

**Minho
Advanced
Computing
Center**

António M. Cunha
University of Minho



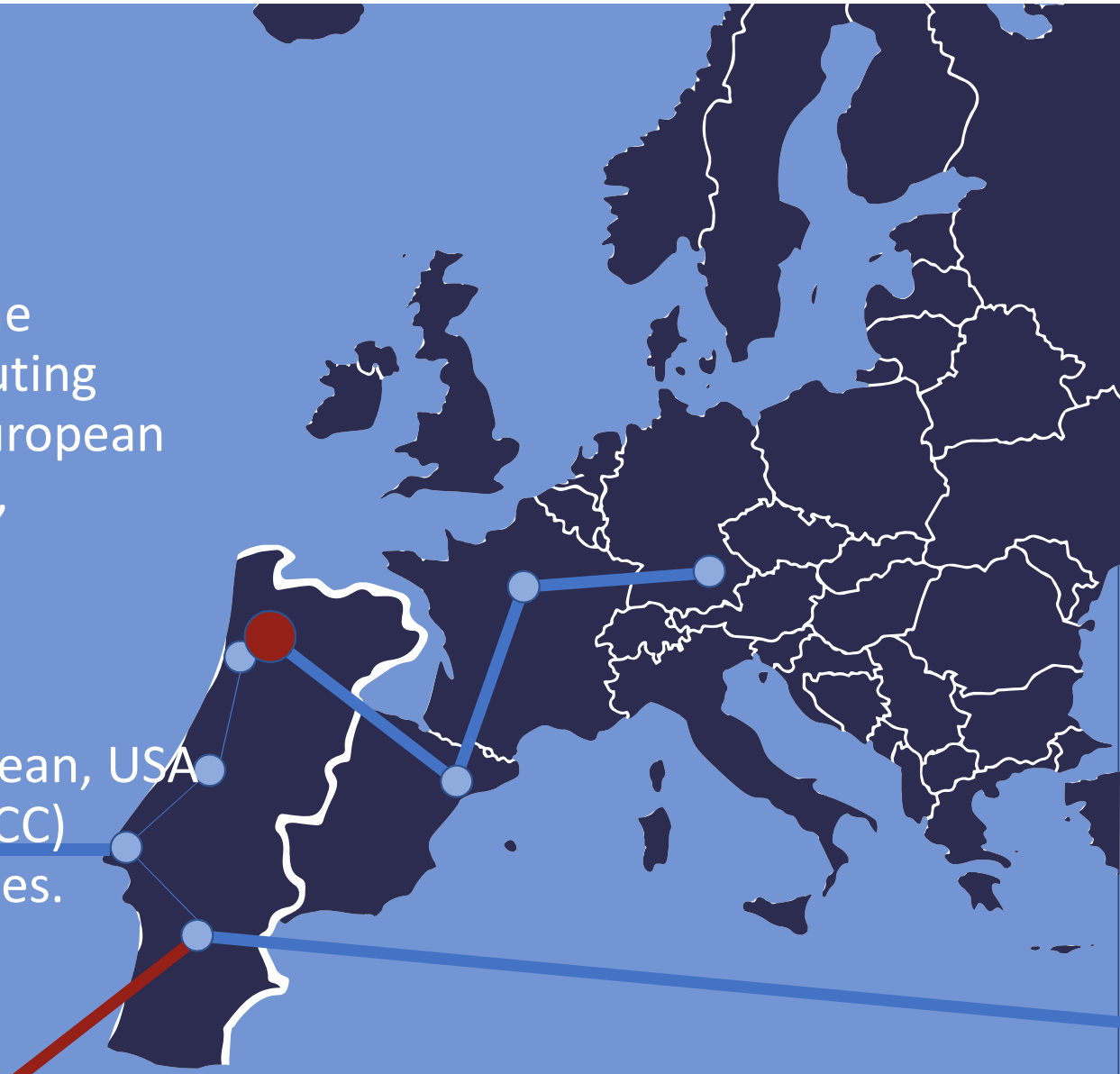
FCT Fundação
para a Ciência
e a Tecnologia

