Grids & E-Science

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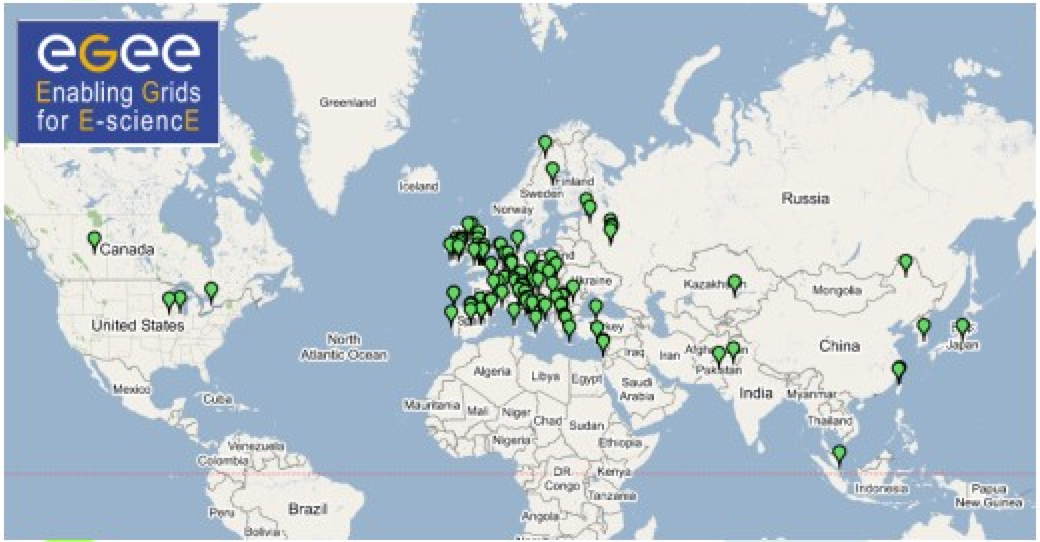
Grid Technologies Trainer, GRNET

University of Athens, October 23rd-24th, 2006

Information Society
and Media

LCG/EGEE collaboration

Grid Projects Collaborating in LHC Computing Grid



Open Science Grid

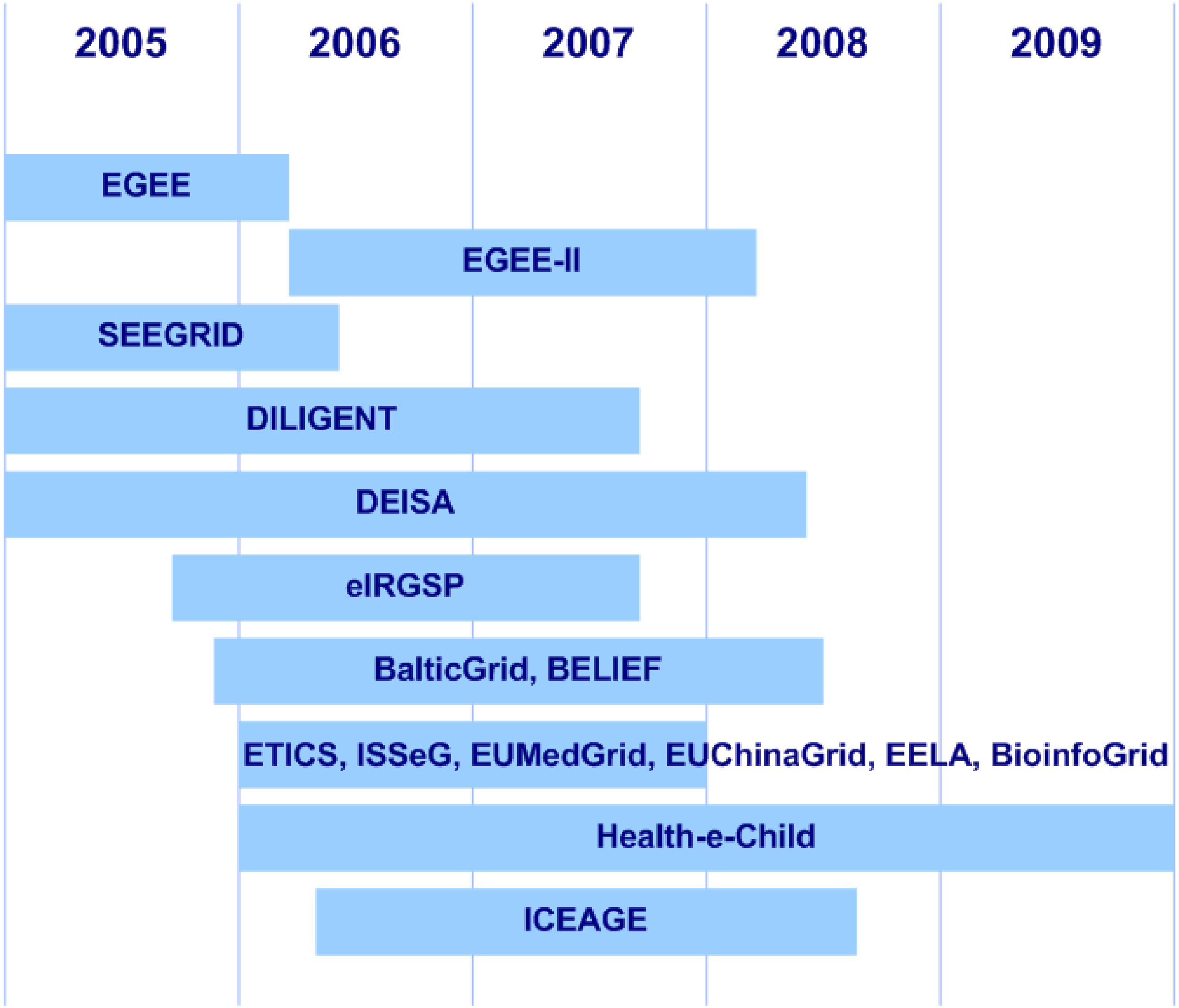
DARTMOUTH
BUFFALO
ALBANY
BU
MIT
UWM
WAYNE
WISC
BINGHAMTON
BNL
UIOWA
FNAL
CHICAGO
PURDUE
PSU
UNL
IU
NERSC
SLAC
HAMPTONU
VANDERBILT
CALTECH
SDSC
UNM
OU
TTU
UTA
UFL
UTEXAS
RICE
FIU

Mon Feb 20 10:38:05 GMT 2006

EGEE Operations Information

Active Sites	~200
Available CPU	~30000
Available Storage (TB)	~10PBytes

European Grid projects, a timeline



Computationally Intensive Science

- **Science is becoming increasingly digital and needs to deal with increasing amounts of data**

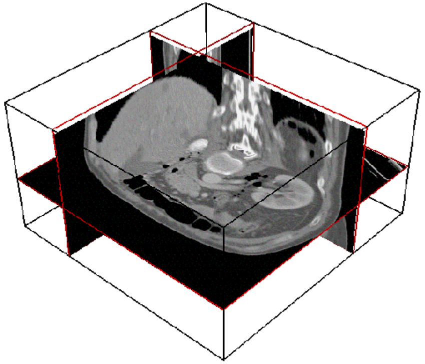
- **Simulations get ever more detailed:**
  - Nanotechnology – design of new materials from the molecular scale
  - Modelling and predicting complex systems (weather forecasting, floods, earthquakes)
  - Decoding the human genome

- **Experimental Science uses ever more sophisticated sensors to make precise measurements**
  - → Need high statistics
  - → Huge amounts of data
  - → Serves user communities around the world

Initial Grid cases: HEP & Biomed

High-Energy Physics (HEP)

- Requires computing infrastructure (LCG)
- Challenging:
  - thousands of processors world-wide
  - generating petabytes of data
  - ‘chaotic’ use of grid with individual user analysis (thousands of users interactively operating within experiment VOs)

