



# Helix Nebula The Science Cloud

Workshop on Best Practices for Data Management & Sharing  
Ispra – 15 April 2014

Bob Jones (CERN)

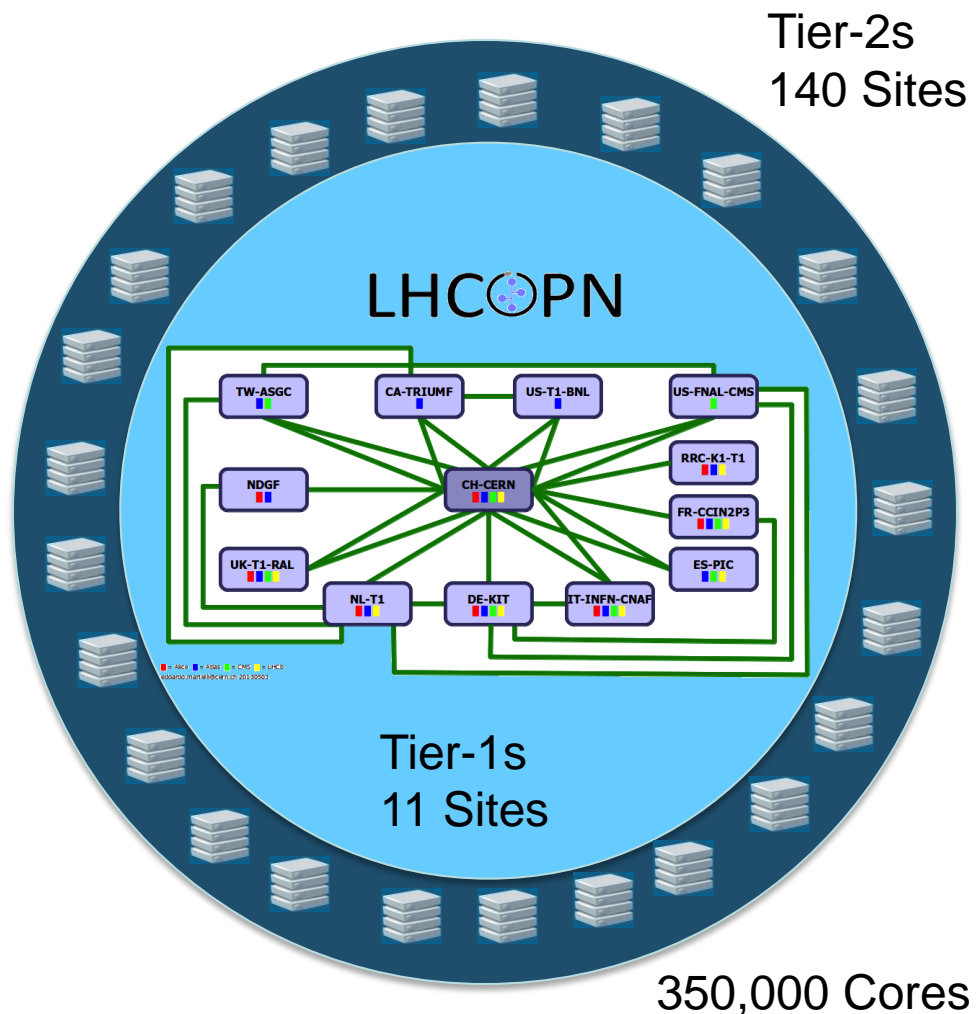
# Worldwide LHC Computing Grid

Running jobs: 246791  
Transfer rate: 13.98 GiB/sec



Data SIO, NOAA, U.S. Navy, NGA, GEBCO  
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US Dept of State Geographer  
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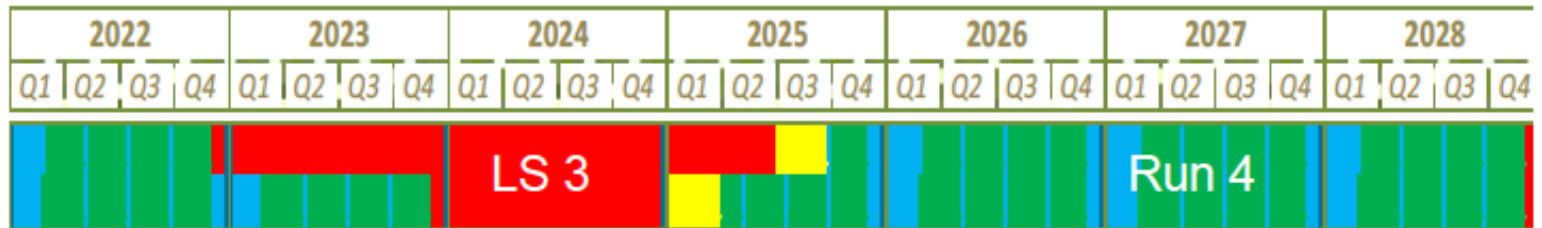
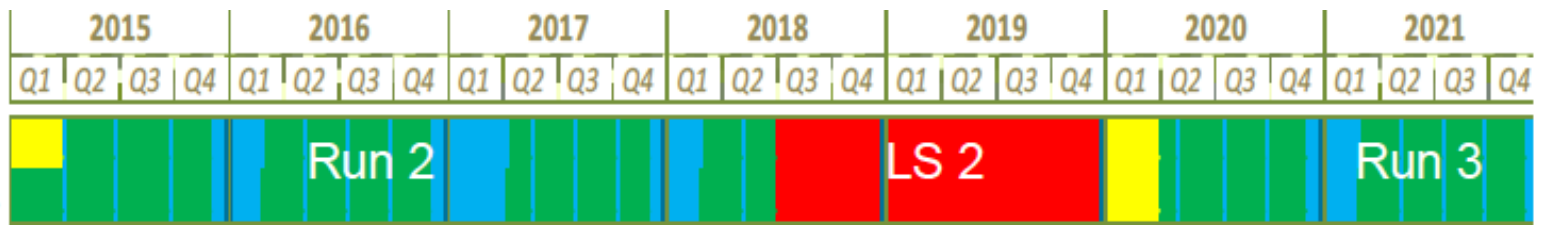
Google



