



Enabling Grids for E-scienceE

Application Building on LCG & EGEE Grids

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www.eu-egEE.org



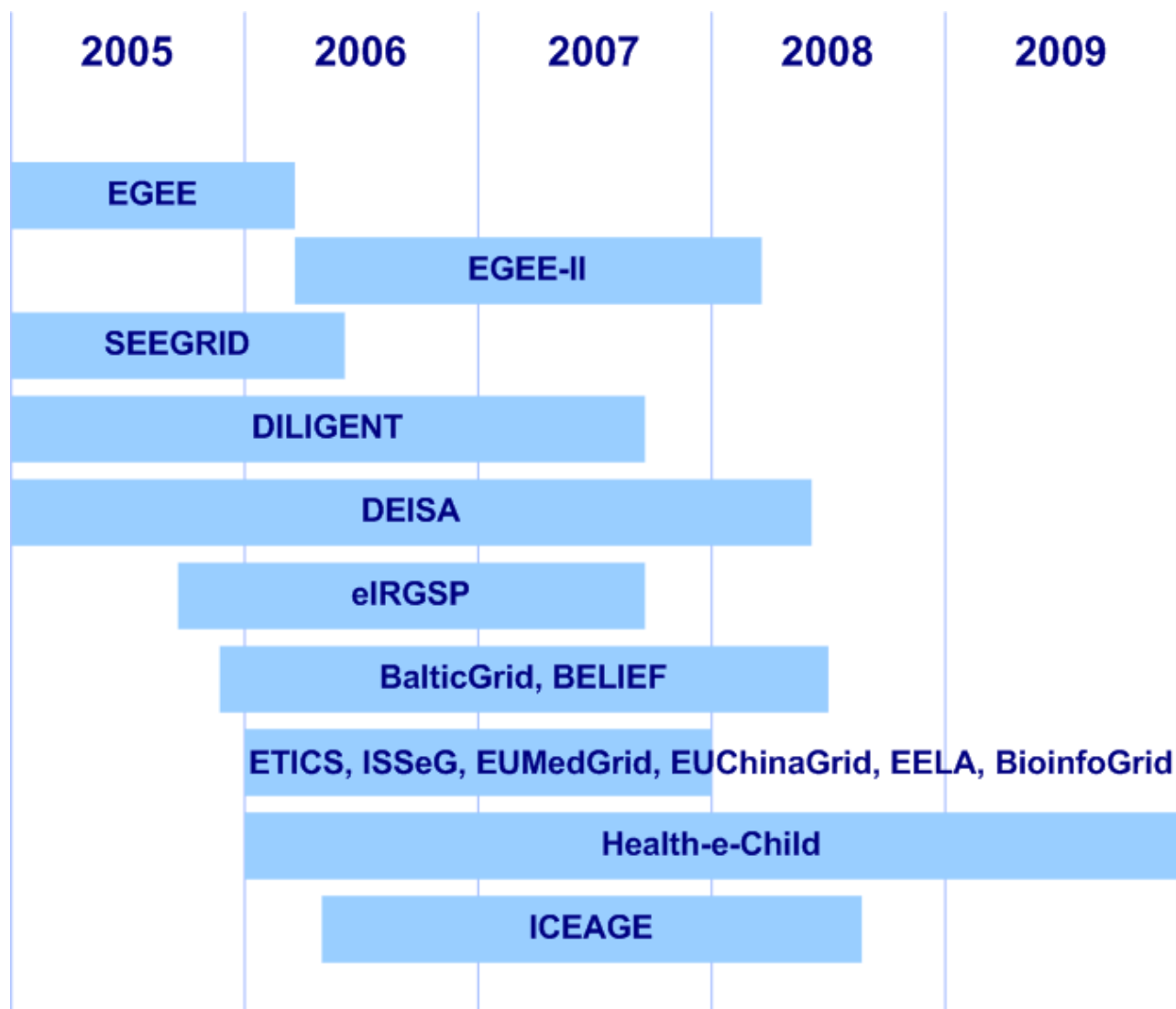


Grid Projects Collaborating in LHC Computing Grid



EGEE Operations Information	
Active Sites	~180
Available CPU	~30000
Available Storage (TB)	~8PBytes





- ▶ **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

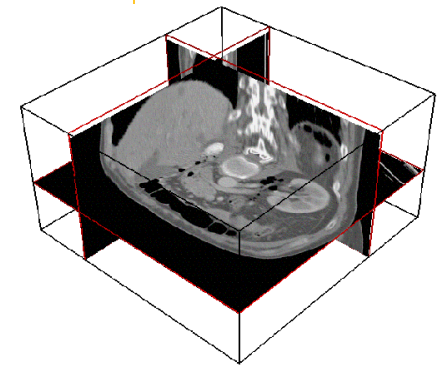
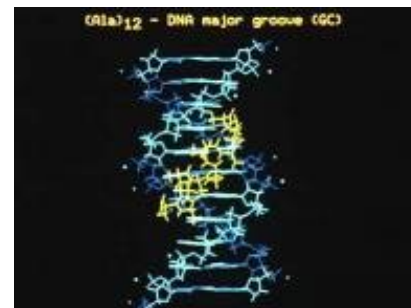
▶ High-Energy Physics (HEP)

- 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)