Objectives

- National collaborative infrastructure to promote and support **Open Science initiatives on super computing, data science and visualization;**
- Sustainable computing and data infrastructure **catering to national scientific and industrial communities** and complementary to international partners;
- Prominent node of the **AIR Centre Data Intelligence Network;**
- Node of the **EuroHPC Joint Undertaking.**

Global locus

- Effective participation in the European advanced computing initiatives: EuroHPC and European Exascale Computer, PRACE, European Cloud Initiative;
- Reinforcement of global collaboration on advanced computing between European, USA (TACC), South America (LNCC) and Asia (PRAGMA) facilities.



Global locus



MACC

Riba d'Ave
28.mar.19



Activity

- High Performance Computing "as a Service"
 - Traditional job submission queues
 - Specific application domain portals
 - Program parallelization and optimization research and consultancy
- Data Science
 - Life-cycle dataset management
 - SaaS for statistics, machine learning, deep learning, etc.
 - Cognitive computing portals
 - Jupyter Notebooks
- Cloud Computing
 - Computing resources – persistent and on-demand
 - Data storage – file-oriented, *tuple* e *object stores*
 - System and application “cloudification” development and consultancy
- Visualisation
 - Visualization “*as a service*”
 - Research and Education Support Facility
 - Data Visualization Tools and ResourcesCognitive Visualization Portals

Activity - HPC

- **Bioinformatics:** Molecular Dynamics, MPI-HMMER, mpiBLAST
- **Fluid Dynamics:** ReFresco, OpenFOAM
- **Environment:** EC-Earth, WRF, MM5, POP, ROMS, GADGET
- **Materials:** Gamess, Octopus, VASP, Alya
- **Molecular:** Desmond, GROMACS, NAMD, OpenAtom, SIESTA, LAMMPS, CHARMM, Amber
- **Physics:** ALPGEN, CLHEP, CORSIKA, DataMelt, DD4Hep, EGS, fads, FLUKA, FREEHep, Gaudi, GEANT4, GenFit, HepMC, HepSim, HERWIG, LarSoft, Lattice QCD, LHAPDF, MADGRAPH, npfinder, ProMC, PYTHIA, Rivet, ROOT, SHERPA, StatShape, TMVA, UrQMD, VDT
- **Chemistry:** Gaussian, Molpro, CP2K

Suggestions to:
rmv@di.uminho.pt

Activity – Data Science

- **Storage:** HDFS, HiBD
- **Database:** Apache HBase, MongoDB, Riak, Apache/DataStax Cassandra, Redis, ElasticSearch, Neo4J, CouchDB, HiBD, InfluxDB
- **Distributed Computing:** Map Reduce, Spark, Storm, Flink, Tez, Apache Flume, HiBD
- **Message Queues:** Kafka, RabbitMQ, ActiveMQ, Krestel
- **Data Warehouse:** Snowflake, RedShift, Apache Hive, Spark SQL, Cloudera Impala, Facebook Presto, Apache Tajo, Apache Drill
- **Modeling:** R, MathWorks, Pandas, Julia, NumPy, SAS, SciPy
- **AI/ML/DL :** Apache Mahout, Weka, TensorFlow, Caffe2, Keras, Apache MXnet, Theano, HiDL
- **Visualization:** Qlik, Tableau, Dataiku

Suggestions to:
rmvilaca@di.uminho.pt

AIR Center focused

- Digital Modelling
 - Earth, Ocean and Atmospheric Sciences
 - Space oriented advanced materials, nanostructures and Nanofabrication
 - Isolated and small-scale island energy systems
- Data Science
 - Climate data, ocean geo data, fisheries, Earth observation, etc.
- Secure Analytics
 - Confidentiality-aware analytics over federated data
- AIR Data Foundry

AIR Data Foundry

INTEGRATED DATA SERVICES

Data products, Data/Metadata Catalogue, Knowledge Spaces, Open APIs, Thematic and Contextual analytics, Cognitive Discovery

DATA
COLLECTION

DATA
PROCESSING,
& STORAGE...

