EGEE Tutorial

Welcome!!

www.eu-egee.org

Information Society

- http://agenda.cern.ch/fullAgenda.php?ida=a061960

What is Grid Computing?

Mike Mineter
Training Outreach and Education
National e-Science Centre, UK

mjm@nesc.ac.uk

Contents

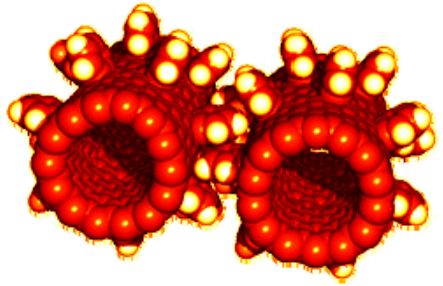
- **Introduction to**
  - e-Infrastructure
  - e-Research and e-Science
- **Some examples from the EGEE project**
  - EGEE: Enabling Grids for E-sciencE
  - EGEE is an EU-funded project that is running the largest international Grid
- **Grid concepts**
- **Grids - Where are we now?**

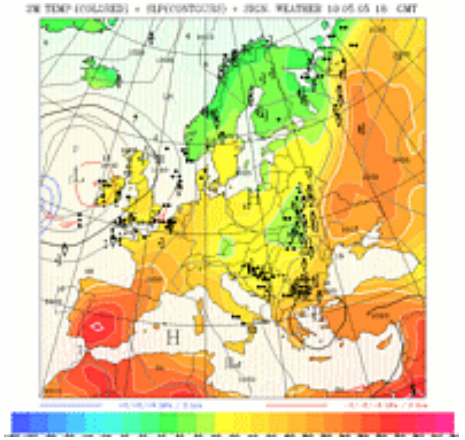
Computing intensive science

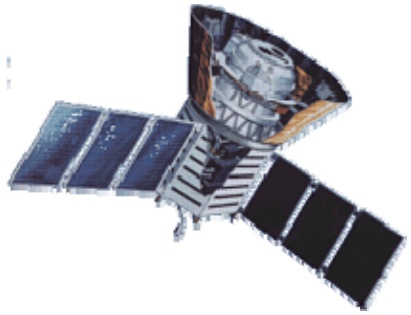
- **Many vital challenges require community effort**
  - Fundamental properties of matter
  - Genomics
  - Climate change
  - Medical diagnostics
- **Research is increasingly digital, with increasing amounts of data**
- **Computation ever more demanding**

e.g.: experimental science uses ever more sophisticated sensors

  - Huge amounts of data
  - Serves user communities around the world
  - International collaborations







e-Infrastructure

*'e-Science is about global collaboration in key areas of science, and the **next generation of infrastructure** that will enable it.'*

John Taylor

Director General of Research Councils

Office of Science and Technology

UK

e-Infrastructure = Networks + Grids

– *Networks connect resources*

– *Grids enable "virtual computing" across administrative domains*

e-Science: the invitation

Collaborative
"virtual computing"

Sharing data, computers, software
Enabled by Grids:
National, regional (BalticGrid)
International: EGEE grid

Improvised cooperation

Email
File exchange
ssh access to run programs
Enabled by networks:
national, regional and
International: GEANT

People with shared goals

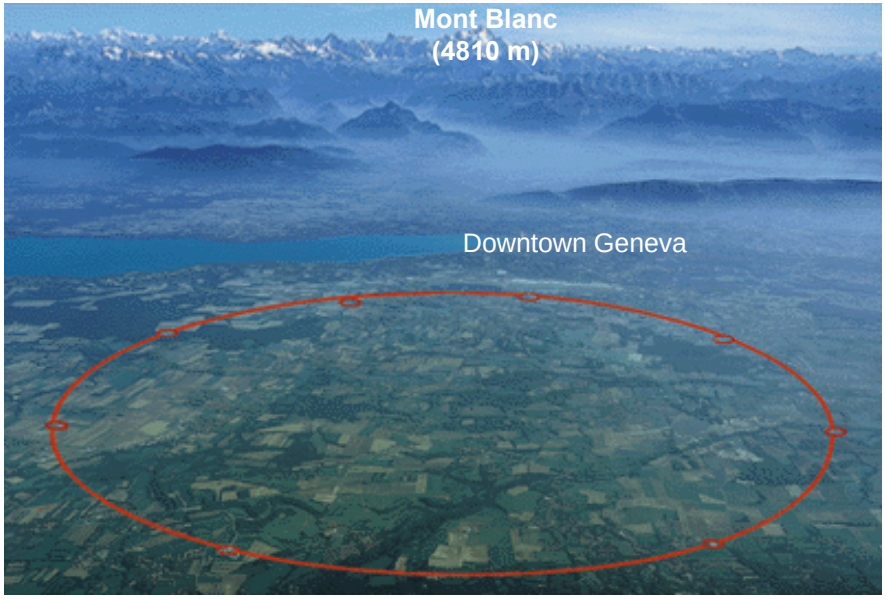
"e-Science" and "e-Research"

