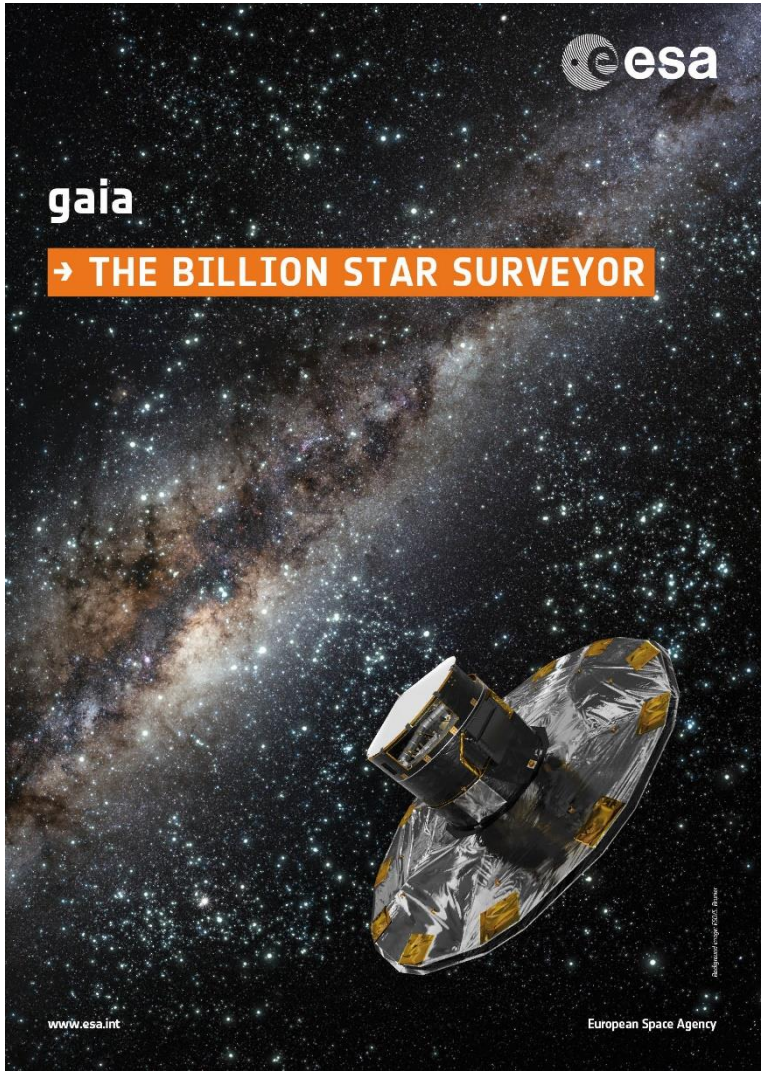
- Race towards Exascale
- HPC and Big Data convergence
- Artificial Intelligence era
- Multiple architectures for different applications domains

Human Brain Project

- 10-year, 1000M€ FET flagship project
- Goal: to pull together all existing **knowledge about the human brain** and to reconstruct the brain in supercomputer based models and simulations.

- **Expected outcomes**: new treatments for brain disease and new brain-like computing technologies
- **BSC role**: Provision and optimisation of programming models to allow simulations to be developed efficiently
- **MareNostrum** part of the HPC platform for simulations

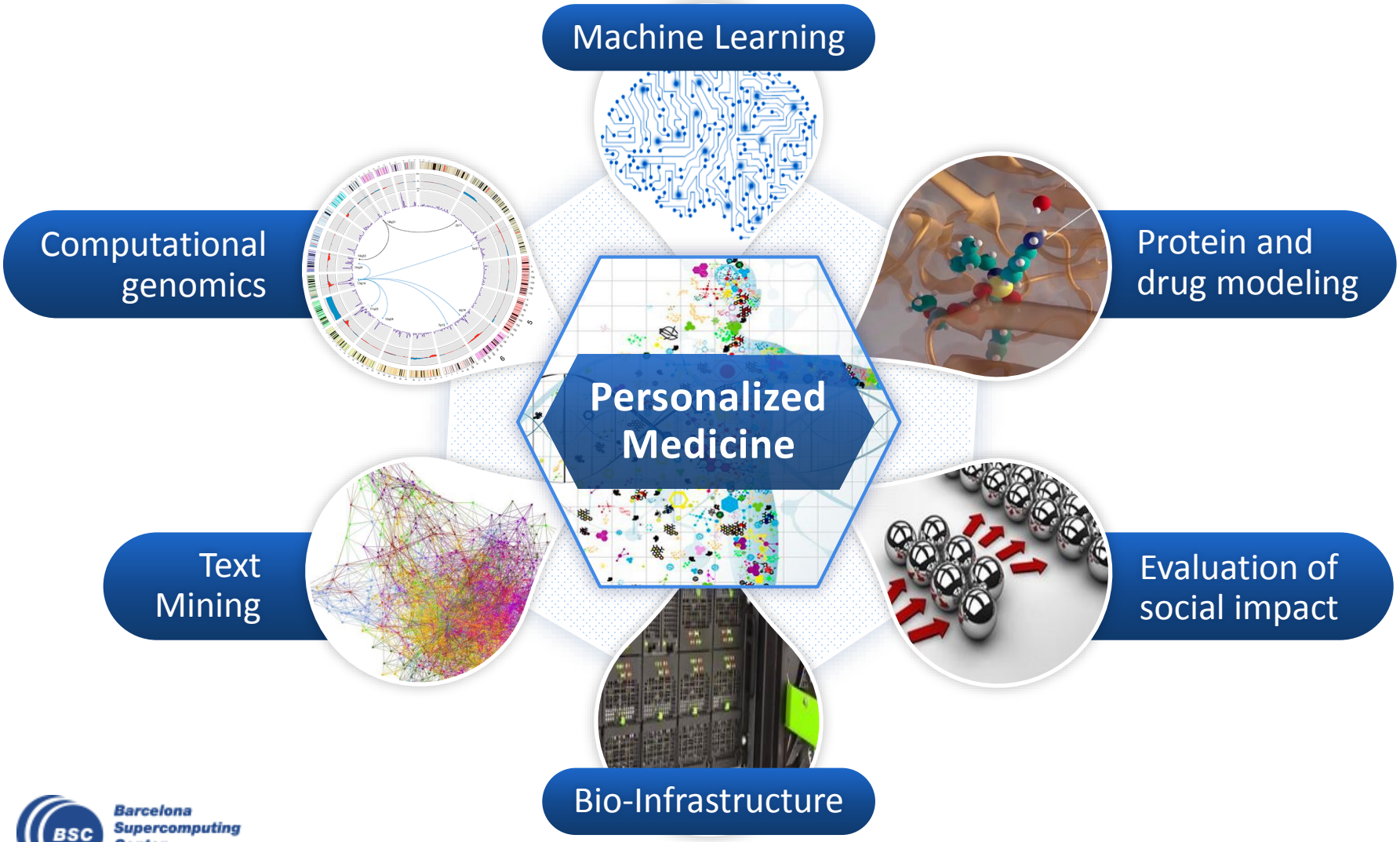
Gaia ESA Mission



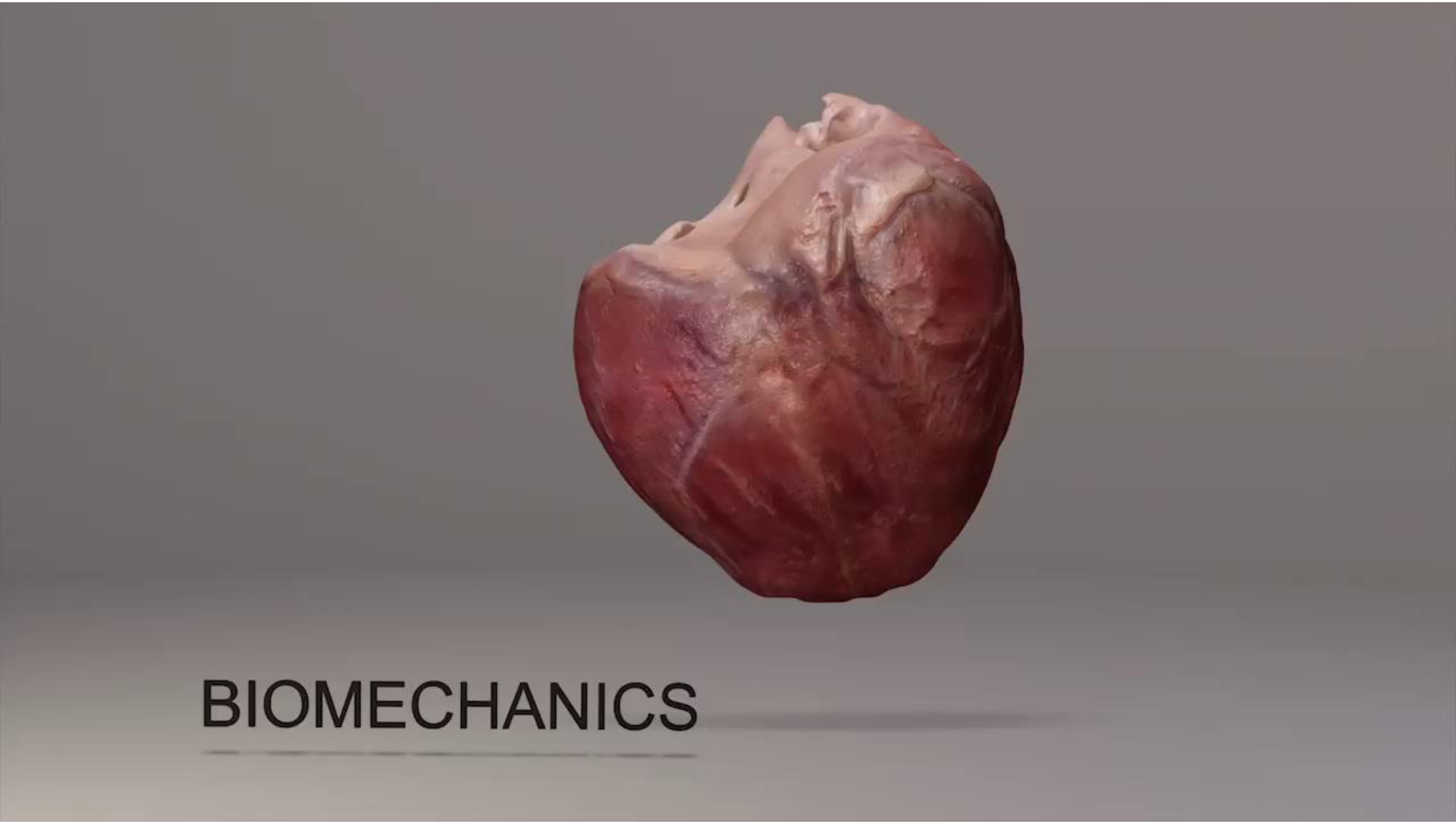
About 3PBytes of data, coming from 1.700.000.000 stars

Life Sciences

Understanding living organisms by theoretical and computational methods



Heart simulator



Detecting genome alterations

Chronic Lymphocytic Leukemia

We set up a Sequencing pipeline for the **Chronic Lymphocytic Leukemia (CLL) Genome Project,** that aims to generate a comprehensive catalogue of genomic alterations involved in the development and progression of the disease.