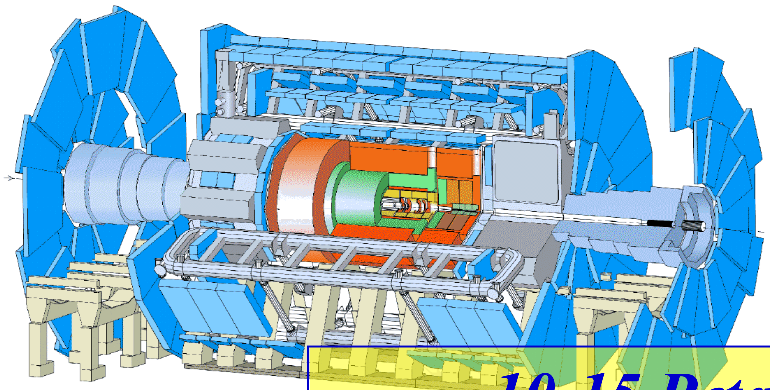


Biomedical Applications

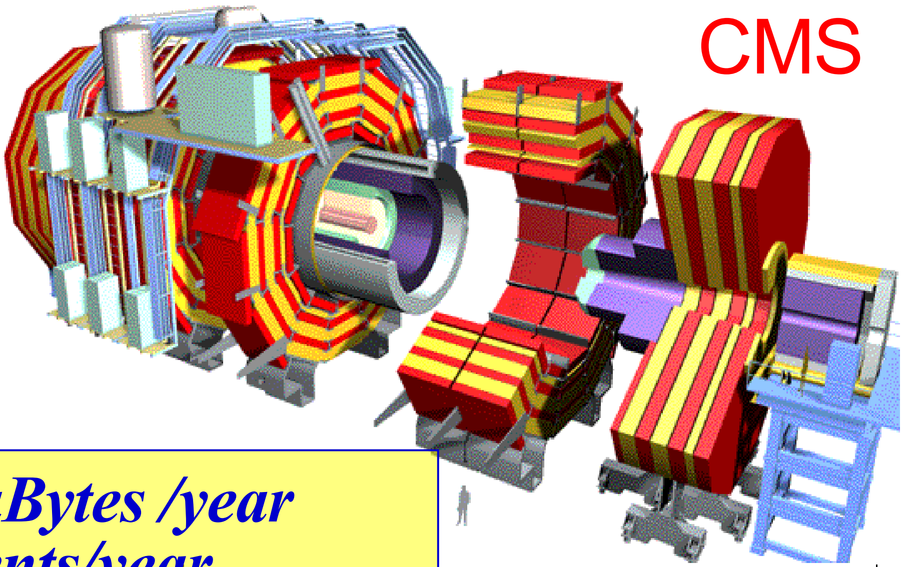
- Similar computing and data storage requirements
- Major additional challenge: security & privacy

HEP: LHC collaborations

ATLAS



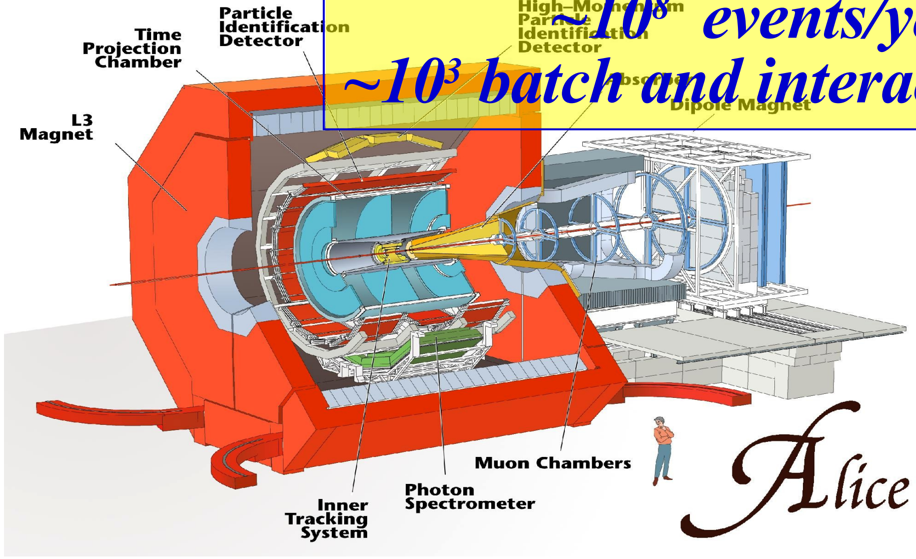
CMS

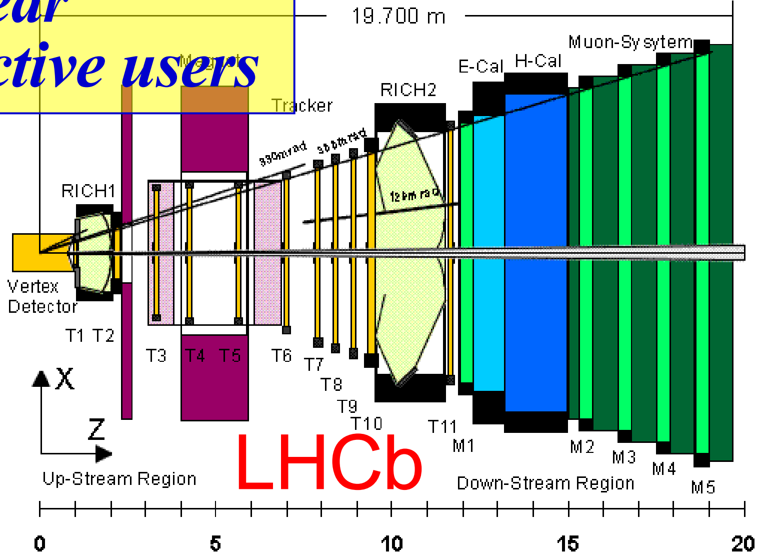


~10-15 PetaBytes /year

~10^8 events/year

~10^3 batch and interactive users

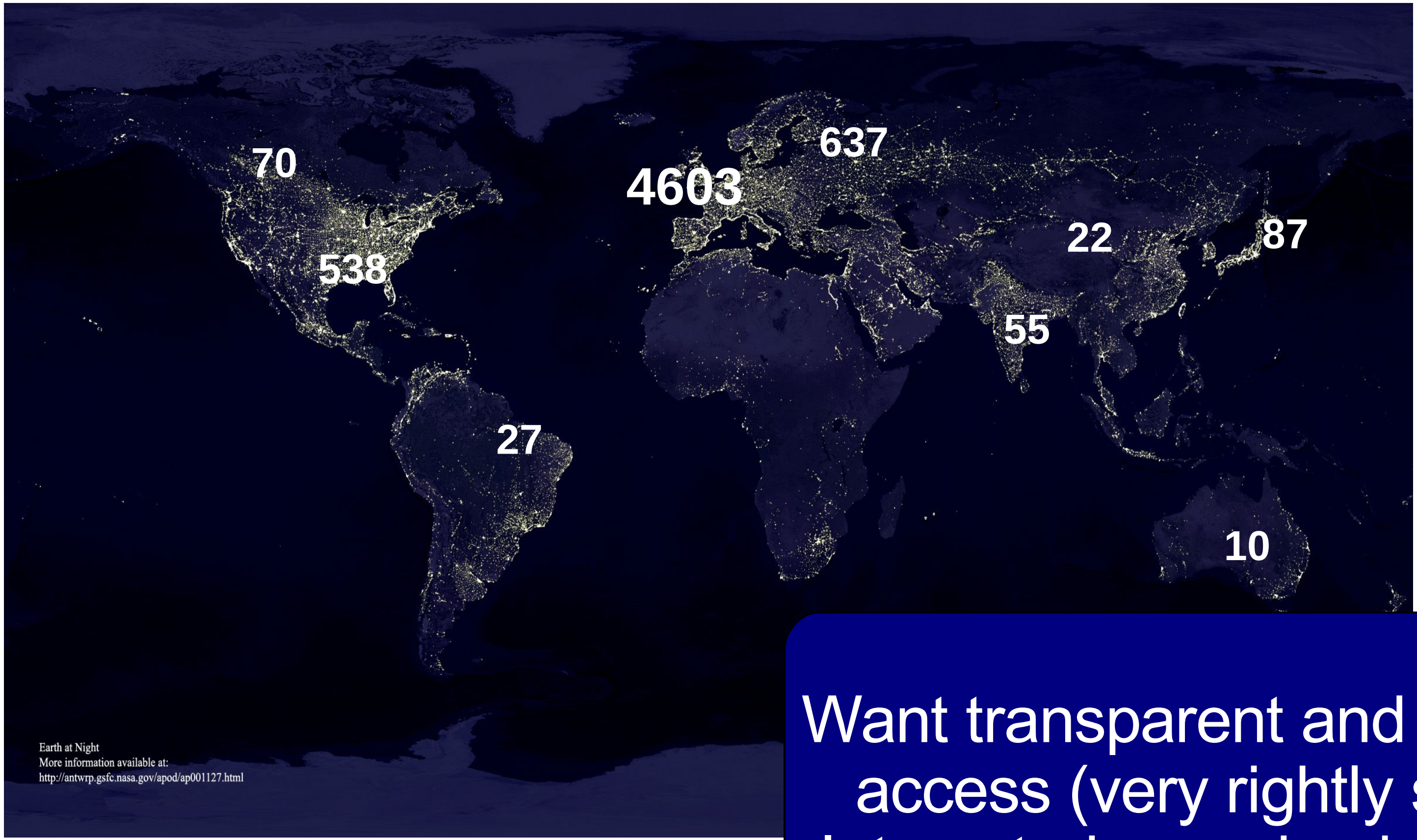




LHCb

LHC: Big "Big Science"