- **Collaborative research that is made possible by the sharing across the Internet of resources (data, instruments, computation, people's expertise...)**
  - Crosses organisational boundaries
  - Often very compute intensive
  - Often very data intensive
  - Sometimes large-scale collaboration
- **Early examples were in science: "e-science"**
- **Relevance of "e-science technologies" to new user communities (social science, arts, humanities…) led to the term "e-research"**

Particle Physics

- **Large amount of data**
- **Large worldwide organized collaborations**
- **Computing and data management resources distributed world-wide owned and managed by many different entities**

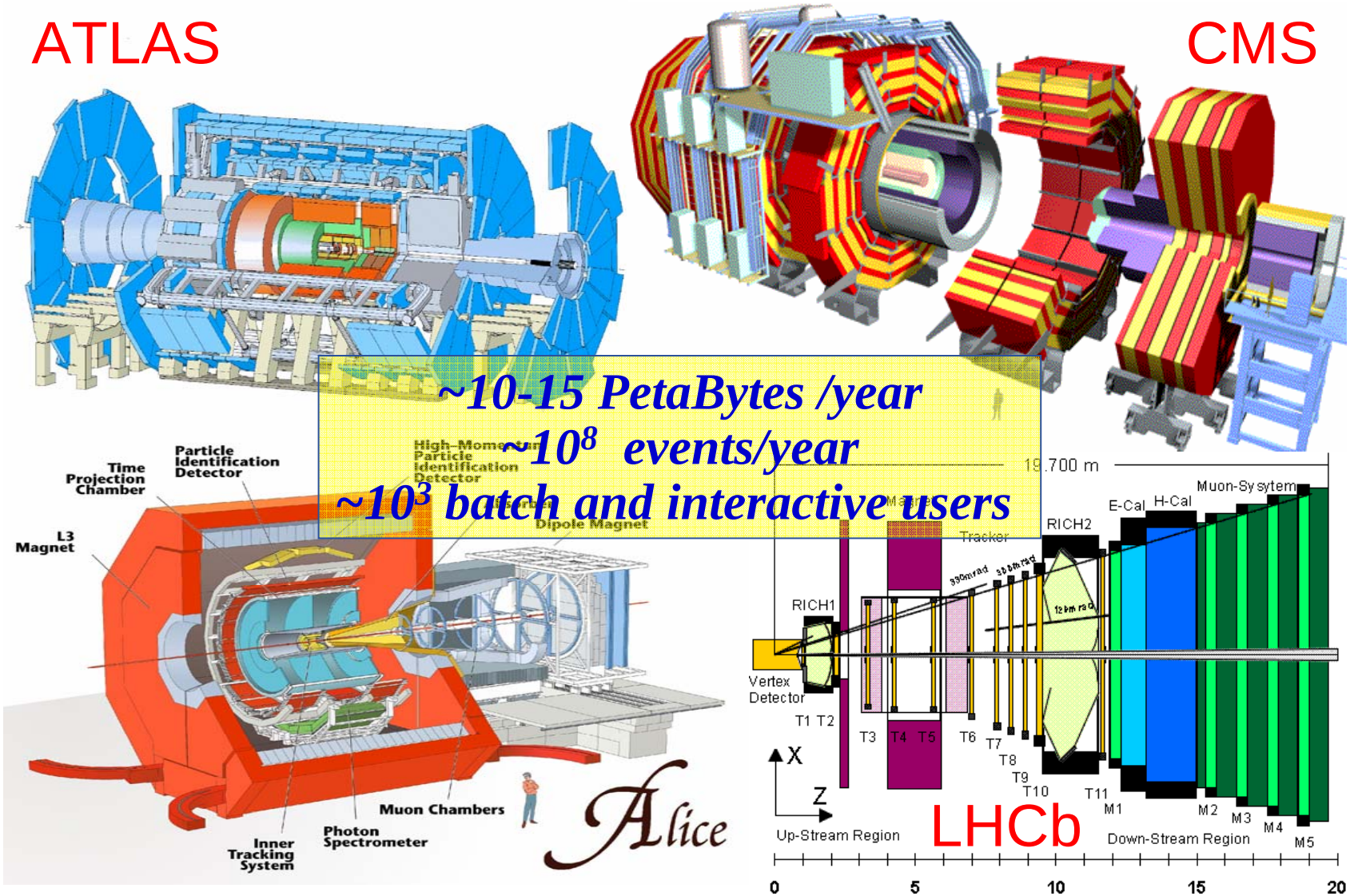
- **Large Hadron Collider (LHC) at CERN in Geneva Switzerland:**
  - One of the most powerful instruments ever built to investigate matter