DATA
REPOSITORIES

DATA
CATALOGUE

THEMATIC DATA SERVICES

Virtual Research Environments (VREs)

Atmospheric Science and Climate Change,
Energy Systems, Ocean Science and
Technology, Space Science and Technology

AIR Data Foundry

AIR CENTER DATA COLLECTION

**Sensors and
Data
Generator**

Data processing, storage and retrieval

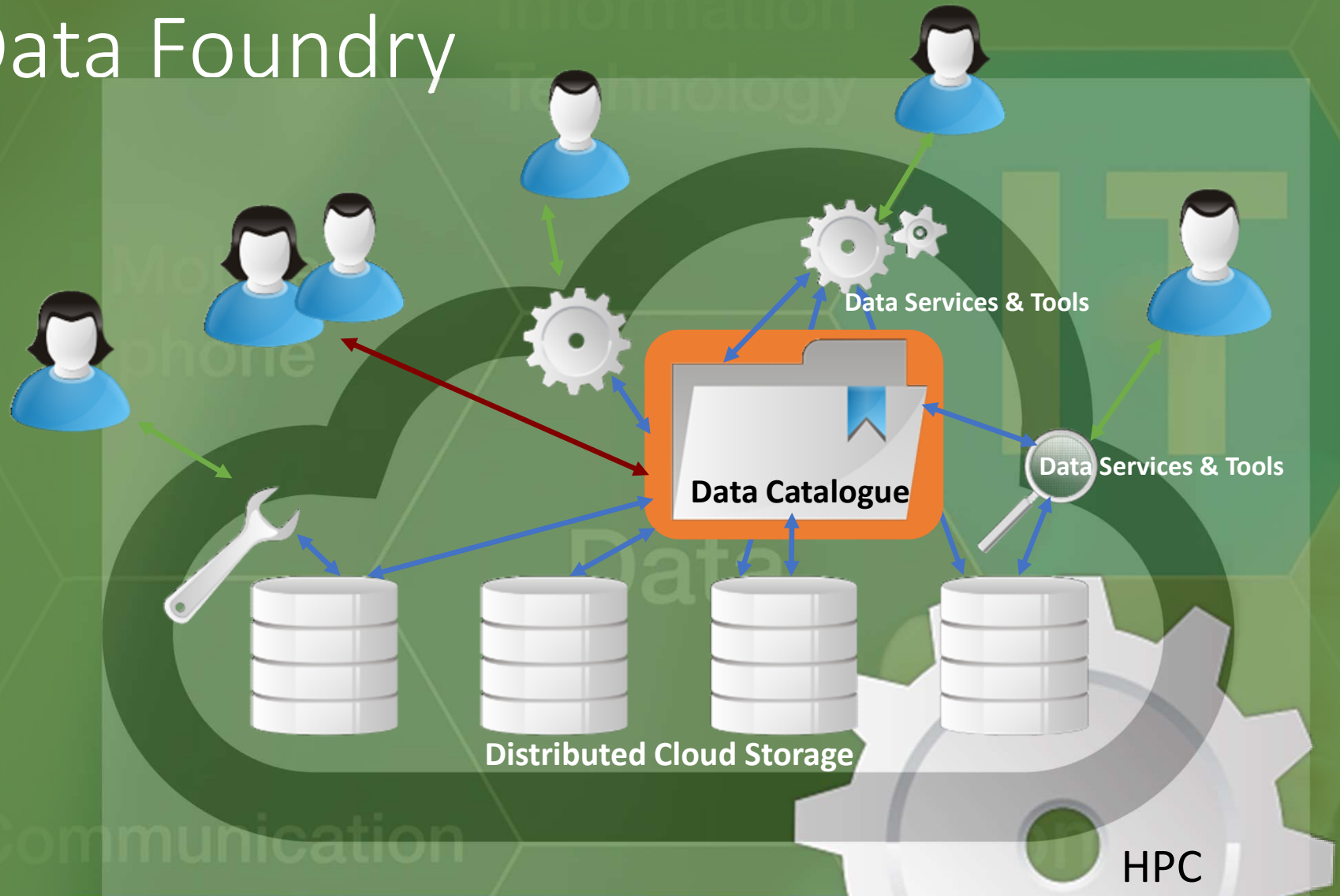
**Services and
Tools (VREs)**

Data Catalogue

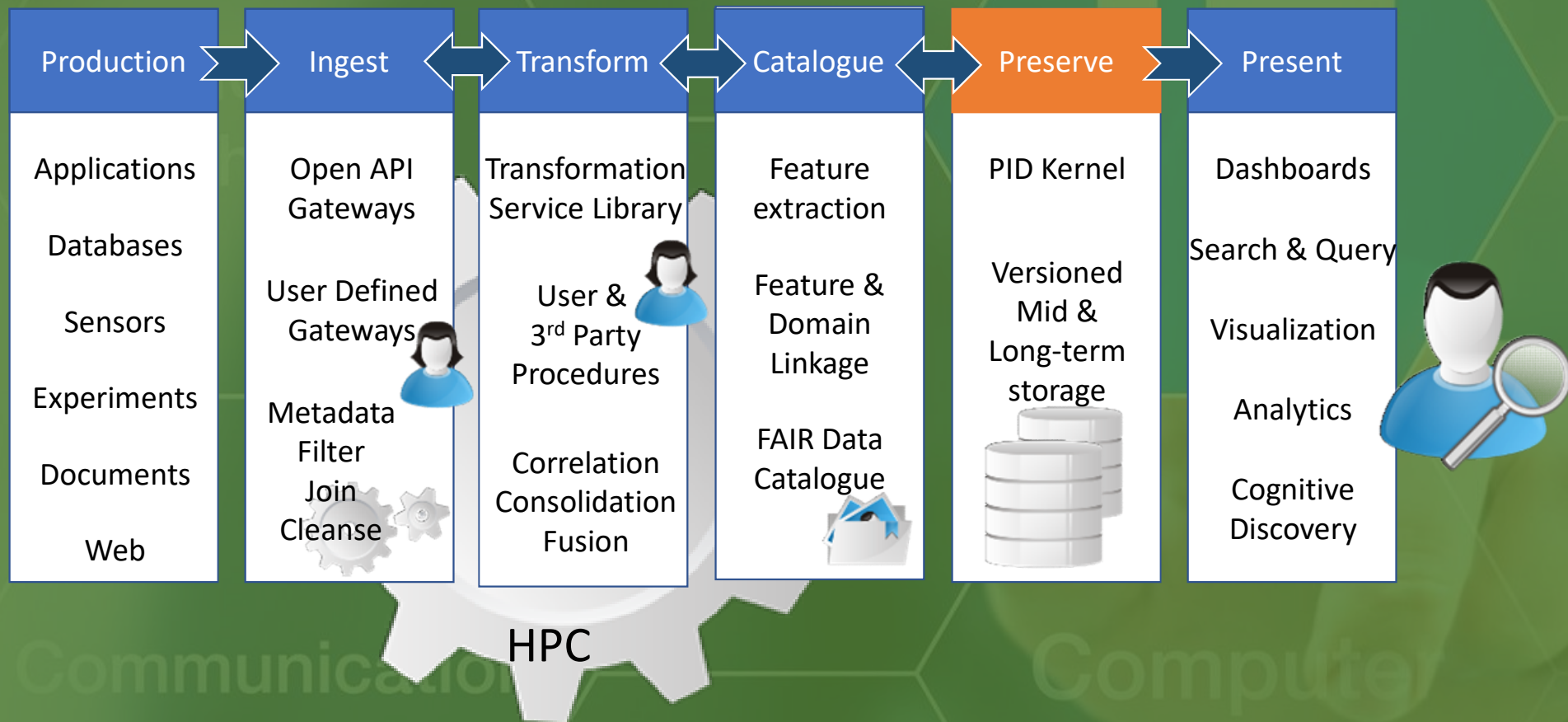


FAIR data/metadata catalogue

AIR Data Foundry



AIR Data Foundry



Resources – Petascale System (possible configuration)

Backup



X86 HPC/HPAI

High speed
Interlink

ARM HPC/HPAI

High speed
Interlink

Cloud Computing
system

High speed
Interlink

Storage