Genome Sequencing (CNAG)

500 Patients
1 Patient = less than a day

BSC
Data Management
Around 1.5 Pb

HPC Computing
Sustained 10-15%
BSC MareNostrum-II

Experimental Validation

Puente et al. Nature 2011
Quesada et al. Nature Genetics 2012
Kulis et al., Nature Genetics 2012
Puente et al., Nature under review

International Cancer Genome Consortium

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Earth Sciences

Environmental modelling and forecasting, with a particular focus on weather, climate and air quality

Modeling **air quality** and **Sand and Dust Storms** Processes from urban to Global and the impacts on weather, health and ecosystems

Research and Forecasts

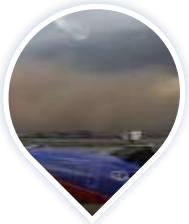
Climate predictions system from subseasonal-to-decadal forecasts

Service Users Sectors


Infrastructures


Solar Energy

Urban development


Transport


Wind Energy


Agriculture

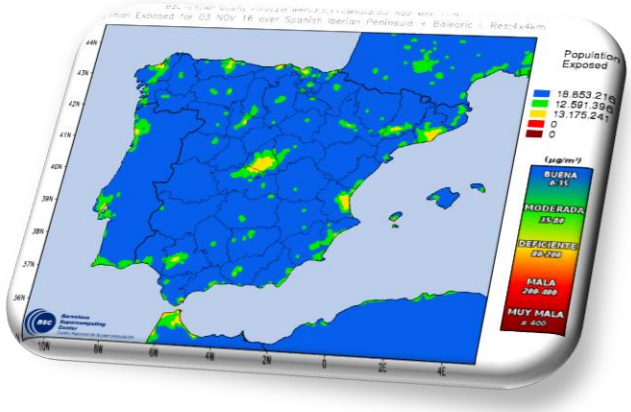

Insurance

CALIOPE Real-time Air Quality forecasts

Provides air quality related information for the coming days and for the application of short term action plans for air quality managers

Information is delivered using both online or custom applications

www.bsc.es/caliope



Smart city platform

vodafone IBM

Air quality index & population exposed

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Maritime emission modelling and prediction

From AIS and fog computing data using convolutional neural networks

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Collaboration with David Carrera's team

Wind Farms Simulation

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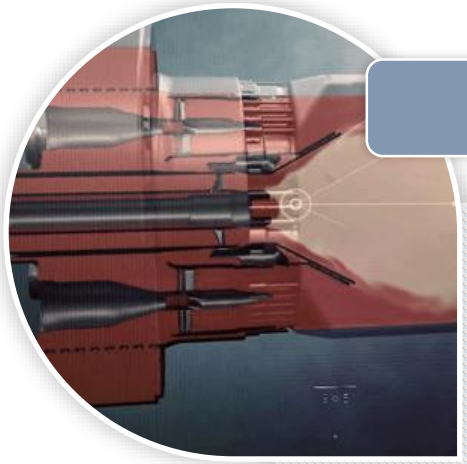
Centro Nacional de Supercomputación