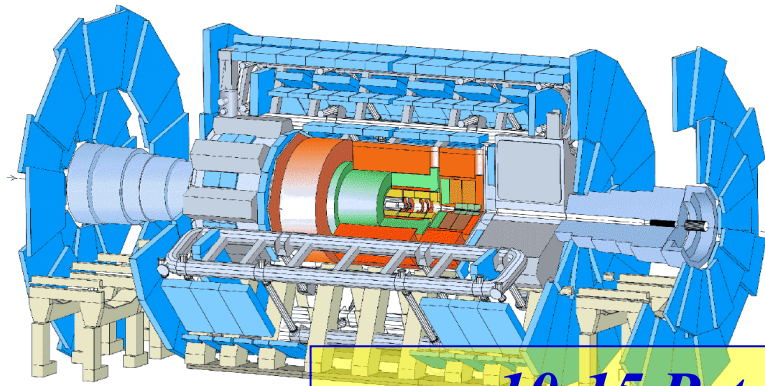


▶ Biomedical Applications

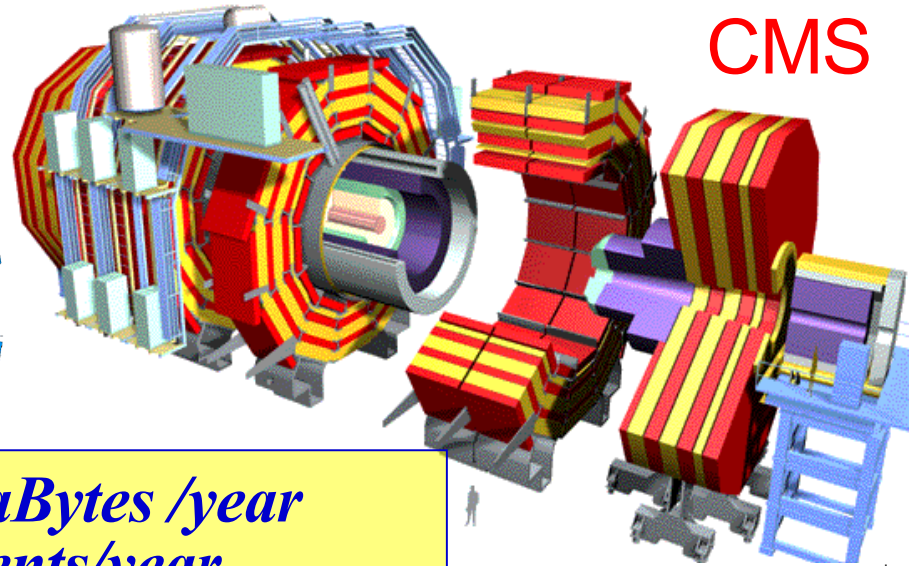
- Similar computing and data storage requirements
- Major additional challenge: **security & privacy**



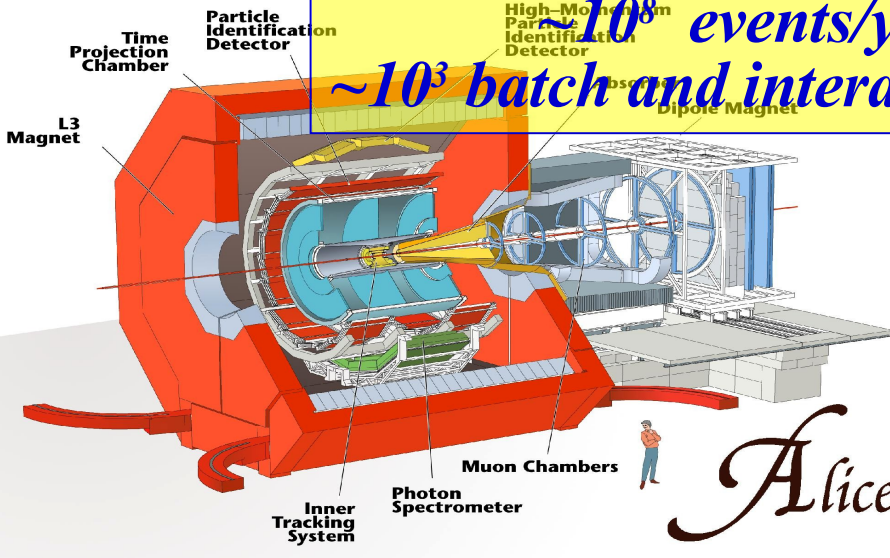
ATLAS



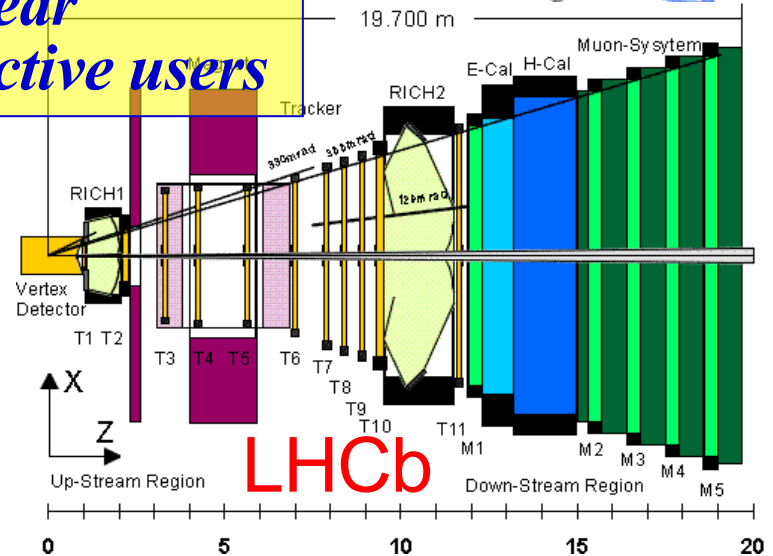
CMS



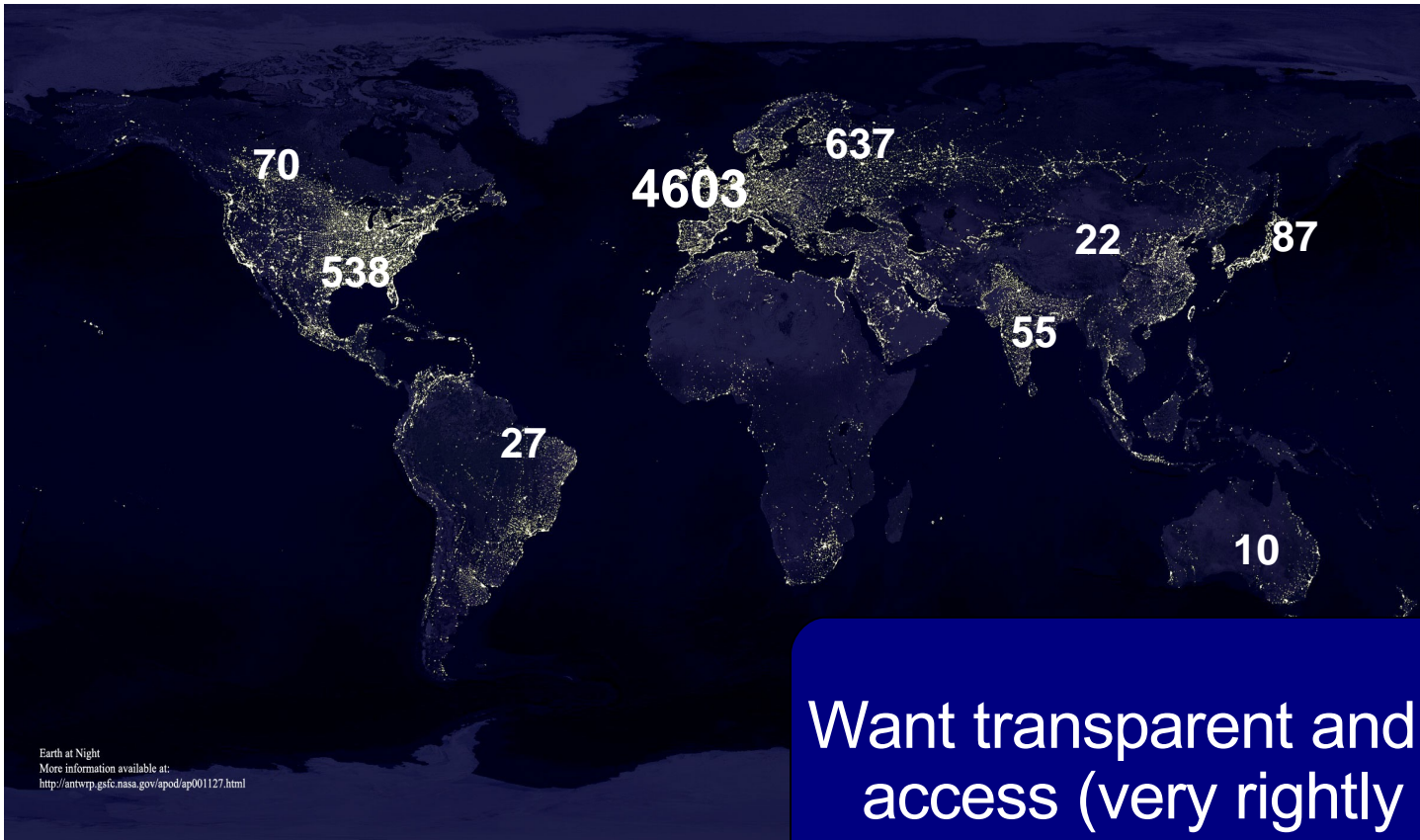
~10-15 PetaBytes /year
~10⁸ events/year
~10³ batch and interactive users