Over 6000 LHC Scientists world wide



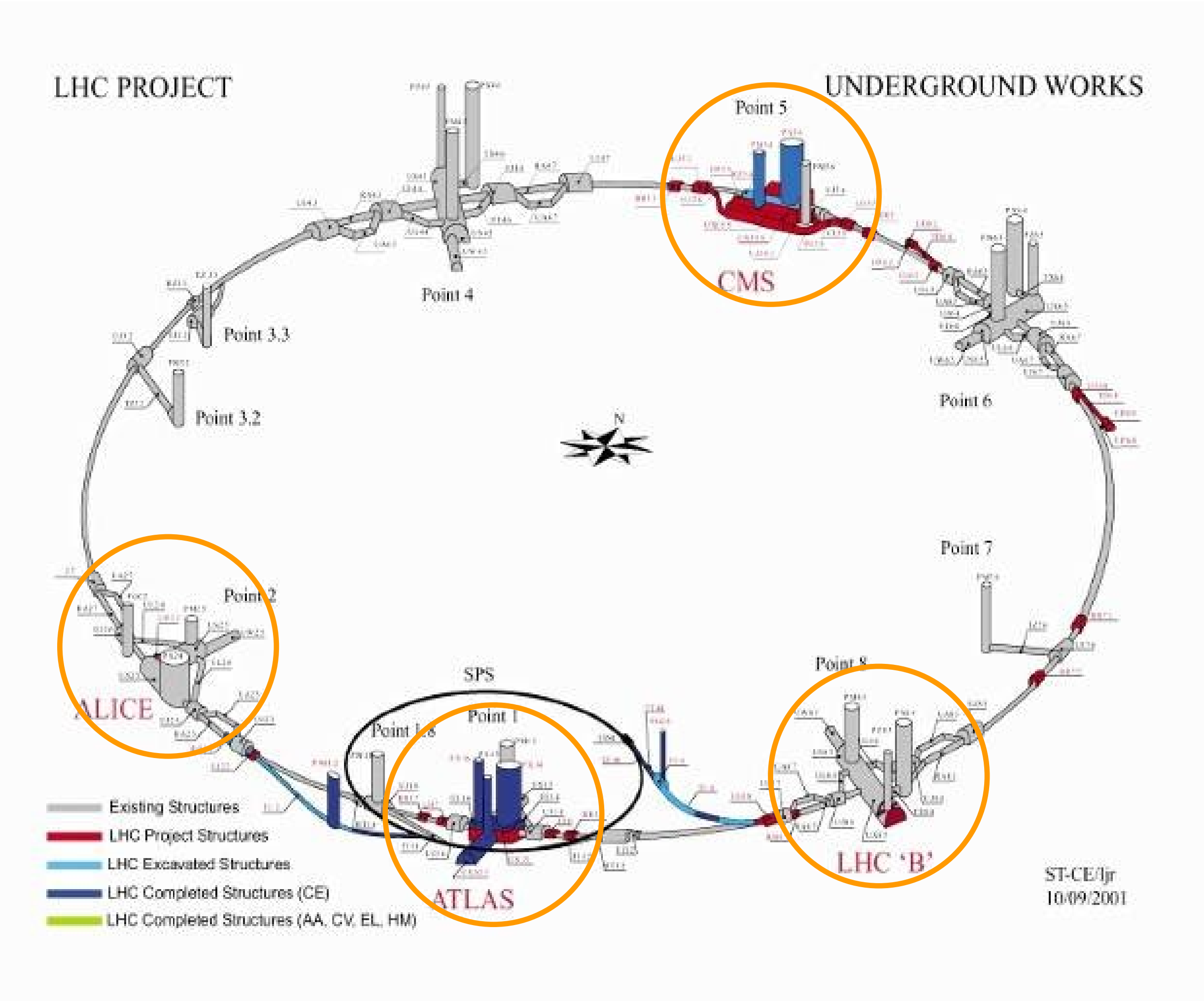
Earth at Night
More information available at:
http://antwrp.gsfc.nasa.gov/apod/ap001127.html

Want transparent and quick access (very rightly so). Interested more in physics results, than computing revolutions

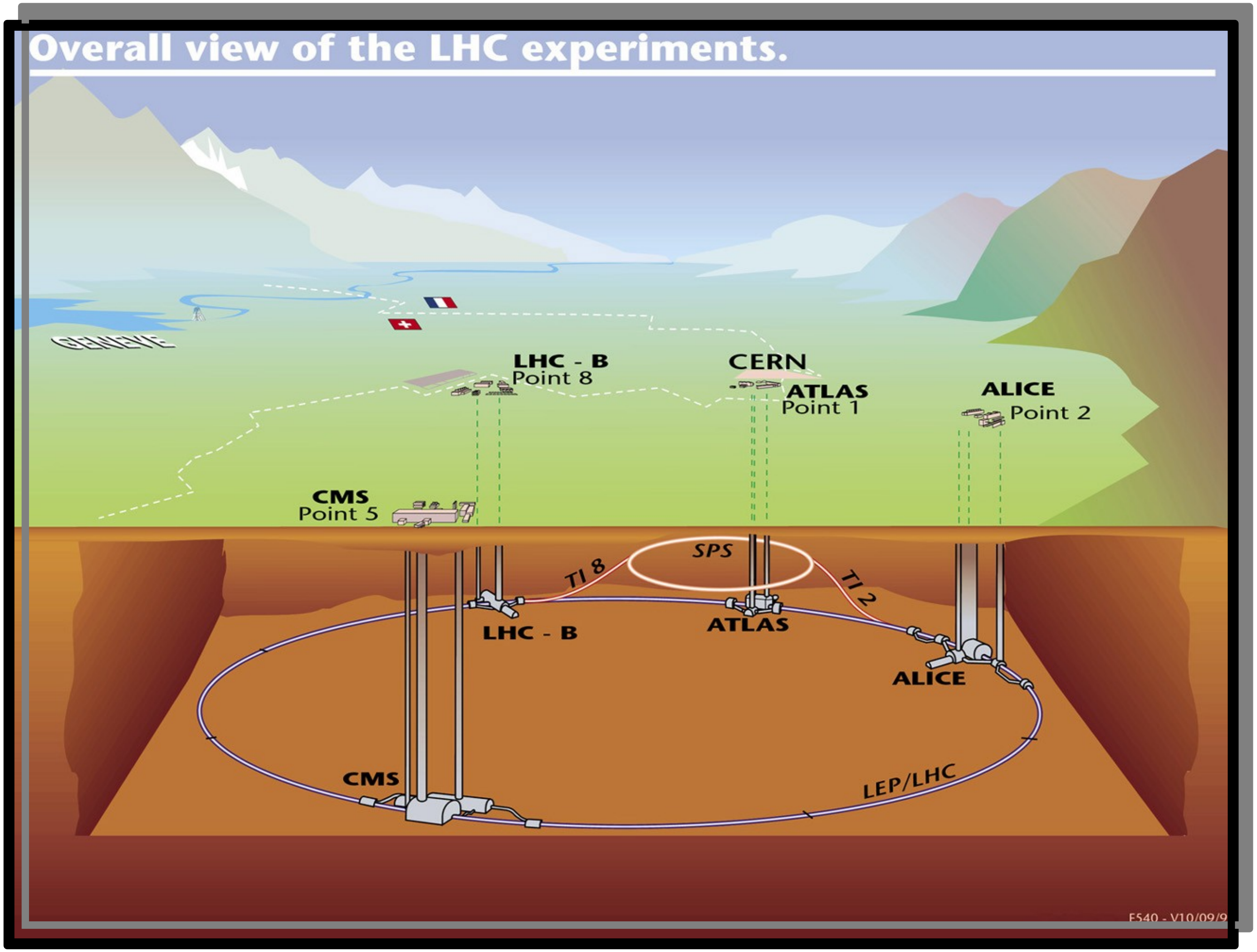
Europe: 267 Institutes, 4603 Users
Other: 208 Institutes, 1632 Users