UEP
+
Mgmt



Resources – Petascale System

PHASE I – April 2019
(StampUM HW)

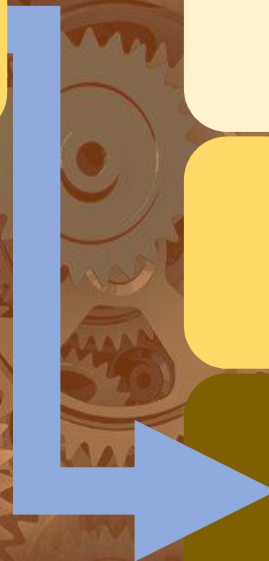
PHASE II – 1Q 2020

x86 HPC
(~1PFlop)

X86 HPC/HPAI

ARM HPC/HPAI

Cloud Computing
system



Resources – Visualisation

- Visualization Computing cluster
 - render raw data /intermediate representation into high resolution multidimensional visual representations
- 100 Mpixel multiview display
 - Data exploration, collaborative work, demonstration
- AR / touchless interfaces
 - e.g., Oculus Rift, Leap Motion, Hololens, ...



April 2019

Visualization Lab

April 2019

Data and Scientific Visualization :

the art and science of creating visual representations of complex data, rendering it intelligible, navigable and usable, facilitating the gaining of insight on the processes and phenomena represented by that data.

Visualization Lab: Mission

- to **promote and support** research, education, knowledge transfer on **data visualization and visual analytics**;
- to **foster adoption of visualization** techniques among **industrial and corporate communities**;
- **Visualization infrastructure and services** catering to **national scientific and industrial communities**;

Visualization Lab: Activity

- Visualization “*as a service*”
- Research and Education Support Facility
- Data Visualization Tools and Resources
- Cognitive Visualization Portals
- Visualization Applications Development and Consulting