Alice



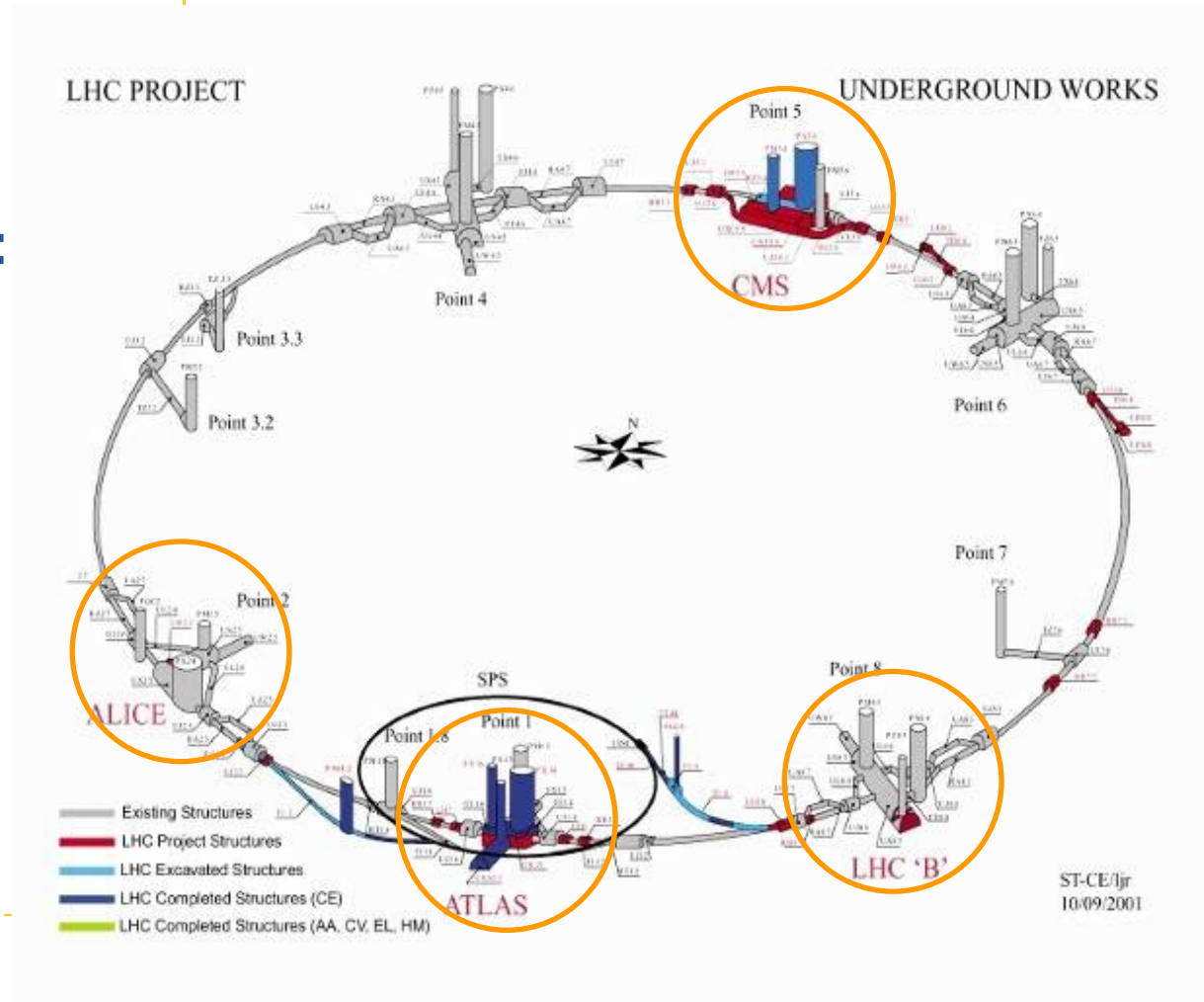
Over 6000 LHC Scientists world wide

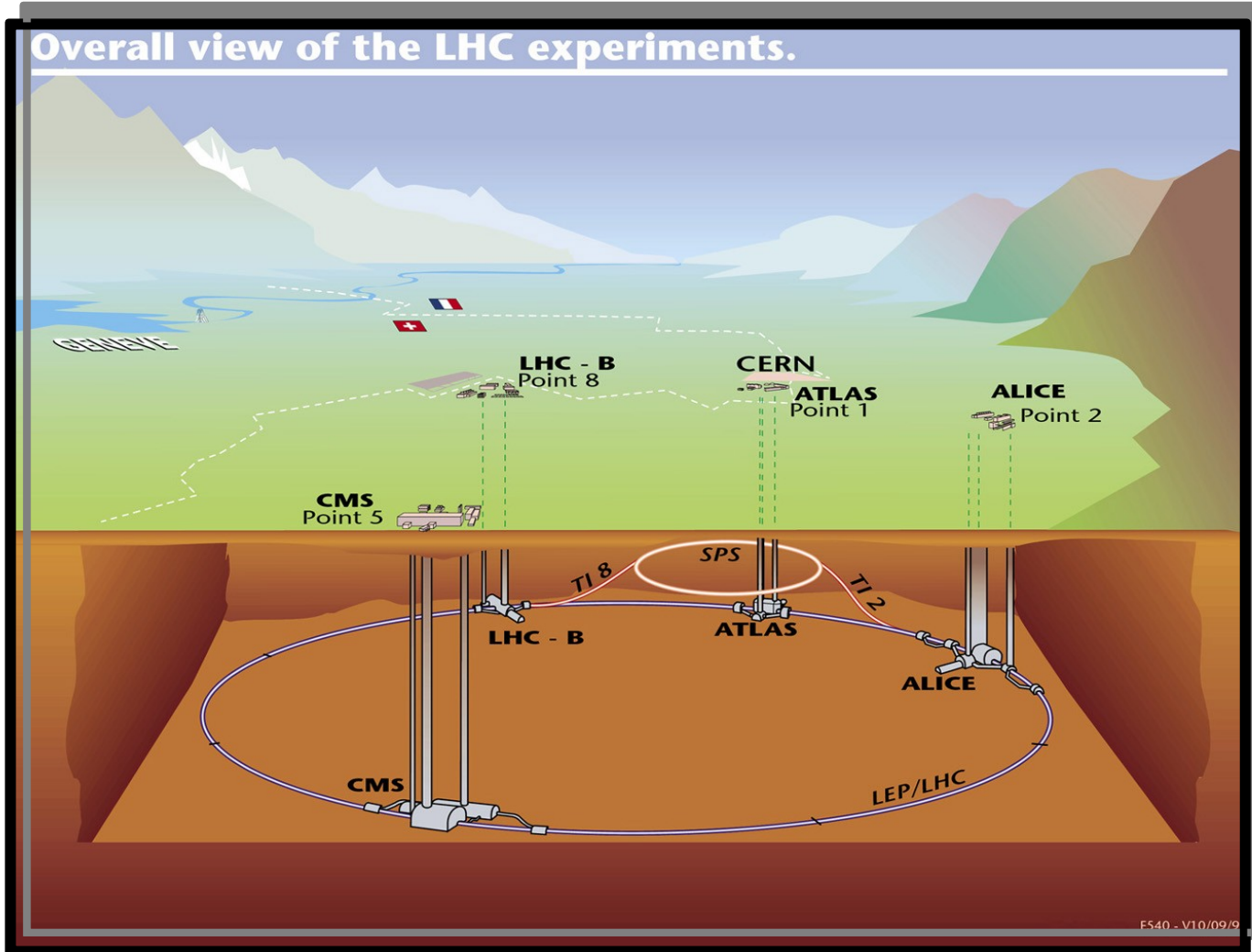


Europe: 267 Institutes, 4603 Users