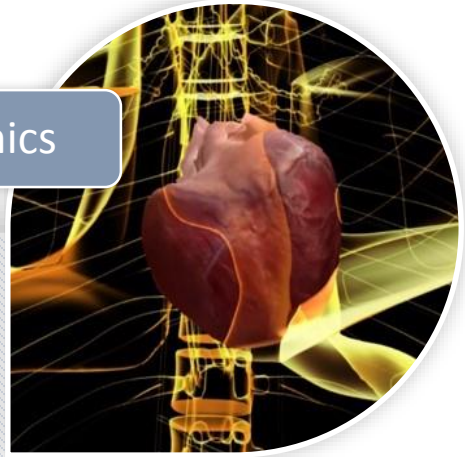
IBERDROLA

Computional Applications for Science and Engineering



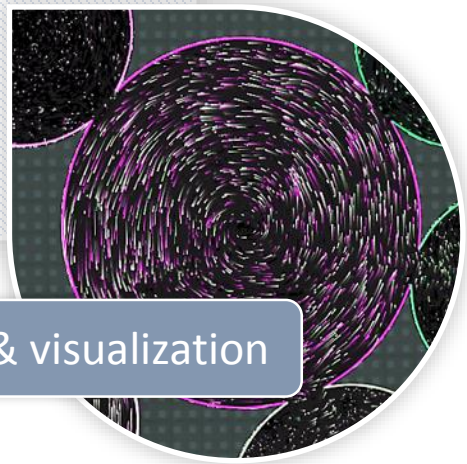
Energy

Biomechanics



INDUSTRY ORIENTED DEPARTMENT

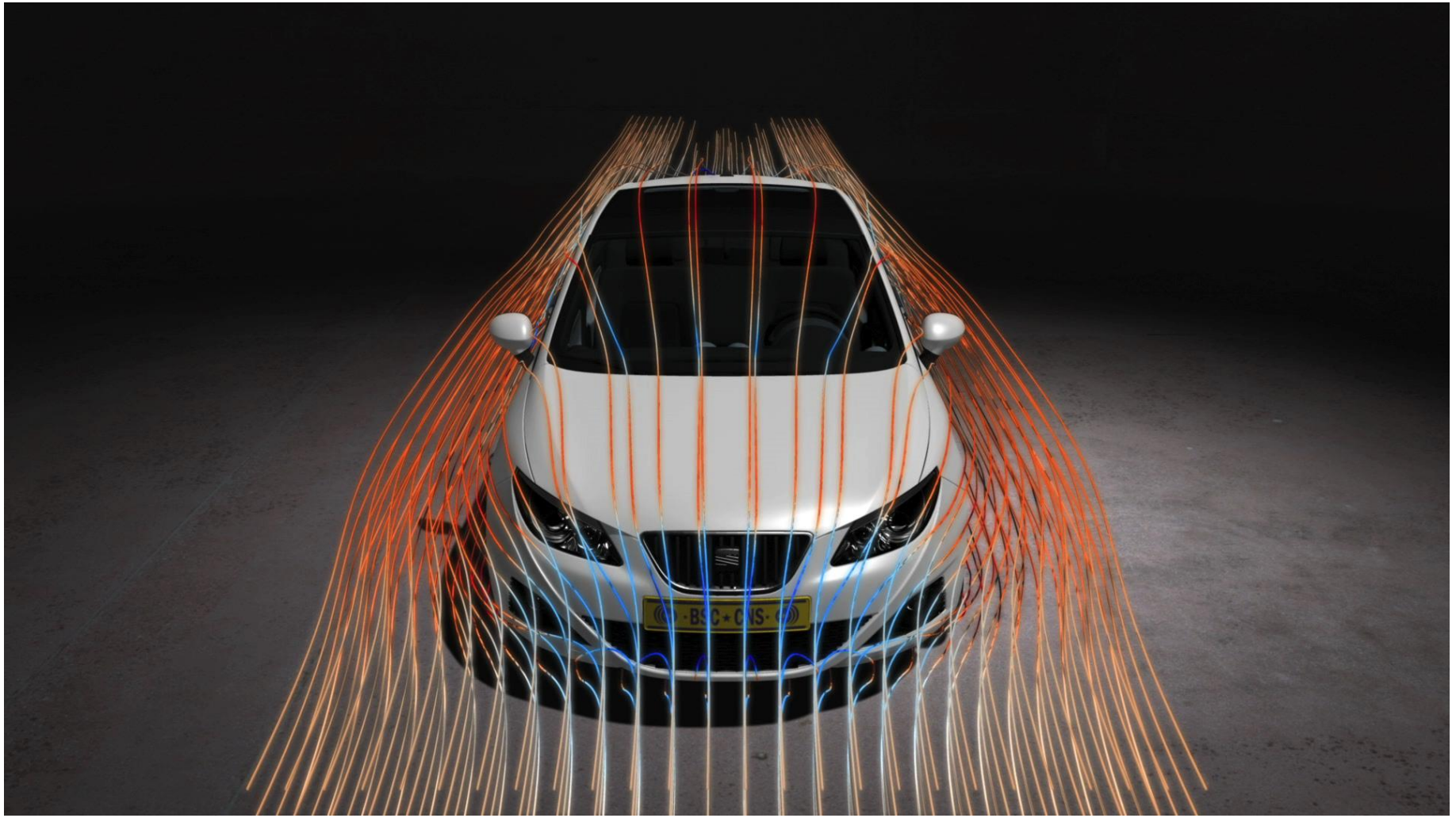
Smart & resilient cities



Data analytics & visualization

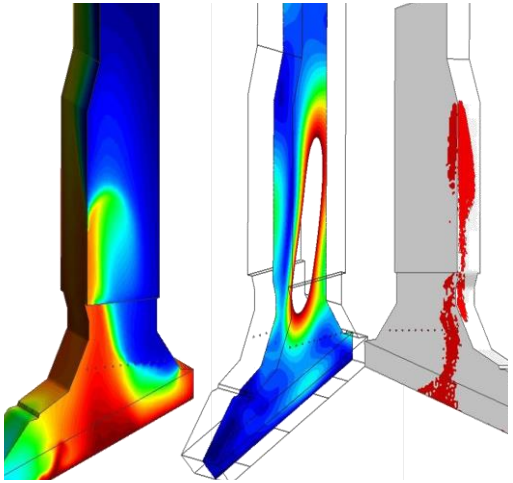
Geo Physics

External Aerodynamics



Machine Learning for Industry

Physical Modelling

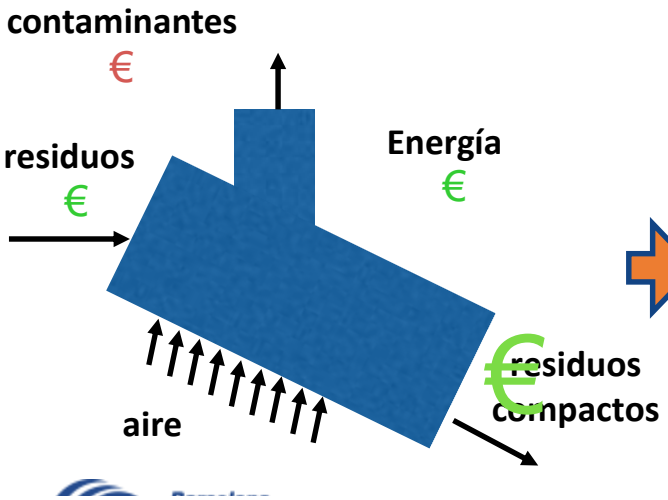


Computer simulations

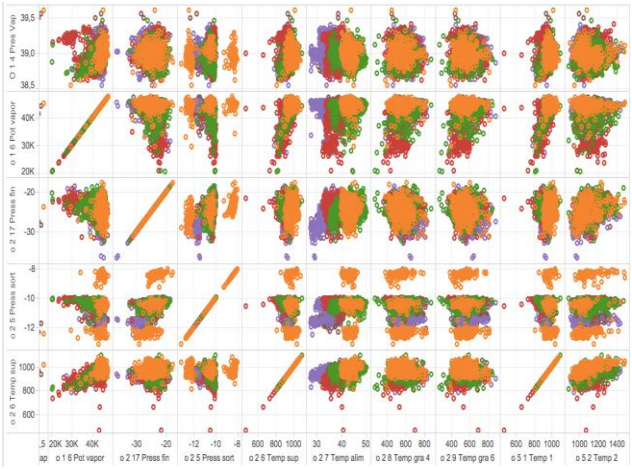
Prediction of unknown conditions

Machine Learning

Validation/support

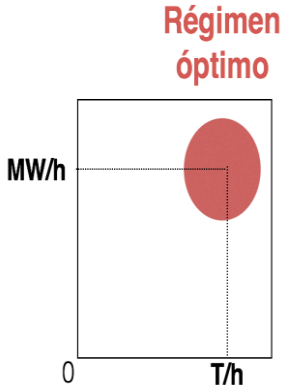


Data gathering/modelling



Information retrieval/display

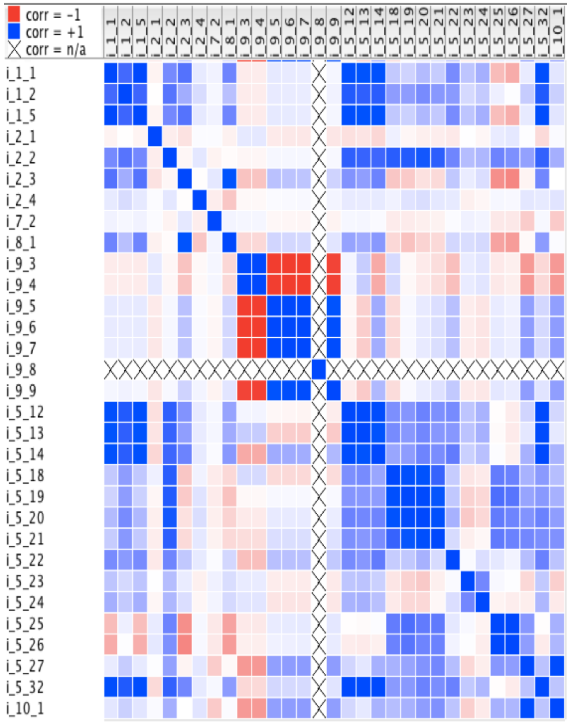
Automatic machine control



Machine Learning for Industry

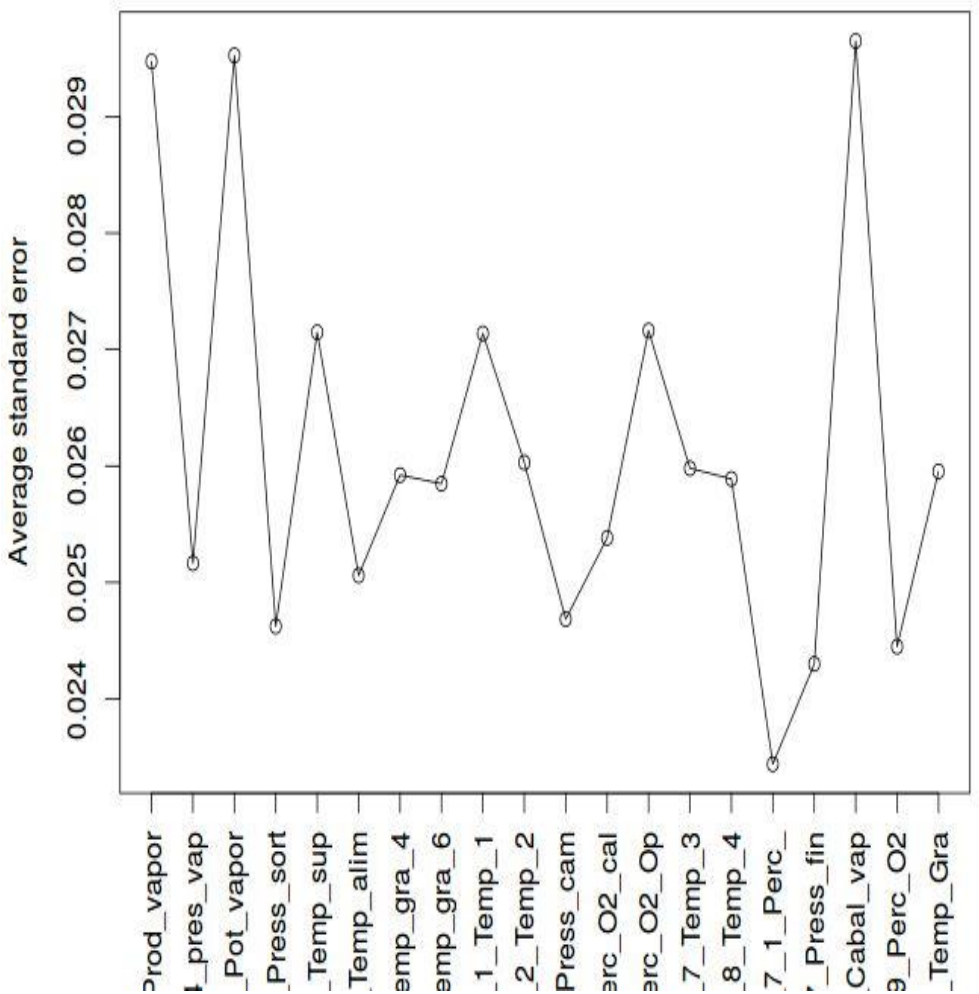
Data cleaning

- 156 variables every 5 seconds
- Storage (SQL, Cassandra)
- Parallel Pipeline
- Redundant data reduction



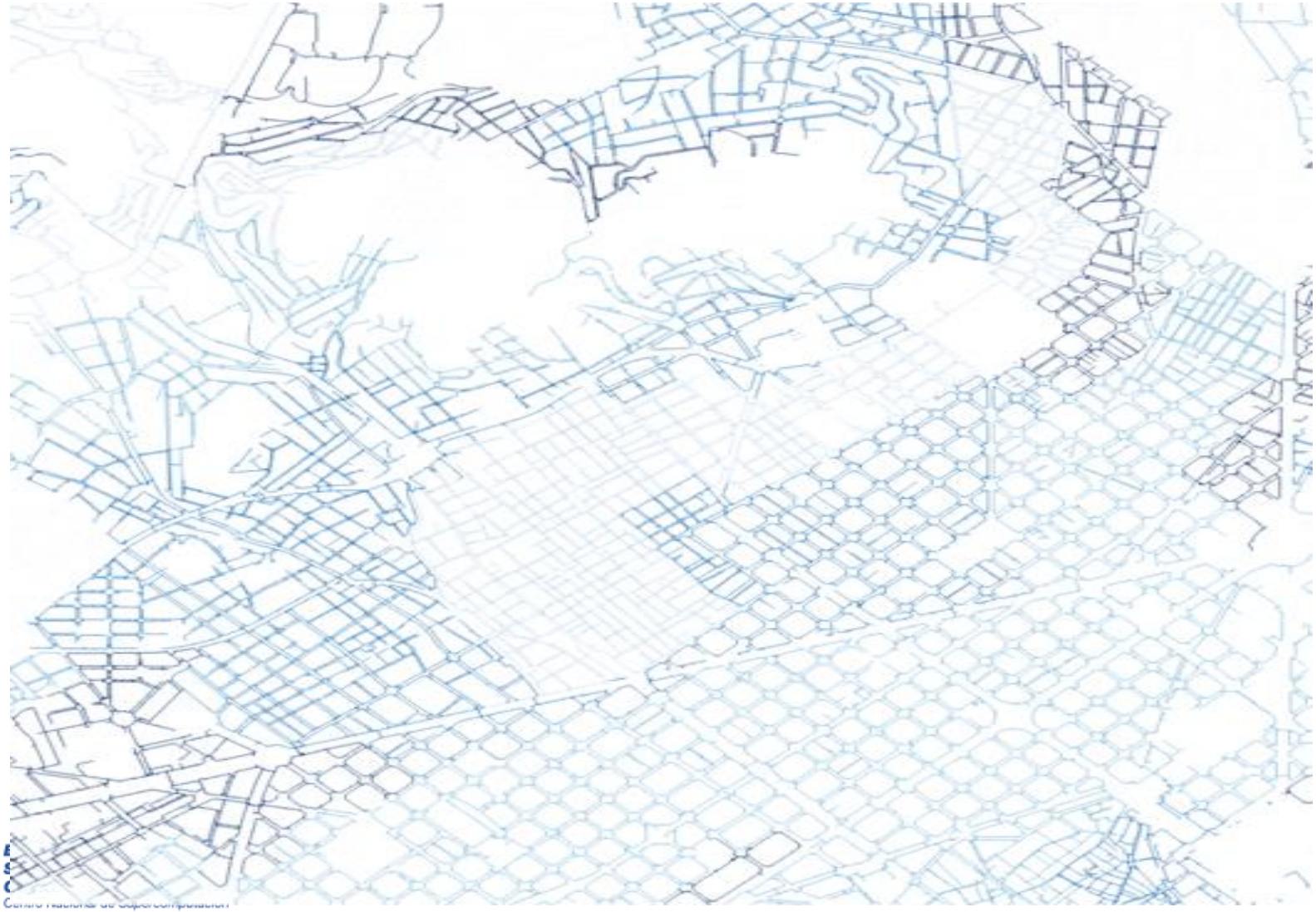
Input-input correlation matrix
(Pearson's coefficient)

Predictive Capacity



Predictive Maintenance: Water distribution network

Agbar



Open Project Portfolio December 2018

(includes H2020 projects in negotiation and national projects beginning soon)

234 running projects, total budget of over 97M€*

106 H2020/FP7 projects running or in negotiation (11 as coordinator)	62M€
39 running contracts, mostly with companies	12M€
52 projects with Spanish and Catalan public funding	16M€
17 projects funded through other EU programmes (incl. Copernicus)	3M€
17 projects funded through other sources	3M€
3 strategic self-funded projects	1M€