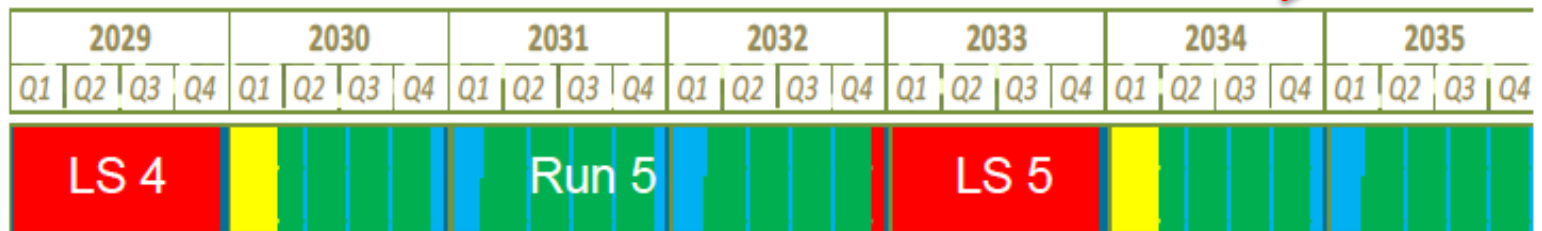
# LHC schedule beyond LS1

Run 1 – which led to the discovery of the Higgs boson – is just the beginning. There will be further data taking – possibly for another 2 decades or more – at increasing data rates, with further possibilities for discovery!