 Other: 208 Institutes, 1632 Users

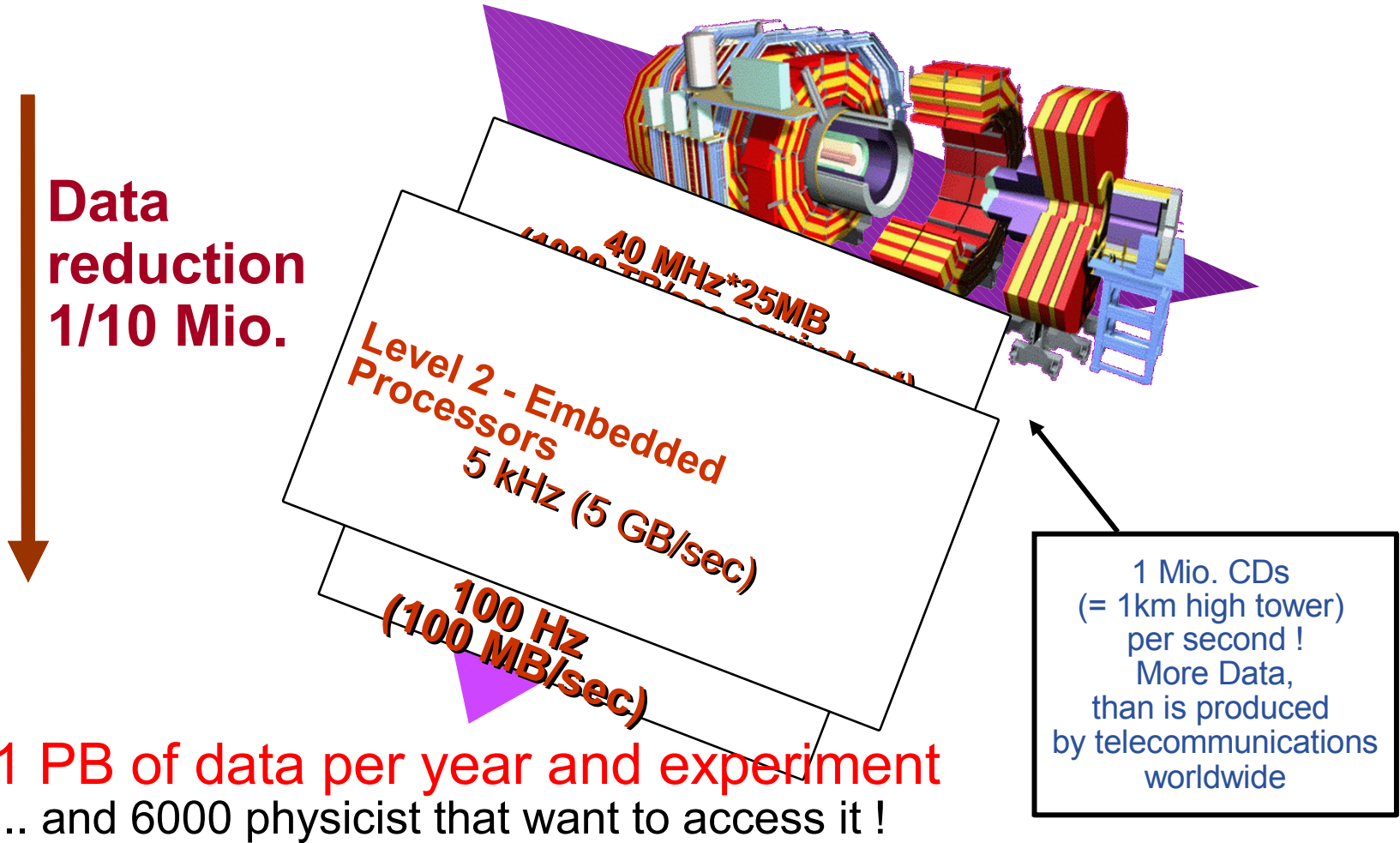
Want transparent and quick access (very rightly so). Interested more in physics results, than computing revolutions