The LHC Experiments

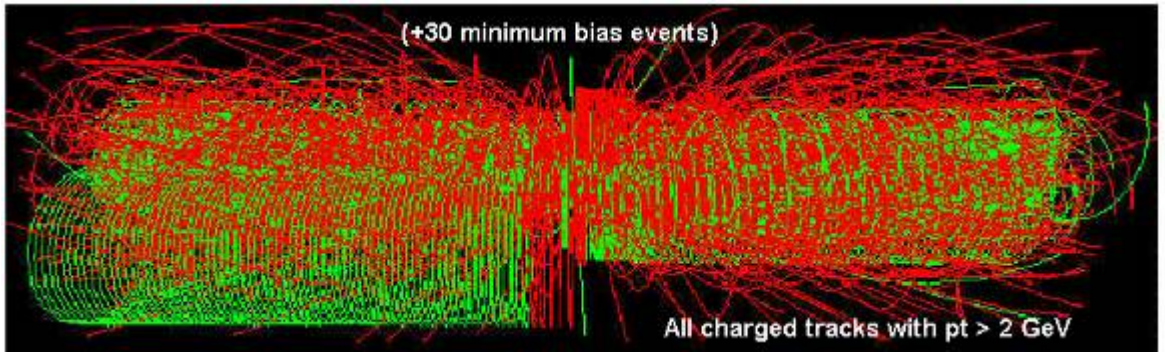
ATLAS

CMS

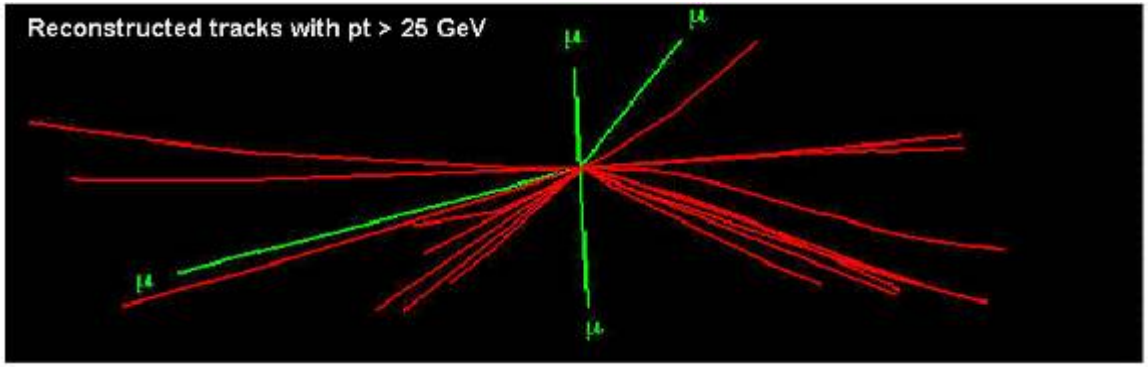


The LHC Data Challenge

Starting from this event



Looking for this "signature"

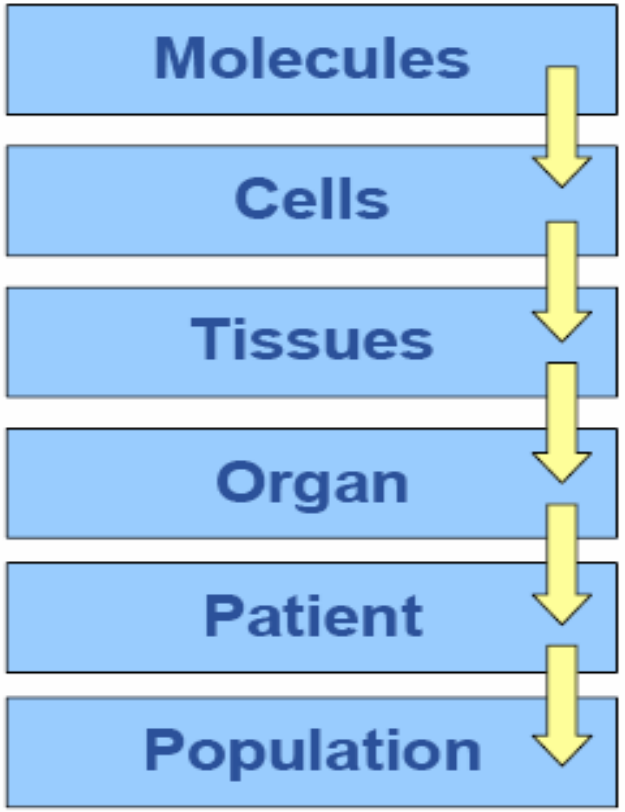


→ **Selectivity: 1 in 10^{13}**

(Like looking for a needle in 20 million haystacks)

