Scientific Computing : Perspectives, Funding, European Model and Future

A. Zoccoli - INFN and University of Bologna

Perugia: School on Open Science Cloud

Outline

- Introduction
- The European scenario
- Italian Infrastructure: HTC & HPC
- The Infrastructure evolution
- A possible future

Credits: S. Bassini , L. Benini, I. Bird, A. Cavalli, F. Fava., D. Lucchesi, D. Salomoni, and many others. Thanks !!

Introduction / History

Introduction

Three different types of scientific computing :

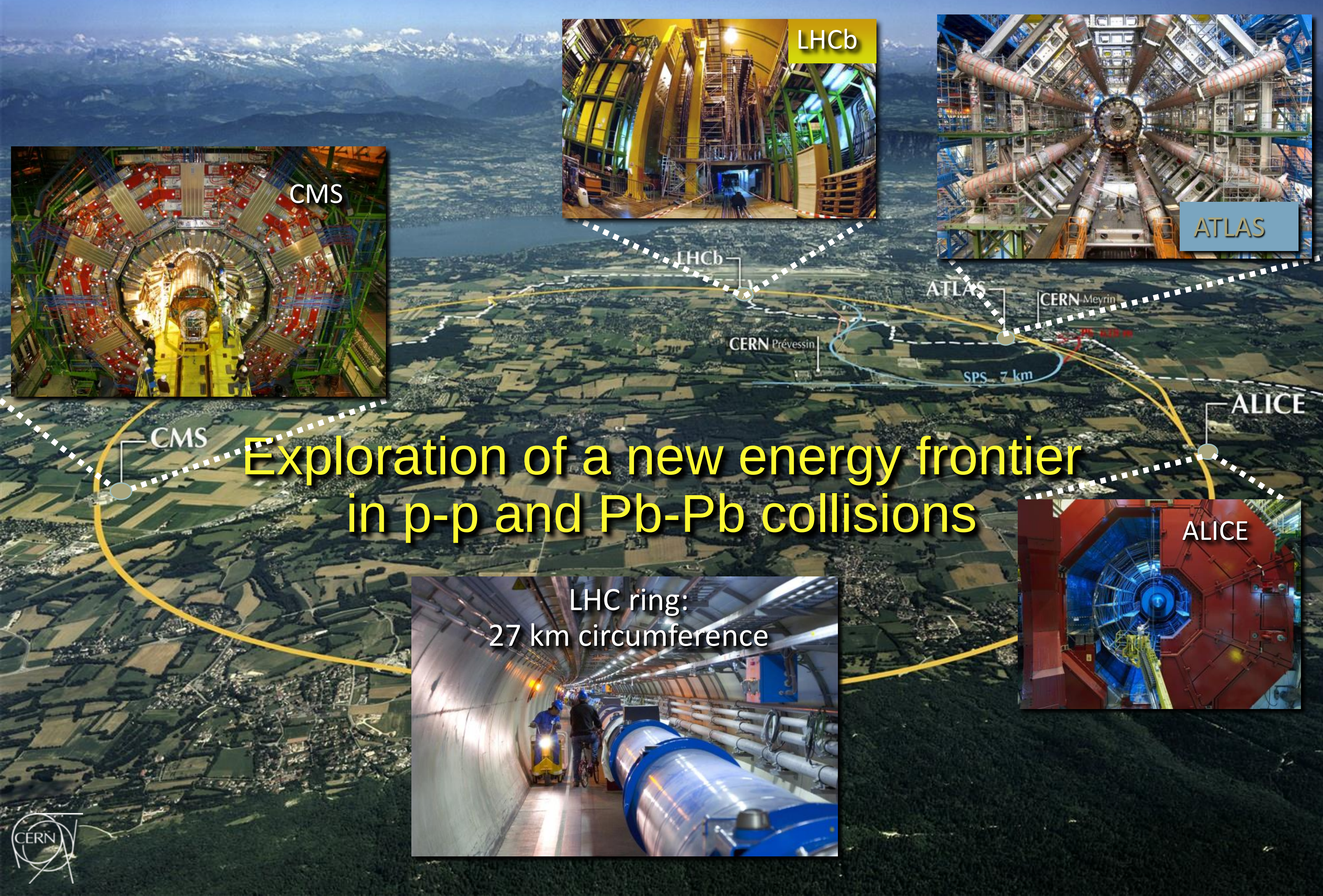
1) High Throughput Computing (HTC) for experimental physis (LHC @ CERN)
2) High Performance Computing (HPC) for theoretical physics, materials studies, weather forecast, fluido-dynamics,deep learning ….
3) "Traditional" Computing for small experiments or scientific initiatives

High Energy Physics developed a worldwide HTC computing infrastructure based on the GRID technology to analyse the data produced at the 4 LHC experiment at CERN.

→ Italian (INFN) national HTC infrastructure

A. Zoccoli

INFN involvement in the LHC project



Exploration of a new energy frontier in p-p and Pb-Pb collisions

The problem: LHC data handling

After filtering, LHC detectors select >200 interesting collisions per second.
Several MBs of data to be stored for each collision...

→ more than 25 Petabytes/year of data!

→ The GRID paradigm

8 Megabyte (8MB)
A digital photo

1 Gigabyte (1GB)
= 1000MB
A DVD movie

1 Terabyte (1TB)
= 1000GB
World annual book production

> 25 Petabytes (25PB)
= 25000TB
Annual LHC data output

The solution: the GRID

At the end of 90's some important initiatives from the Physics community have provided the foundation for the GRID infrastructure:

1. The CERN action to prepare an EC project for the LHC computing
2. The launch of the eScience program in UK
3. The action of the INFN Management setting up the CNTC the Committee for the new IT technologies for LHC
4. ……….

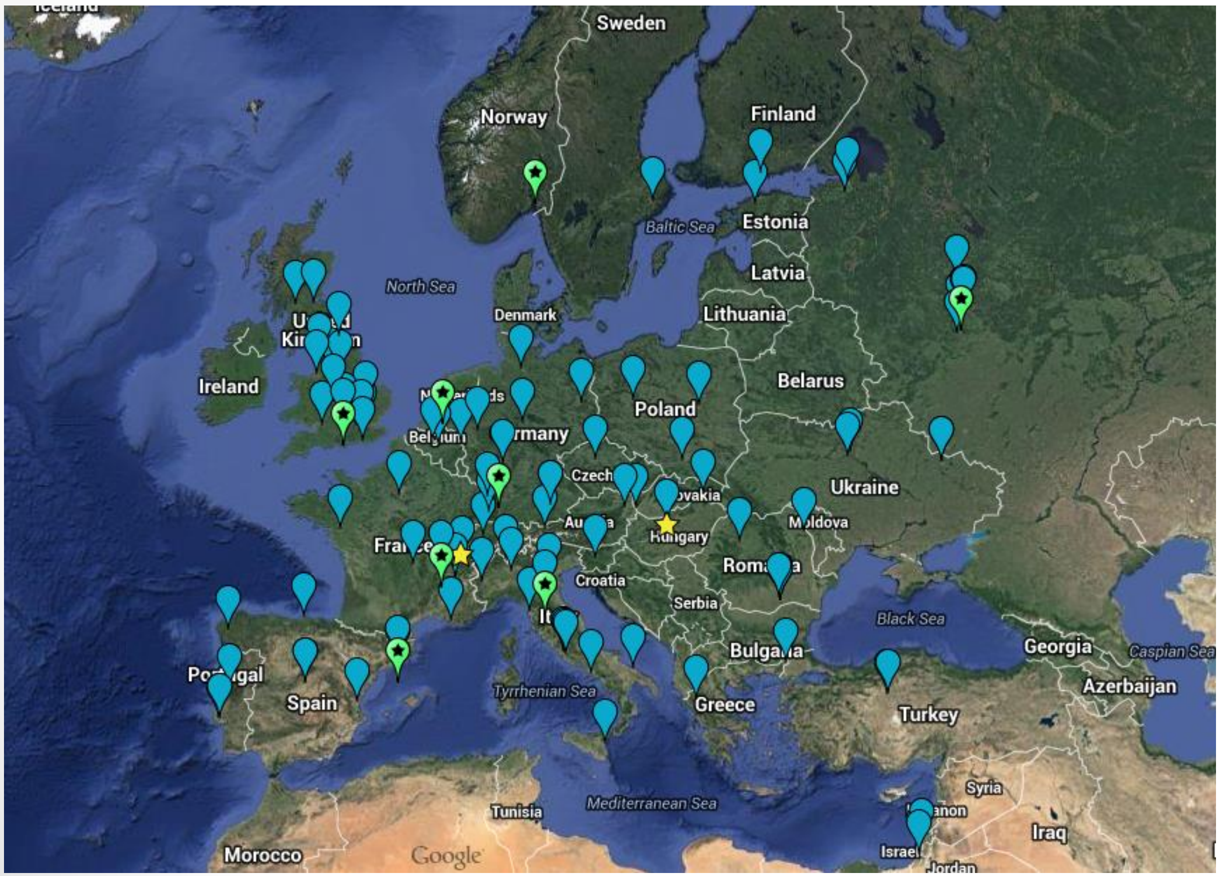
The GRID development and INFN

Active participation in all the development steps like for example:

1. DataGrid (2000) with CERN, INFN, CNRS, PPARC, NIKEHF
2. egee (2003)" Enabling GRID for E-Science in Europe": definition of the European Grid operation model
3. WLCG (2004) designed for the LHC data analysis based on GRID
4. EGI (2010) "European Grid Infrastructure": probably we know what it is or should be..

The e-infrastructure

During the past years INFN + other FA + CERN with large contributions of EC has constructed and consolidate a large computing infrastructure



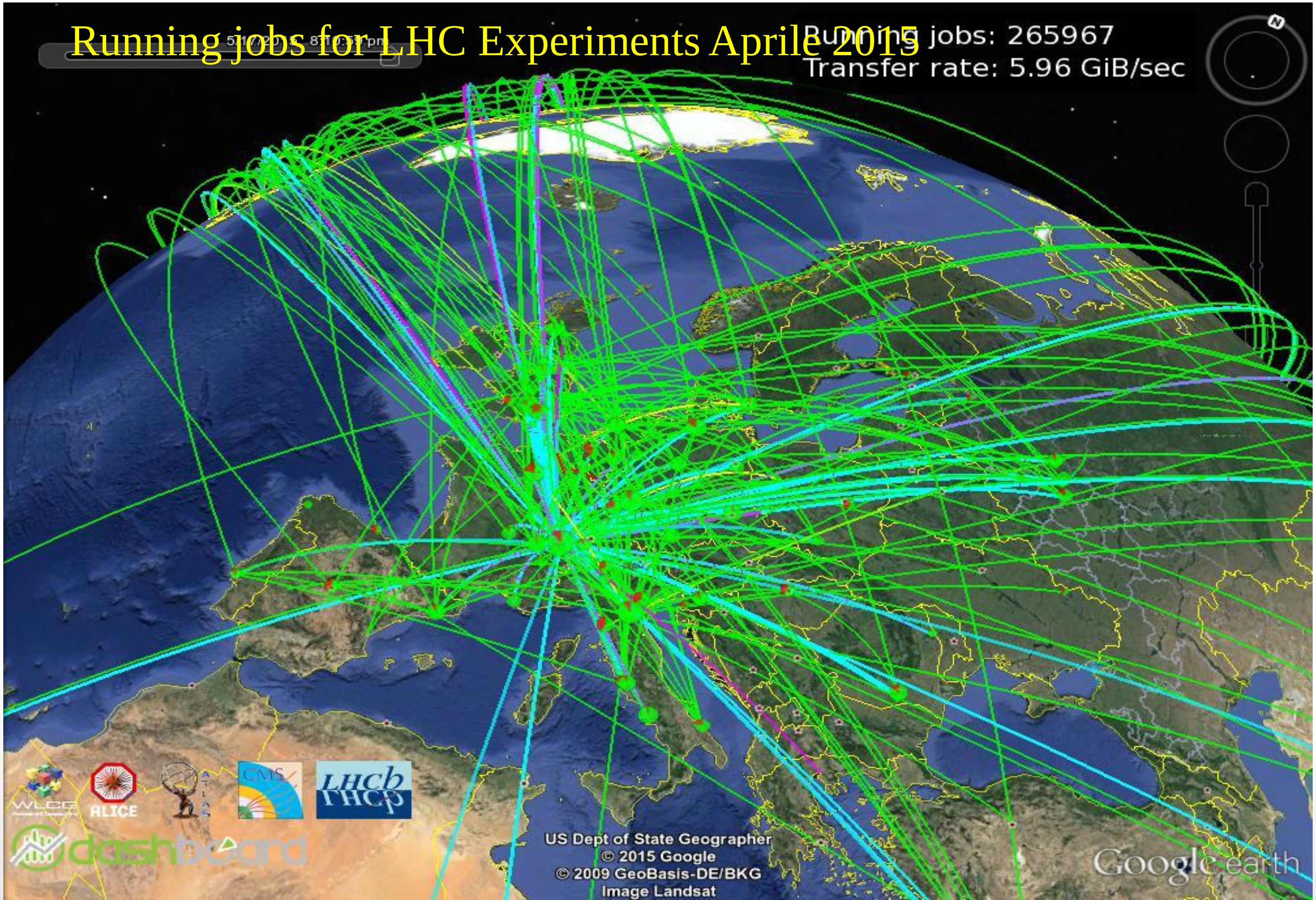
☆ Tier-0 ☆ Tier-1 ☆ Tier-2

Nearly 170 sites in 40 Counties:
~500.000 cores
~1000 PB storage (400 disk + 600 Tape)
~ 2M jobs/day
in 2017

Half of the resources are sitting in Tier-1

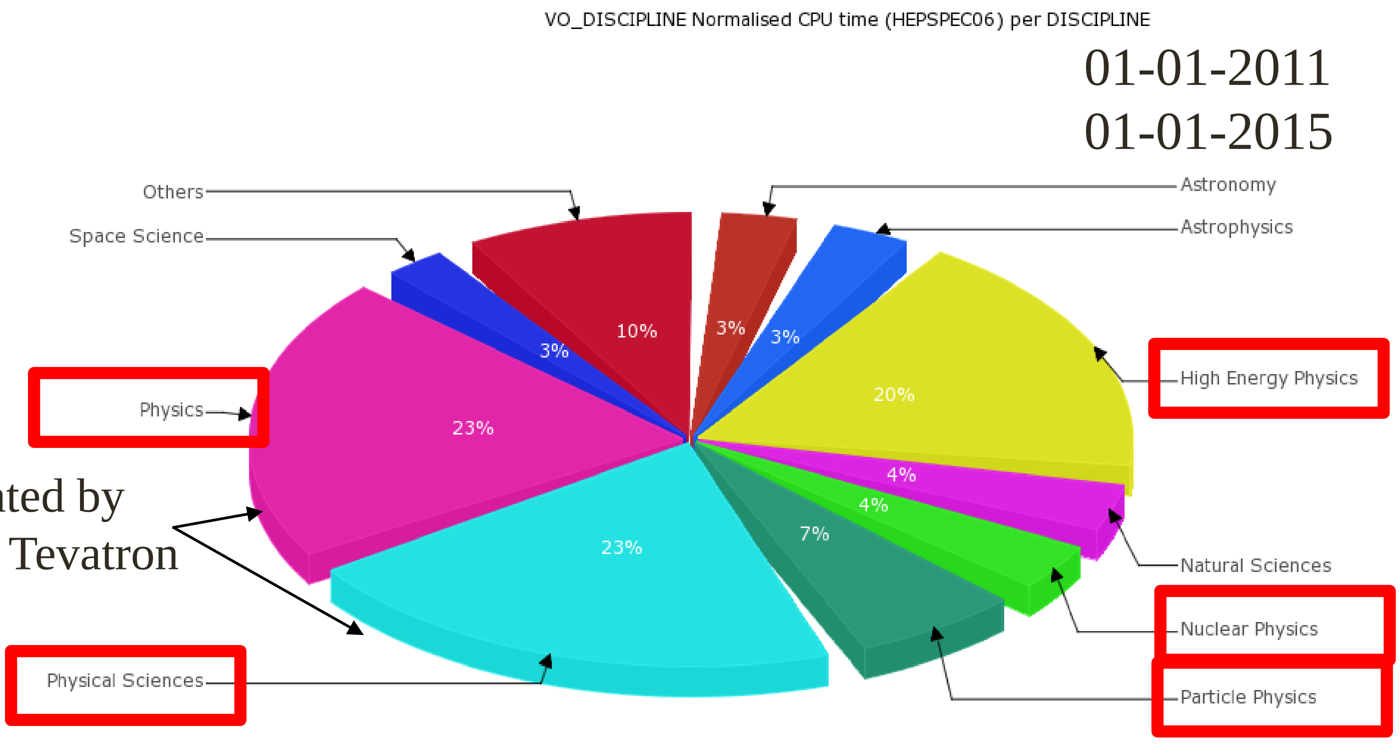
The GRID

Besides the computing centers the infrastructure rely on network which has modified the major experiments computer models