We are here

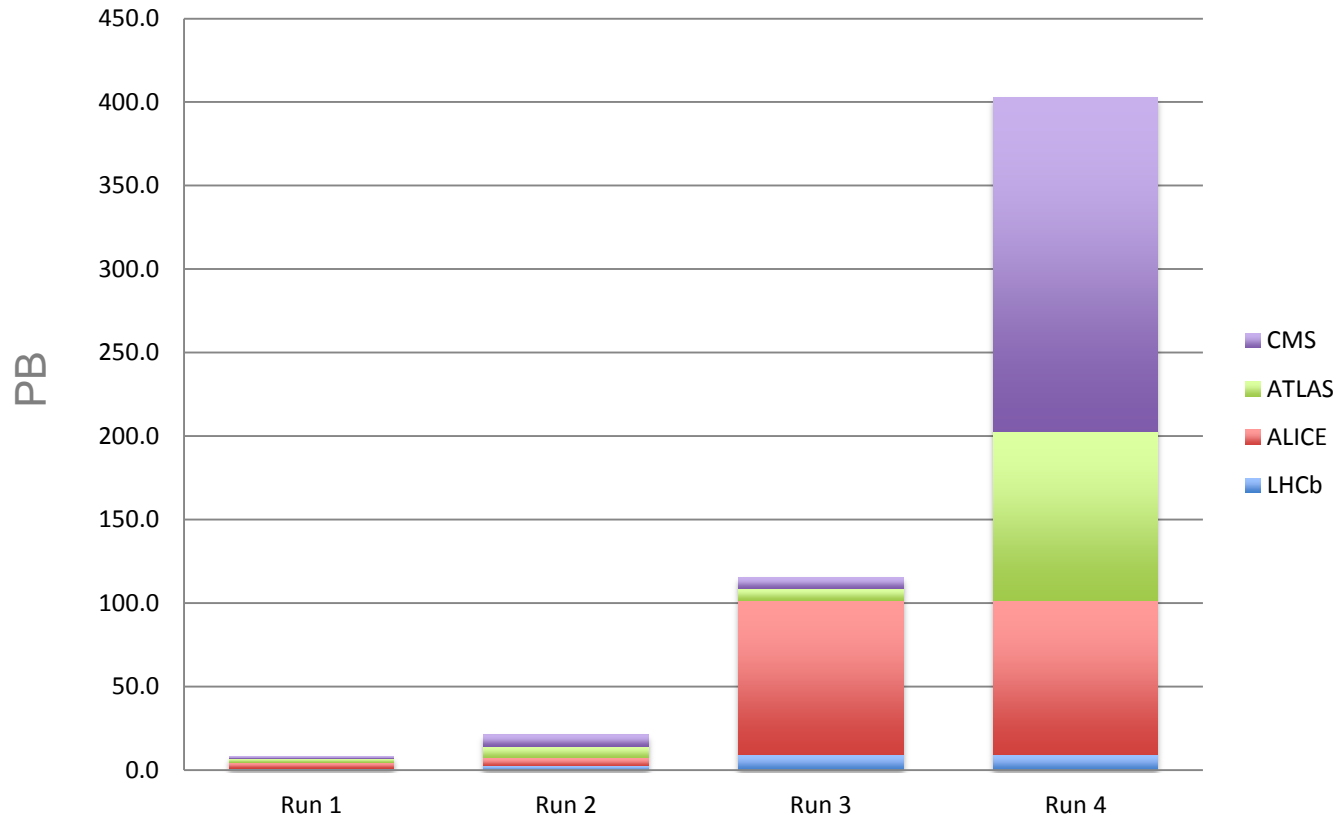


HL-LHC





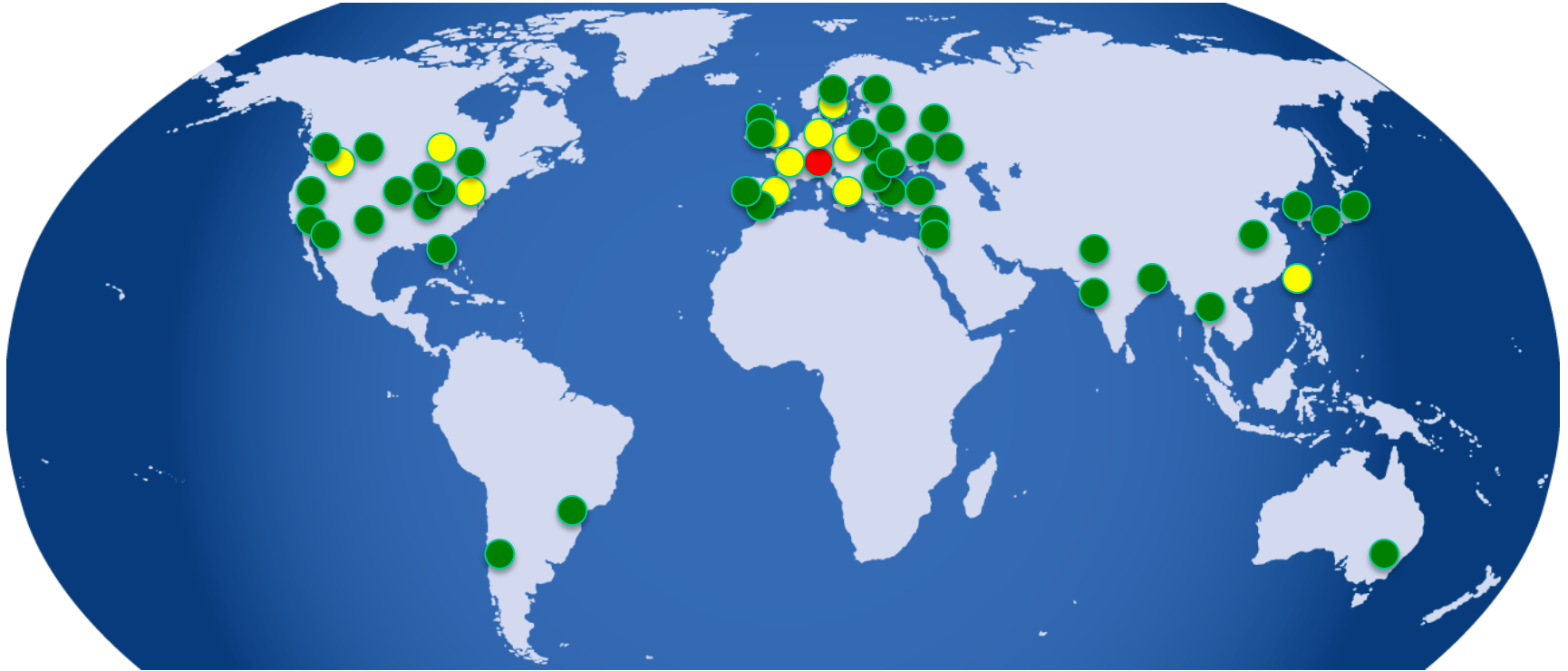
# Data: Outlook for HL-LHC



- Very rough estimate of a new RAW data per year of running using a simple extrapolation of current data volume scaled by the output rates.
  - To be added: derived data (ESD, AOD), simulation, user data...
- **0.5 EB / year is probably an under estimate!**