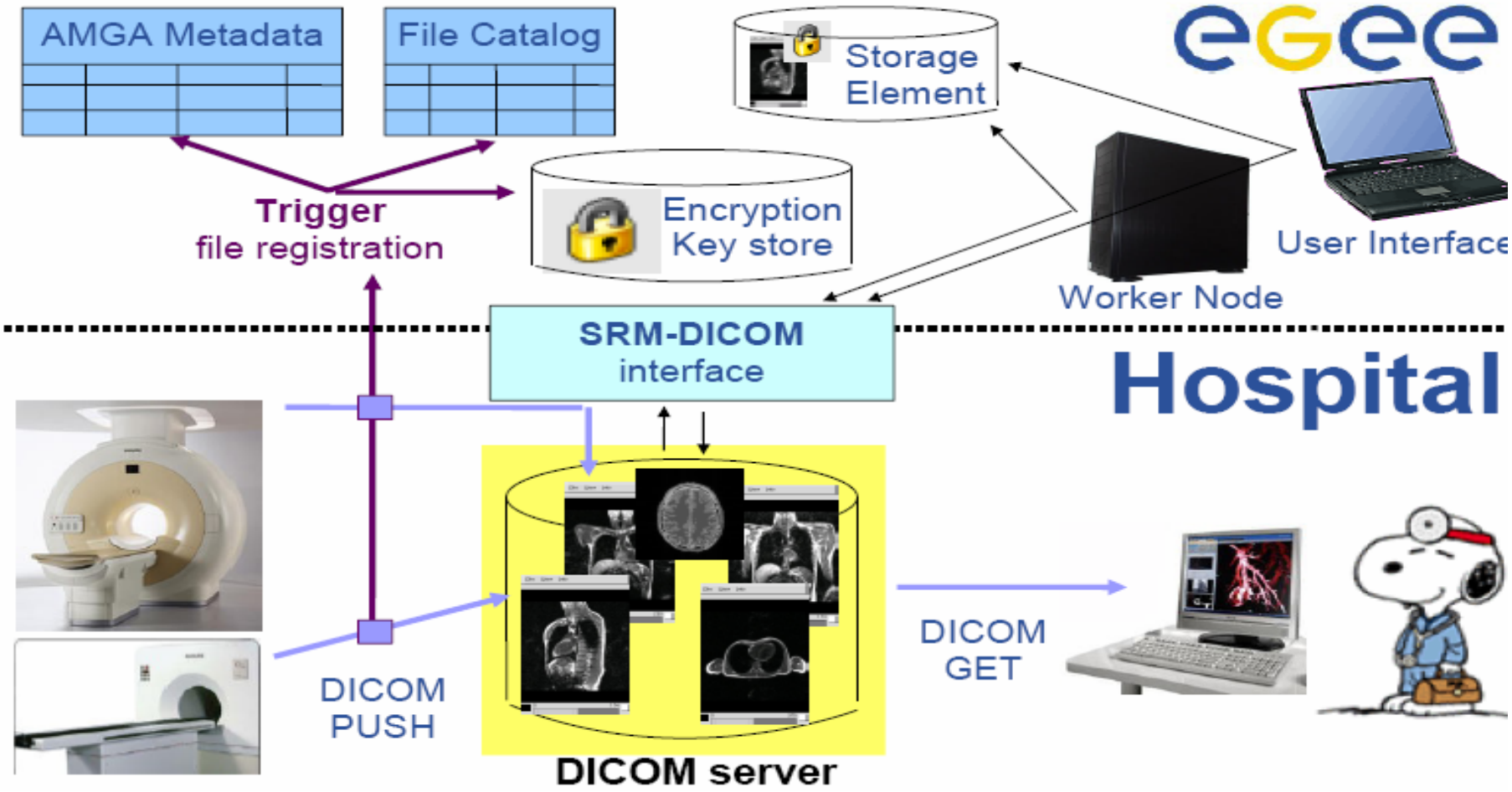
Biomedical applications

- **Bioinformatics**
  - Genomics
  - Proteomics
  - Phylogeny…
- **Medical imaging**
  - Medical imaging
  - Computer Aided Diagnosis
  - Therapy planning
  - Simulation…
- **Life sciences**
  - Drug discovery
  - Epidemiology
  - …



Biomedical community and the Grid, EGEE User Forum, March 1st 2006, I. Magnin

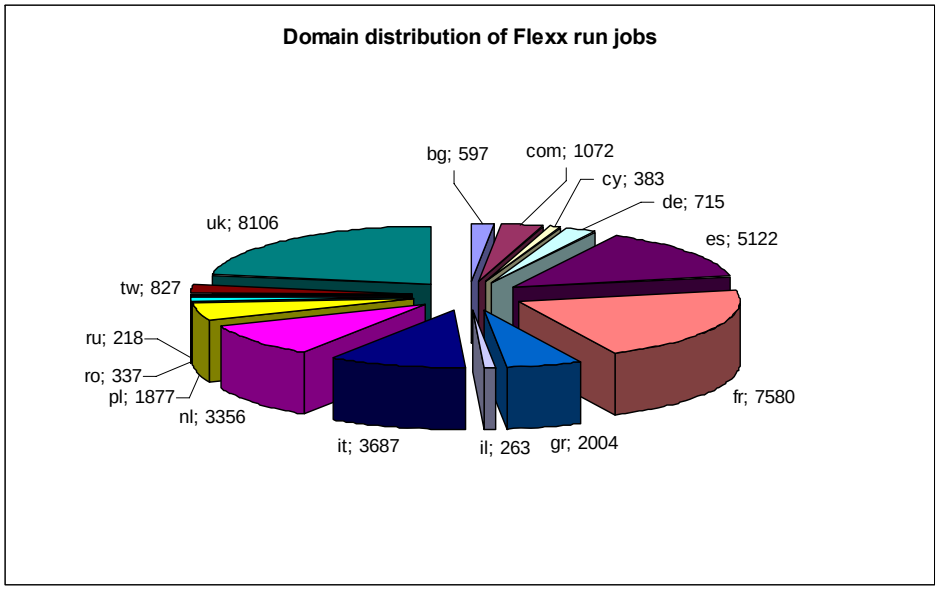
Data management – medical images



Biomedical community and the Grid, EGEE User Forum, March 1st 2006, I. Magnin

First biomedical data challenge: World-wide In Silico Docking On Malaria (WISDOM)