Plus:

65 personnel grants (national funding plus CONACYT programme)	7M€

Does not include ICREA, UPC, MSC,

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*** Budget for full term of project – normally multi-annual**

TOP-10 Catalan Organizations in Horizon 2020

Legal name	EU Contribution (€)	Project Participations
Barcelona Supercomputing Center	68,326,411 €	123
Universitat Pompeu Fabra	53,189,145 €	96
Universitat Politècnica de Catatalunya	52,595,046 €	147
ICFO	50,390,271 €	72
Universitat Autònoma de Barcelona	46,478,150 €	99
Universitat de Barcelona	43,292,105 €	120
CRG	36,333,838 €	62
LEITAT	26,988,611 €	60
EURECAT	25,713,104 €	60
IDIBAPS	17,874,593 €	35

Source:
European Commission, Participant Portal H2020 Projects
Updated March 2019

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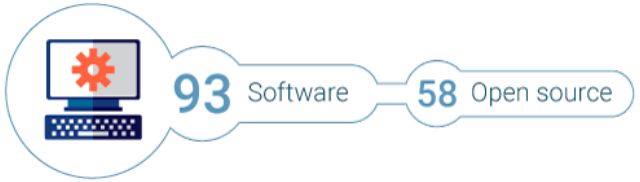
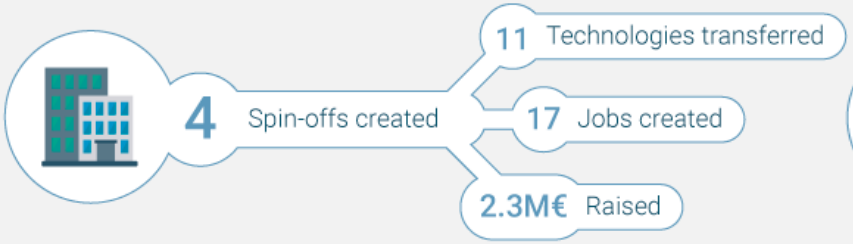
European Commission

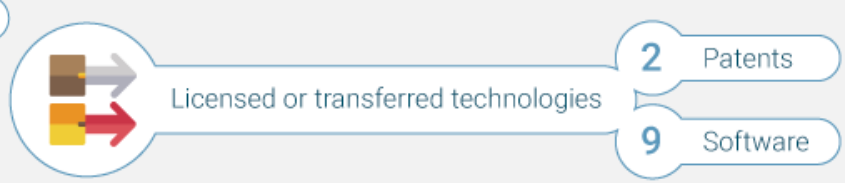
TECHNOLOGY TRANSFER

BSC IPR PORTFOLIO



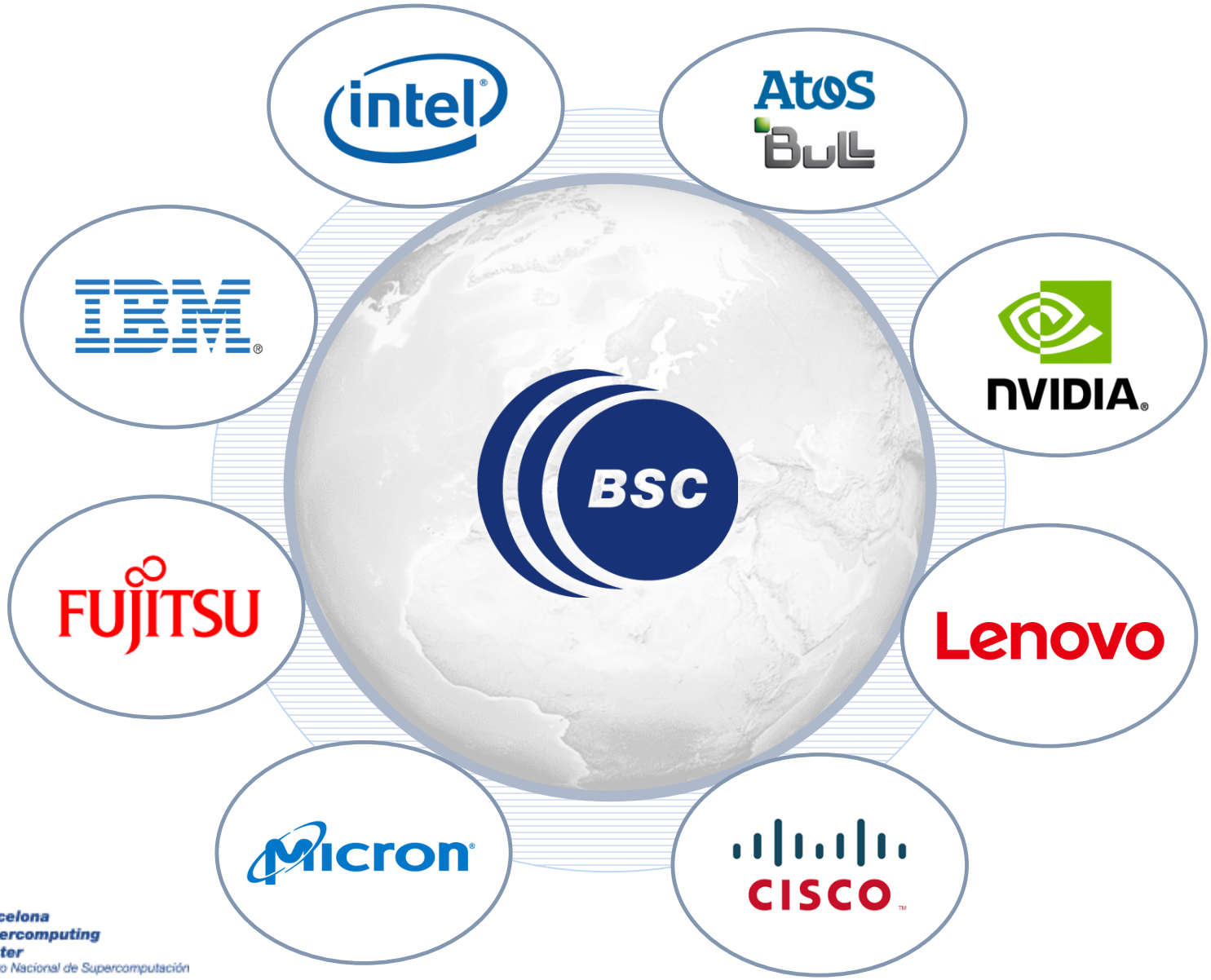
SPIN-OFFS AND LICENCING





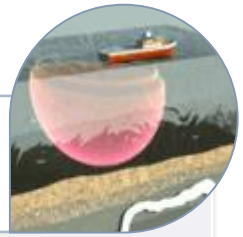
BILATERAL COLLABORATION WITH COMPANIES

BSC & The Global IT Industry 2018



Collaborations with Industry

REPSOL



Research into advanced technologies for the exploration of hydrocarbons, subterranean and subsea reserve modelling and fluid flows

IBERDROLA

Research on wind farms optimization and wing energy production forecasts

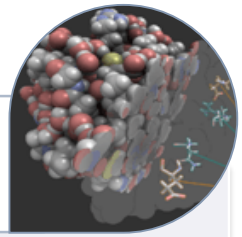
CaixaBank

Collaboration agreement for the development of advanced systems of deep learning with applications to banking services

Rockwell Collins

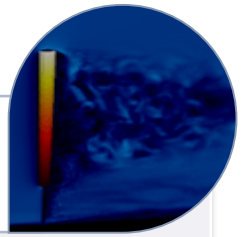
BSC's dust storm forecast system licensed to be used to improve the safety of business flights.

AstraZeneca



Research on the protein-drug mechanism of action in Nuclear Hormone receptors and developments on PELE method to perform protein energy landscape explorations

VORTEX Bladeless



Simulation of fluid-structure interaction problem with the multi-physics software Alya

BSC's spin-offs in brief

NOSTRUM BIODISCOVERY, S.L.	MITIGA SOLUTIONS, S.L.	ELEM BIO, S.L.	NEARBYCOMP, S.L.
Supercomputing **to speed up drug discovery**	Supercomputing **to minimize the impact of volcanic ash hazards**	Supercomputing **for biomechanics simulations.** Sas simulation tool focused on cardiovascular and respiratory systems	**FOG computing for IOT.** Customization services for different scenarios

“MareNostrum” by Macedònia

Today's menu

- **Let's understand the role of HPC & AI in the current and future European Challenges**
  - Evolution of computing power
  - Evolution of AI technologies
  - Impact on Research (and the role of the BSC)
  - Impact on Industry

- **Let's discuss the role of Europe in the future revolutions**
  - In HPC
  - In AI
  - In Quantum

Antecedents

2004

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Generalitat de Catalunya

Gobierno de España · Ministerio de Ciencia, Innovación y Universidades

Universitat Politècnica de Catalunya · BarcelonaTech

2006

RES
Red Española de Supercomputación

Barcelona Supercomputing Center · CESGA · IFCA Instituto de Física de Cantabria · Universidad de Málaga · Universitat de València · Instituto de Astrofísica de Canarias

SCAYLE Supercomputación Castilla y León · CénitS · bifi Instituto Universitario de Investigación de Biocomputación y Física de Sistemas Complejos Universidad Zaragoza · UAM Universidad Autónoma de Madrid · CSUC

2009

Ingrés a PRACE. Cinc Estats són considerats "*Hosting members*"