# WLCG



# Strategic Plan for a Scientific Cloud Computing infrastructure for Europe

- Establish a sustainable multi-tenant cloud computing infrastructure in Europe
- Initially based on the needs for the European Research Area & space agencies
- Based on commercial services from multiple IT industry providers
- Adhere to internationally recognised policies and quality standards
- Governance structure involving all stakeholders

## Contacts

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# Timeline

2011

- Endorse the Common **Strategy**
- Agree on the **Partnership**
- Select **flagships** use cases
- Define **governance** model

2012-2013

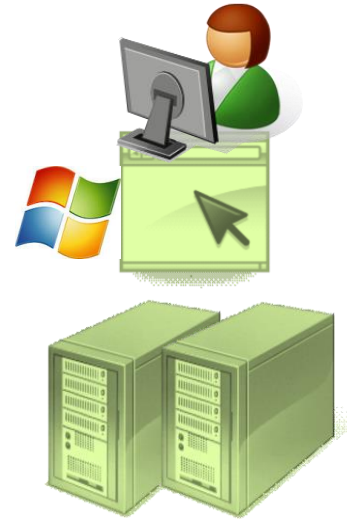
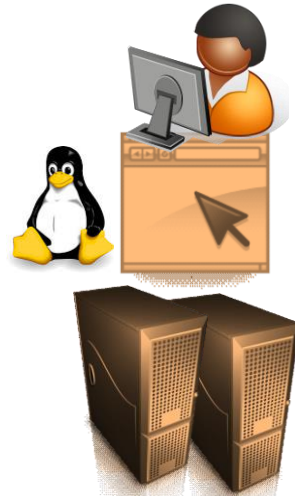
- **Pilot** Phase
- **Deploy** flagships,
- **Analysis** of functionality, performance & financial model

2014 ...

Towards an **open market for Science**



# Cloud Services: *virtualisation*

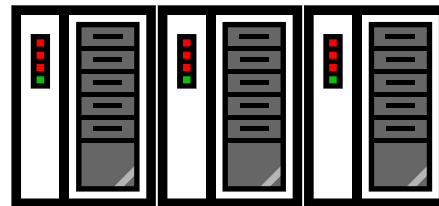


User  
Application  
Server

**Lower Cost**  
**Faster Maintenance**  
**More Flexibility**



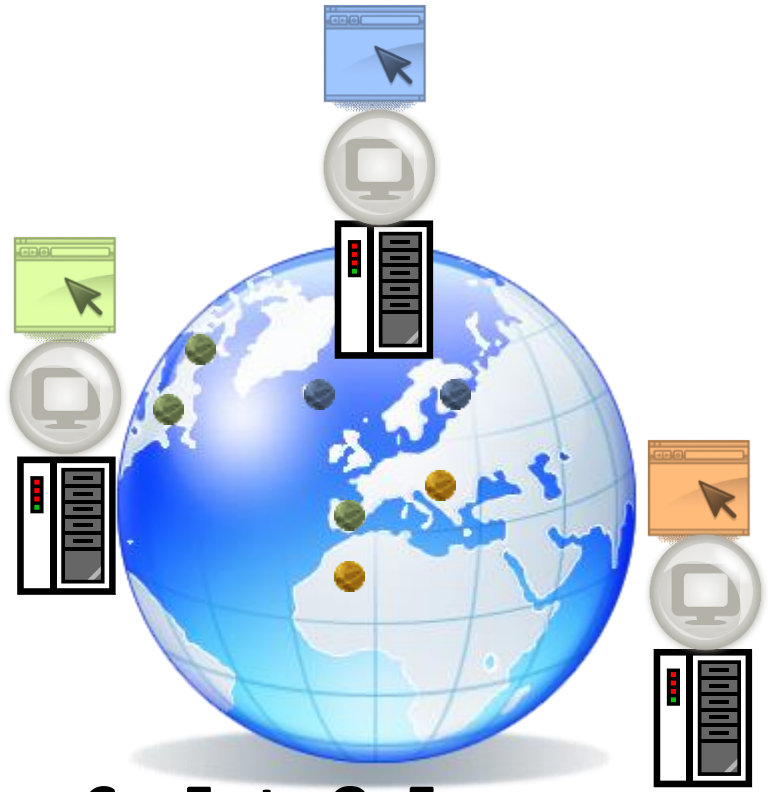
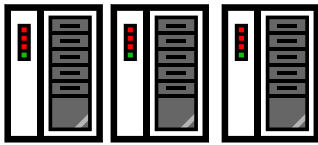
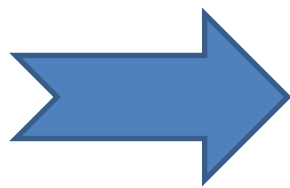
Hypervisor