- **Significant biological parameters**
  - two different molecular docking applications (Autodock and 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 to 1000 computers in 15 countries used simultaneously for a total of about 80 CPU years
- **Significant results**
  - Best hits to be re-ranked using Molecular Dynamics

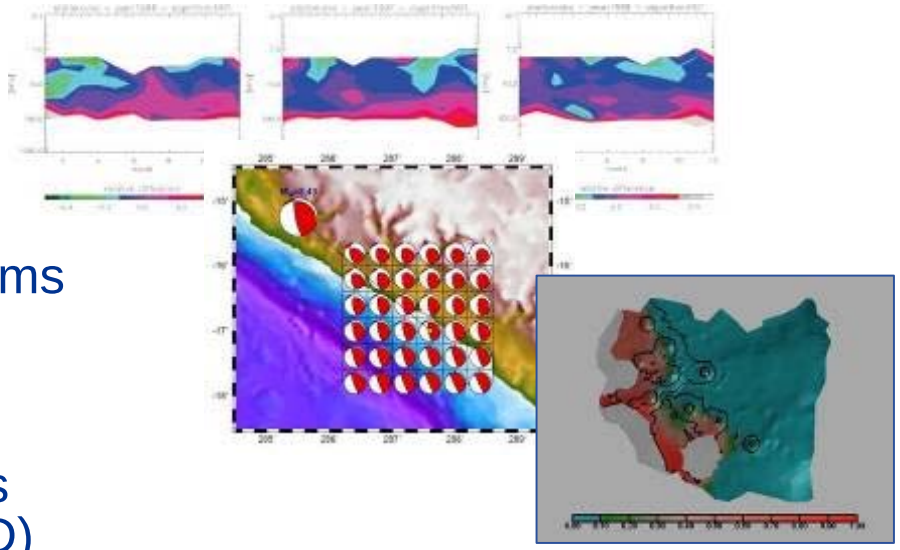


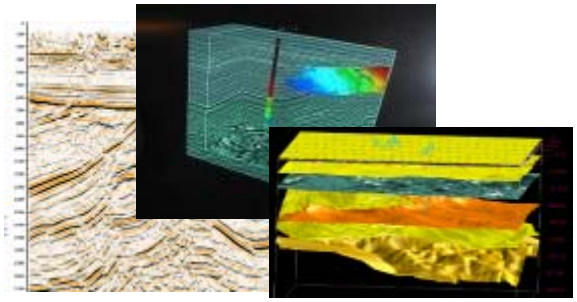
New data challenge in the fall of 2006
New malaria targets
Focus on other neglected diseases
Enlarged collaboration
(possibly including related projects)

Roberto Barbera, 1st EGEE User Forum, CERN, 1st March 2006

Earth sciences applications

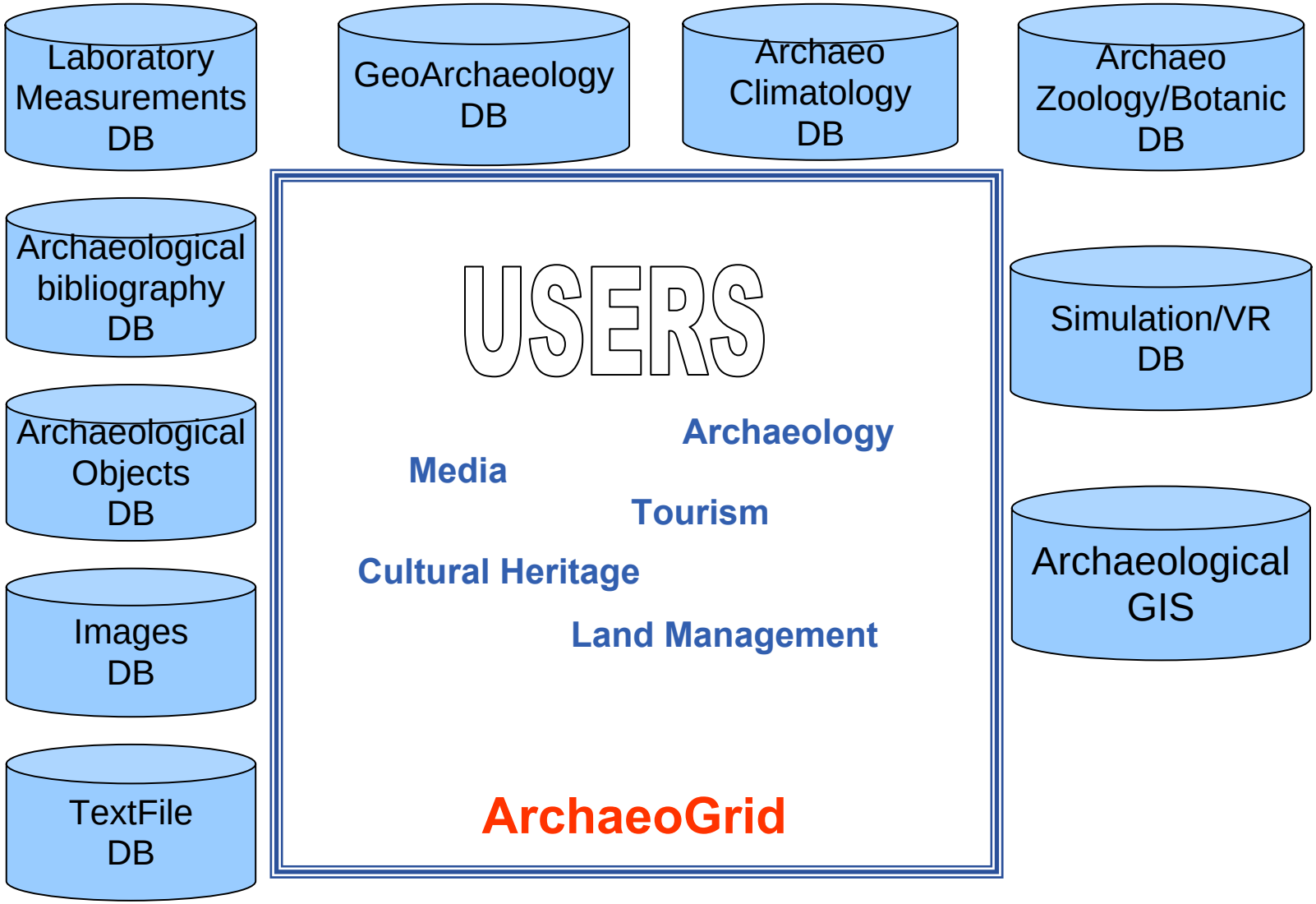
- **Earth Observations by Satellite**
  - Ozone profiles
- **Solid Earth Physics**
  - Fast Determination of mechanisms of important earthquakes
- **Hydrology**
  - Management of water resources in Mediterranean area (SWIMED)
- **Geology**
  - Geocluster: R&D initiative of the Compagnie Générale de Géophysique