The Users

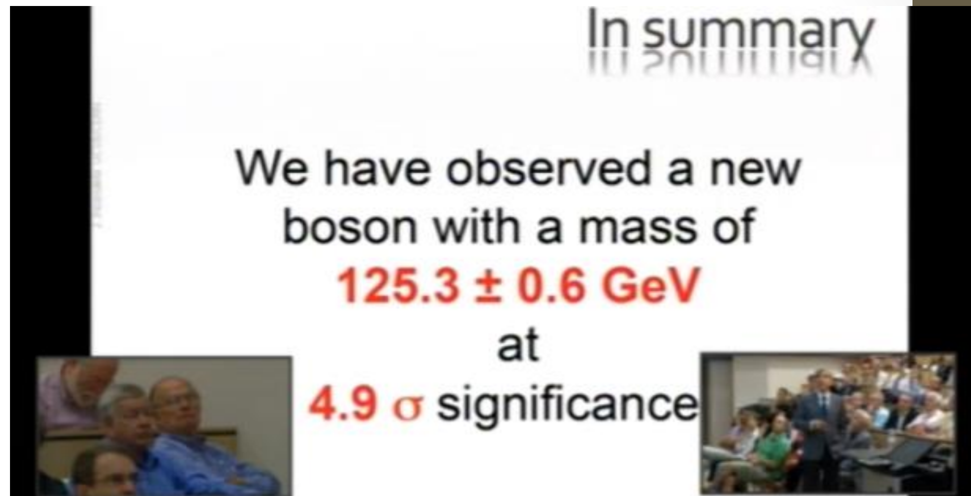
This infrastructure has served several disciplines but mainly high energy physics (> 75%)

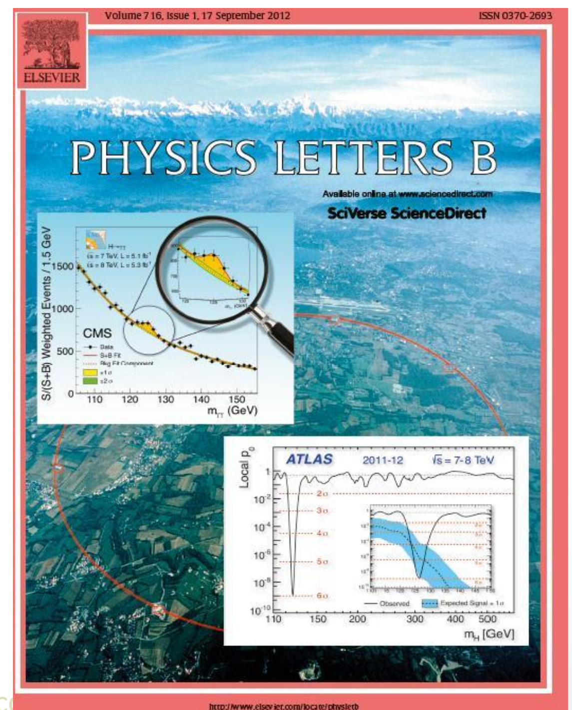


Form EGI accounting portal

A successful GRID story

On 4 July 2012 both of the CERN experiments ATLAS and CMS announced they had independently made the same discovery

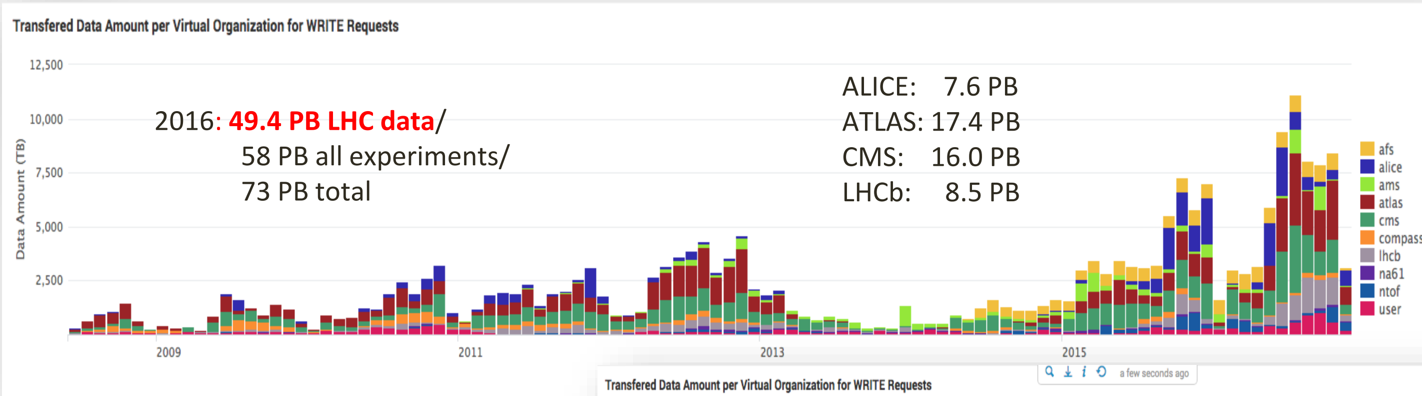


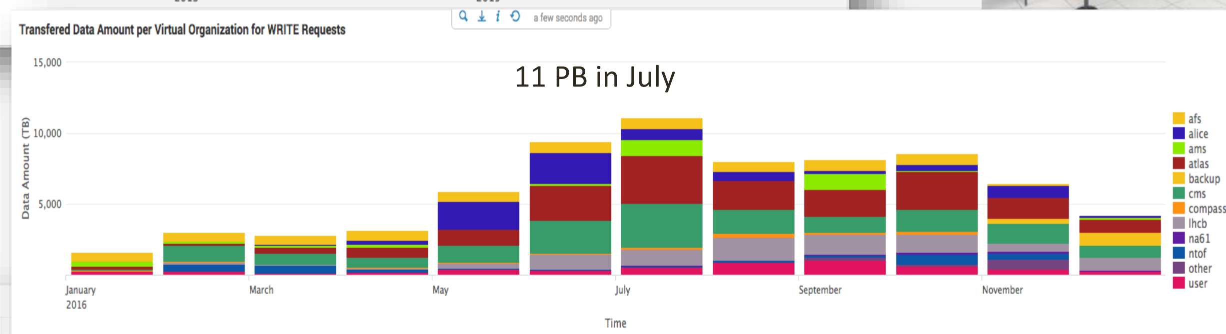


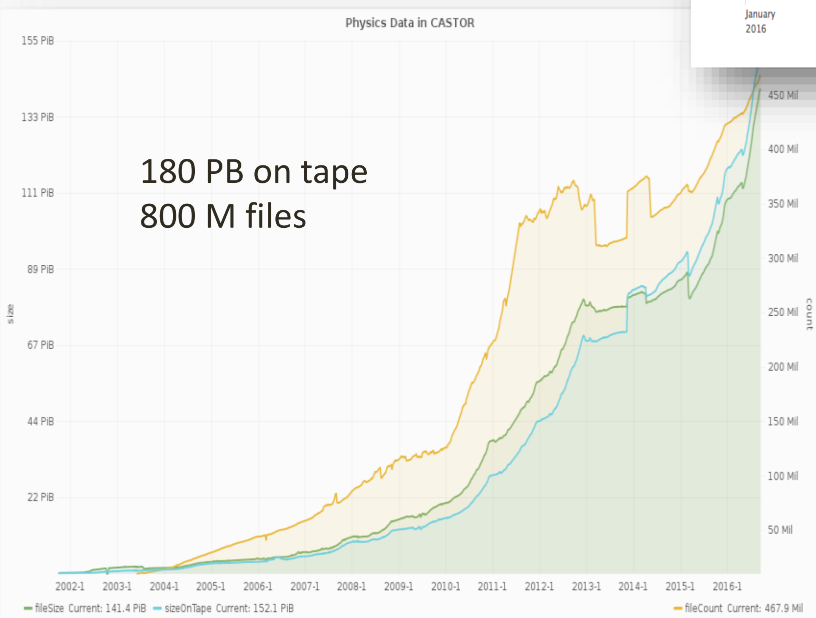
A successful GRID story lasting an year

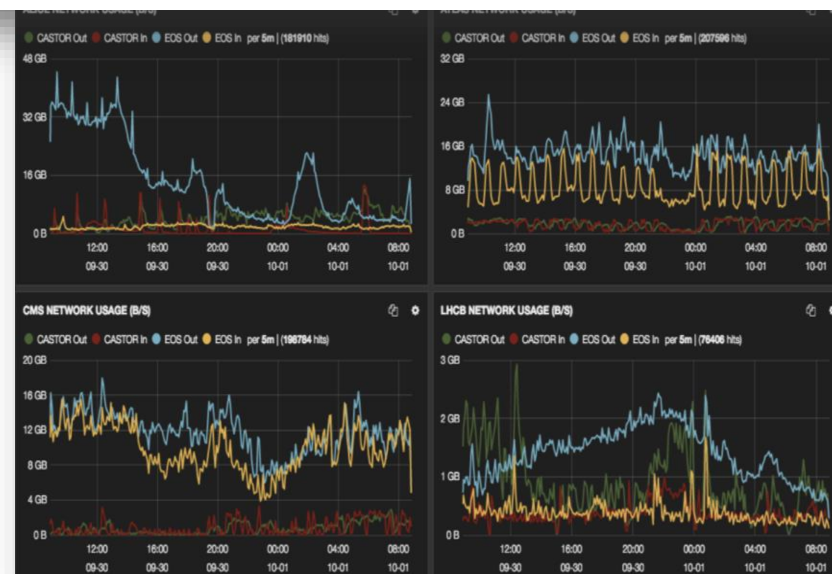
On 14 March 2013 CERN confirmed that:
"CMS and ATLAS have compared a number of options for the spin-parity of this particle, and these all prefer no spin and positive parity [two fundamental criteria of a Higgs boson consistent with the Standard Model]. This, coupled with the measured interactions of the new particle with other particles, strongly indicates that it is a Higgs boson." (wikipedia)