The LHC experiment

- **Large Hadron Collider**
  - Four experiments:
    - ALICE
    - ATLAS
    - CMS
    - LHCb
  - 27 km tunnel
  - Start-up in 2007

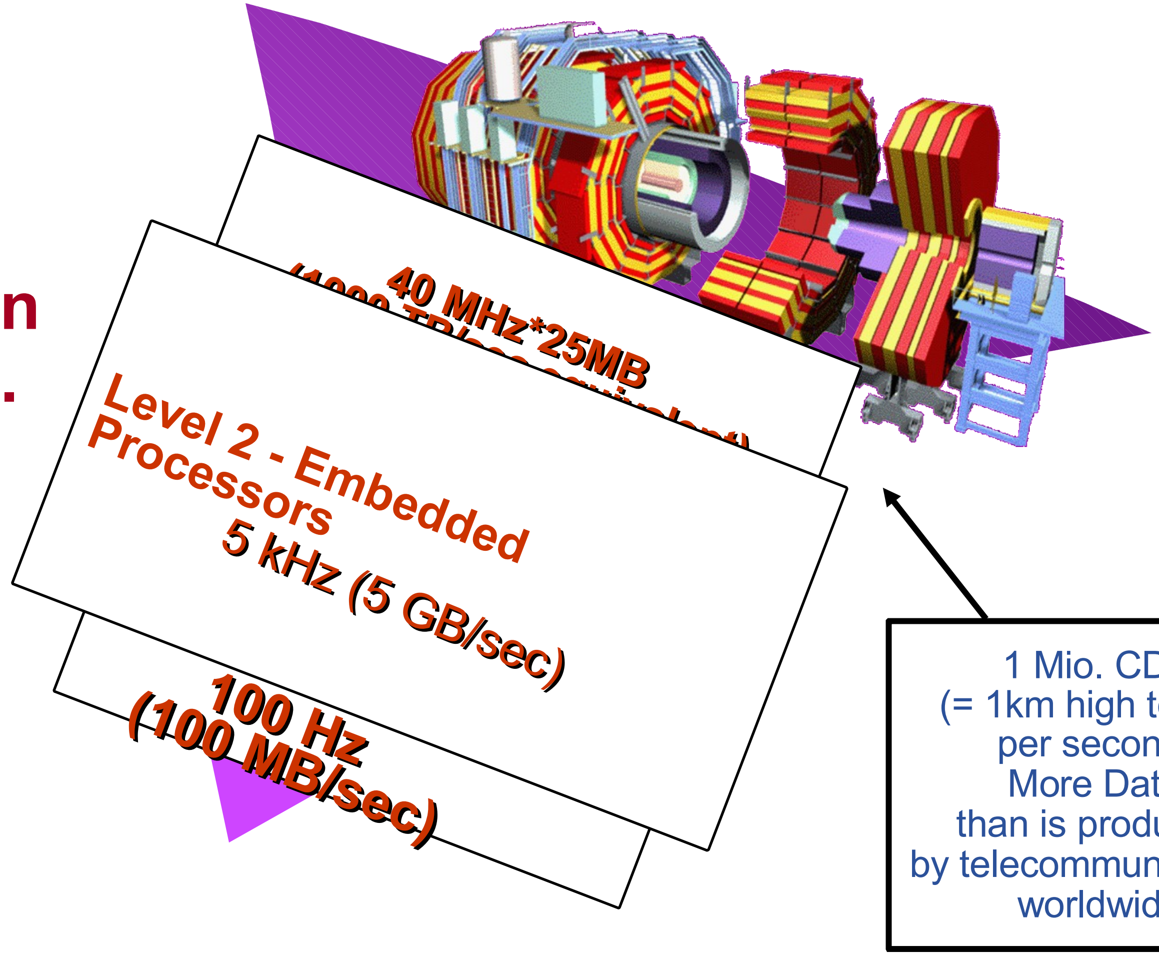


The underground LHC facility



LHC, the CMS detector

Data reduction 1/10 Mio.



40 MHz*25MB
(1000 TB/sec equivalent)

Level 2 - Embedded Processors
5 kHz (5 GB/sec)

100 Hz
(100 MB/sec)

1 Mio. CDs
(= 1km high tower)
per second !
More Data,
than is produced
by telecommunications
worldwide

1 PB of data per year and experiment

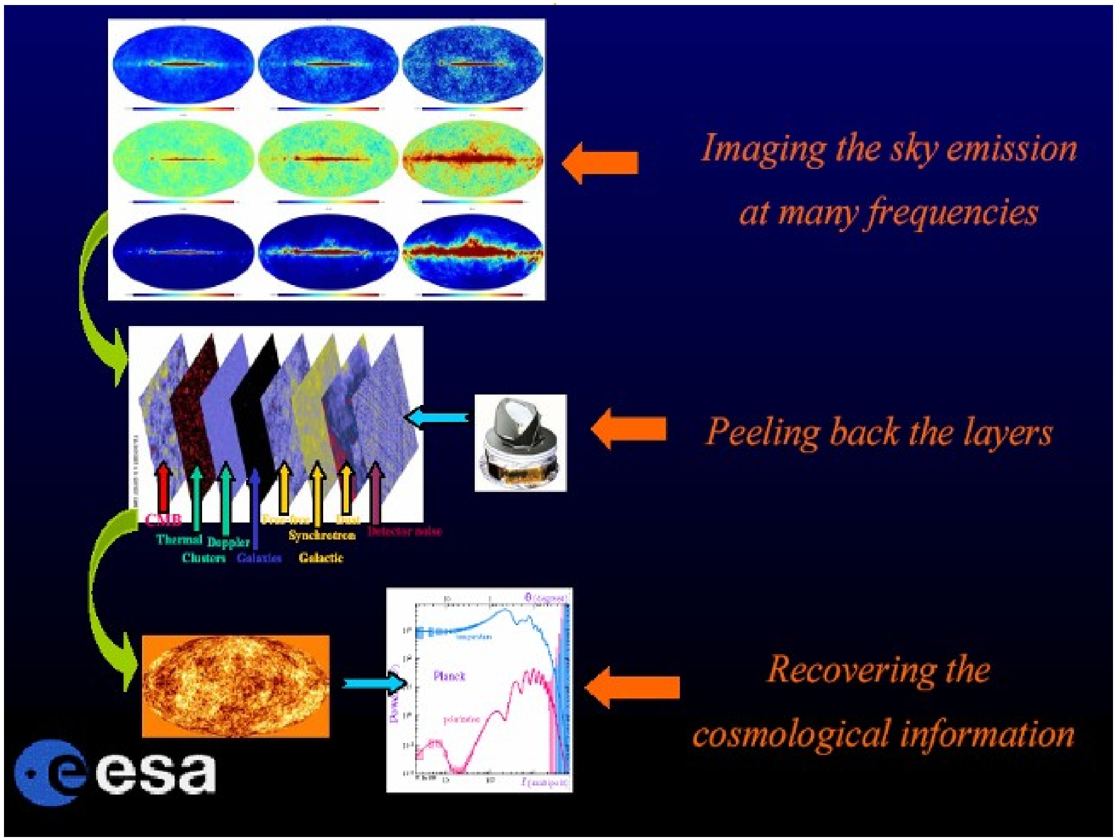
... and 6000 physicist that want to access it !