# Cloud Services: *outsourcing & offshoring*



**From CapEx to OpEx**  
**Procurement Process**  
**Terms and Conditions**  
**Jurisdiction and Legislation**



# Cloud Services: *contracts*

- **Liability** - *Exclusion, Limits and Remedies for Breach of Warranties & Indemnities*
- **Service Levels** - *Data integrity, resilience and business continuity, transparency*
- **Regulatory Issues** - *Data location and data export*
- **Confidentiality** - *Rights to Monitor, Access, Disclose or Use Customer Data*
- **Security** - *Requirements, Audit Rights, Security Incidents and Response*
- **Vendor Lock-In** - *Data retention, deletion and data portability*
- **Term and Termination**
- **Changing Service Description or Features**
- **Intellectual Property Rights**

Source: Cloud legal project, Queen Mary College London

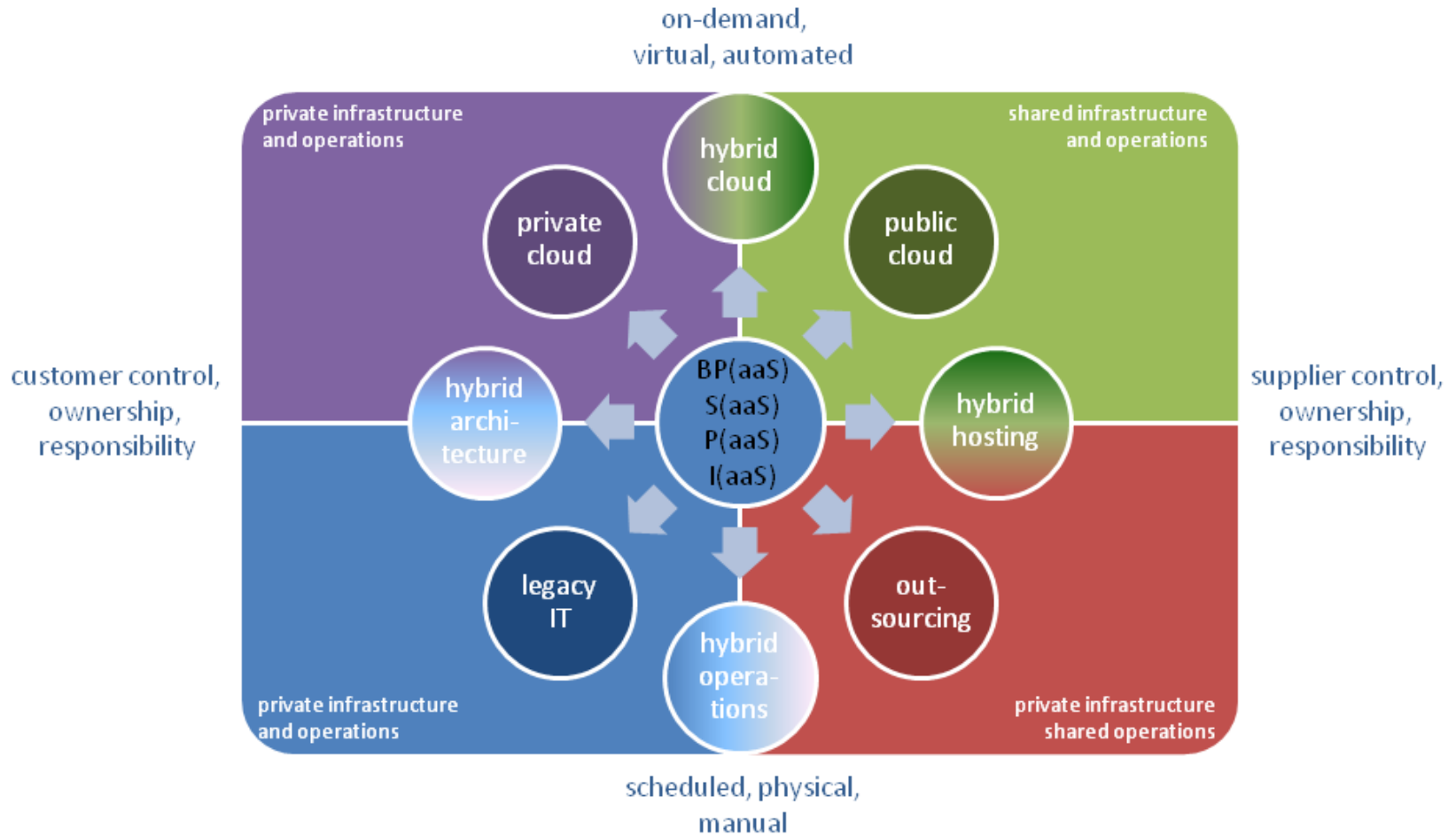
<http://www.cloudlegal.ccls.qmul.ac.uk/>

Webcast lecture from CERN on 13 May:

<https://indico.cern.ch/event/306750/>



# Hybrid clouds



Our preferred model is a hybrid cloud that combines commercial cloud services with resources managed by public organisations