Data in 2016 - updated



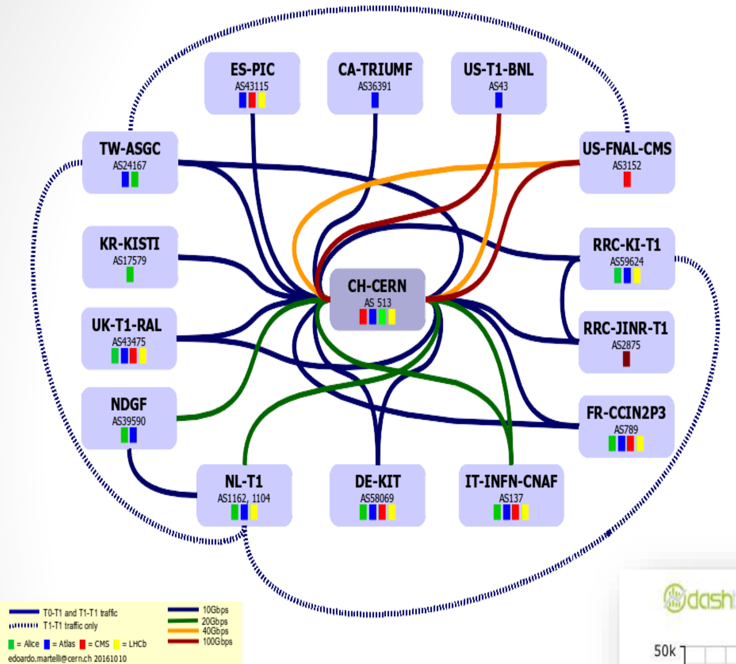


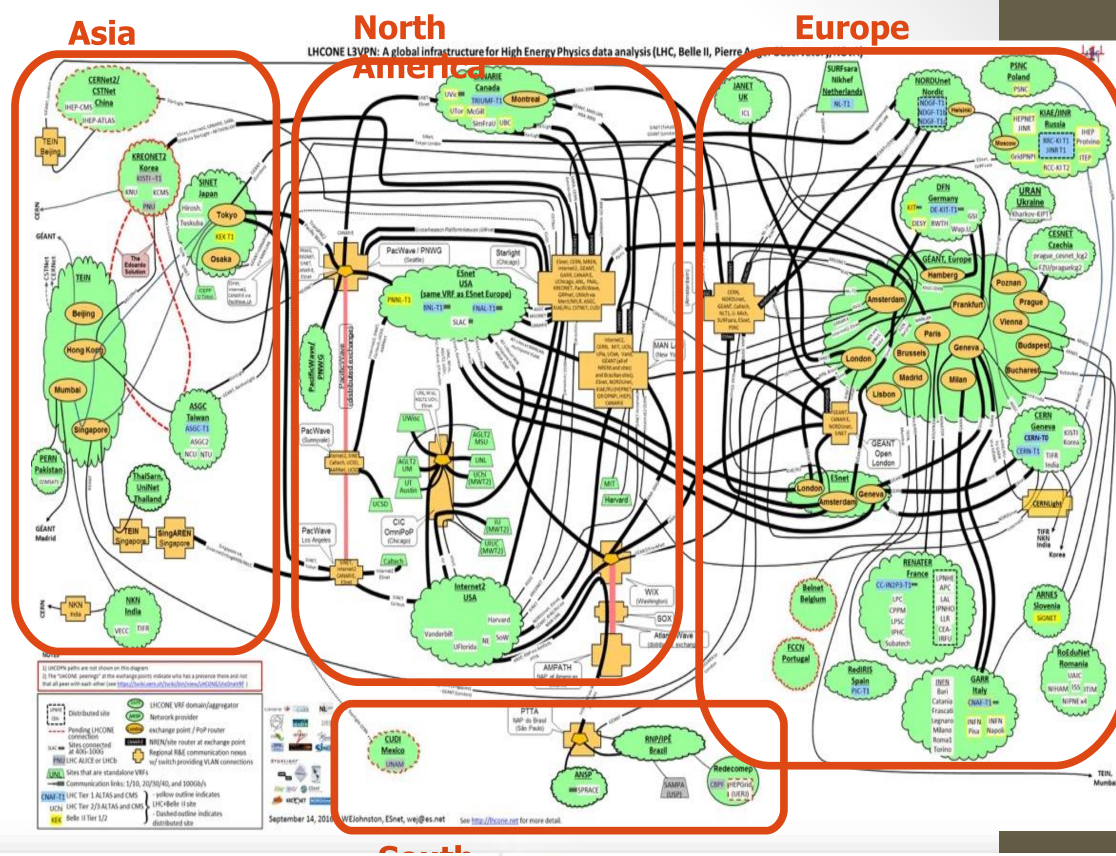


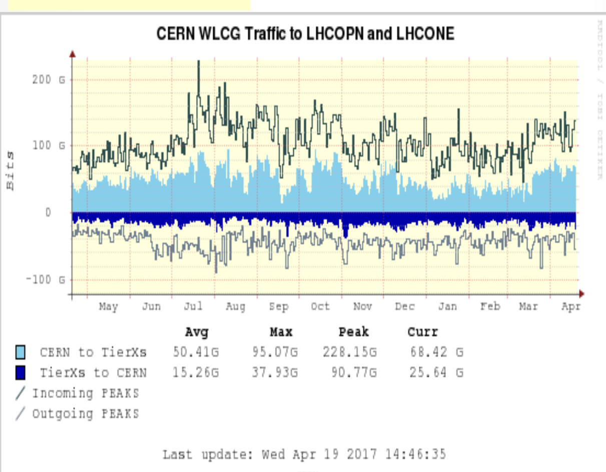


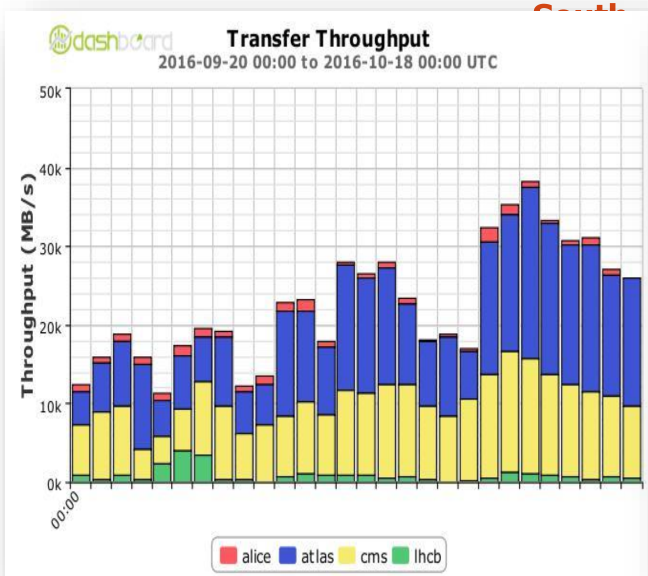
Data transfers

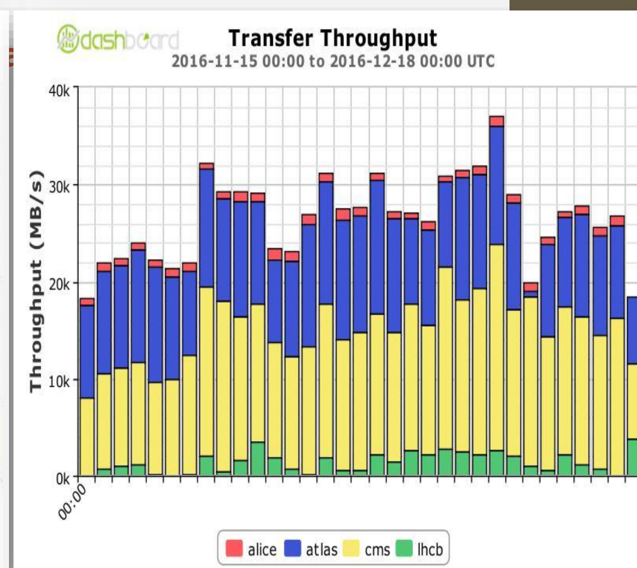
LHCOPN



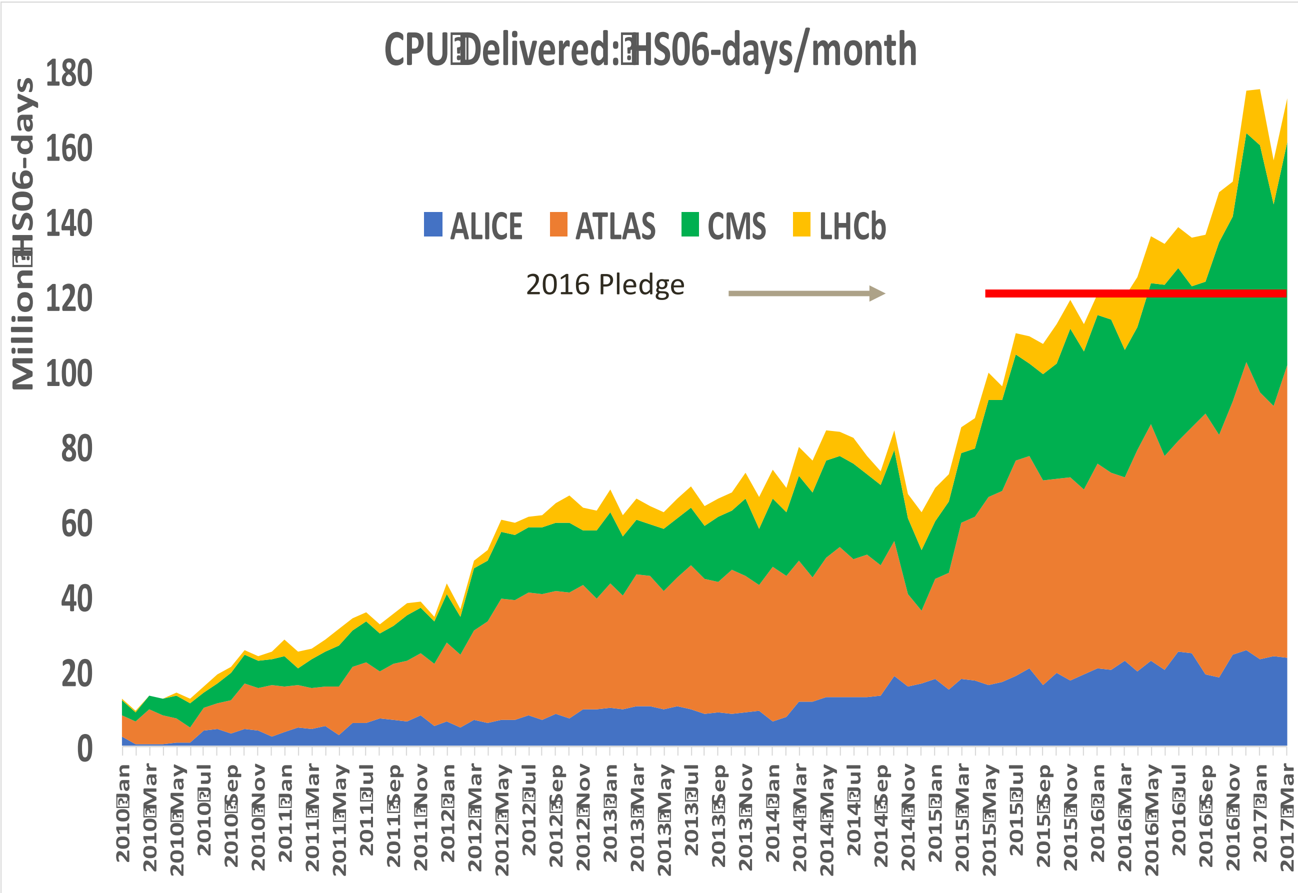








CPU Delivered



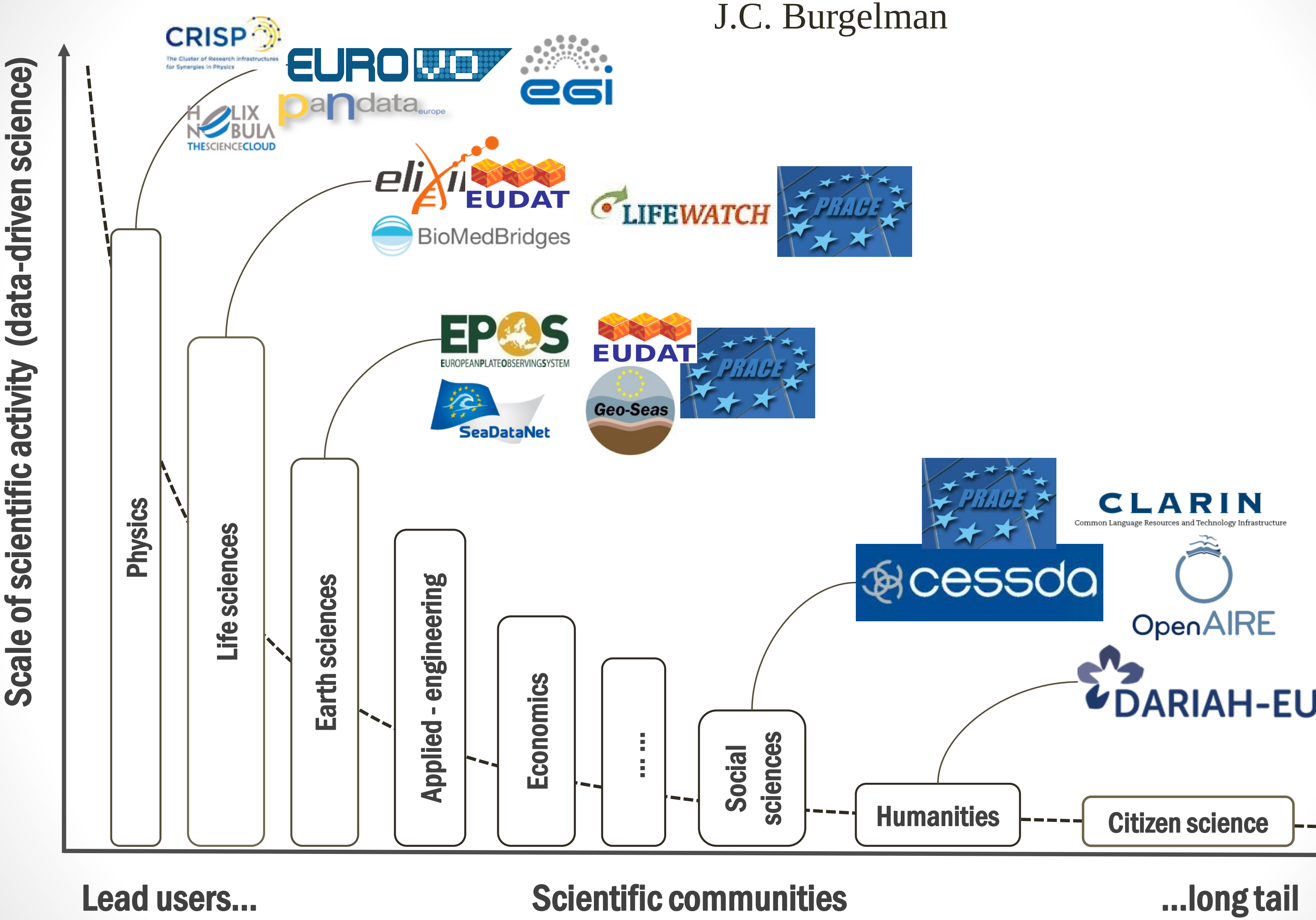
New peak: ~180 M HS06-days/month

~ 600 k cores continuous

The European Scenario

European Computing Landscape

J.C. Burgelman



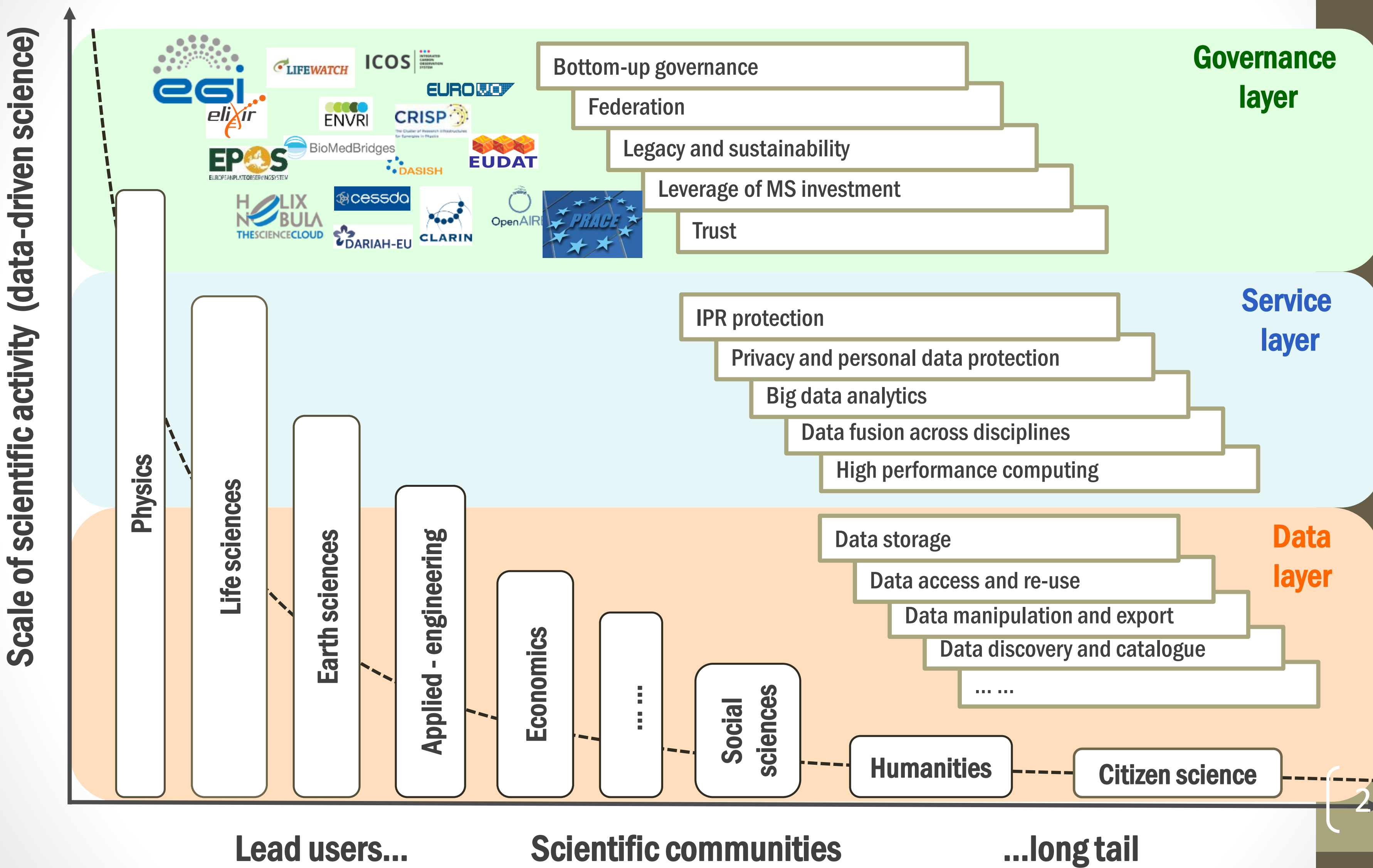
European Computing e-infrastructures

EGI is a federated e-Infrastructure set up to provide advanced computing services for research and innovation.
The EGI e-infrastructure is publicly-funded and comprises over 300 data centres and cloud providers spread across Europe and worldwide. The federation is coordinated by the EGI Foundation (also known as EGI.eu)

PRACE Partnership for Advanced Computing in Europe, an international not-for-profit association with 24 member countries. A pan-European supercomputing infrastructure, providing access to computing and data management resources and services for large-scale scientific and engineering applications at the highest performance level.

EUDAT Collaborative Data Infrastructure consists of a European e-infrastructure of integrated data services and resources to support research.