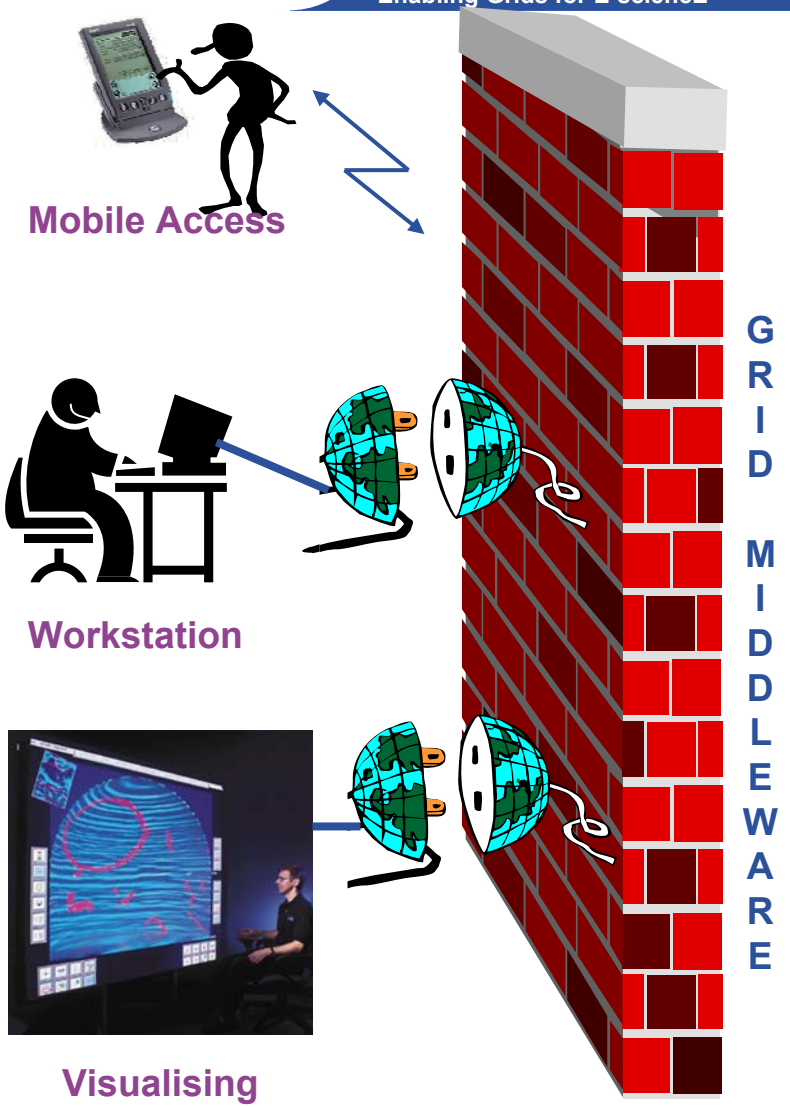


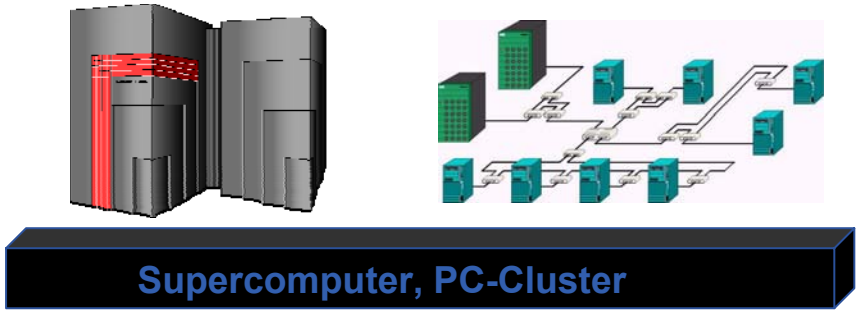
➢ **A large variety of applications ported on EGEE**