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





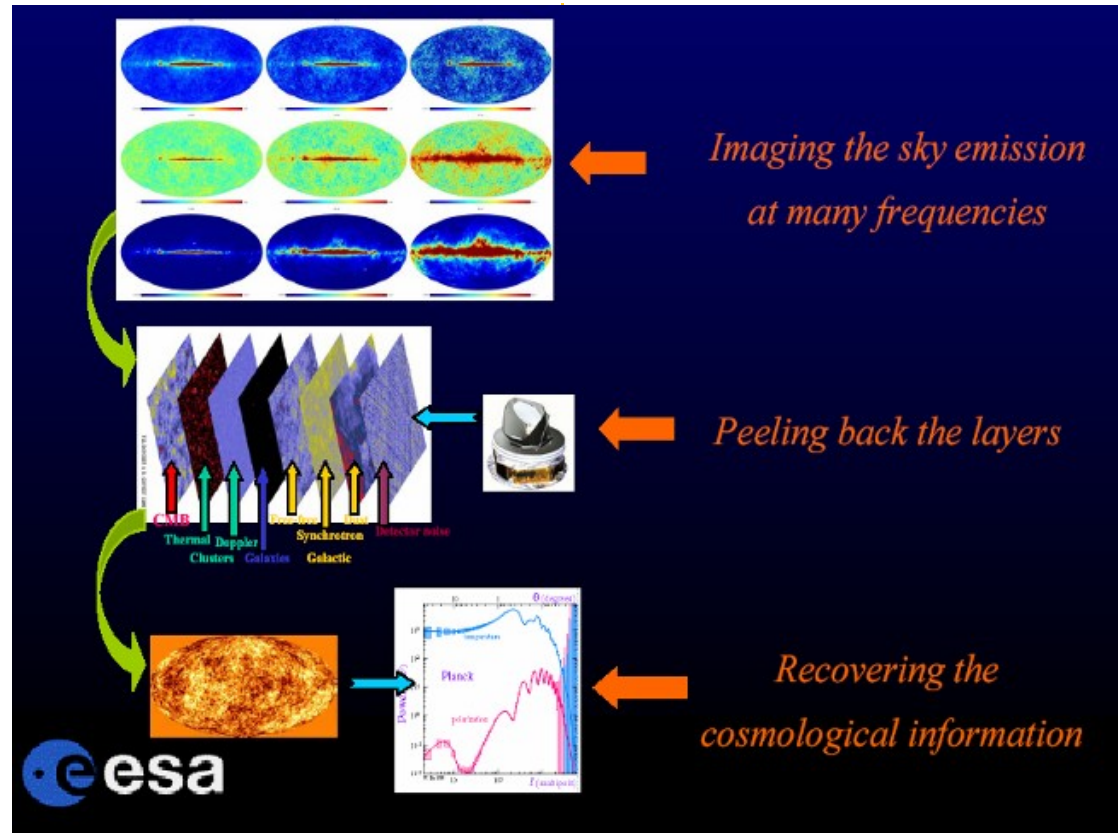
LHC, the CMS detector



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

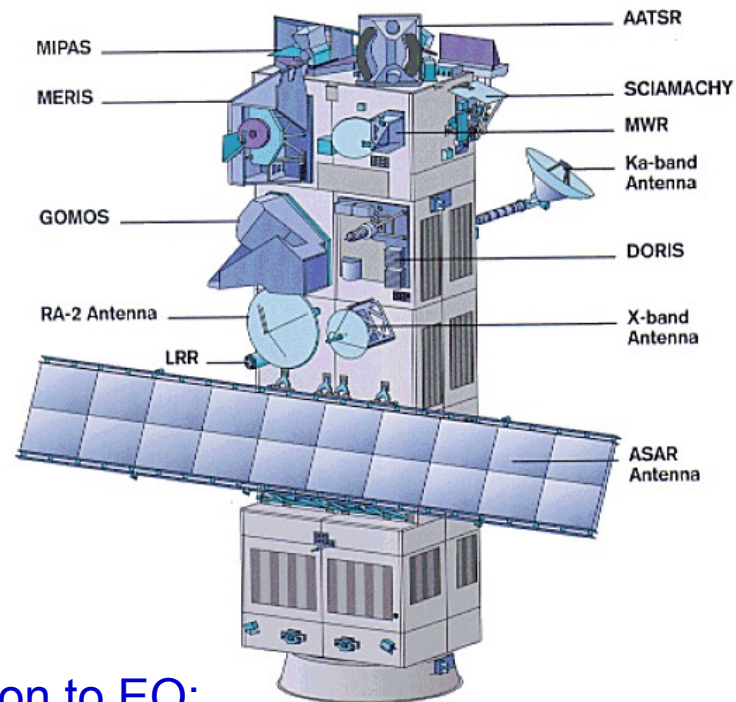
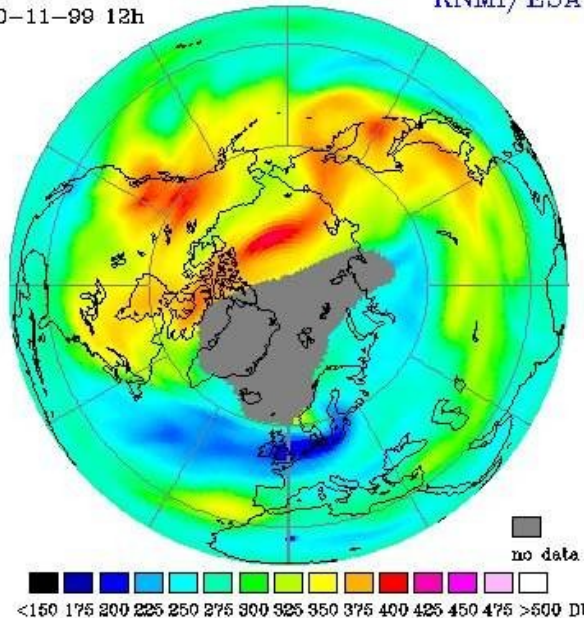
- ▶ **Complex data structure**
 - data handling important

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



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

Assimilated GOME total ozone
30-11-99 12h
KNMI/ESA



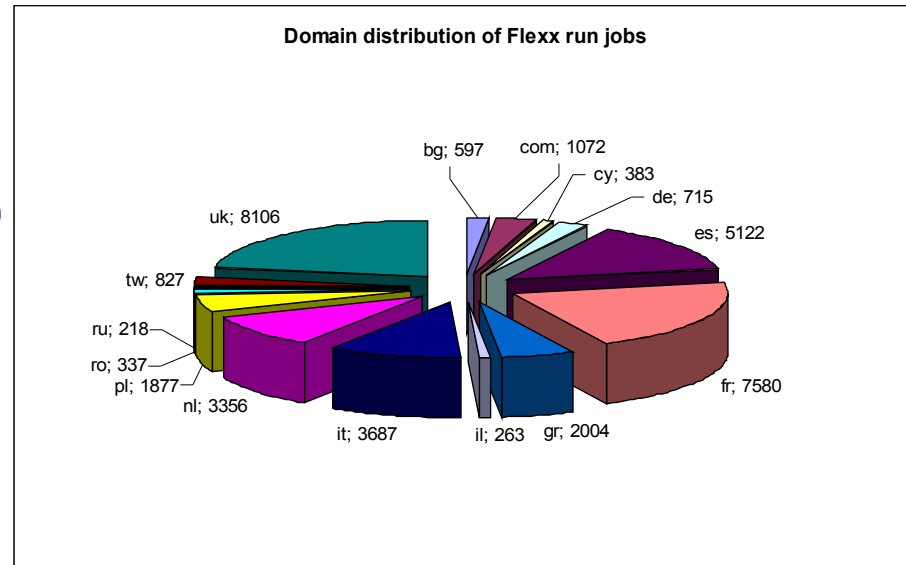
Grid contribution to EO:
Enhance the ability to access high level products
Allow reprocessing of large historical archives
Improve Earth science complex applications
(data fusion, data mining, modelling ...)