European Computing Landscape Evolution



Eureopean Cloud Initiative

19 April 2016 Blueprint of EC

European Open Science Cloud (EOSC)

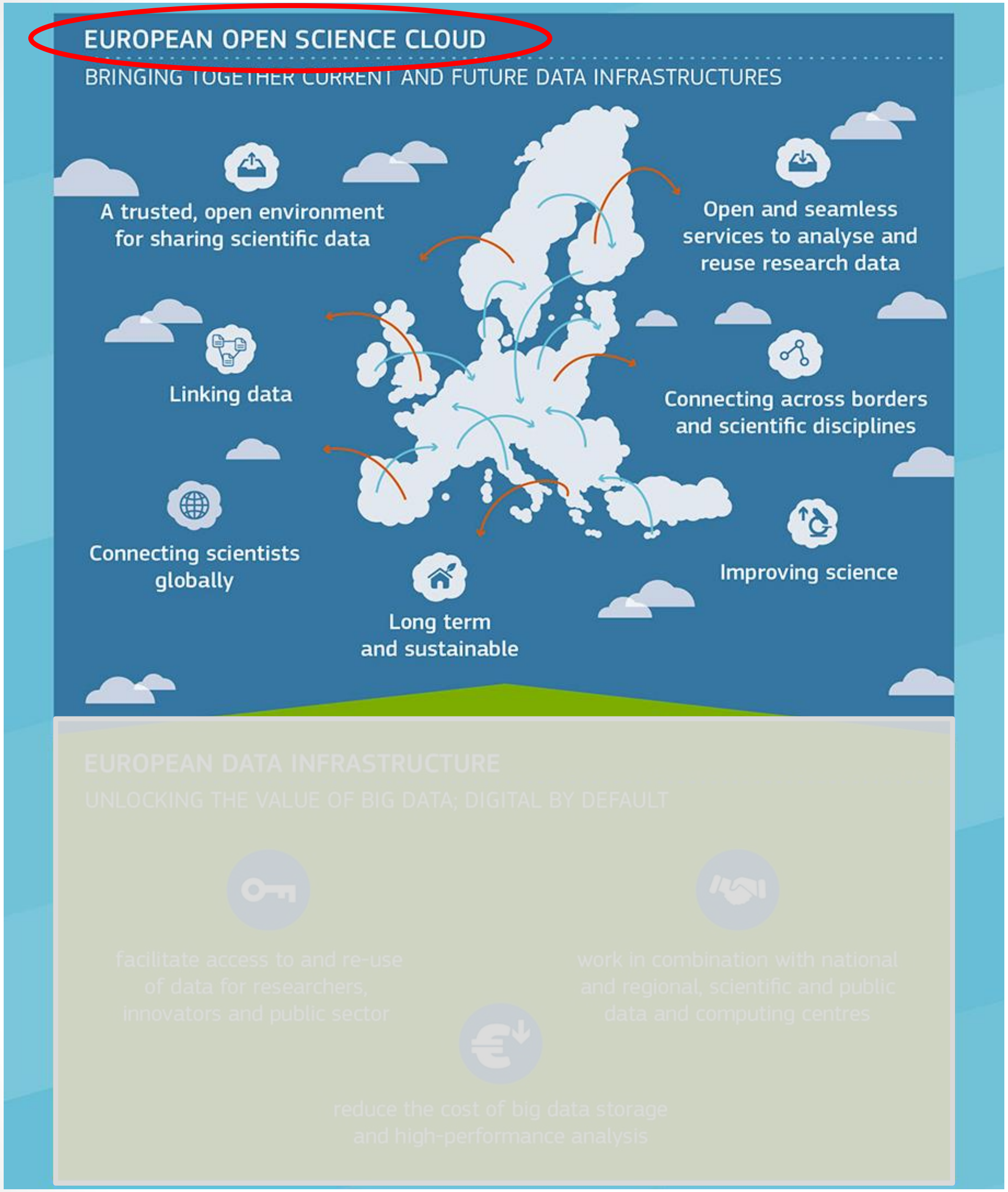
Carlos Moedas – Commissioner for Research, Science and Innovation

Submitted by alim on 18 Sep 2015

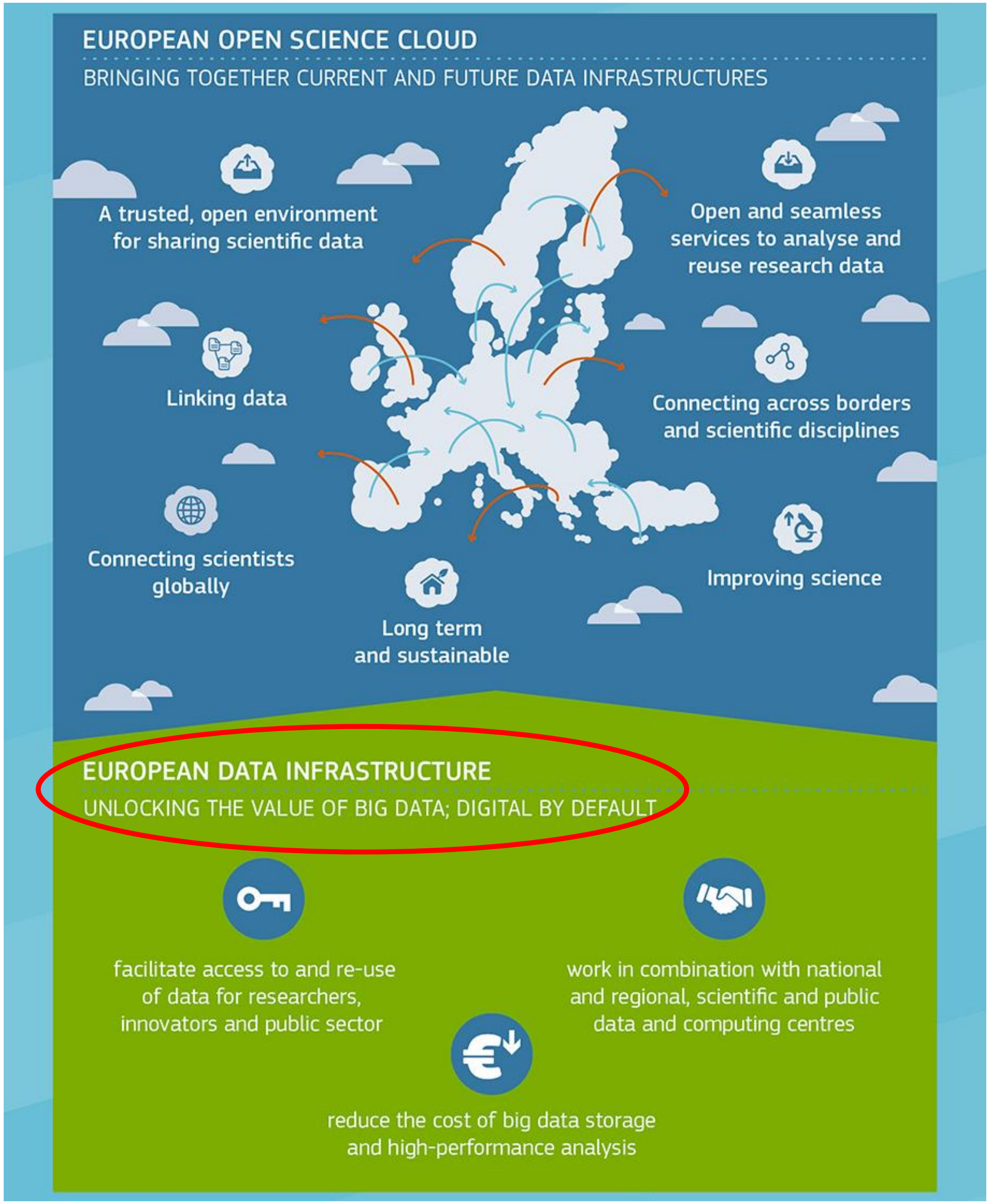
European Commission - Speech - [Check Against Delivery]

First, we are preparing a call for European Science Cloud Project in order to identify the possibility of creating a cloud for our scientists. We need more open access to research results and the underlying data. Open access publication is already a requirement under Horizon 2020, but we now need to look seriously at open data.

Launched directly by Commission
Formed an High Level Expert Group
October 11 released a first report
HLEG Report



H2020 call Infradev-04-2016: Proposal EOSCPilot on European Open Science Cloud for Research


EUROPEAN OPEN SCIENCE CLOUD
BRINGING TOGETHER CURRENT AND FUTURE DATA INFRASTRUCTURES
A trusted, open environment for sharing scientific data
Open and seamless services to analyse and reuse research data
Linking data
Connecting across borders and scientific disciplines
Connecting scientists globally
Improving science
Long term and sustainable
EUROPEAN DATA INFRASTRUCTURE
UNLOCKING THE VALUE OF BIG DATA; DIGITAL BY DEFAULT
facilitate access to and re-use of data for researchers, innovators and public sector
work in combination with national and regional, scientific and public data and computing centres
reduce the cost of big data storage and high-performance analysis

European Data Infrastructure

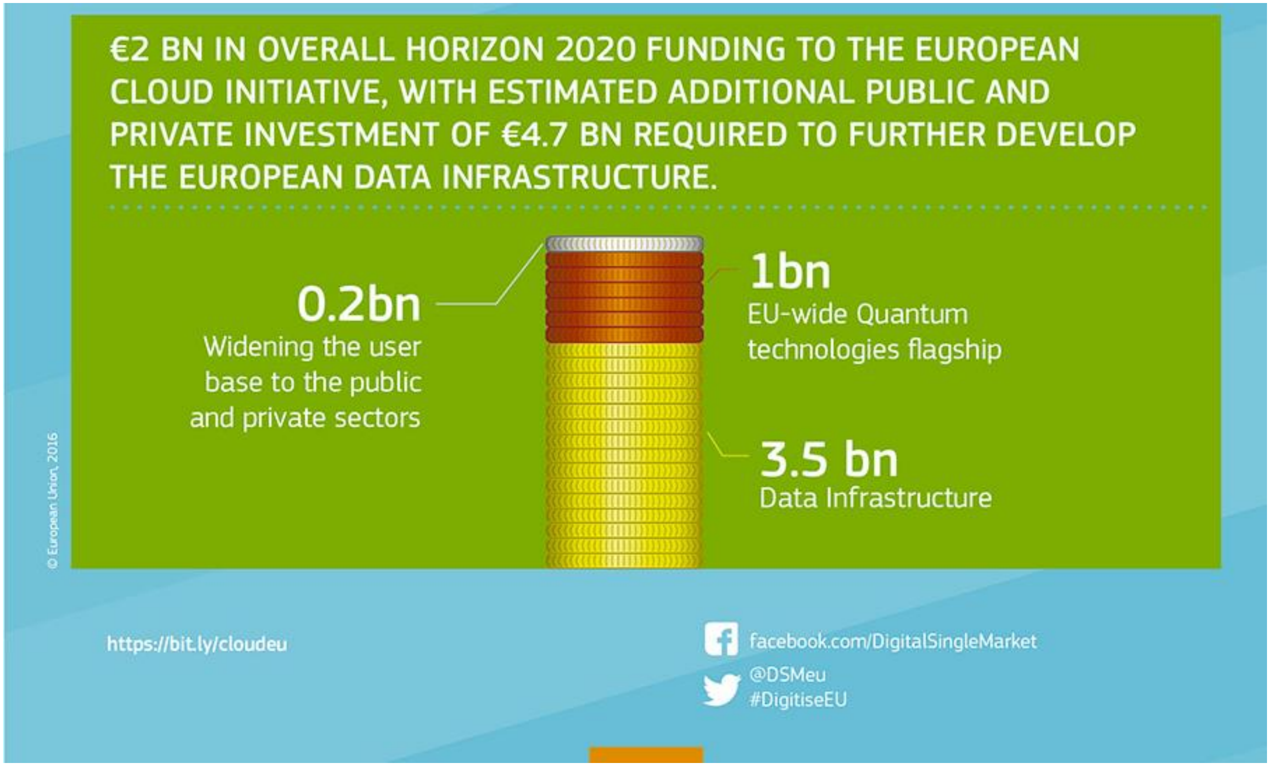
Pilot project
***Important Project of Common European Interest* IPCEI**

IPCEI *on* ***High Performance Computing and Big Data Enabled Applications***

1. **European exa-scale technology**
   prove the capacity of the European industry to answer the challenges of building an exa-scale machine by 2023 via a prototype to be ready by 2020.

2. **Large test beds and applications**
   Establish Centers of Excellence, starting from research, to develop and test HPC-enabled and big data based applications in specific and strategic sectors at regional, national and pan-European scale;
   Deploy application test beds on:
   Personalized Medicine, Smart Space, Industry 4.0 and Smart Manufacturing, New advanced Materials,Fintech,
   Smart Agrifood and Smart City Applications.

European Cloud Initiative Business Model



Declaration
Cooperation Framework on High Performance Computing

Bundesrepublik Deutschland

and

República Portuguesa

and

République française

and

Reino de España

and

Repubblica Italiana

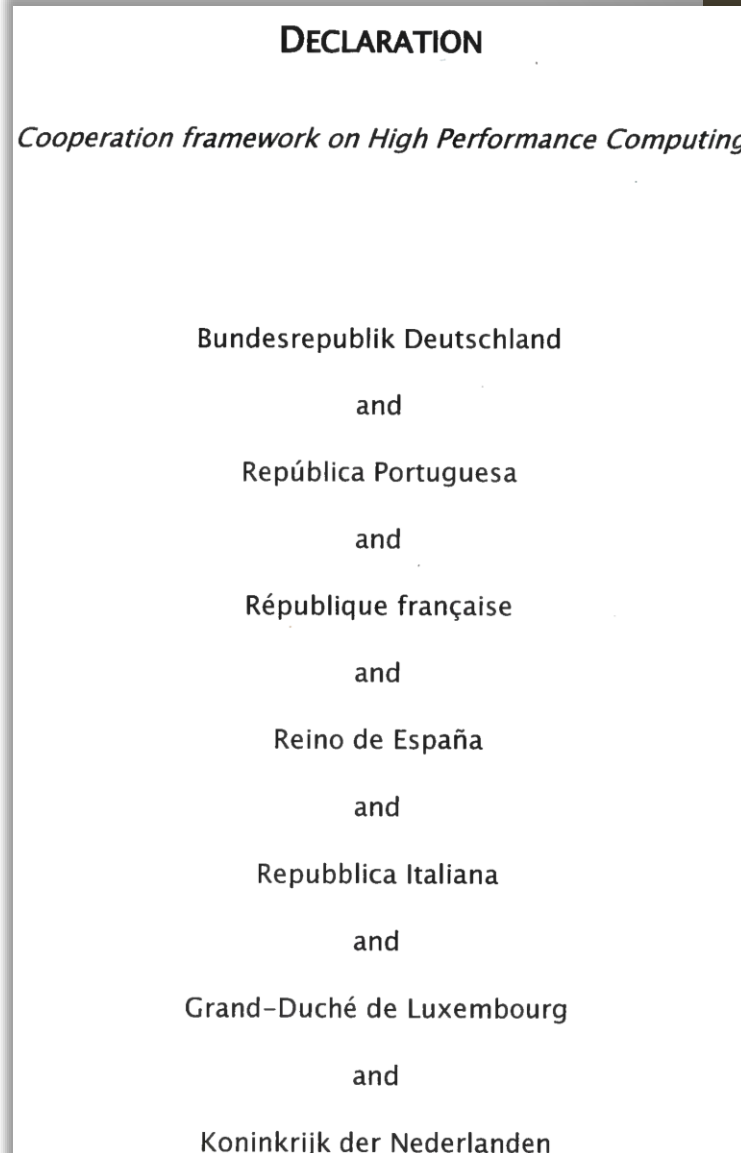
and

Grand-Duché de Luxembourg

and

Koninkrijk der Nederlanden

Agree to work together towards making available across EU an integrated world class computing (HPC) infrastructure which in combination with European data and network infrastructures would upraise Europe Scientific capabilities and industrial competitiveness.