PRACE

Barcelona Supercomputing Center — Espanya

CINECA — Itàlia

ETH zürich — *Suissa

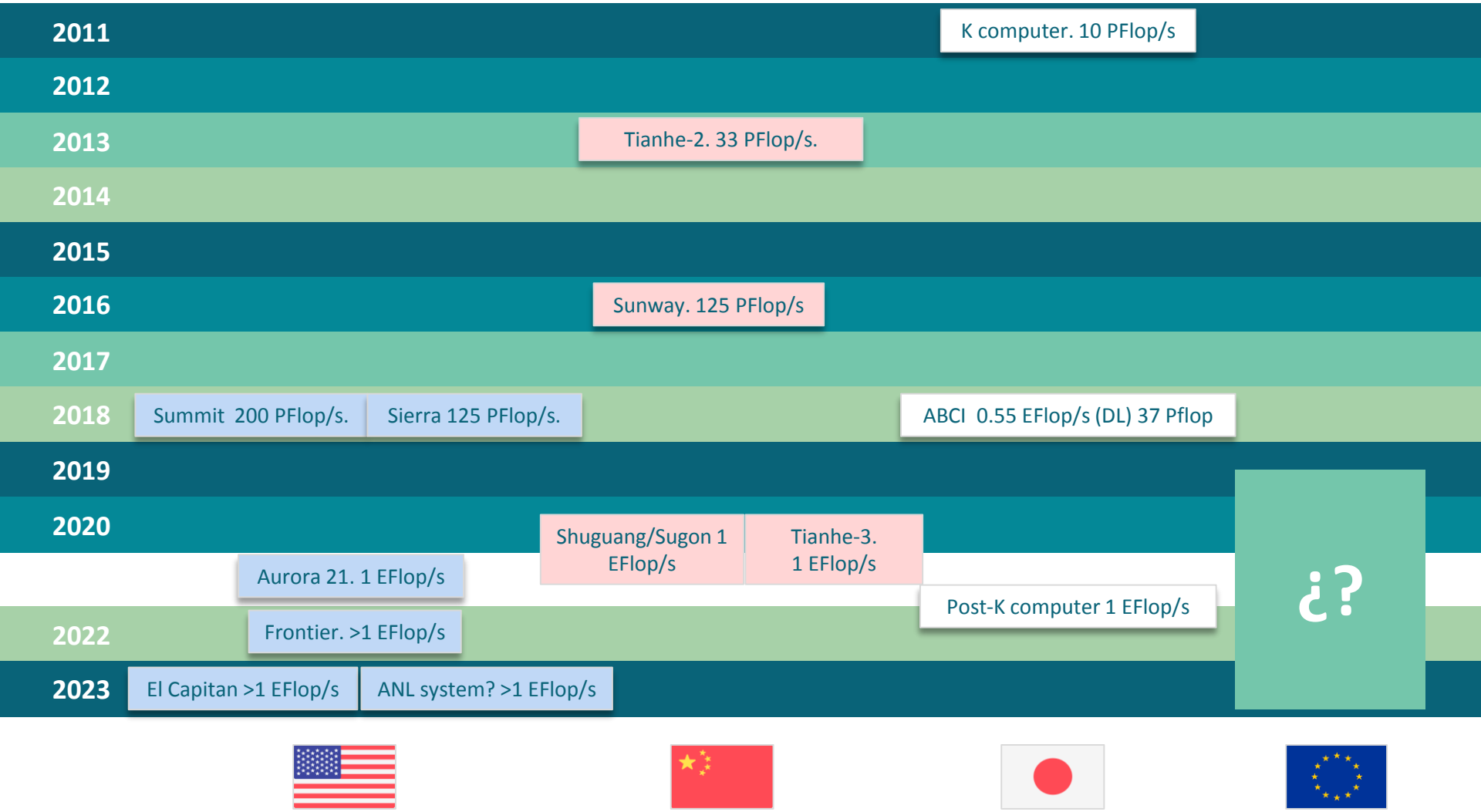
GCS Gauss Centre for Supercomputing — Alemanya

GENCI — França

2017

Neix la iniciativa **EuroHPC**

The roadmap to the Exascale (10^18)



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The European HPC puzzles

EuroHPC: to European HPC technologies

EuroHPC-Ju members:

Austria, Belgium, Bulgaria, Croatia, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Ireland, Italy, Latvia, Lithuania, Luxembourg, the Netherlands, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, Switzerland and Turkey

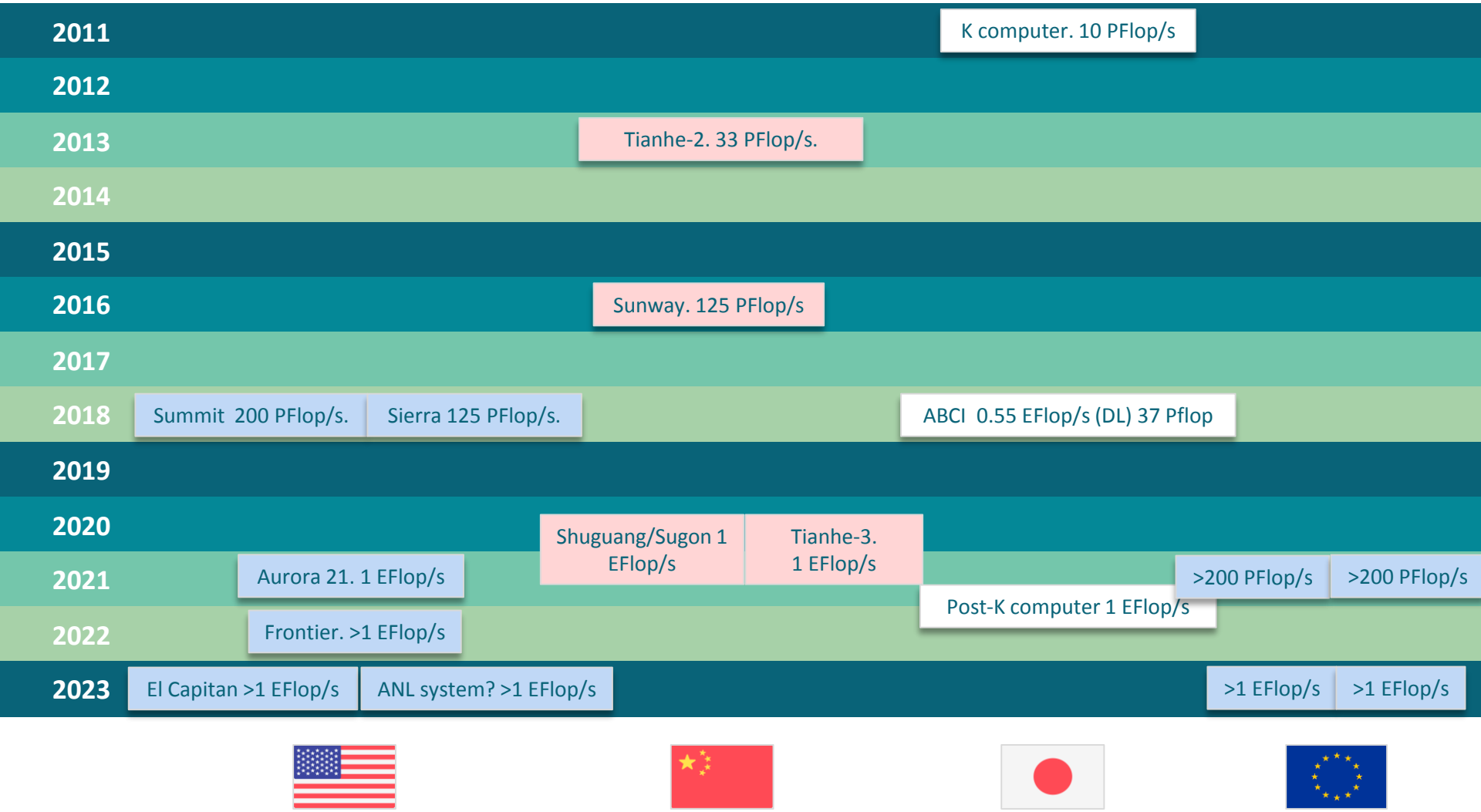
ETP 4 HPC

BDV

"A new legal and funding structure – the EuroHPC Joint Undertaking – shall acquire, build and deploy across Europe a world-class High-Performance Computing (HPC) infrastructure.

It will also support a research and innovation programme to develop the technologies and machines (hardware) as well as the applications (software) that would run on these supercomputers."

La hoja de ruta internacional hacia la exaescala



Suport a la candidatura del BSC

Patrons BSC-CNS

Generalitat de Catalunya
Departament d'Empresa i Coneixement

GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

UPC
UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Altres Estats adherits a EuoHPC

REPÚBLICA PORTUGUESA

Rialtas na hÉireann
Government of Ireland

Government of the Republic of Croatia

PRESIDENCY OF THE REPUBLIC OF TURKEY

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Where Europe needs to be stronger

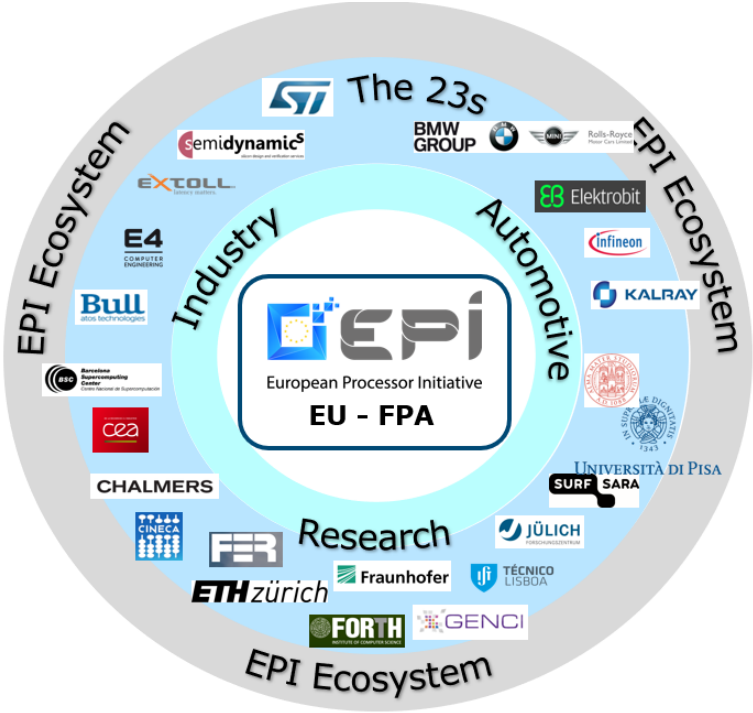
- Only 1 of the 10 most powerful HPC systems is in the EU
- HPC codes must be upgraded
- Vital HPC hardware elements are missing: General Purpose