Federico.Carminati , EU review presentation, 1 March 2002

- ▶ 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 on the grid!**



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>

▶ **Earth Observations by Satellite**

- Ozone profiles

▶ **Solid Earth Physics**

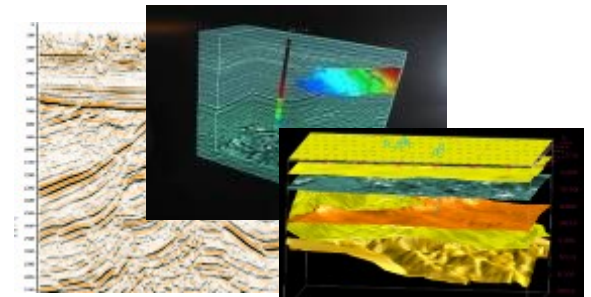
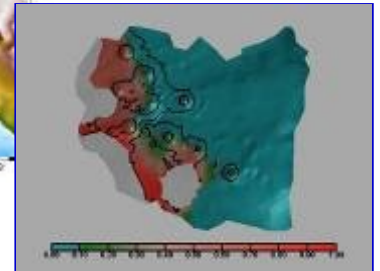
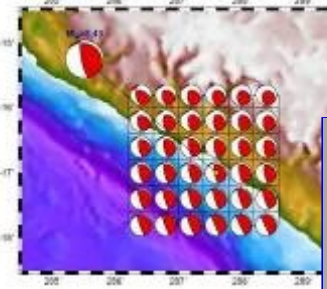
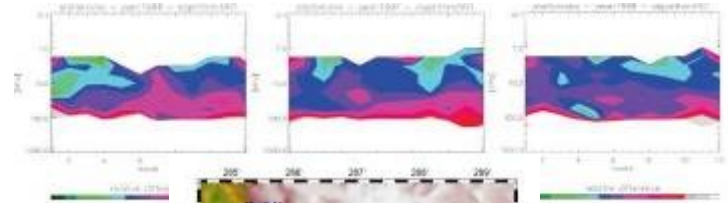
- Fast Determination of mechanisms of important earthquakes

▶ **Hydrology**

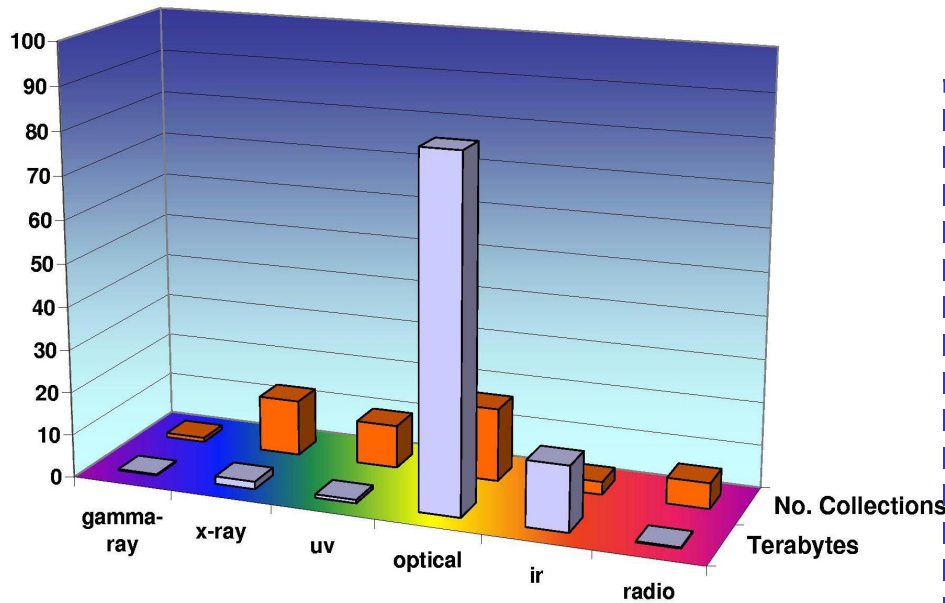
- Management of water resources in Mediterranean area (SWIMED)

▶ **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**



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

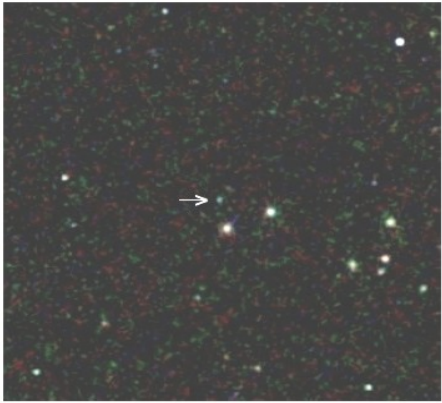
Doubling every 12 months

Largest catalogues near 1B objects

2MASSW J1217-03

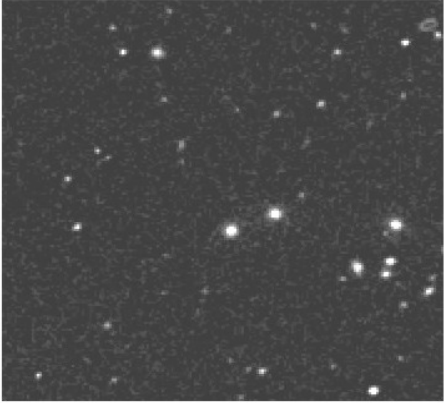
A methane (T-type) dwarf in the constellation Virgo

The near-infrared view




2MASS Composite JHK_s Atlas Image

The optical view



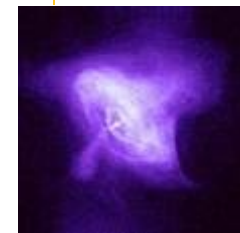
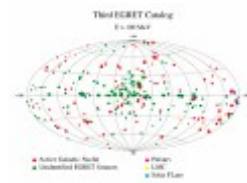
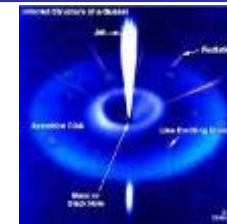
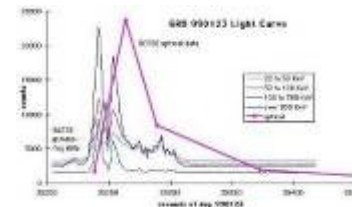
Palomar Digitized Sky Survey