DECLARATION

Cooperation framework on High Performance Computing

Bundesrepublik Deutschland

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Grand-Duché de Luxembourg

and

Koninkrijk der Nederlanden

Member states

- Agree to work towards the establishment of a cooperation framework – EuroHPC- for acquiring and deploying an integrated exascale supercomputer

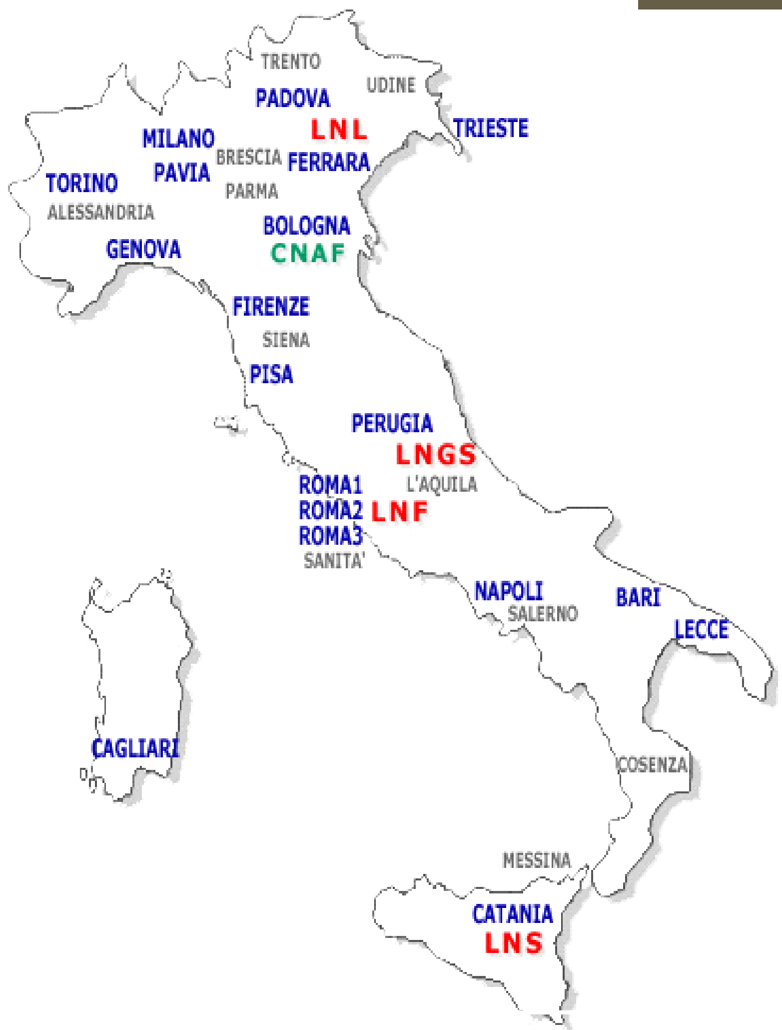
- Agree to work together and with EC to prepare by the end of 2017 a roadmap to address:
  - Technical requirements and financial resources needed
  - Definition of legal and financial instruments
  - Procurements process for acquisition of 2 world-wide pre-exascale computer in 2019-2020 and 2 exascale computers by 2023
  - Development of high quality competitive European technology and its optimization through co-design approach
  - Development of test-beds for HPC and big data applications for scientific, public administration and industrial purposes

- Agree to enable the development of application and services for example those proposed in the IPCEI

Italian infrastructure (INFN)

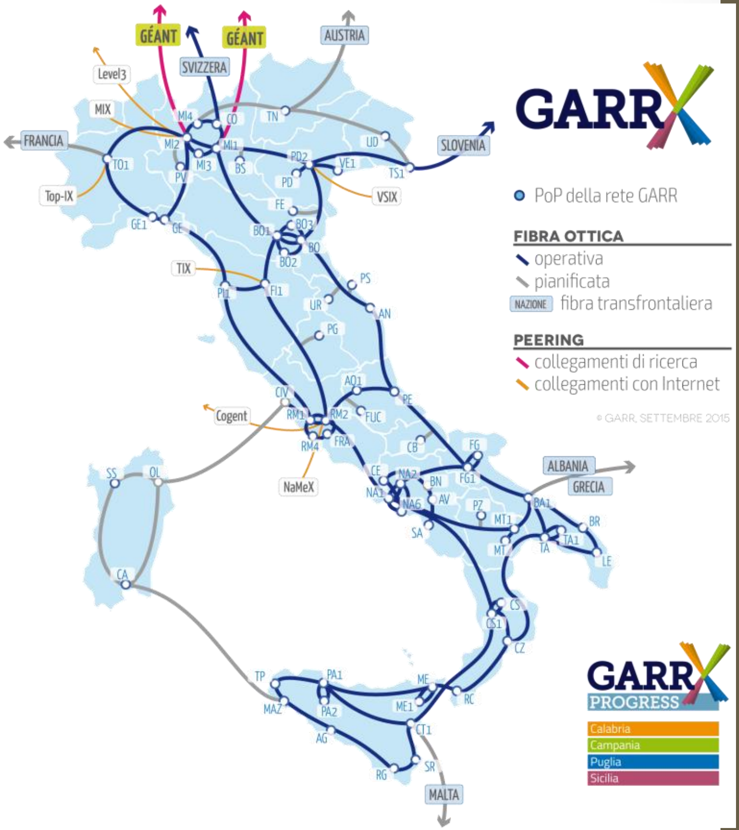
L'Istituto Nazionale di Fisica Nucleare

The National Institute for Nuclear Physics (INFN) is the Italian research agency dedicated to the study of the fundamental constituents of matter and the laws that govern them, under the supervision of the Ministry of Education, Universities and Research (MIUR). It conducts theoretical and experimental research in the fields of subnuclear, nuclear and astroparticle physics.



The Italian Network for Research, Education …

- 100 Universities, Conservatories and art Academies
- 350 Research Institutes and Laboratories
- 60 Biomedical Research Institutes
- 65 Libraries, Museum and Cultural Institutions
- More than 300 schools



MINISTERO DELL'ISTRUZIONE DELL'UNIVERSITA' E DELLA RICERCA

Ministero della Salute

Ministero dello Sviluppo Economico

Ministero delle politiche agricole alimentari e forestali

MiBAC Ministero dei beni e delle attività culturali e del turismo

Current INFN e-Infrastructure

Network provided by GARR
- All Tiers updating to 100 Gbps

1 Tier-1 hosting
- four LHC experiments
- Astro-particle experiments
- Any other HEP experiment that need tape and/or large resources

10 Tier-2: large centers are multi-disciplinary (~half)

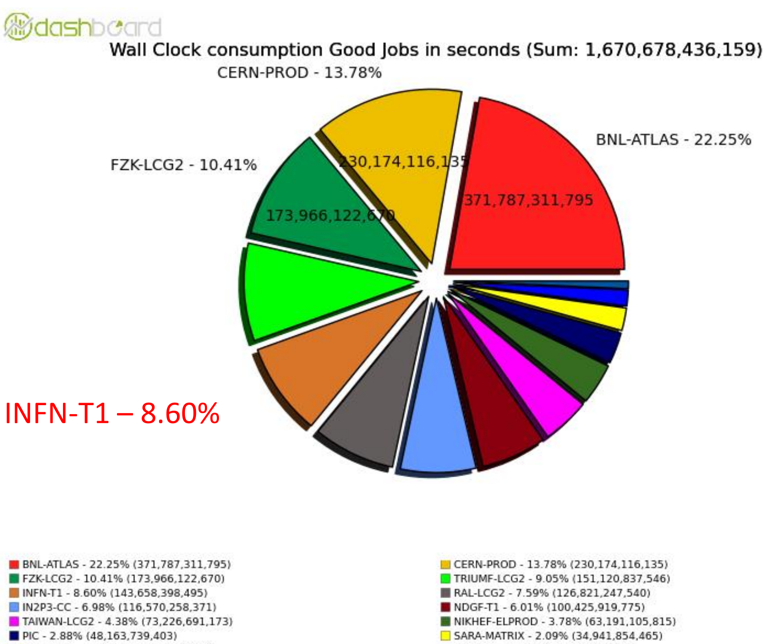
	CPU(KHS06)	Disk(TB)	Tape(TB)
WLCG	5142	396,000	590,000
INFN	439	37,180	57,000
% INFN	9	9	10

The INFN Tier1 @ CNAF

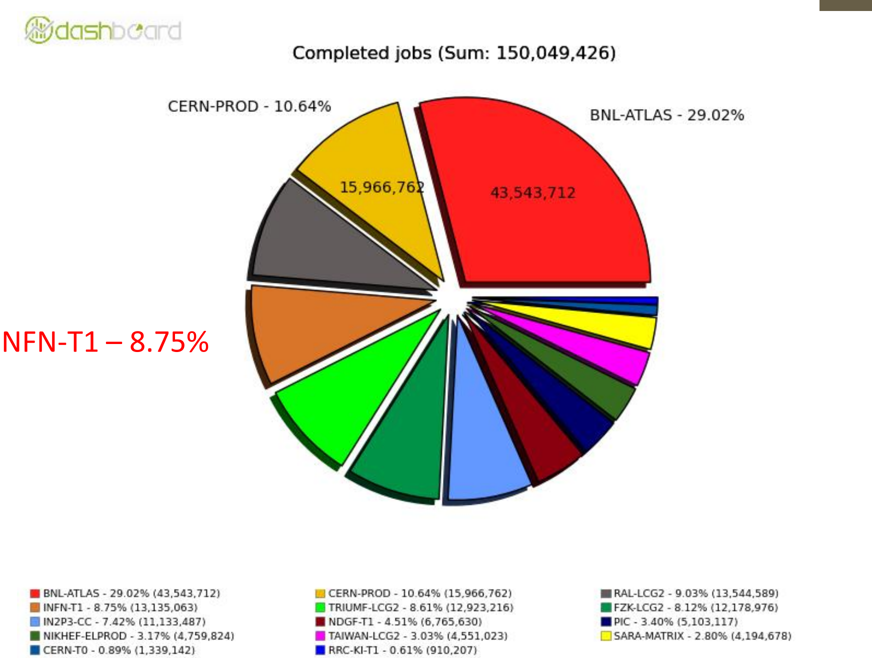
- Main Italian computing centre for LHC experiments and several others:
  - Particles: Kloe, LHCf, Babar, CDF, Belle2
  - Astroparticles: ARGO, AMS, PAMELA, MAGIC, Auger, Fermi/GLAST, Xenon ….
  - Neutrino: Icarus, Borexino, Gerda
  - Gravitation: Virgo

- Available resources: ~250 kHS06, ~20 PB of disk, ~57 PB of tape

Typical T1 contribution to LHC activities (ATLAS)



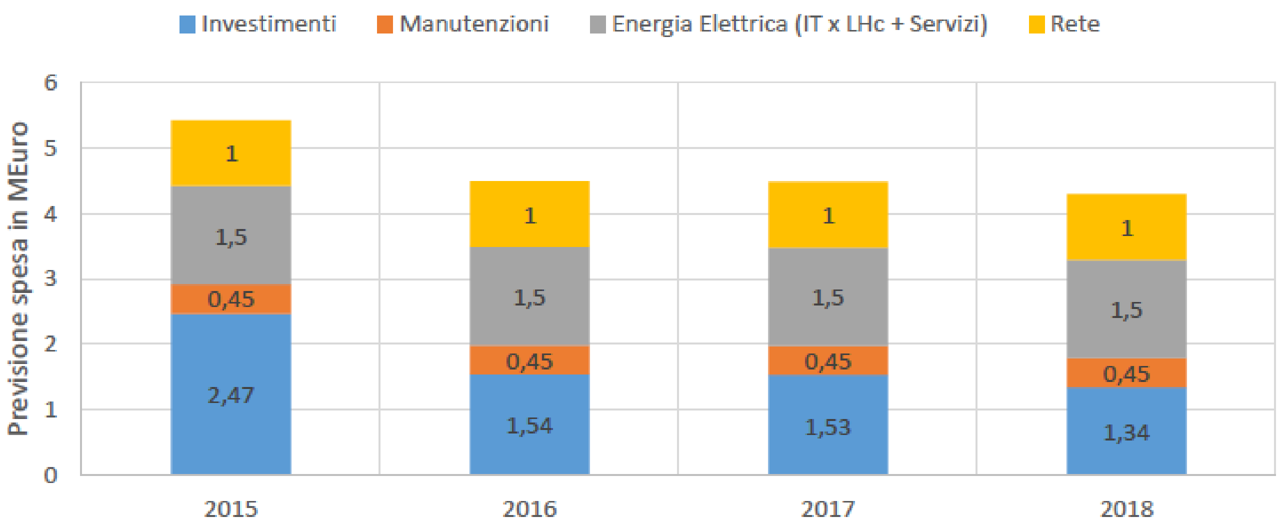
INFN-T1 – 8.60%



INFN-T1 – 8.75%

The Business model

- Hardware costs: ≈5 M€/year
- Running costs: ≈ 4 M€/year (wo personnel)
- Personnel: ≈ 50 FTE/year



Tier1 - CNAF

- Indirect/direct costs for software development and maintenance → INDIGO DATA CLOUD

Computing Funds are coming from "external" sources, most important examples of the latest years:

- Italian minister, *High performance data network*,

- Projects with National and Regional funds
  - RECAS
  - PRISMA and OCP for Public administration

- EC H2020 projects
  - Indigo-DataCloud
  - EGI-Engage
  - European Open Science Cloud Pilot, EOSCPilot

- In 2017 INFN is participating to:
  - EOSC-Hub the second part of EOSCPilot
  - eXtremeDataCloud, still related to EOSCPilot
  - DEEP-HybridDataCloud, still related to EOSCPilot

The next steps for distributed computing

INDIGO - DataCloud

1. Ease of access and use for small and big collaborations alike.
2. Software and economic sustainability.
3. Robustness (no single points of failure).
4. Modular, scalable architecture.
5. Open source software, vendor independence, hybrid infrastructures.



INDIGO - DataCloud

Our objective

- The development of an **easy-to-use, Cloud-based open source software platform**, without restrictions on the e-Infrastructure(s) to be accessed (public or commercial, GRID/Cloud/HPC) or its underlying software, **targeted at scientific communities**, addressing current technology gaps linked to specific use cases.
- Wherever possible, we will **exploit existing solutions**, learning, re-using and extending them according to user requirements, and having in mind the expected evolution of technology.

High Performance Computing (HPC)

Towards a digital infrastructure

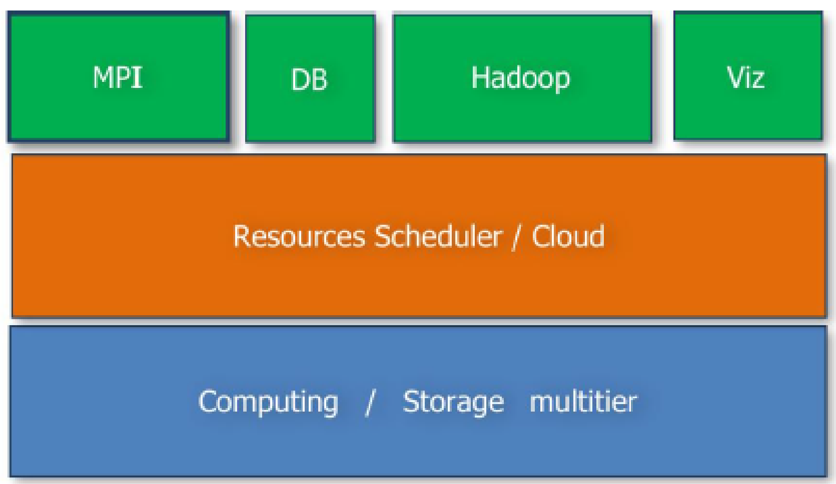
Challenges and treats to create a national research hub

Roadmap

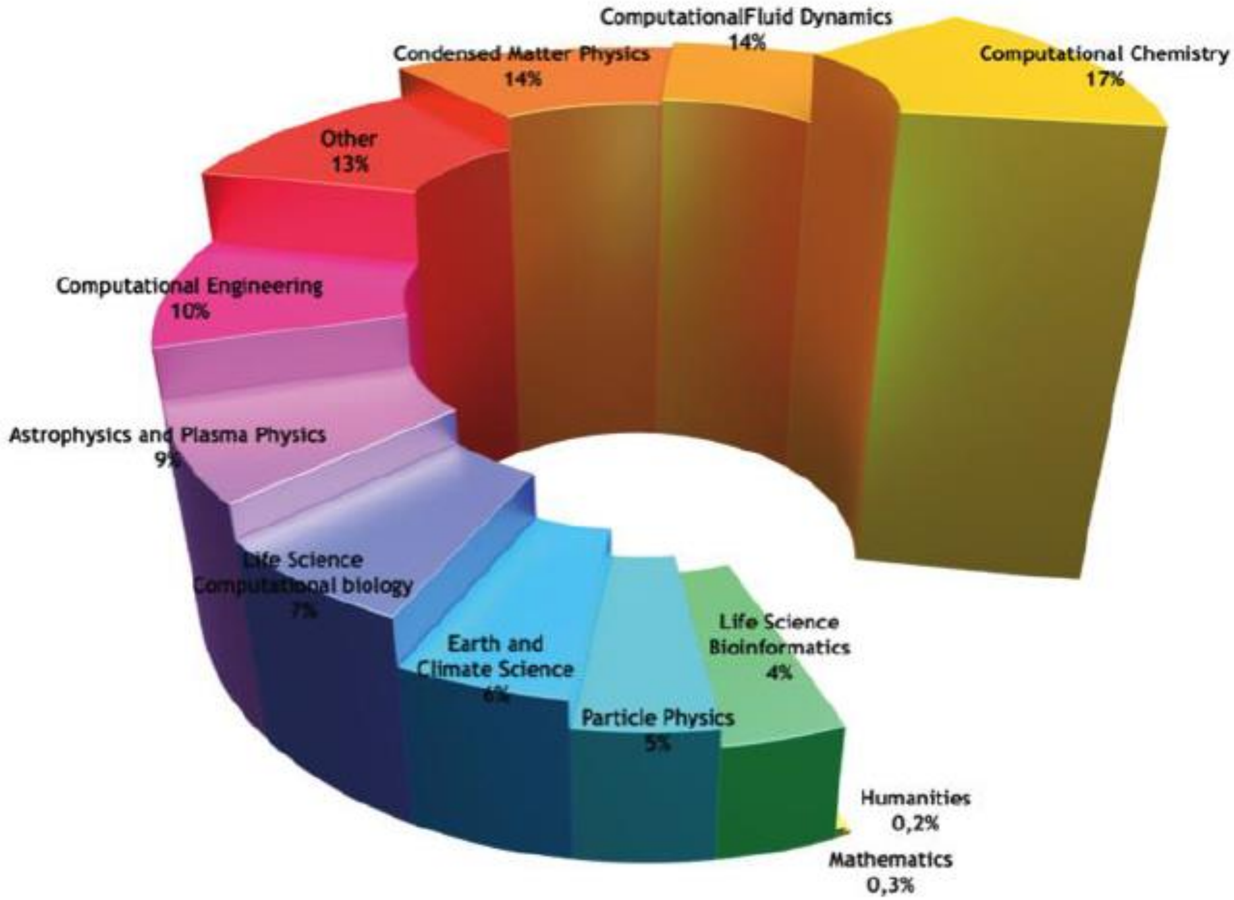
Logical Name	Tier 0 - FERMI (June 2012)	Tier 1 - GALILEO (December 2014)	Big data - PICO (October 2014)
Peak Performance	~ 2 Pflops; ~ 5 PByte	~ 0,5 PFlops	~ 0,3 Pflops; ~ 15 Pbyte