Processor and Accelerators

EU needs its own source of as many of the system elements as possible

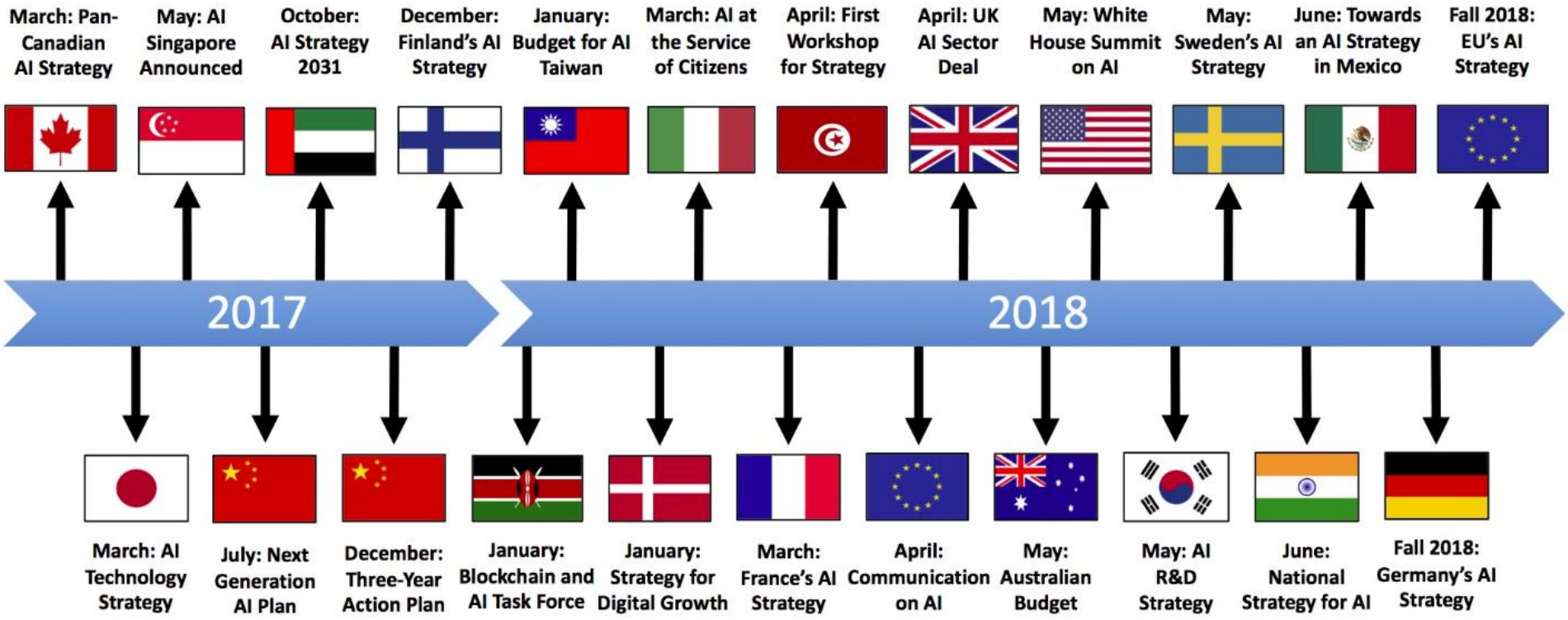
EuroHPC & EPI (European Processor Initiative)

- High Performance General Purpose Processor for HPC
- High-performance RISC-V based accelerator
- Computing platform for autonomous cars
- Will also target the AI, Big Data and other markets in order to be economically sustainable



Images courtesy of European Processor Initiative

Some relevant AI national initiatives



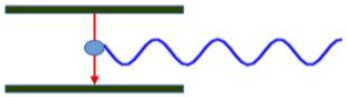
What about Quantum Computing?

$$|\psi\rangle = \underbrace{|000\rangle}_{0} + \underbrace{|010\rangle}_{2} + \underbrace{|110\rangle}_{6}$$

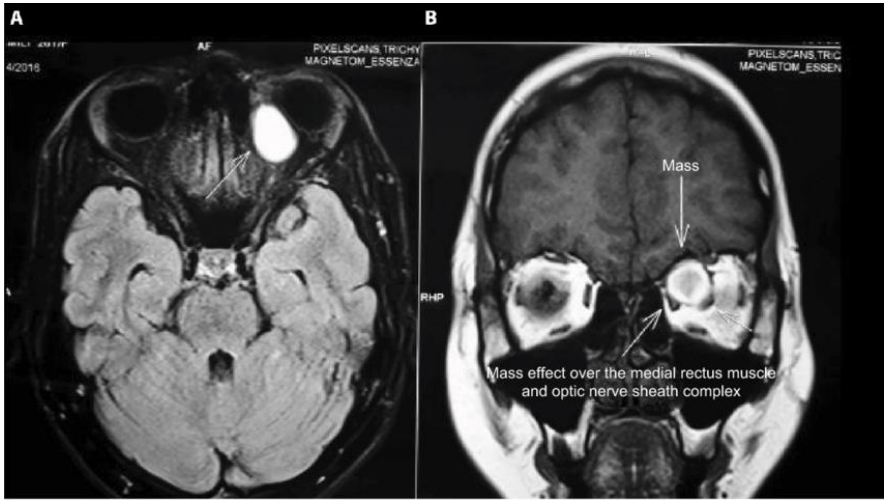
$$U_{+1}|\psi\rangle = U_{+1}|000\rangle + U_{+1}|010\rangle + U_{+1}|110\rangle$$

$$= \underbrace{|001\rangle}_{1} + \underbrace{|011\rangle}_{3} + \underbrace{|111\rangle}_{7}$$

Quantum things are pretty old…



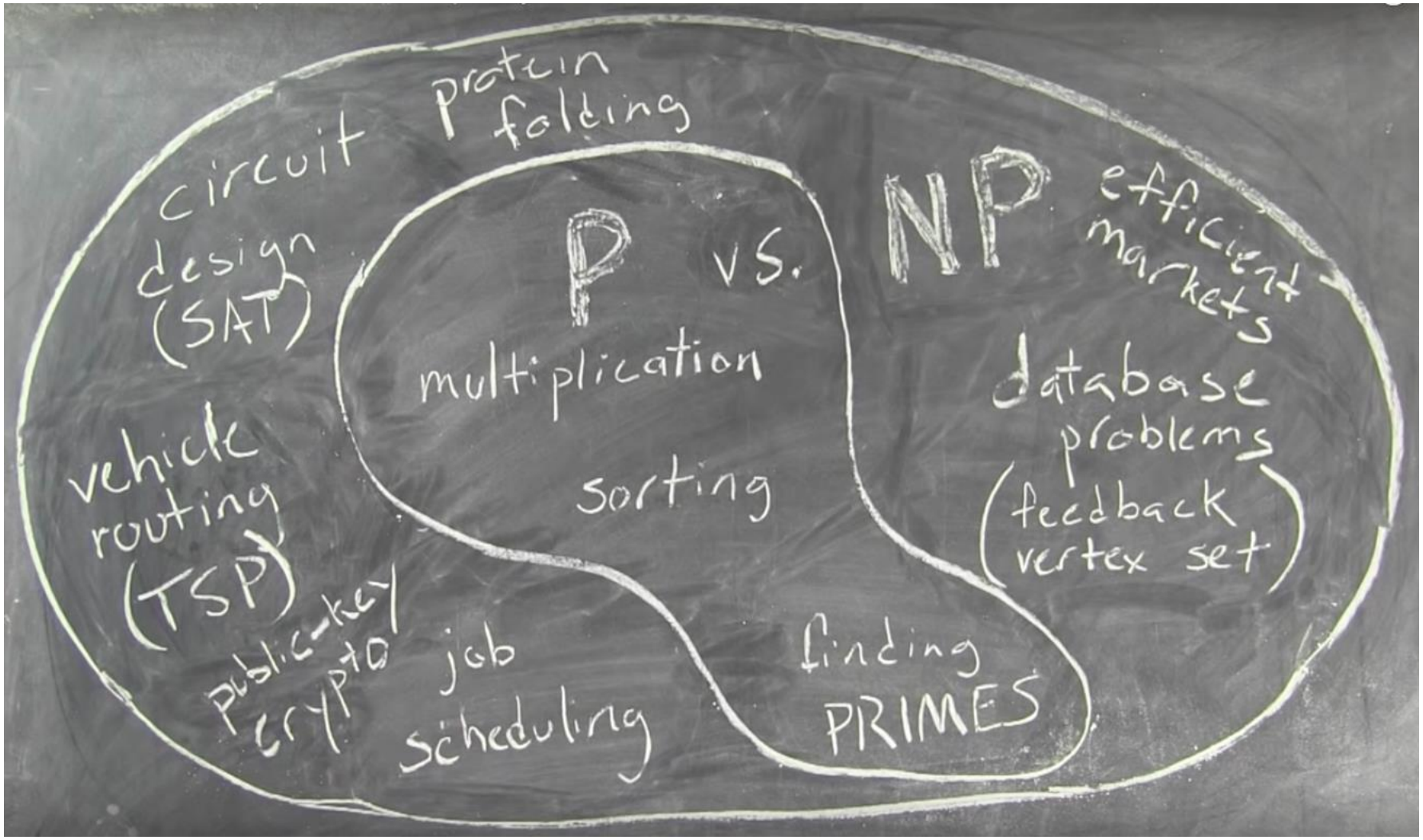
Reloj ultrapreciso, 1 parte en 10^{13}



Why now?

- Sistemas cuánticos bajo control
  - niveles atómicos en trampas de iones
  - polarizaciones de fotones
  - gases ultrafríos
  - corrientes superconductoras (DWAVE2)
- Manipulación
  - láseres
  - cavidades electromagnéticas
  - bajas temperaturas
- Decoherencia
  - control del entorno + algoritmos de corrección