HEP case: Planck experiment

- **On the Grid:**
  > 12 time faster
  (only ~5% failures)

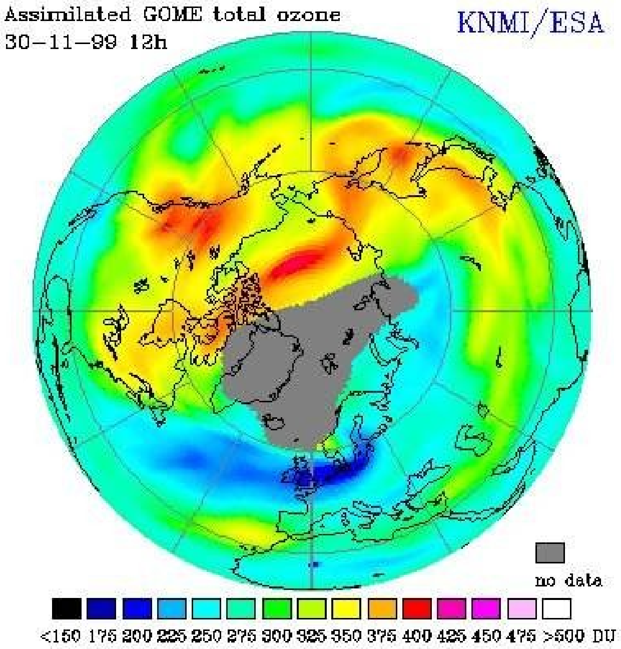
- **Complex data structure**
  → data handling important

- **The Grid as**
  - Collaboration tool
  - common user-interface
  - flexible environment
  - new approach to data and S/W sharing

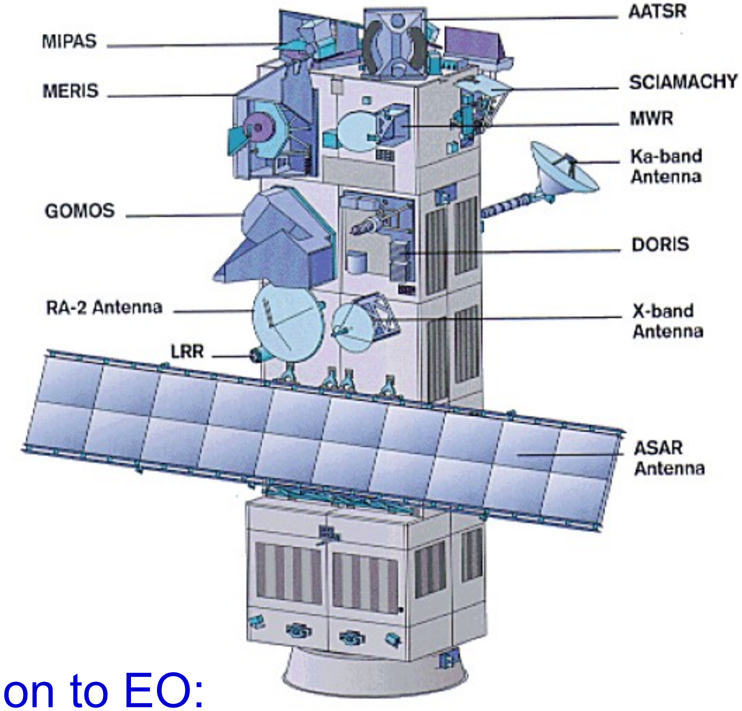


Earth Observation: success cases

ESA missions:
100’s of Gbytes of data per day


Assimilated GOME total ozone
30–11–99 12h
KNMI/ESA
no data
<150 175 200 225 250 275 300 325 350 375 400 425 450 475 >500 DU

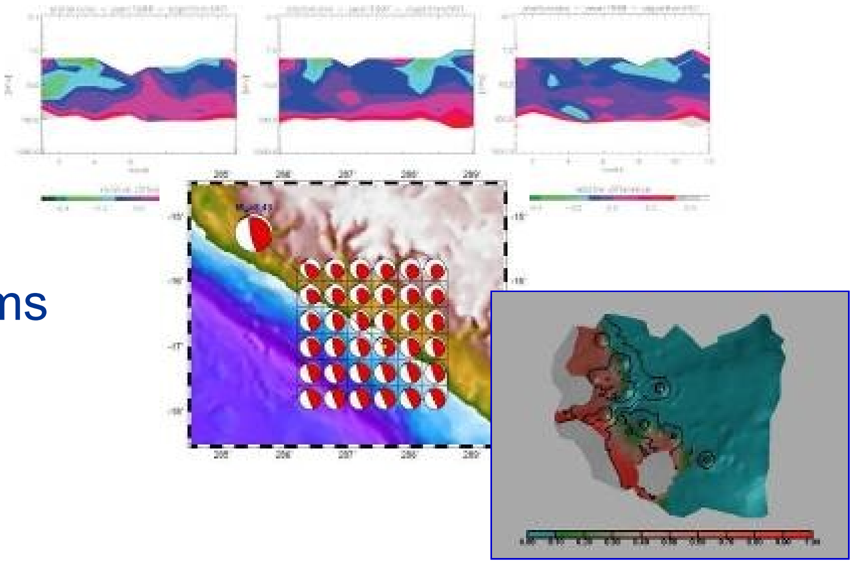
Federico.Carminati , EU review presentation, 1 March 2002



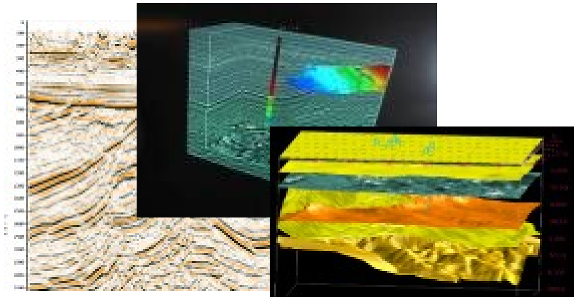
Grid contribution to EO:
Enhance the ability to access high level products
Allow reprocessing of large historical archives
Improve Earth science complex applications
(data fusion, data mining, modelling …)

Earth Sciences

- **Earth Observations by Satellite**
  - Ozone profiles



- **Solid Earth Physics**
  - Fast Determination of mechanisms of important earthquakes
- **Hydrology**
  - Management of water resources in Mediterranean area (SWIMED)
- **Geology**
  - Geocluster: R&D initiative of the Compagnie Générale de Géophysique

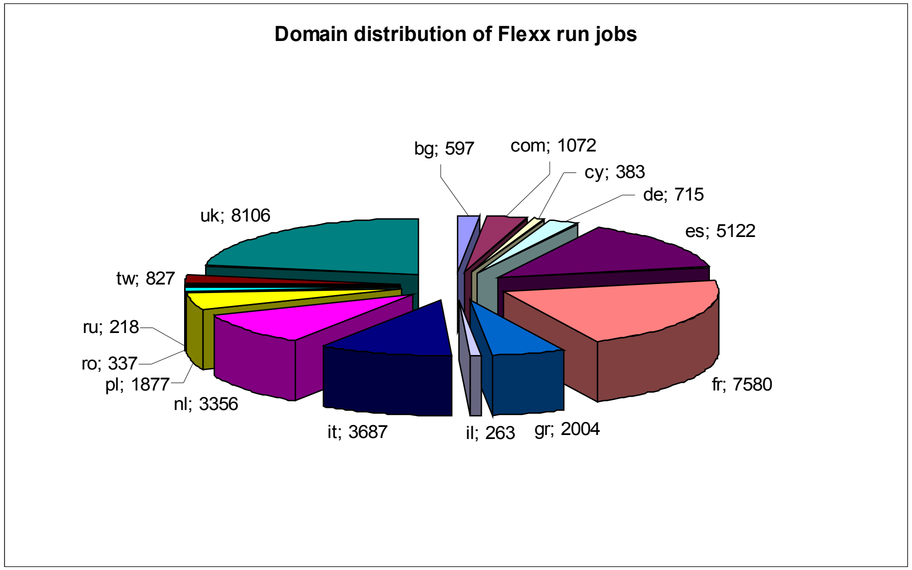


- **A large variety of applications ported on EGEE which incites new users**
- **Interactive Collaboration of the teams around a project**

Biomed case: WISDOM

World-wide In-silico Docking on Malaria

- Significant biological parameters
  - two different molecular docking applications (Autodock & FlexX)
  - about one million virtual ligands selected
  - target proteins from the parasite responsible for malaria
- Significant numbers
  - Total of about 46 million ligands docked in 6 weeks
  - 1TB of data produced
  - Up 1000 computers in 15 countries used simultaneously corresponding to about 80 CPU years
- **Next case:**
  SARS, H5N1 research on the grid!