Logical Name	MARCONI (2016 / 2017)	BIG DATA (2016)
Peak Performance	~ 20 Pflops; ~ 15 Pbyte	~1 Pflops; ~ 20 Pbyte

Logical Name	Tier 0 BIG DATA (2019 – 2020)
Peak Performance	< 50 Pflops; < 50 Pbyte on line storage; < 50 Pbyte repository

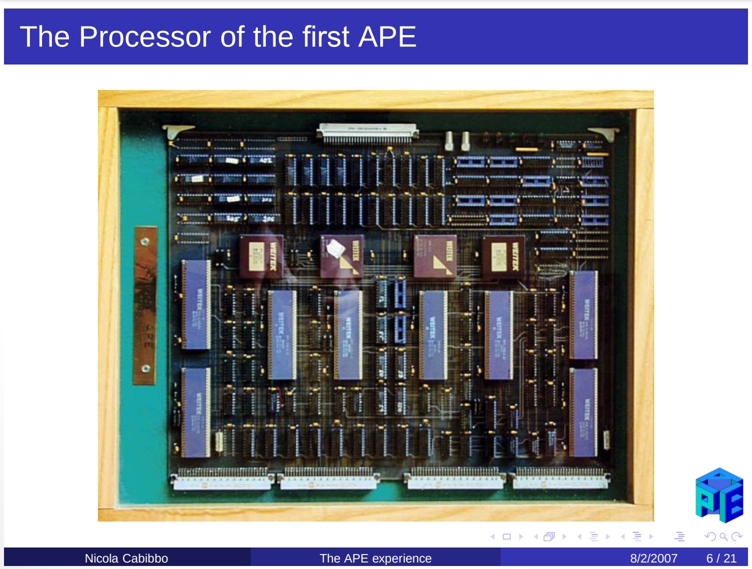


Enabling science – 2015 discipline distribution



HPC, a crumb of history

In 1984 Nicola Cabibbo, Giorgio Parisi and young students participated at a workshop on Lattice Gauge Theory.
The formal conclusions of the workshop were that even thinking to build a computer for Lattice Gauge Theory was insane.
Despite the official conclusions of the meeting, after a few hours of discussion the basic ideas of APE (Array Processor Experiment) were sketched. In the following months it was quickly organized a scientific collaboration led by Nicola Cabibbo and Giorgio Parisi involving INFN of Padua, Pisa and Rome, and the CNAF.



HPC today in Europe and Italy

System Name	Hosting Center	Architecture	Capacity
CURIE	GENCI@CEA	Bull x86	2 PFlop/s
MARCONI	CINECA	Intel Broadwell	13 PFlop/s
HAZEL HEN	HLRS	Cray XC40	7.42 PFlop/s
JUQUEEN	GCS@FZJ	IBM BlueGene/Q	5.87 PFlop/s
MareNostrum	BSC	IBM iDataPlex	1 PFlop/s
Piz Daint	CSCS	Cray XC30	7.8 Pflop/s

HPC has already European dimension

- INFN has an agreement with CINECA renewed every three years
- INFN participates to H2020 HPC project:
  - ExaNeSt, to study network and storage for exa-scale facilities
  - EuroExa, to build a prototype of exa-scale machine with new network

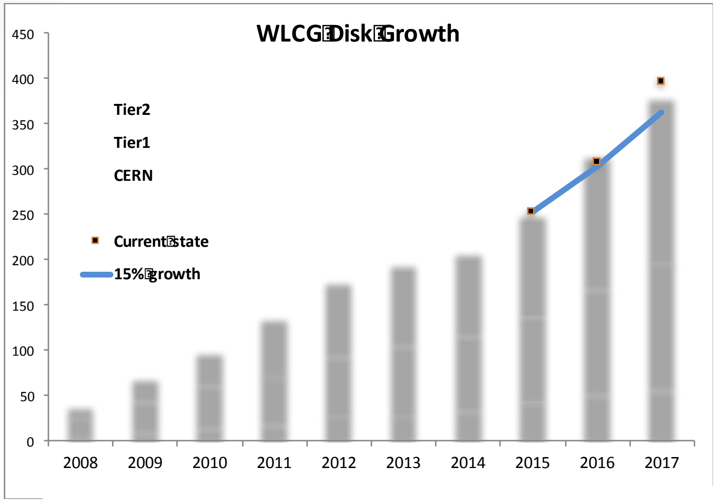
The evolution in the next years

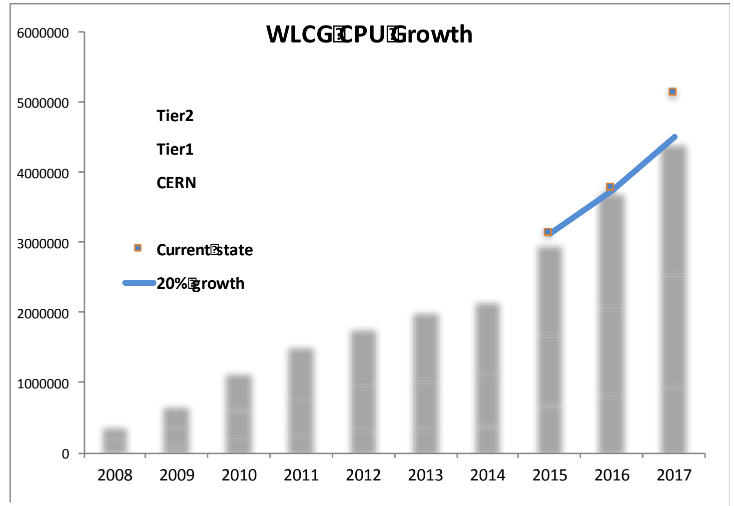
The evolution of scientific computing

The evolution of scientific computing is mainly driven by the necessity to process unprecedented data samples and by the needs from different disciplines (astroparticle, biology, science of materials, medicine, industry etc. etc.)

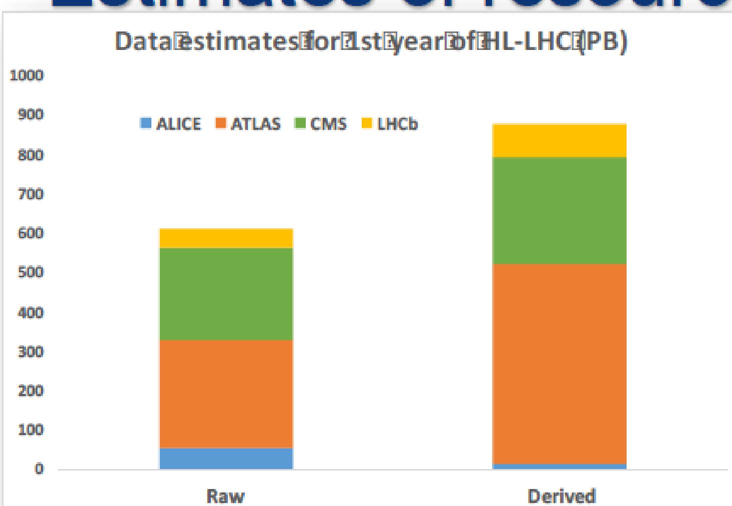
- → New computing models for LHC experiments
- → Fast networking
- → New concepts for e-infrastructures
- → Cloud computing

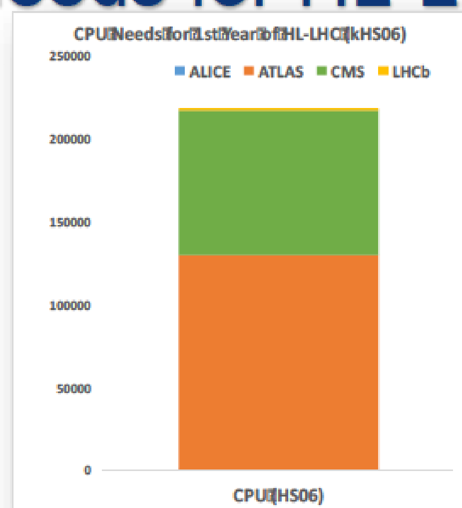
The increase of resources





Estimates of resource needs for HL-LHC

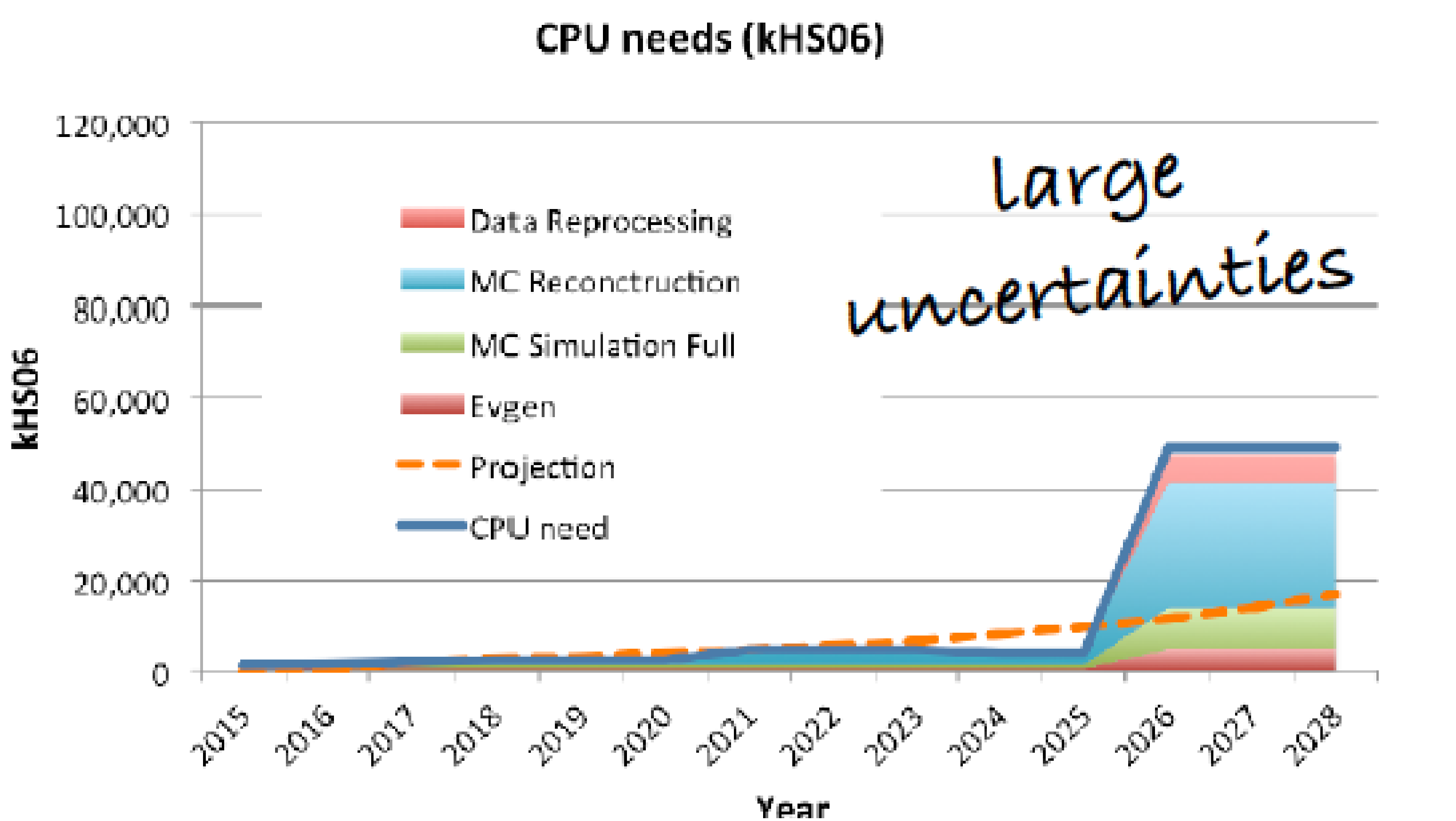




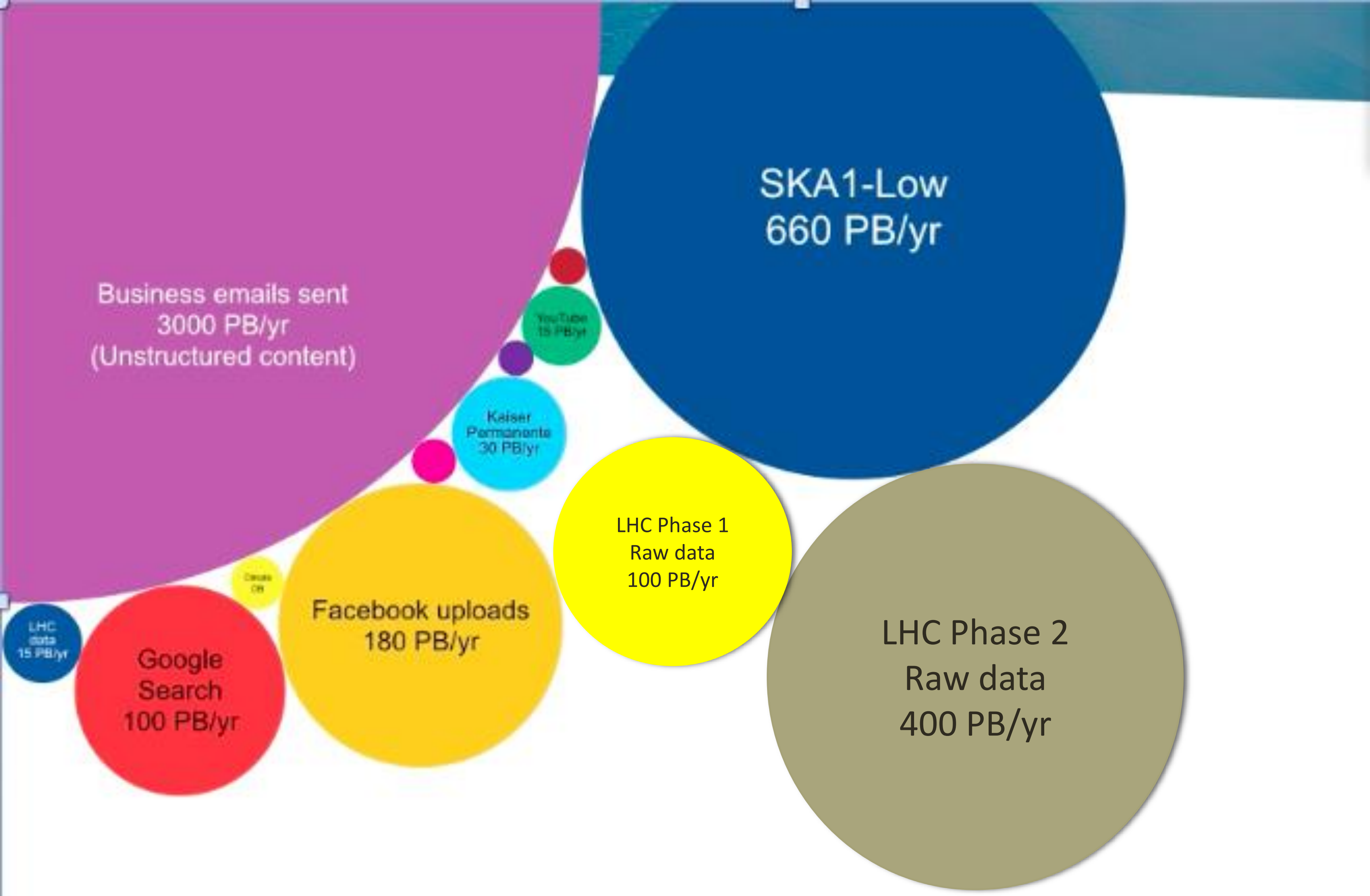
Data:
- Raw 2016: 50 PB → 2027: 600 PB
- Derived (1 copy): 2016: 80 PB → 2027: 900 PB