P and NP problems



Factorization

Ordenador clásico

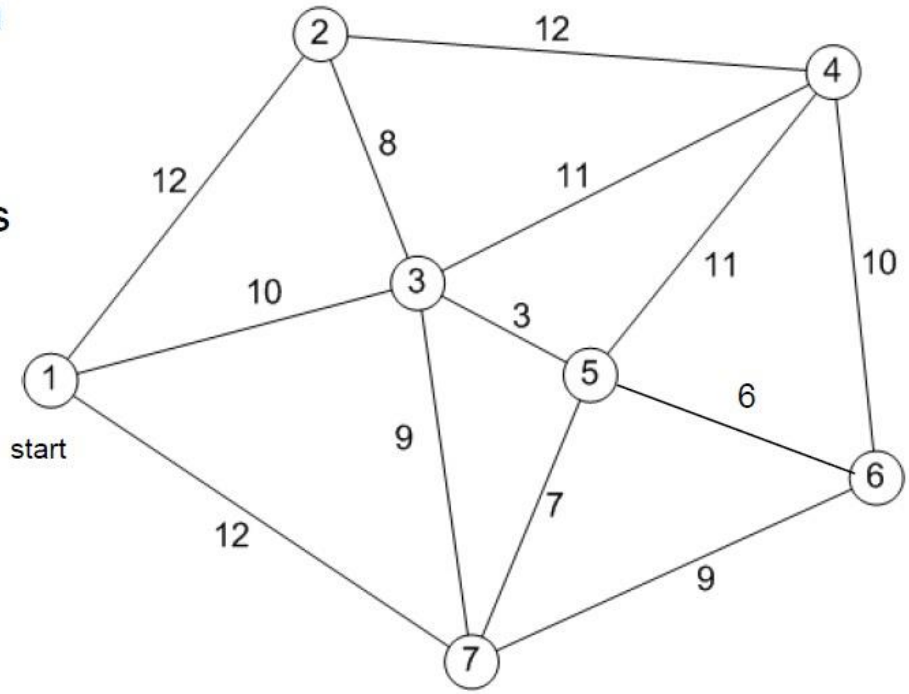
$$e^{ct\,n^{1/3}(\log n)^{2/3}}$$

Ordenador cuántico

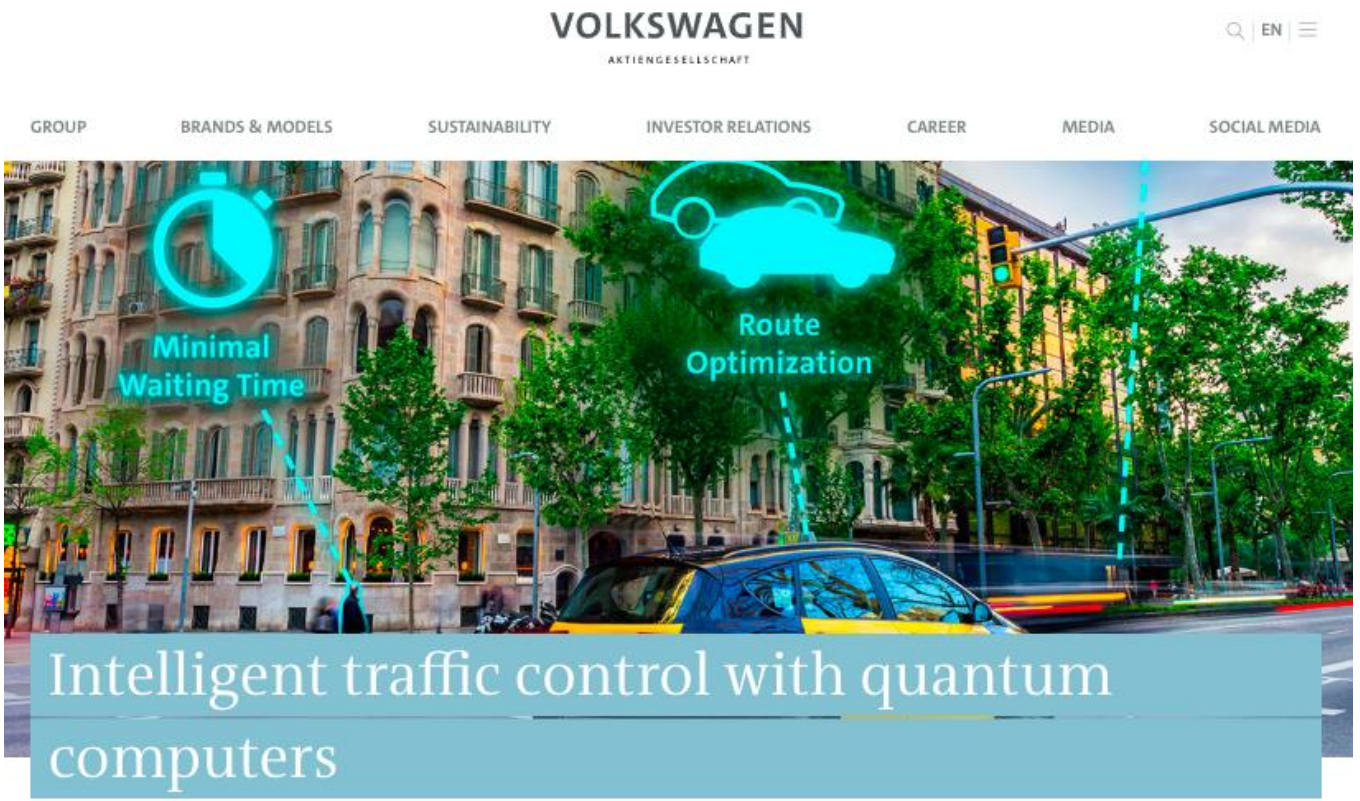
$$n^2(\log n)(\log(\log n))$$

The Traveling Salesman Problem

- Starting from city 1, the salesman must travel to all cities once before returning home
- The distance between each city is given, and is assumed to be the same in both directions
- Only the links shown are to be used
- Objective - Minimize the total distance to be travelled

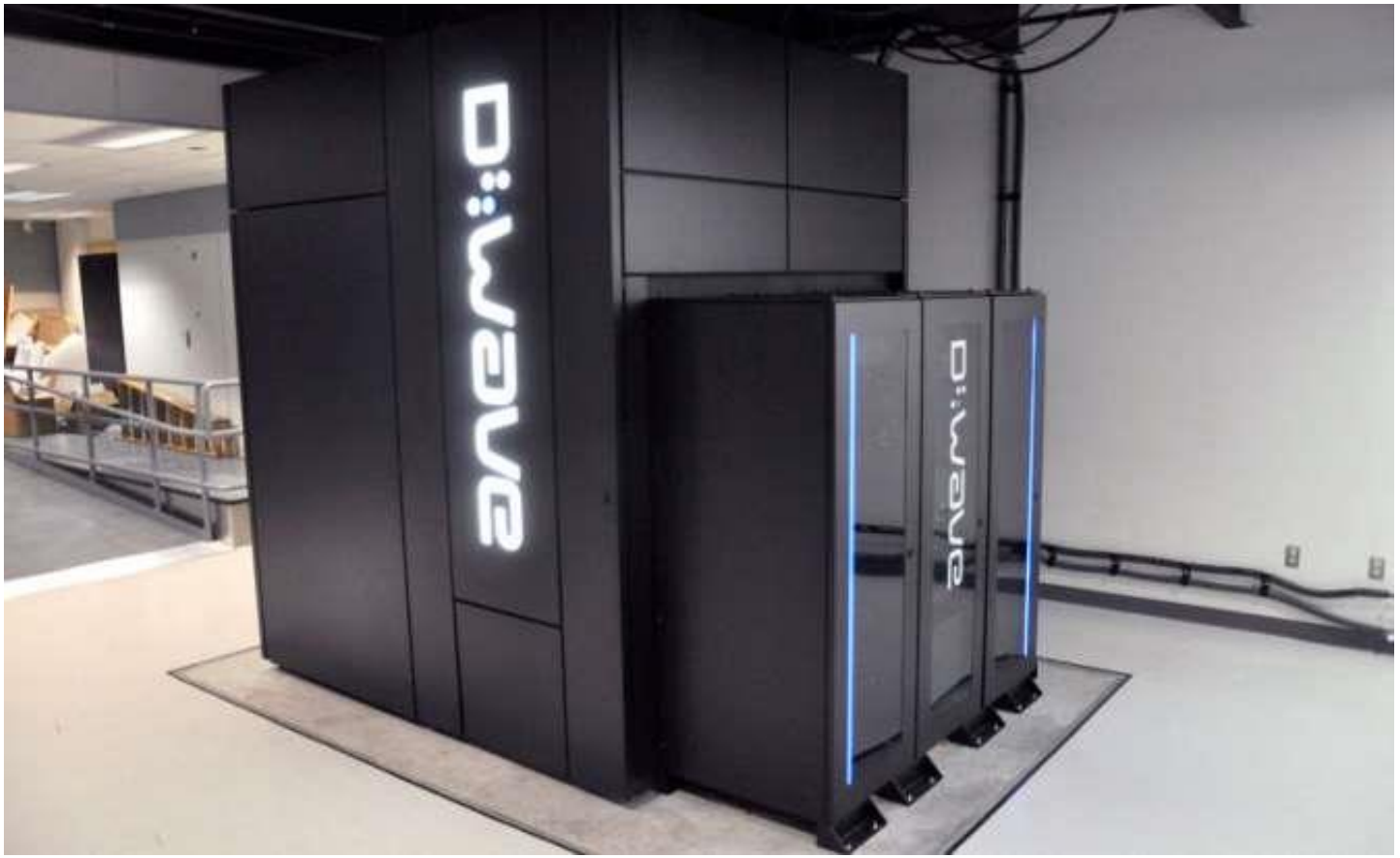


The Traveling Salesman Problem



Traffic control is one of the many areas where quantum computers could be used. An innovative project by Volkswagen: Avoiding traffic jams and shortening waiting times using quantum algorithms.

Example 1: D-Wave



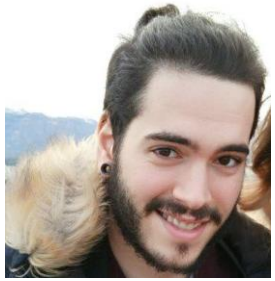
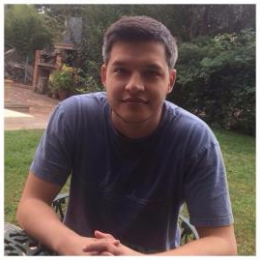
Example 2: IBM - Q

Towards a south-European Q processor

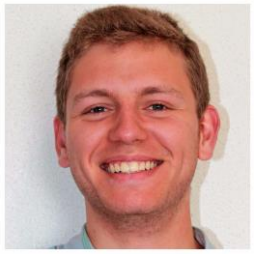
- QUANTIC Group launched: https://quantic.bsc.es

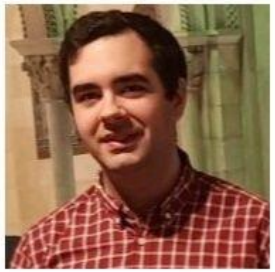








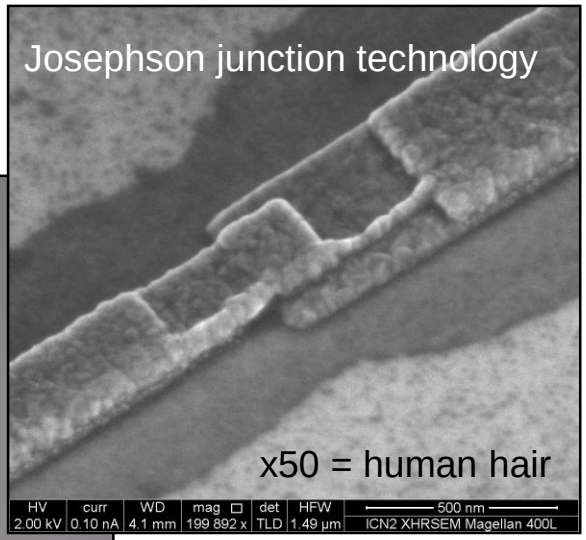
… and growing!