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

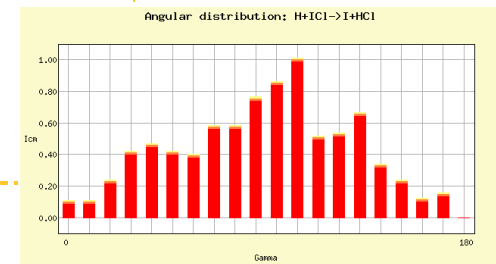
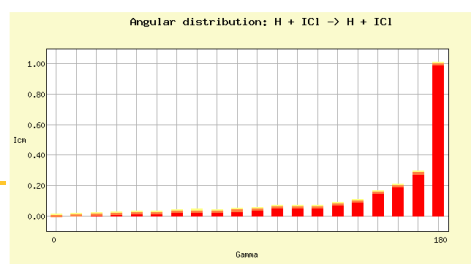
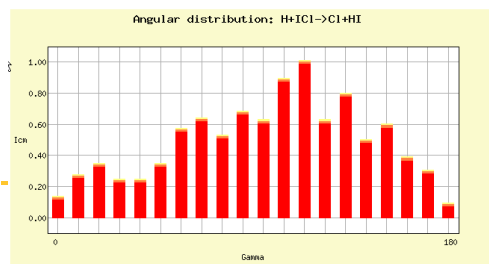
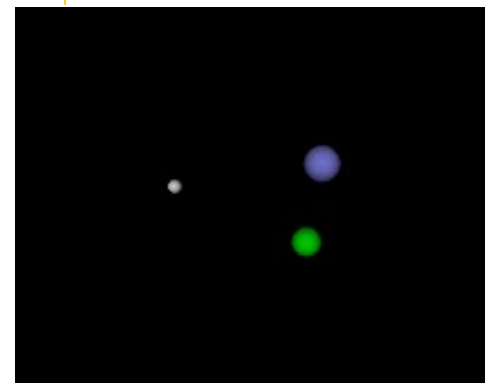
Data and images courtesy Alex Szalay, John Hopkins University

- ▶ **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



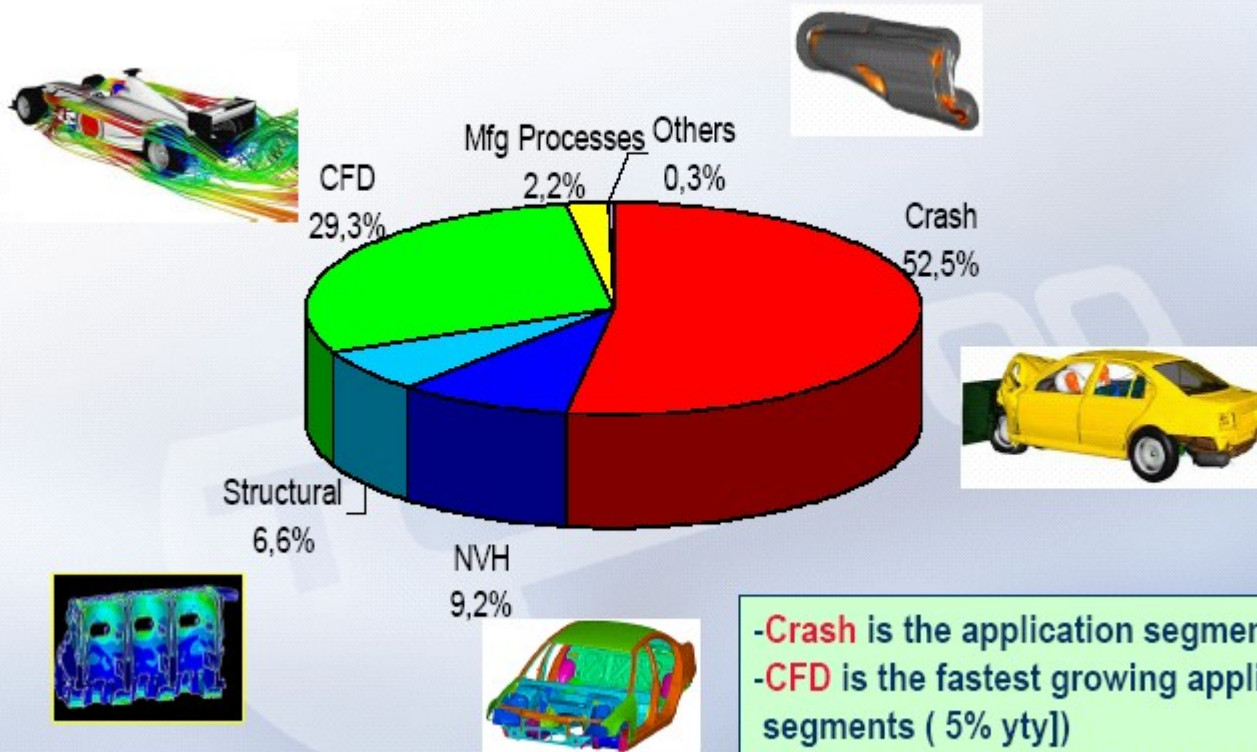
► The Grid Enabled Molecular Simulator (GEMS)