# A European cloud computing partnership: big science teams up with big business



## Strategic Plan

- ▶ Establish multi-tenant, multi-provider cloud infrastructure
- ▶ Identify and adopt policies for trust, security and privacy
- ▶ Create governance structure
- ▶ Define funding schemes



To support the computing capacity needs for the LHC experiments



Setting up a new service to simplify analysis of large genomes, for a deeper insight into evolution and biodiversity



To create an Earth Observation platform, focusing on earthquake and volcano research



To improve the speed and quality of research for finding surrogate biomarkers based on brain images

## Suppliers



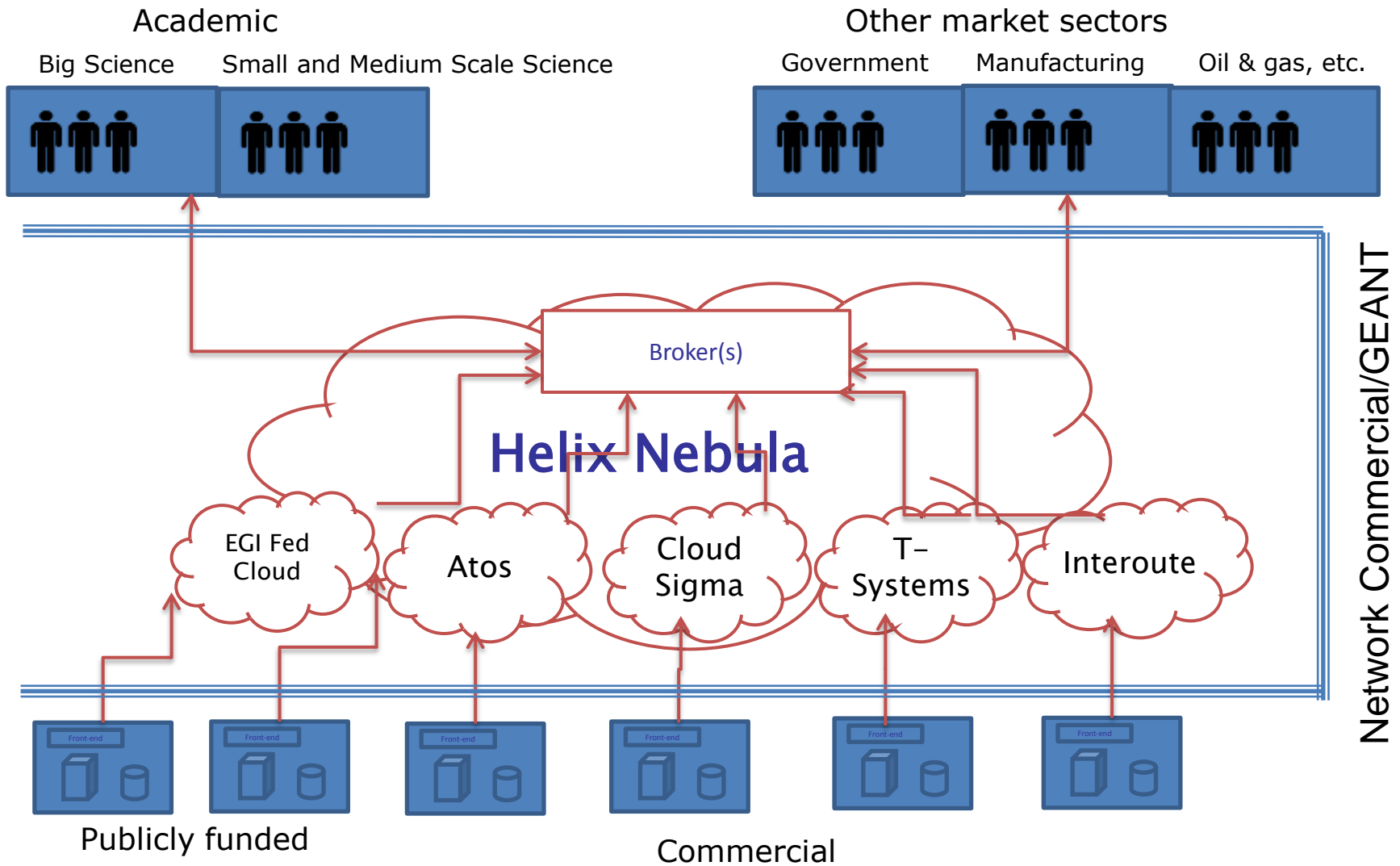
## Adopters



# Flagship use cases

	ATLAS H.E.P. Cloud Use (CERN)	Genomic Assembly in the Cloud (EMBL)	SuperSites Exploitation Platform (ESA/CNES/DLR)
Scientific goal/society impact/photogenic	•	•	•
Scale of resources used	•	•	
Federation/Aggregation of datasets		•	•
Long-term archiving of data			•
On-demand processing	•	•	•
Impact on community & benefits	•	•	•
Potential increase of users	•	•	•
Interoperability	•	•	•
Data security	•	•	•
Maturity	•	•	•
Access to license-controlled sw			•