Towards a south-European Q processor

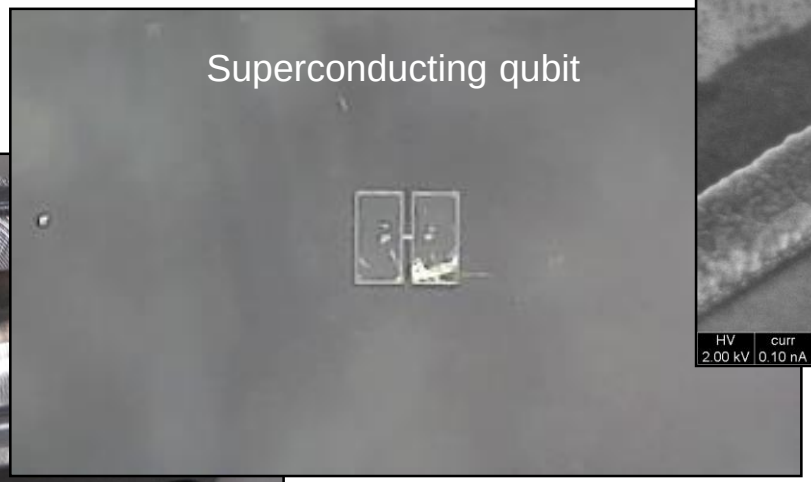
- A Quantum Computer is **hardware**
  - Building hardware: New paradigm at BSC
  - Need a lab (space)

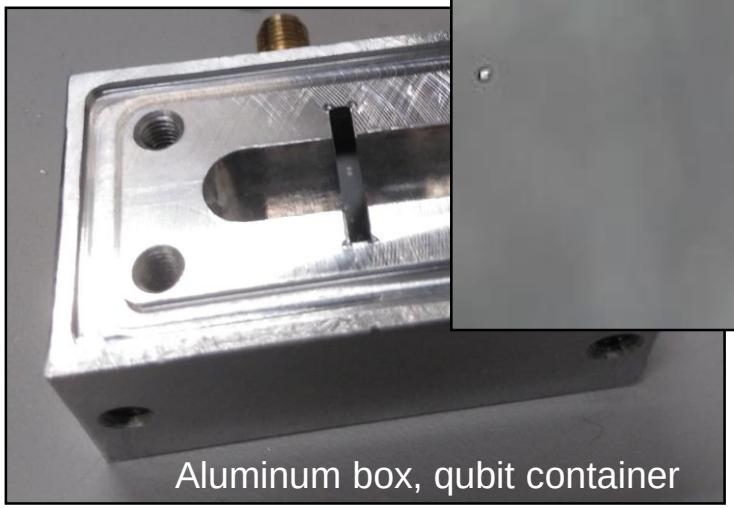
Towards a south-European Q processor

- A Quantum Computer is **hardware**
  - Building hardware: New paradigm at BSC
  - Need a lab (space)
  - Need quantum devices



SEM image





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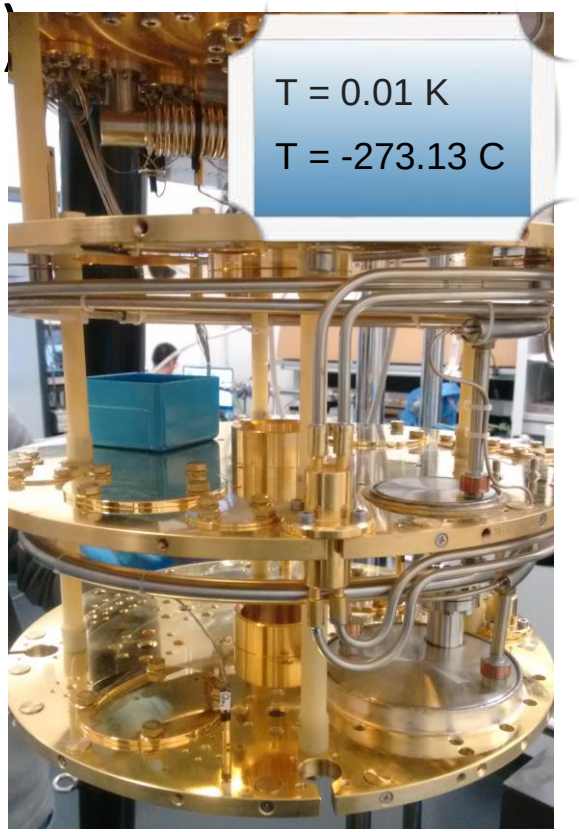
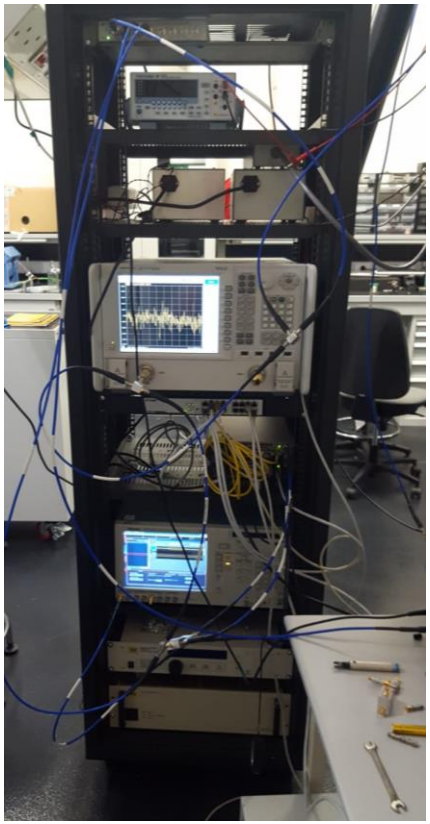
Karlsruher Institut für Technolog

Towards a south-European Q processor

- A Quantum Computer is **hardware**
  - Building hardware: New paradigm at BSC
  - Need a lab (space)
  - Need devices
  - Need equipment



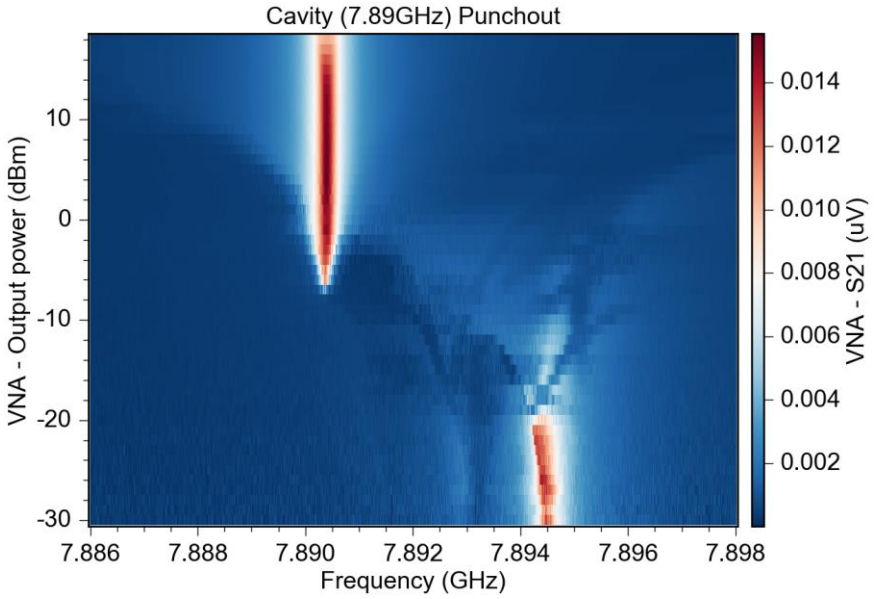
Dilution refrigerator



Quantum Control Unit

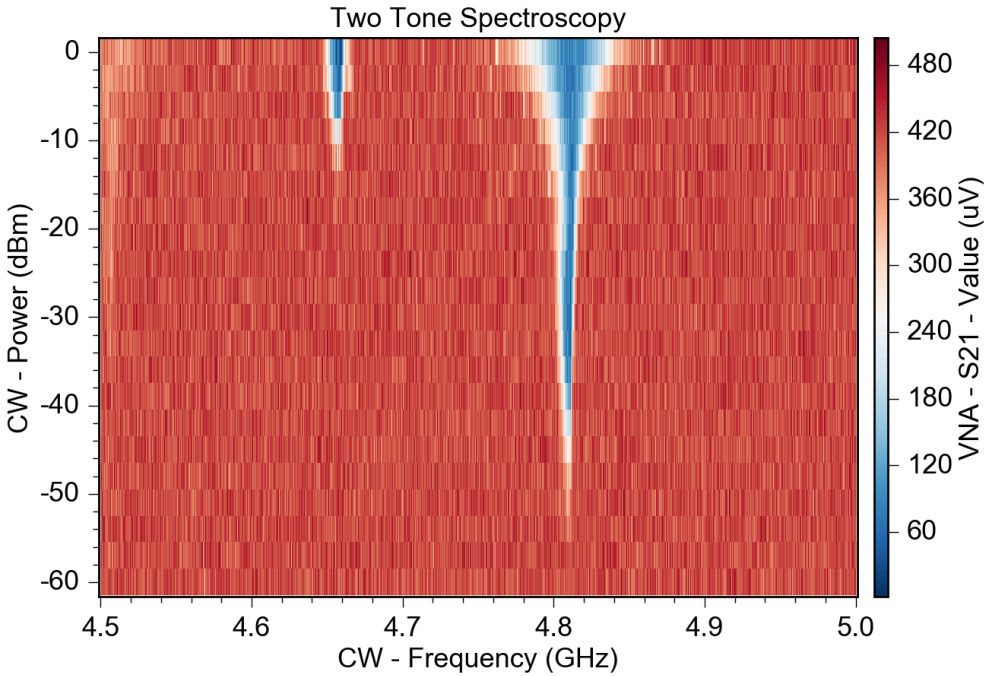
Towards a south-European Q processor

OUR FIRST 1-QUBIT QUANTUM PROCESSOR



Cavity resonance modulated by qubit

Microwave fields excite qubit transitions



First superconducting qubit in the **South of Europe**!

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Geopolitics, again!

- Propietary Technology

- Applicatons to
  - Communications, security
  - Mobility, logistics,
  - Pharma
  - Financial forecast

  … Very strategic!

The European future wager

Quantum Flagship in a nutshell.

01

1b €

Quantum Technology will be funded with at least one billion Euro by the European Commission.

02

10+ yrs

Flagship's timescale

03

5000+

researchers residing in all EU and associated countries involved

04

140

Research and Innovation Actions (RIA) proposals submitted in response of the first Quantum Flagship call

The European long-term vision

The long-term horizon is a "Quantum Web": Quantum computers, simulators and sensors interconnected via quantum networks distributing information and quantum resources such as coherence and entanglement.

On the corresponding time scale – which is in fact longer than 10 years – the performance increase resulting from Quantum Technologies will yield unprecedented computing power, guarantee data privacy and communication security, and provide ultra-high precision synchronization and measurements for a range of applications available to everyone locally and in the cloud.

Wrapping-up

- **Let's understand the role of HPC & AI in the current and future European Challenges**
  - Evolution of computing power
  - Evolution of AI technologies
  - Impact on Research (and the role of the BSC)
  - Impact on Industry

- **Let's discuss the role of Europe in the future revolutions**
  - In HPC
  - In AI
  - In Quantum

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EXCELENCIA SEVERO OCHOA

Thank you

martorell@bsc.es

martorellBSC

06/2019