Domain distribution of Flexx run jobs

WISDOM open day

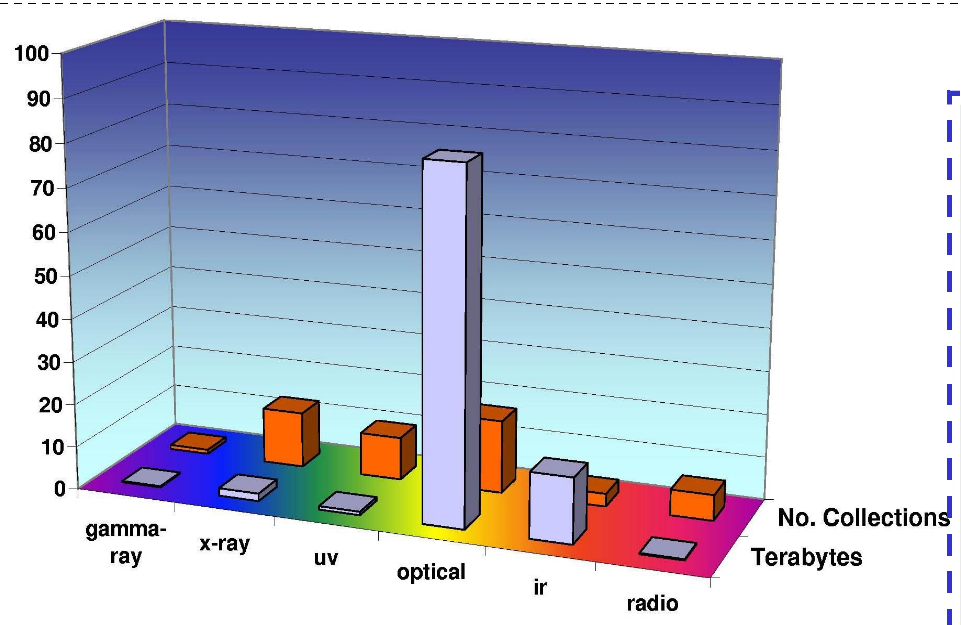
December 16th, 2005, Bonn (Germany)

Discuss Data Challenge results

Prepare next steps towards a malaria Grid (EGEE-II, Embrace, Bioinfogrid)

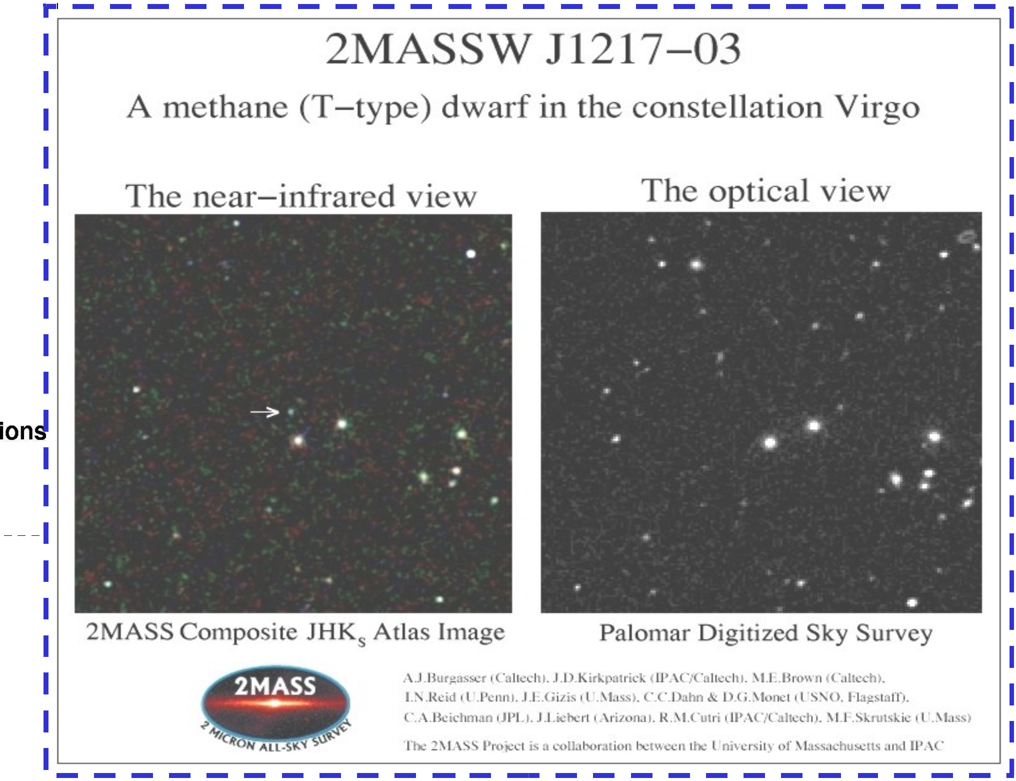
Information: http://wisdom.eu-egee.fr

Astronomy



No. & sizes of data sets as of mid-2002, grouped by wavelength

- 12 waveband coverage of large areas of the sky
- Total about 200 TB data
- Doubling every 12 months
- Largest catalogues near 1B objects



2MASSW J1217−03

A methane (T−type) dwarf in the constellation Virgo

The near−infrared view

The optical view

2MASS Composite JHK$_s$ Atlas Image

Palomar Digitized Sky Survey

2MASS
2 MICRON ALL-SKY SURVEY

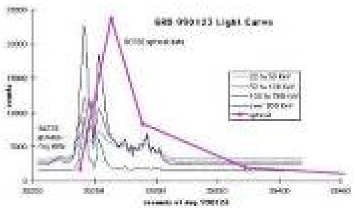
A.J.Burgasser (Caltech), J.D.Kirkpatrick (IPAC/Caltech), M.E.Brown (Caltech), I.N.Reid (U.Penn), J.E.Gizis (U.Mass), C.C.Dahn & D.G.Monet (USNO, Flagstaff), C.A.Beichman (JPL), J.Liebert (Arizona), R.M.Cutri (IPAC/Caltech), M.F.Skrutskie (U.Mass)

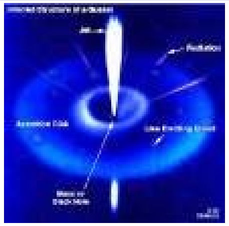
The 2MASS Project is a collaboration between the University of Massachusetts and IPAC

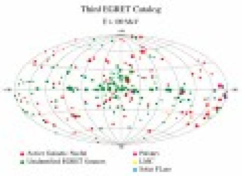
Data and images courtesy Alex Szalay, John Hopkins University

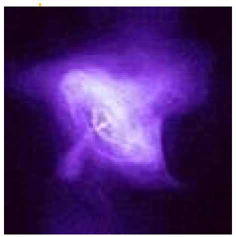
MAGIC telescope and VO

- **Ground based Air Cerenkov Telescope 17 m diameter**
- **Physics Goals:**
  - Origin of VHE Gamma rays
  - Active Galactic Nuclei
  - Supernova Remnants
  - Unidentified EGRET sources
  - Gamma Ray Burst
- **MAGIC II will come 2007**
- **Grid added value**
  - Enable “(e-)scientific” collaboration between partners
  - Enable the cooperation between different experiments
  - Enable the participation on Virtual Observatories







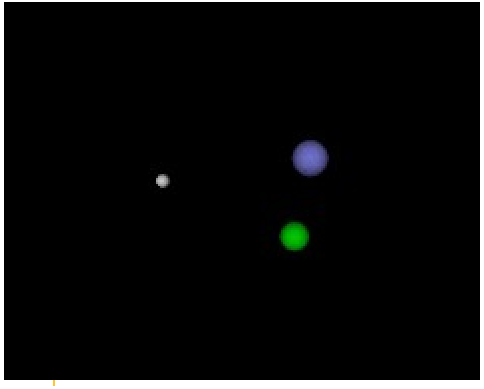


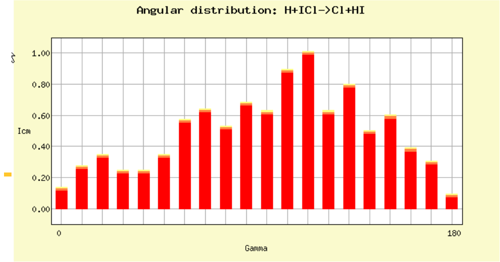
Computational Chemistry

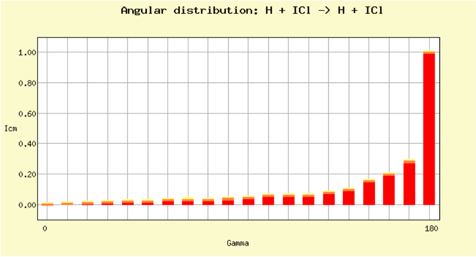
The Grid Enabled Molecular Simulator (GEMS)