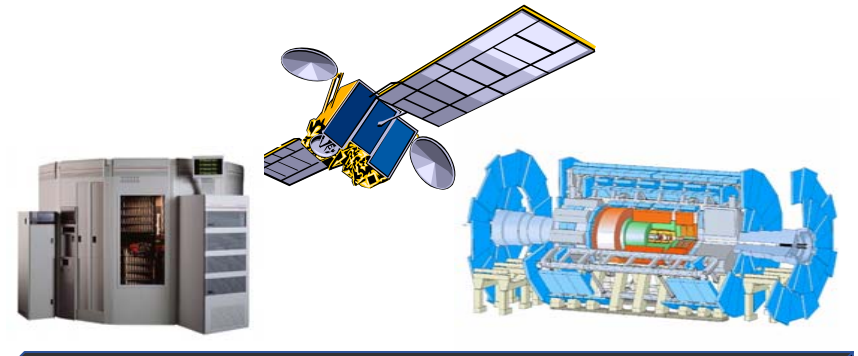
The newest EGEE application: Archaeology

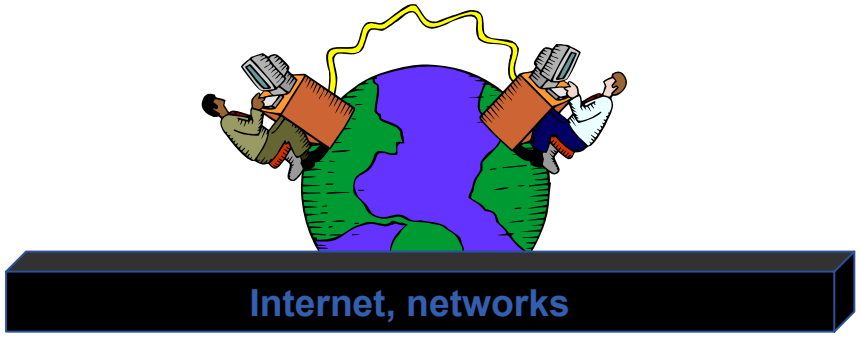


The Grid Metaphor



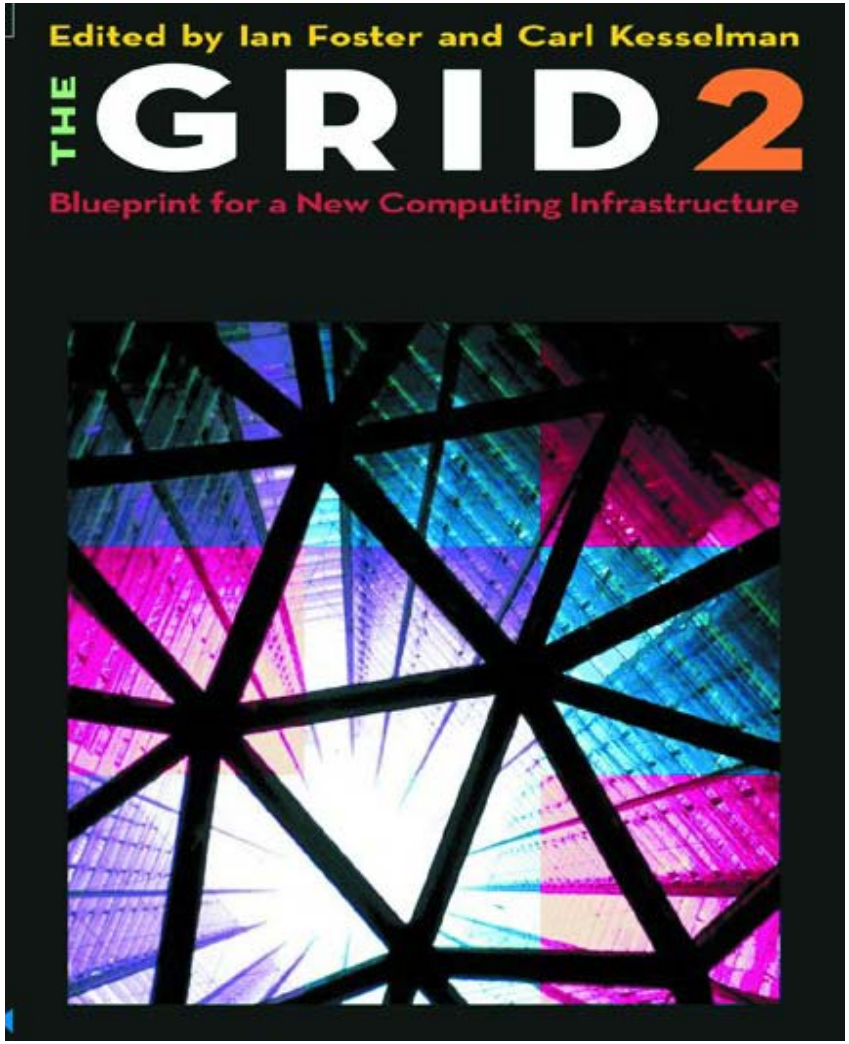






What is Grid Computing?