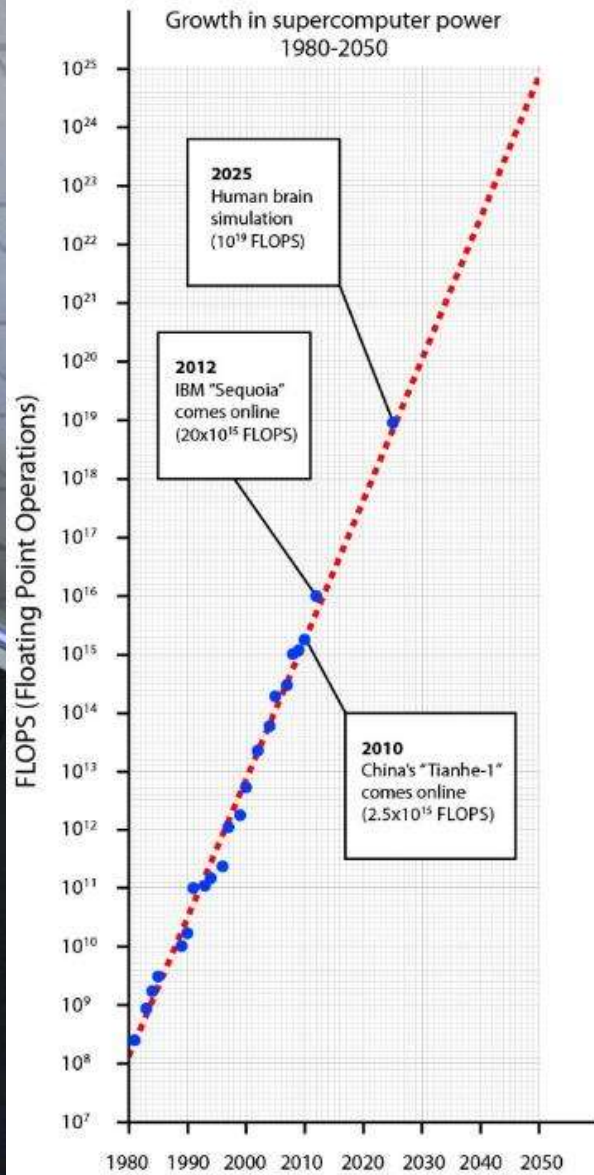
Visualization Lab: Resources

- Visualization Computing cluster
 - render raw data /intermediate representation into high resolution multidimensional visual representations
- Mega resolution multiview display
 - Data exploration, collaborative work, demonstration
- AR / touchless interfaces
 - e.g., Oculus Rift, Leap Motion, Hololens, ...