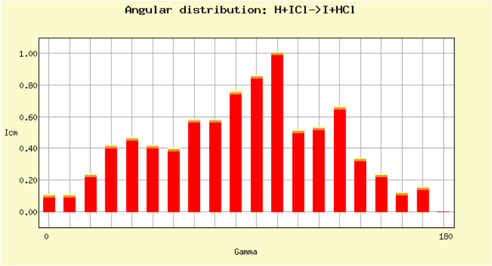
- Motivation:
  - Modern computer simulations of biomolecular systems produce an abundance of data, which could be reused several times by different researchers.
    → data must be catalogued and searchable

- GEMS database and toolkit:
  - autonomous storage resources
  - metadata specification
  - automatic storage allocation and replication policies
  - interface for distributed computation

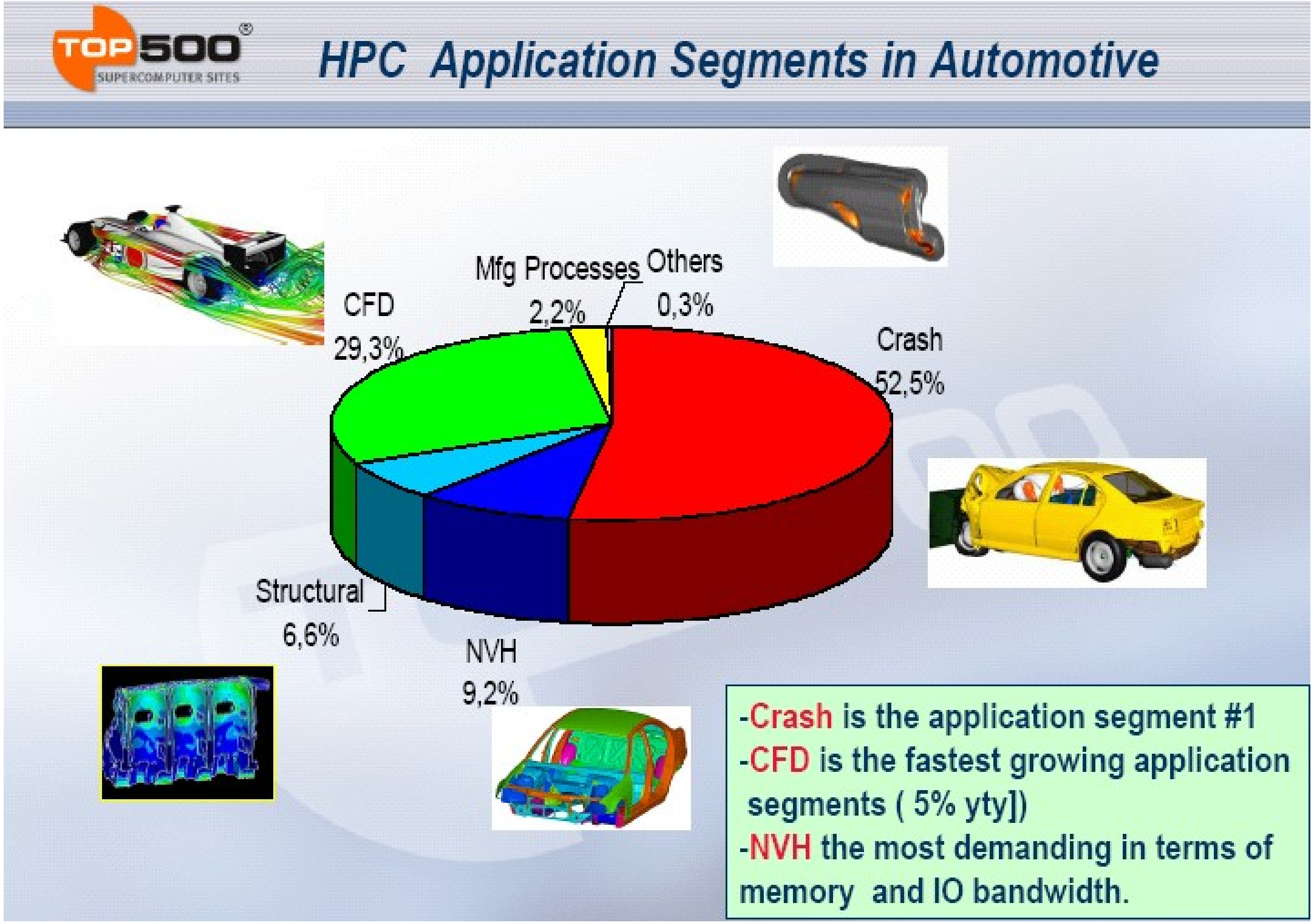








Automotive Industry: Grid potential



HPC Application Segments in Automotive

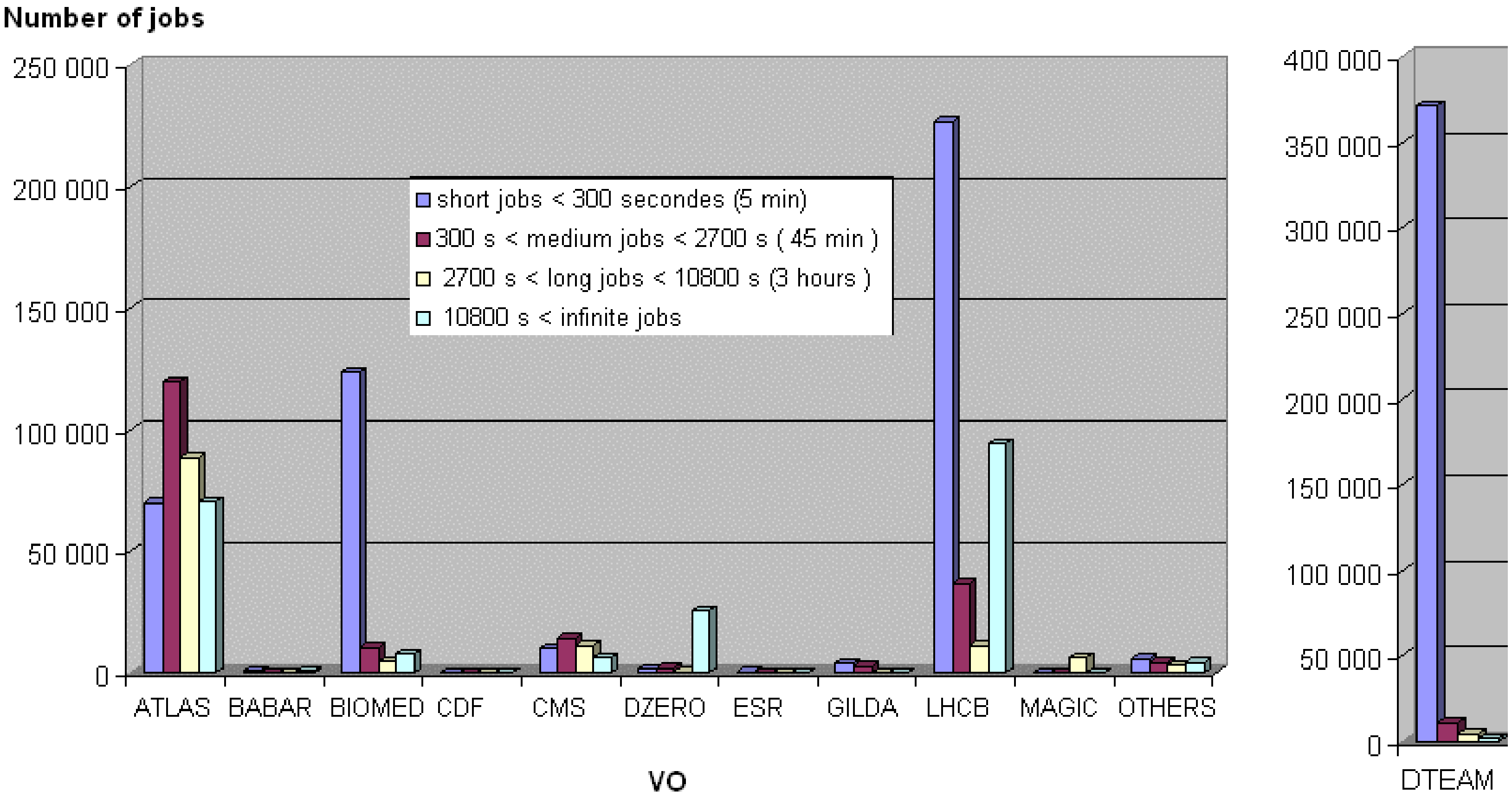
-Crash is the application segment #1

-CFD is the fastest growing application segments (5% yty])