# Hybrid Public-Private Cloud Model



# Helix Nebula Marketplace (HNX)



- Builds upon the work of the Helix Nebula Initiative and EC support action
- Supported by European cloud providers
- Integrates with existing e-Infrastructures to form a hybrid cloud Market Place and reach out to Europe's research communities
- Trusted cloud services through compliance with EU regulations and legislation
- Simplifies procurement process across multiple services providers



Atos

CloudSigma



••T••Systems•



CGI



# Relevance of HNX to H2020

## HORIZON 2020 WORK PROGRAMME 2014 – 2015

### 4. *European research infrastructures (including e-Infrastructures)*

- Introduction:

- “production-level e-infrastructures are able to serve the computing and data needs of any project in the framework programme fostering economies of scale in the use of ICT systems by projects supported by Horizon 2020.”
- “A related new element in Horizon 2020 is the use of Data Management Plans (DMPs) detailing what data the project will generate, whether and how it will **be exploited or made accessible for verification and re-use**, and how it will be **curated and preserved**.”

- INFRADEV:

- “Proposals should build upon the state of the art in ICT and e-infrastructures for data, computing and networking and work in cooperation with e-infrastructure service providers.”





# What have we learnt?

**Public organisations see value and opportunities in making use of commercial cloud services**

**The production usage of commercial cloud services by public organisations has already started**

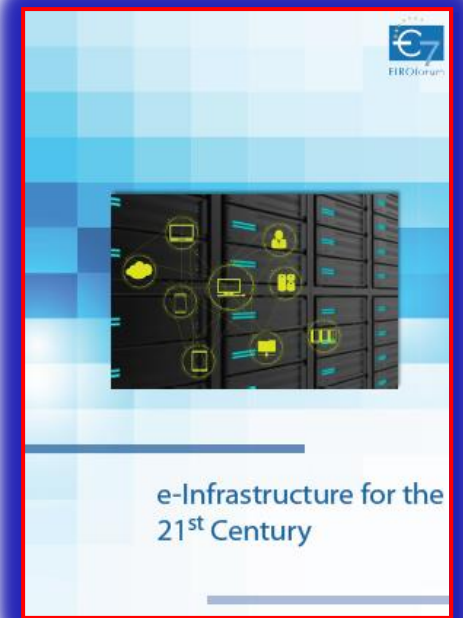
**The public sector is a potentially profitable market for commercial cloud service providers**

**The procurement and use of commercial cloud services poses a number of legal questions**

**A coordinated approach by public organisations will help structure the market and reduce the burden on individual organisations**

# E-Infrastructure for the 21<sup>st</sup> Century

- The goal is to transform existing Distributed Computing Infrastructures (DCIs) based on a range of technologies into a *service-oriented platform* for the *global research community* that can be *sustained* through *innovative business models*
- Prepared by CERN on behalf of the EIROforum IT Working Group



DOI:[10.5281/zenodo.7592](https://doi.org/10.5281/zenodo.7592)