CPU:
- x60 from 2016

A case study for
Demands in Computing for HL-LHC



Technology at ~20%/year will bring x6-10 in 10-11 years


SKA1-Low
660 PB/yr
Business emails sent
3000 PB/yr
(Unstructured content)
YouTube
15 PB/yr
Kaiser
Permanente
30 PB/yr
LHC Phase 1
Raw data
100 PB/yr
Facebook uploads
180 PB/yr
LHC
data
15 PB/yr
Google
Search
100 PB/yr
LHC Phase 2
Raw data
400 PB/yr

….not only physics …

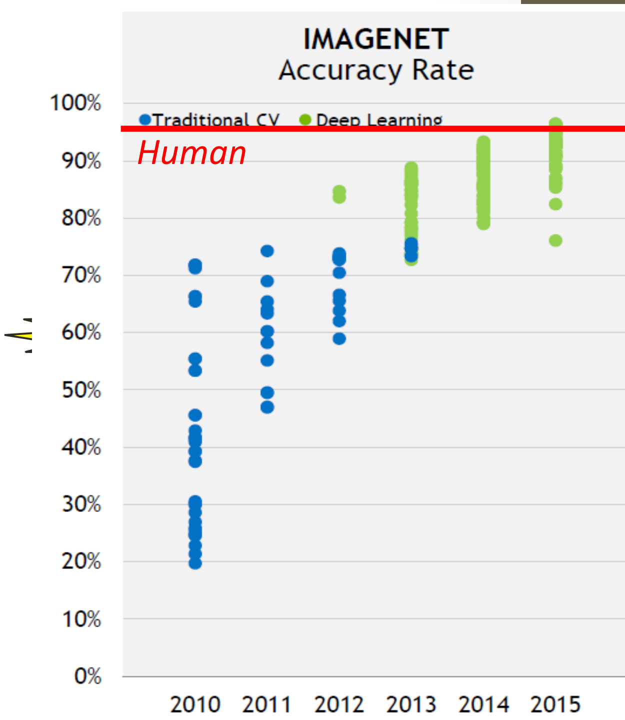
Big data are becoming a key issue in many other disciplines like:

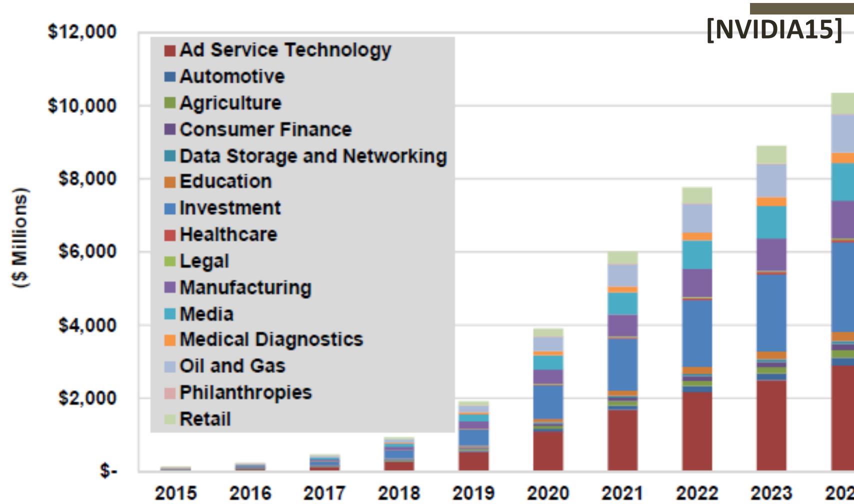
- Public administration
- Industry (mechanics, automotive, ….)
- Medicine and biology
- Materials
- Fintech: banks, insurance companies
- Weather forecast and climate change
- Agricolture
- Space data

Deep Learning

- Why it's a Big Data Problem
  - 1 Exaflop to train a SOA deep network [Baidu]
  - Need fast turnaround time for idea→test→code
  - Unsupervised learning is orders of magnitude more demanding than supervised learning

- Supply chains Pilot
  - **Automatic vision-based quality inspection**

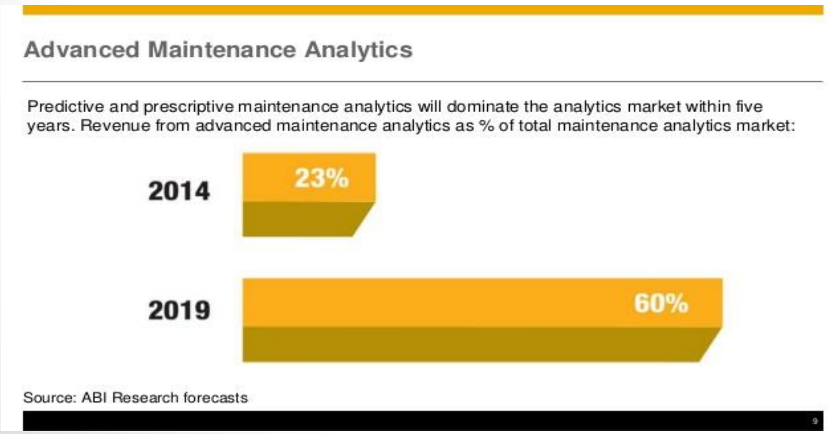


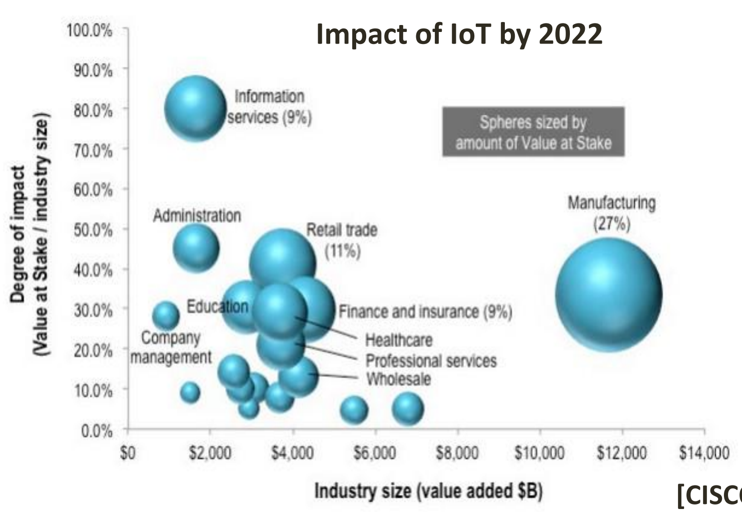


Predictive IoT-Based Analytics

- Why it's a Big Data Problem
  - Huge volume: a A350 aircraft has 6,000 sensors and generates 2.5Tb/day
  - More than 80% of IoT data is not acted on today → dark data [IBM]
  - Advanced Machine Learning on heterogeneous, structured and unstructured knowledge: IoT data, with historical records and logs, social networks graphs, speech, videos, images …

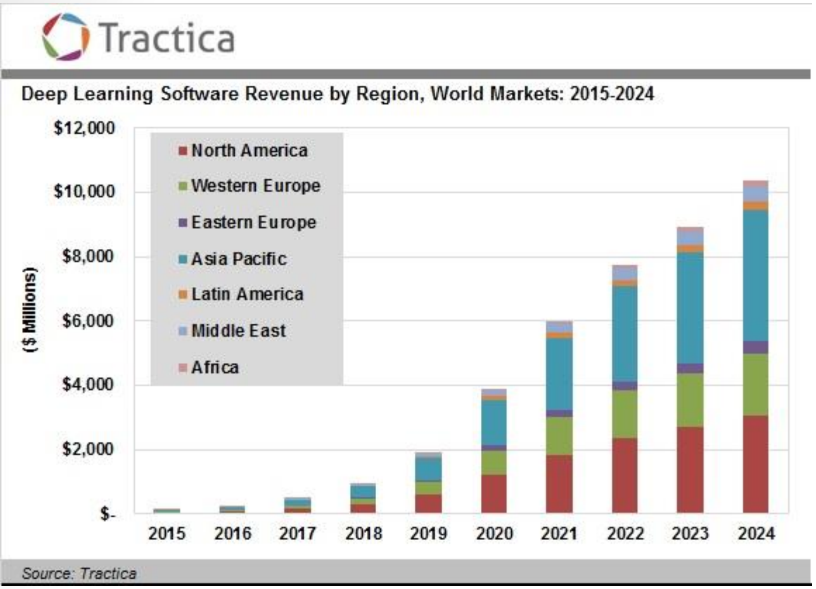
- Supply chains Pilot
  - **Predictive equiment maintenance**



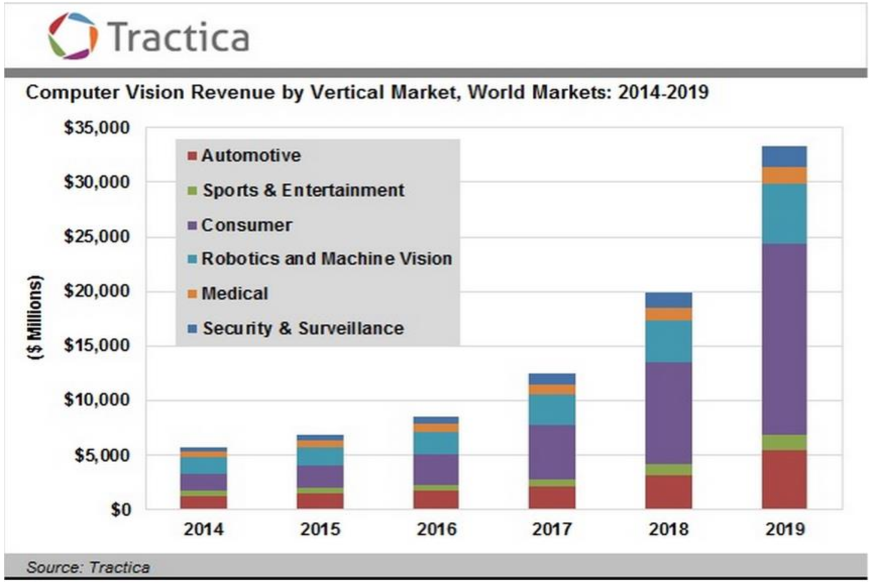


[CISCO15]

Computer Vision and Deep Learning Market



Deep Learning



Computer Vision

The market for **computer vision** technologies will grow from $5.7 billion in 2014 to $33.3 billion by 2019, representing CAGR of 42%

The machine vision market size is estimated to grow from USD 8.08 billion in 2015 to USD 12.49 billion by 2020, at an estimated CAGR of 9.1%.

3D Machine Vision Market Global Forecast to 2020 says, the market is expected to grow at a CAGR of 10.53% during the forecast period between 2015 and 2020

In "**Automated Guided Vehicle Market**", the total market is expected to reach USD 2.81 Billion by 2022, at a CAGR of 10.2%

Big Data for Personalized Medicine

Scientific Objectives

- To collect genomic and clinical data from diseased and healthy patients
- To define best practice for the creation of databases in a standard and exploitable fashion
- To define clear policy for privacy and to create an ethical and transparent program based on consent
- To create reliable correlations between clinical and genomic data
- To exploit genomic and clinical data for patients stratification and clinical trial design

Big Data for Personalized Medicine

Worldwide Situation

- Dozens of projects have been launched worldwide from Asia (China and Japan) to the US through Europe
- 100,000 Genomes Project in UK, announced in July 2013 aimed and completing the sequencing of 100,000 genes by end 2017
- Obama's Precision Medicine Initiative launched in 2015 with the objective of sequencing million patients

Biobanks: constant increase of biological collections:

- end of 2012 about 600 million pieces in USA [1]

Biobanks: global Market:

- Some billion dollars volume [2]
- Technavio report [2] estimates a stable yearly increase of the global market of about 8% in the period 2016–2020, mainly in the nord european area

Evolution of the field due to:

- new technologies for the samples conservation
- new platform to store and analyse the data
- new efficient methods for data analysis

The players:

- public and private companies
- research communities

[1] Monya Baker, "Building better biobanks", Nature 46 (2012), 141–146

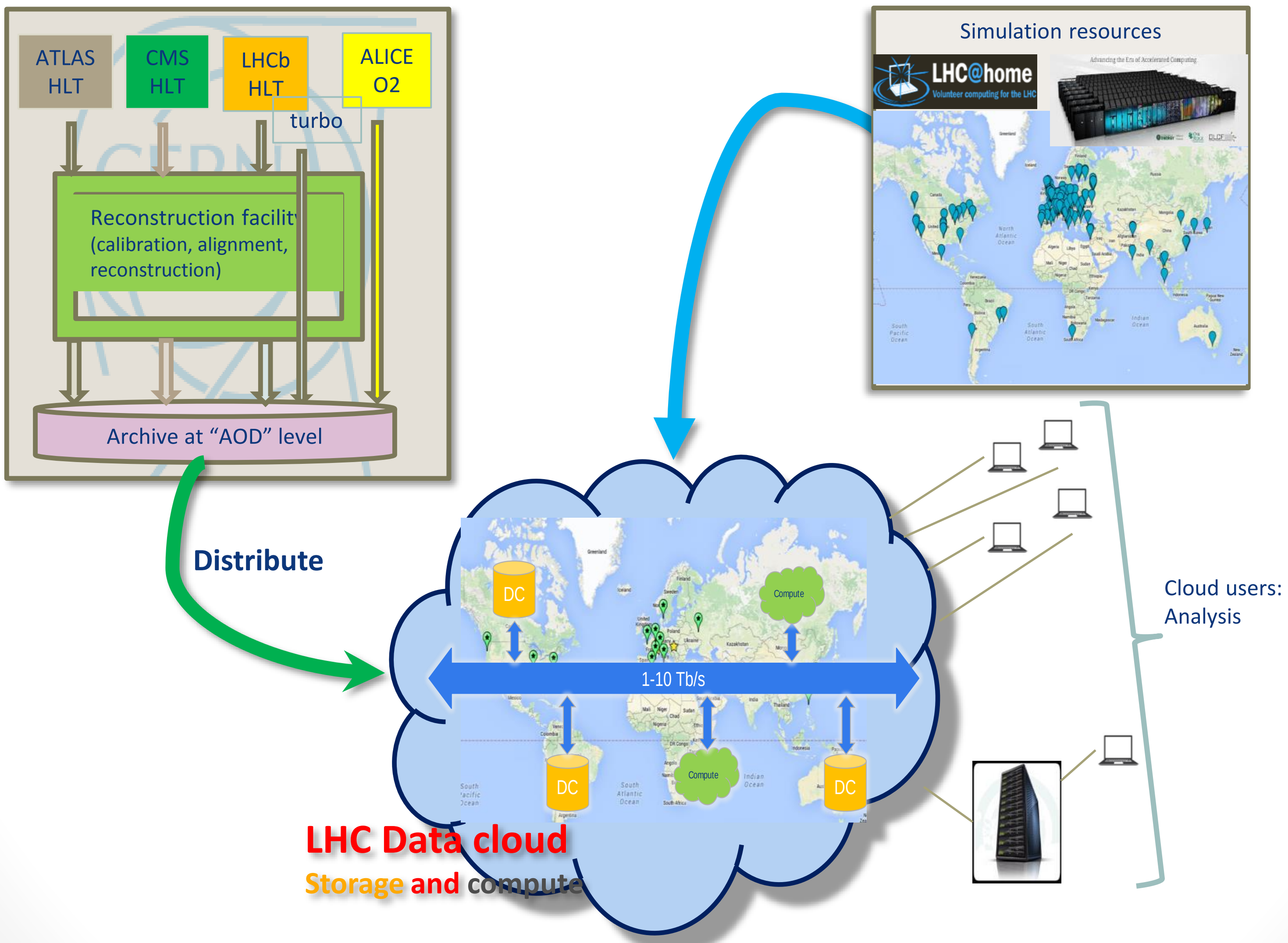
[2] Global Biobanking Market 2016-2020, Technavio Division of Cambridge Healthtech Institute, Tec. Rep. IRTNTR7852 (Nov. 2015), 1–145.