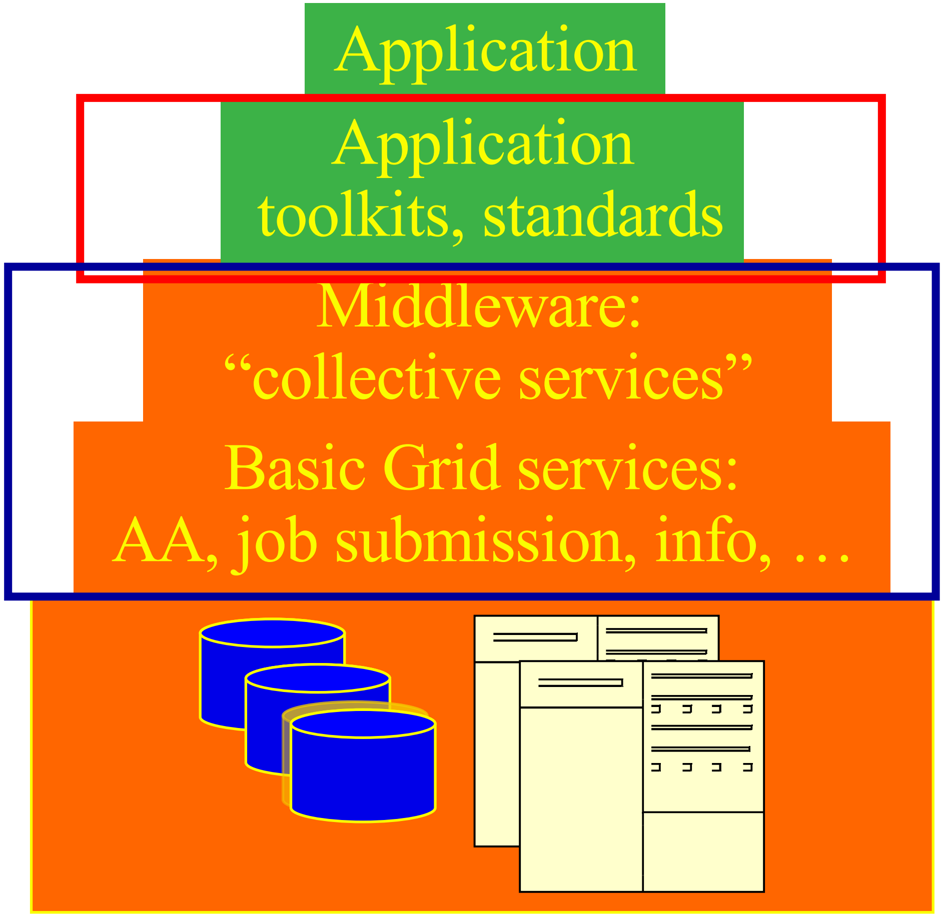
-NVH the most demanding in terms of memory and IO bandwidth.

EGEE infrastructure usage

Average job duration January 2005 – June 2005 for 10 major VOs



Future: Empowering VOs



Application

Application toolkits, standards

Middleware: “collective services”

Basic Grid services: AA, job submission, info, …

VO-specific developments:

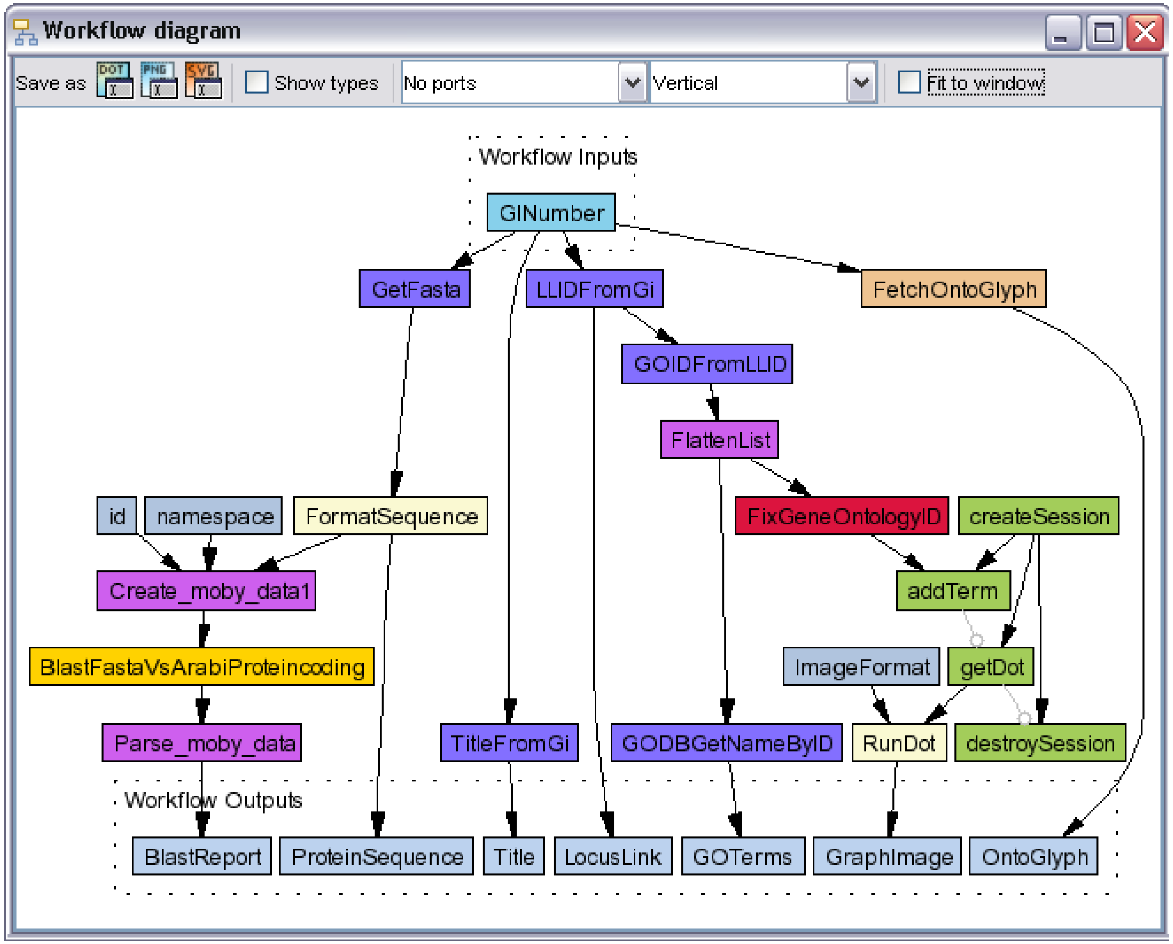
- Portals
- Virtual Research Environments
- Semantics, ontologies
- Workflow
- Registries of VO services

Production grids provide these services.

Develop above these to empower non-UNIX specialists!

Future: Workflow features

- Taverna in MyGrid http://www.mygrid.org.uk/
- “allows the e-Scientist to describe and enact their experimental processes in a structured, repeatable and verifiable way”
- GUI
- Workflow language
- Enactment engine



egee

Enabling Grids for E-sciencE

National Grid initiatives

CroGrid

E-sciencE conclusions...

- We live in a time where the computing infrastructure makes **distributed computation more attractive** than centralised computation – at least for some applications
- Many scientific disciplines, application areas and organisation types create a **demand for a global computing infrastructure**
- **Grid Computing has gained a lot of momentum**, its meaning has started to change
- As explained, this gain in momentum stems from the drastically **increased hardware capabilities and new application types**
- The **theoretical groundwork** for a distributed computing infrastructure has been available since long time – distributed computing and Grid computing is not really a new phenomenon (**only the name is new, plus a couple of facilities**)
- **The challenge in building this infrastructure lies in the large scale and in the need for standardisation and bridge building**

If “The Grid” vision leads us here…

… then where are we now?

Q & A