information technologies





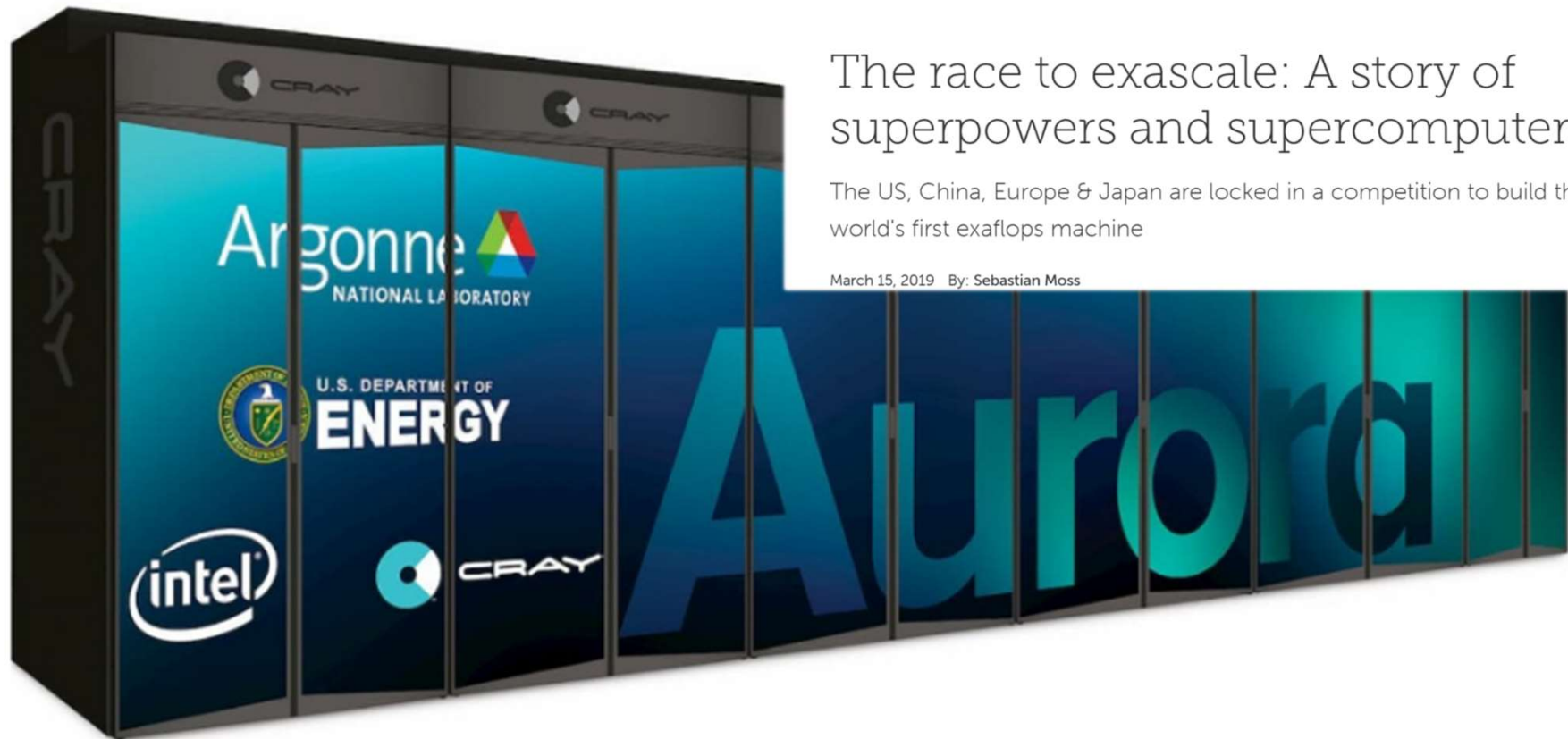


Intel will build the first exascale supercomputer in the US

Aurora will help advance cancer research and climate modeling, Sec. Perry said.



Kris Holt, @krisholt
03.18.19 in [Gadgetry](#)



The race to exascale: A story of superpowers and supercomputers

The US, China, Europe & Japan are locked in a competition to build the world's first exaflops machine

March 15, 2019 By: Sebastian Moss

Proyecto europeo

su primera convocatoria para financiar máquinas de :
para el futuro del continente



**Supercomputing Center-Centro Nacional de
tación (BSC-CNS)** presentará a principios de abril su
construir un **superordenador** cofinanciado por la UE
pa no pierda competitividad respecto a Est
y Japón en capacidad de cálculo.

Más potencia

La capacidad de cálculo del futuro
MareNostrum 5 multiplicará por más de 20 la
de la máquina actual

Apoyo político y económico

La candidatura barcelonesa tiene el apoyo de los gobiernos de Catalunya, España y Portugal

La selección de las candidaturas empezará con una evaluación técnica y continuará con una negociación política antes de la decisión final, que debe anunciarse el 7 de junio.

Para la fase técnica, el BSC-CNS cuenta con la baza de haber sido una de las cinco instituciones fundadoras en 2009 –al igual que la italiana Cineca- de la red europea de supercomputación Prace. A ello se suma que el director del BSC-CNS, Mateo Valero, que ya trabaja más como embajador de la supercomputación que como informático, fue en 2017 uno de los principales artífices de que la CE adoptara la iniciativa EuroHPC.