Where are we going ?

A possible evolution in HEP

- Evolution toward a federated infrastructure with larger installation with integration of HPC and commercial clouds:
  - Economies of scale and improved efficiency
  - Reduction of operating costs
- Evolve the current e-infrastructure and the computing models:
  - serve HEP at large and neighbouring sciences ((astrophysics, astronomy, photon science, chemistry, biology, medicine …)
  - flexible to technological development on datastorage solutions and HPC
- exploit different budget lines

Model for future HEP computing infrastructure



Build a "data cloud"

- Few – O(5-10) - large centres
  - Multi-Tb private (SDN) network between them
  - Treat as a single "virtual data centre"
    - Policy replicates data inside for security and performance
    - Think of RAID across data centres
  - Store all of the "AOD" data here; Do not replicate data to global physics institutes (major cost)
- Pluggable compute capacity:
  - HEP resources at these centres & other large centres
  - Commercial compute
- Model allows commercial data centres
  - For storage – enough redundancy that a commercial centre could unplug
  - For compute
  - Relies on networking and GEANT/Esnet etc. connections to commercial entities, policy
- ☞ Users access data in this cloud remotely
  - Eventually download "ntuples" – or equivalent
  - All organised processing is done in this model
- ☞ Enables new analysis models: all data can be seen as colocated
  - Get away from the "event-loop" → queries, machine-learning, etc.

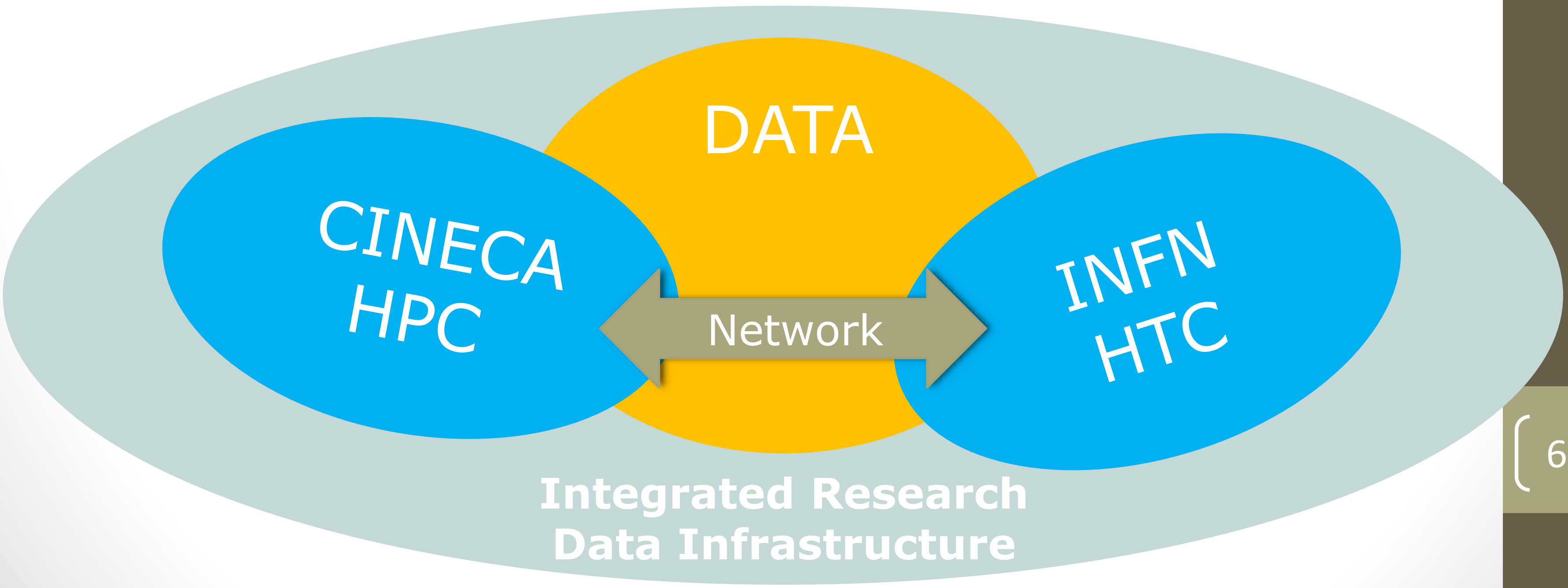
This idea has been discussed in the WLCG community (e.g. see I. Fisk CHEP plenary)

- ❑ Hybrid model:
  - ▪ HEP-resources at a level we guarantee to fill → cost-effective
  - ▪ Commercial resources for "elasticity"
- ❑ Needs new funding models

New italian integrated e-infrastructure

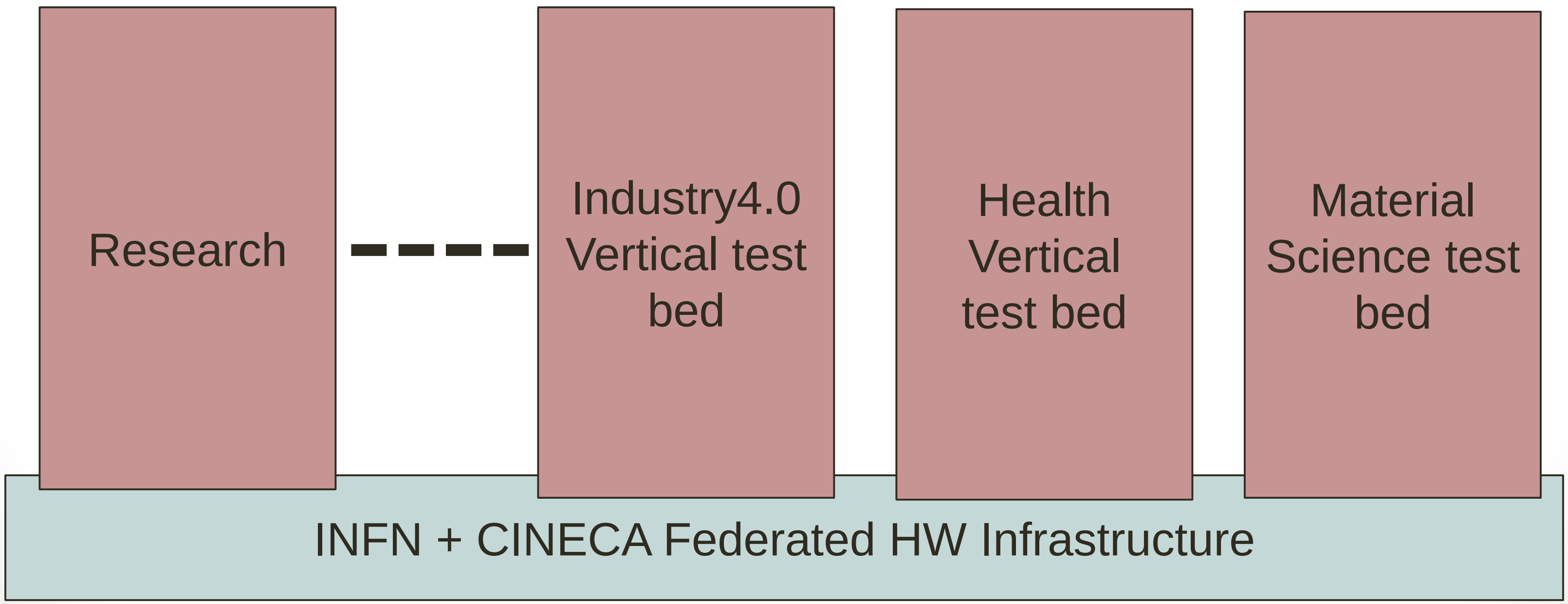
Integration of CINECA-HPC and INFN-HTC computing infrastructure, in connection with the ENEA CRESCO farm, to provide services to:

- Institutional basic and applied research
- Enabling for Public administrations
- Proof of concept and innovation for private organizations and industries



The goal

- provide a common infrastructure to the different research communities (physics, astrophysics, Biology, Medicine, engennering, …)
- but also to public and private sectors (test beds)
- attract National, regional and European funds



INFN Scientific Computing in the next years

Middleware:

- Tools development for EOSC, in collaboration and within European projects
- Development of tools and services pilots to exploit the research e-infrastructure by SMEs

Other initiatives

- IPCEI: INFN leading role in project, focus mainly in HPC and big data integration with involvement of private companies and public administration

Pre-Pilot activity:

- In collaboration with ASI (Italian Space Agency), development and implementation of the **Italian Sentinel Collaborative Data Hub** for the Italian Collaborative Ground Segment. ASI uses LHC infrastructure, necessary services installed on the Bari Tier-2

INFN Scientific Computing in the next years cont'd

- INFN and INAF collaboration/discussion for CTA computing and in the future for SKA and EUCLID

Computing training

- INFN is investing 1 M€ in 12 post-doctoral positions to collaborate with the LHC experiments to the development of:
  - innovative computing workflow and data management solutions for large scale science
  - high performance data analysis and algorithms
  - machine and deep learning techniques

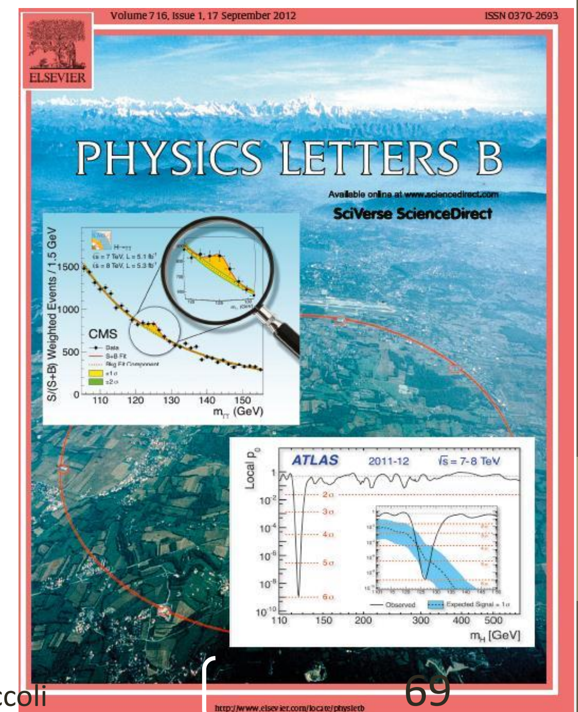
Summary

- INFN is moving towards a integrated cross-disciplinary national e- infrastructure
- Future strategy includes other disciplines like services for astrophysics (CTA, SKA, Euclid), satellites (Copernicus, Cosmoskymed), ….
- Pilot activities are starting within regional and international initiatives to provide services to public private partners
- Evolution of the middleware toward a Cloud vision
- Fund raising from different sources: national, regional, EU

Results

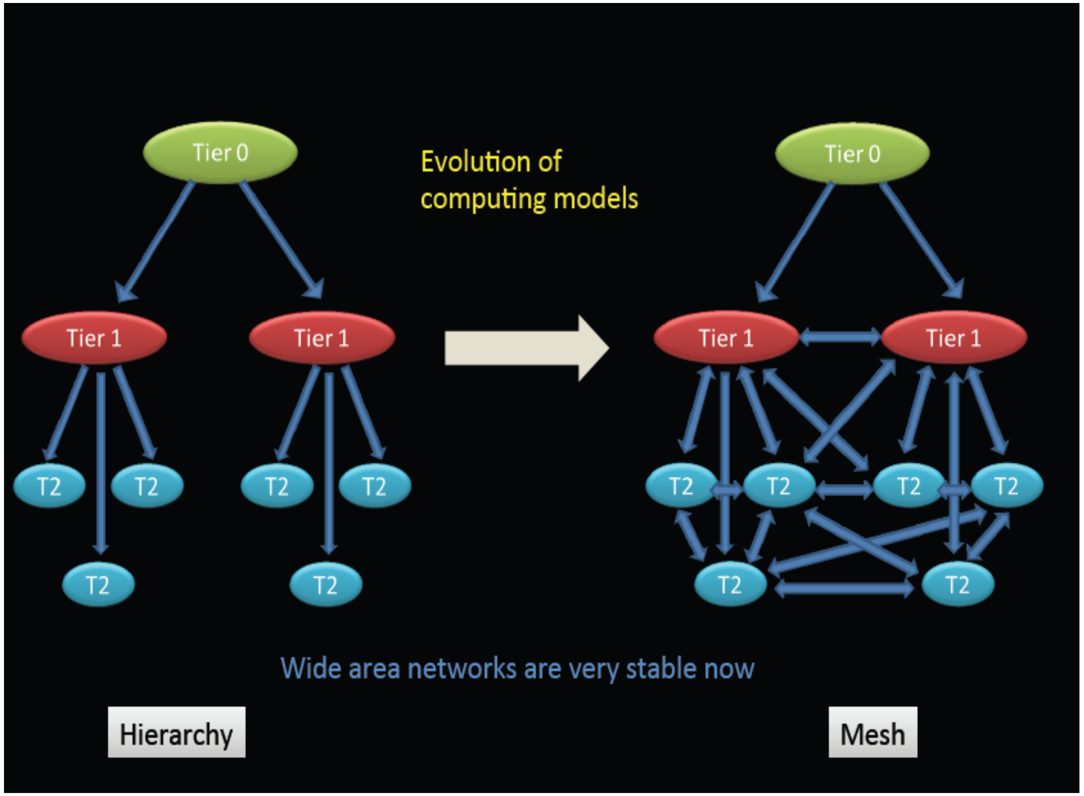
INFN computing based GRID.
"Grid computing combines computers from multiple administrative domains to reach a common goal[...]
One of the main strategies of grid computing is to use middleware to divide and apportion pieces of a program among several computers, sometimes up to many thousands (wikipedia)"

After few analysis months:



New computing models in HEP

- Computing Models are not static. Continuous evolution
  - since the beginning of the data taking, the “ideal” CMs have been replaced by realistic ones exploiting the technology and infrastructure improvements
- In Run-1 the LHC experiments have been able to cope with an unforeseen amount of data transferred and analysed



New middleware: from Grid to Cloud

- Grid:
  - Long, steep learning curve.
  - Difficult to use for real-time analysis, visualization, provisioning of complex virtual environments.
  - Storage management normally at the file/block level, not as distributed objects.

- Cloud:
  - Provide new services; In addition to grid interface
  - Site Virtualisation, for efficiency, service provision, etc
  - Access also to academic infrastructures
  - Possibility to use commercial clouds

New Facts

European Center for Medium-Range Weather Forecasts will be in Bologna. Center employs around 300 staff from more than 30 countries and *the current data centre facility does not offer the required flexibility for future growth and changes in high-performance computing (HPC) technology*
Press kit: Discussions with Bologna to host new data centre

- Supported by Emilia-Romagna Region and Italian government.
- It will be a large data center, 10 MW to upgrade to 20MW
- Timeline: June 2017 ratification agreement, to be ready by end of 2019

INFN Scientific Computing in the next years

Infrastructure:

- Delocalized Tier-1:
  - Off-load Monte Carlo production to Bari Tier-2 where a lot of CPU cycles are available since it is a regional center
  - Integration of CINECA computing into Tier-1: ~half of current CPU power of Tier-1 will be "rented" by CINECA in a transparent way (2018)
- Likely evolution of Tier-1 into the "LHC data center"
- Re-organization of the Tier-2, configuration and number of centers depend on regional funds
- Integrate INFN e-infrastructure with HPC and Network to a single e-infrastructure