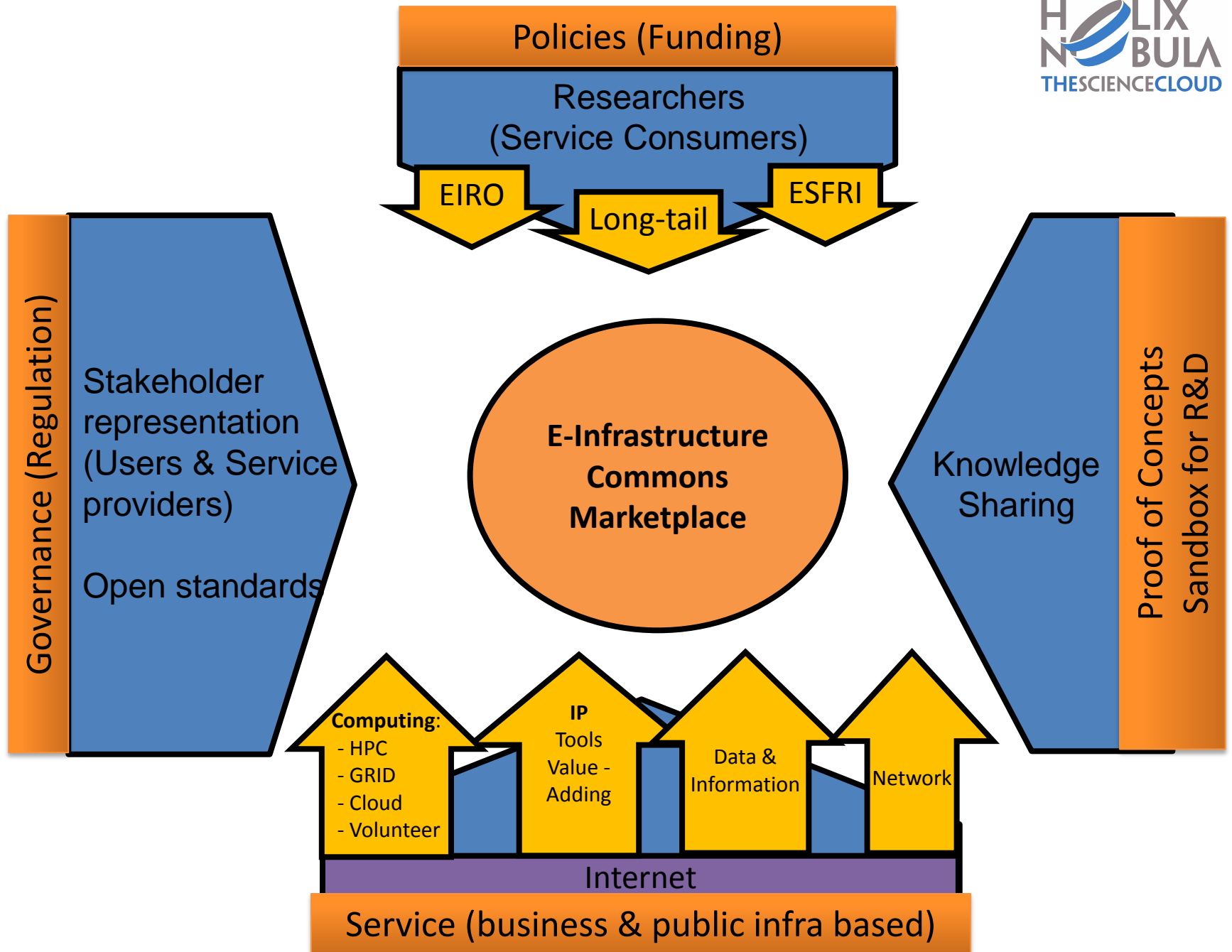
# Vision for the future

The e-Infrastructure commons marketplace will

- Provide access to world class resources through a **dynamic and sustainable marketplace**
- Take a hybrid approach building on public and commercial assets to cover the **entire scientific workflow**
- Offer a broad range of services
- Use **open standards** to ensure **interoperability** of service providers and adhere to **European policies, norms and requirements**

# To get there, we need to

- Driving convergence between existing e-Infrastructure service providers
- Use market mechanisms to attract new service providers & consumers to the Marketplace



# Make it happen in H2020

- Make it possible to **trade** services
  - Services from commercial and public providers offered on a pay-per-usage model should be considered eligible costs for EC projects



**robert madelin** @eurohumph · Feb 17

Data solutions. Help EU clouds and computation networks. Make use of them an allowable cost in EU grant agreements. Cloud/Grid as a service.

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Model GA article13 — Implementation of Action Tasks by Subcontractors

*The beneficiaries must ensure that the majority of the research and development work done by the subcontractor(s) (including the work of the main researchers) is located in the EU Member States or associated countries ('place of performance obligation').*

20 February 2014

Dataset Open access

# Detailed data sets of MMP-cliffs, SAR transfer series, RECAP-MMPs and compound activities

Hu, Ye ; de la Vega de León, Antonio ; Zhang, Bijun ; Bajorath, Jürgen

(show affiliations)

An and up-to-date version of three MMP-based data sets derived from compounds included in the latest release of ChEMBL is presented. These data sets include activity cliffs, structure-activity relationship (SAR) transfer series, and second generation MMPs based upon retrosynthetic rules. The structural data and information are provided in eight different files comprising the data sets of MMP-cliffs, SAR transfer series, and RECAP-MMPs. Compound activities are incorporated in files of RECAP-MMPs. For transfer series, substituted fragments are also provided. All MMP-cliffs, SAR transfer series with approximate or regular potency progression, and RECAP-MMPs are provided in canonical SMILES representation on a per-target basis separately for the Ki and IC50 subsets. The corresponding files are clearly designated.

Files

Name	Date	Size
mmp_data_sets.zip	21 Feb 2014	12.1 MB

**Publication date:**

20 February 2014

**DOI:**

10.5281/zenodo.8418

**Keyword(s):**

data, MMPs, cliff activity, SAR

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F1000Research (on 21 February 2014)

DOI

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Data

Being extended to include citation of software:

<http://www.isgtw.org/spotlight/tool-developed-cern-makes-software-citation-easier>

# Expected impact

- Researchers, supported by large scale long-term research infrastructures, drive the evolution of services for their research needs
- Funding agencies benefit from market forces
- Create a fertile environment that nurtures new scientific ideas and challenges
- Service providers are able to sustain services
- Grow an ecosystem that benefits downstream industries
- Assemble a dynamic market place, building on Information as a Service, based on federation meeting European requirements
- Provide visibility and incentives to industry to invest in new assets (*as a business case but also to use the science communities for testing cutting-edge technology and new services*)



**Helix Nebula *Cloud Productive* event**  
**CERN, Geneva, 14 May 2014**

[http://indico.cern.ch/e/Helix\\_Nebula\\_Cloud\\_Productive](http://indico.cern.ch/e/Helix_Nebula_Cloud_Productive)