- 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



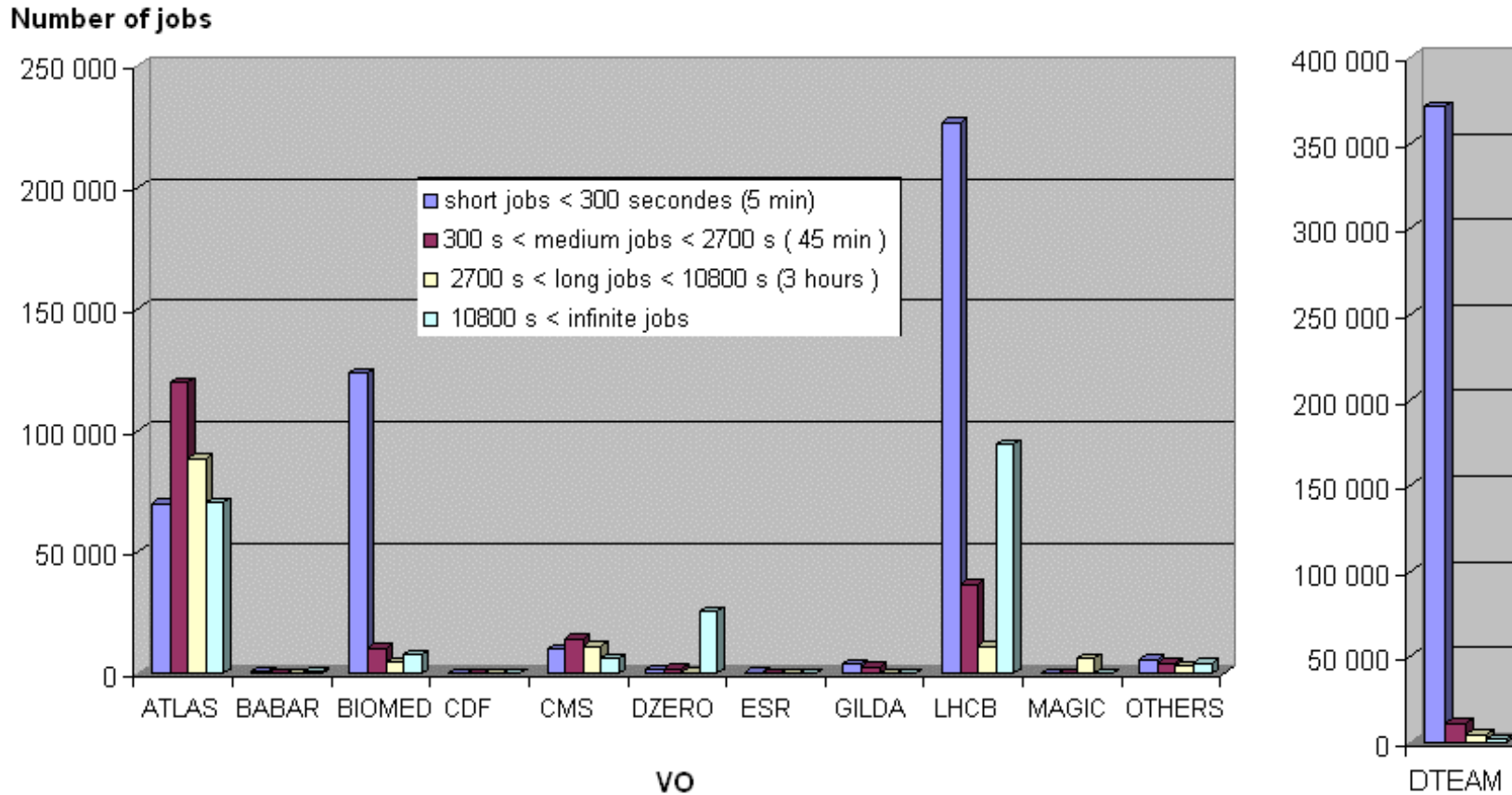


HPC Application Segments in Automotive



- 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.

▶ Average job duration January 2005 – June 2005 for ten major VOs

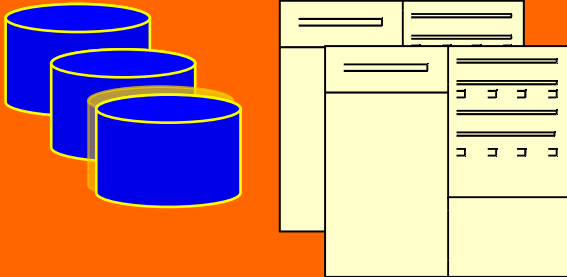


Application

Application
toolkits, standards

Middleware:
“collective services”

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



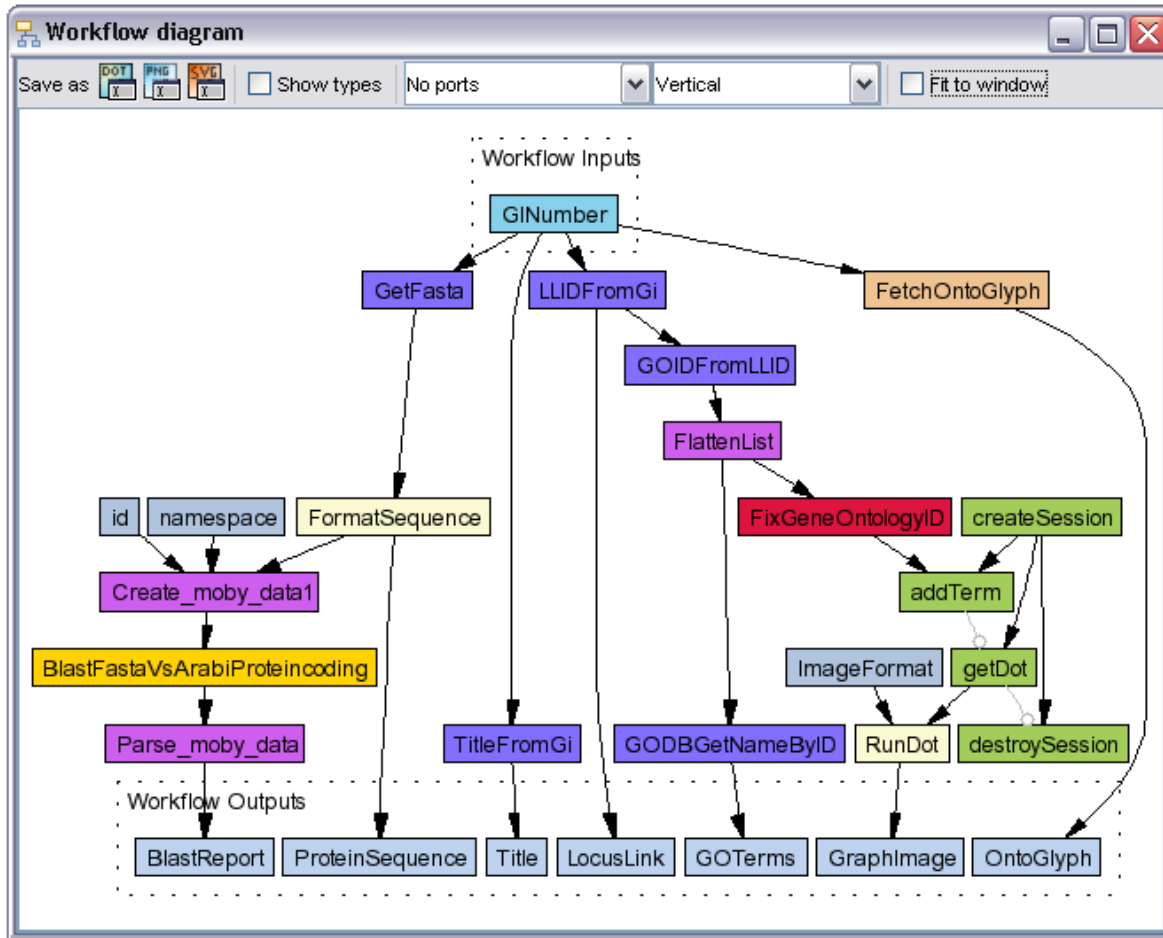
VO-specific developments:

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

Production grids provide these services.

Develop above these to empower non-UNIX specialists!

- ▶ 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





CroGrid



- ▶ 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?