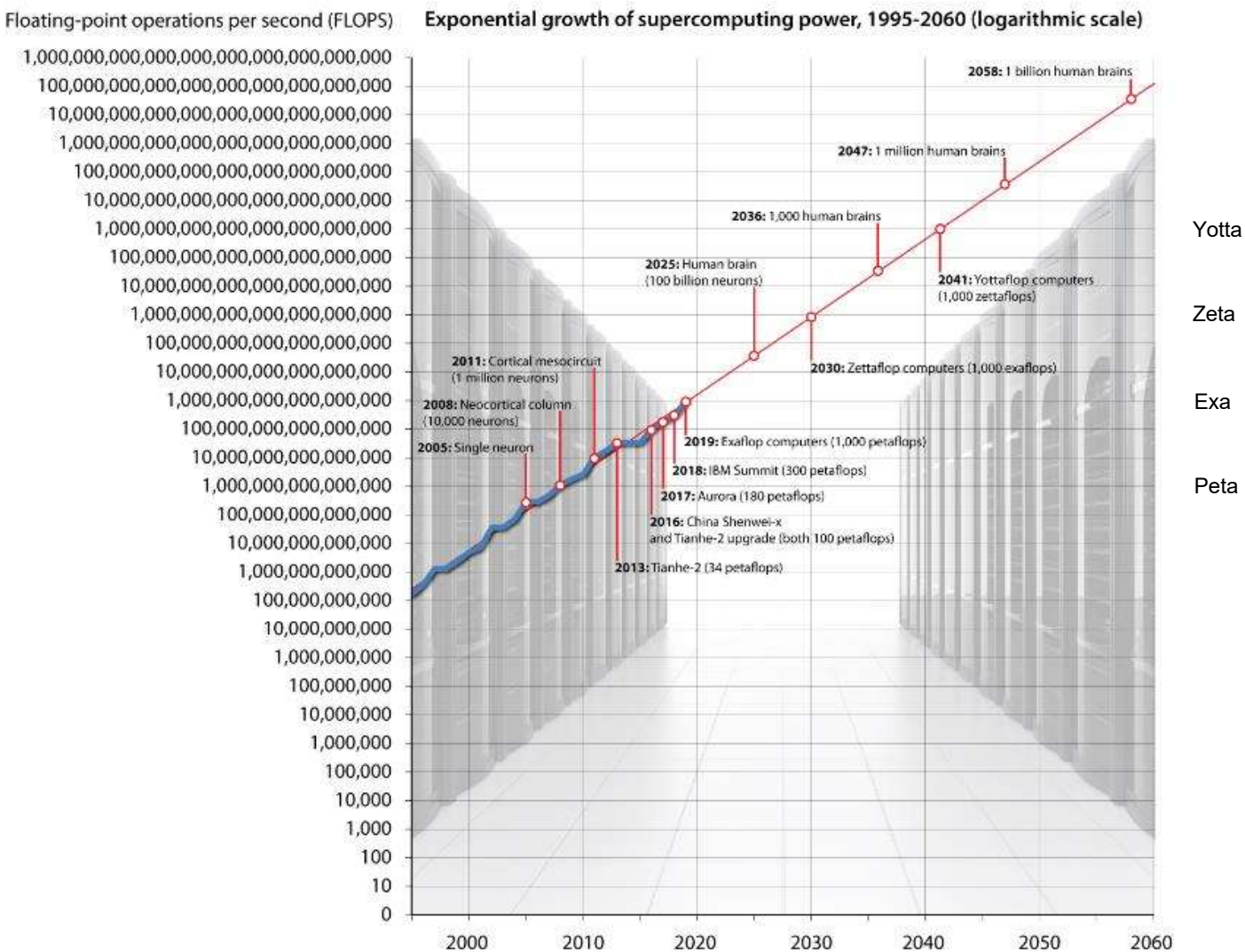
Estratégia Ibérica para a supercomputação

No contexto, dos avisos em curso, ou a abrir brevemente, da iniciativa EuroHPC, o acordo entre os dois países prevê:

- uma candidatura conjunta a uma máquina pre-exascale a instalar em Barcelona
- o apoio do BSC a uma candidatura portuguesa, através da FCT (Fundação para a Ciência e Tecnologia) e do MACC a um supercomputador petascale.

A candidatura ibérica, liderada pelo BSC, terá uma participação portuguesa de 10%, o que se traduzirá num esforço financeiro português deste nível e na correspondente disponibilização de tempo de computação.

Exponential growth of supercomputing power, 1995-2060 (logarithmic scale)



The background is a deep blue with a complex, abstract pattern of glowing lines and small squares, creating a sense of depth and digital connectivity. The lines are mostly horizontal and slightly curved, with small squares scattered throughout, some appearing as if they are floating or moving. The overall effect is reminiscent of a data center or a high-tech digital environment.

MACC

Minho Advanced Computer Center