- **The grid vision is of "Virtual computing" (+ information services to locate computation, storage resources)**
  - Compare: The web: "virtual documents" (+ search engine to locate them)
- **MOTIVATION: collaboration through sharing resources (and expertise) to expand horizons of**
  - Research
  - Commerce – engineering, …
  - Public service – health, environment,…



Grids: a foundation for e-Research

- Enabling a whole-system approach
- A challenge to the imagination
- Effect > Σparts

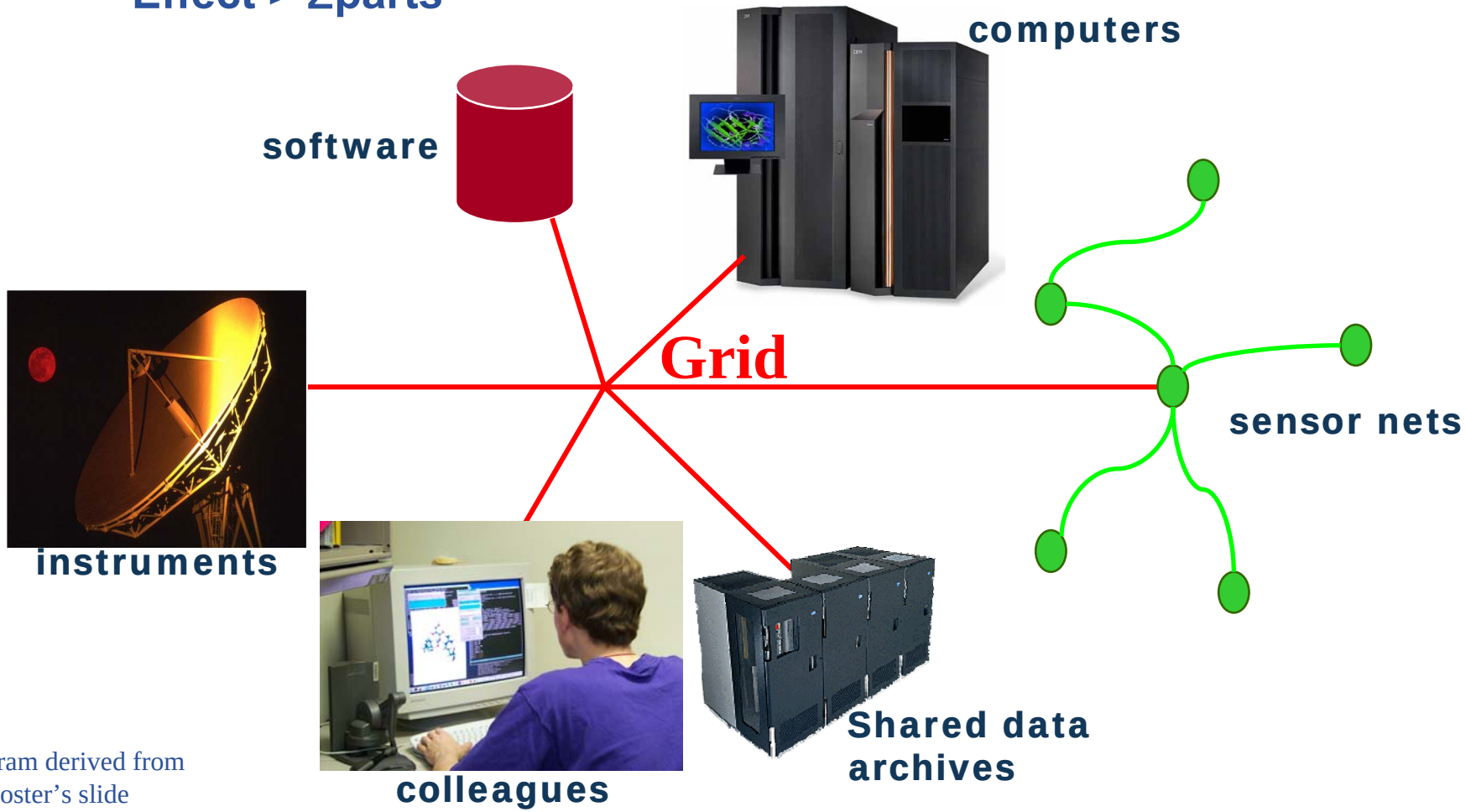


Diagram derived from Ian Foster's slide

"Effect > Σparts"

- **Flexible, simplified orchestration of resources available to a collaboration**
  - Across administrative domains
  - Abstractions hide detail of individual resources
    - Conform to Grid's procedures to gain benefit
  - Operations services (people and software)

- **Increased utilisation**
  - Collaboration shares its resources
  - Collaborations share resources
    - Each can benefit from
      - *Heterogeneity*
      - *Scale*

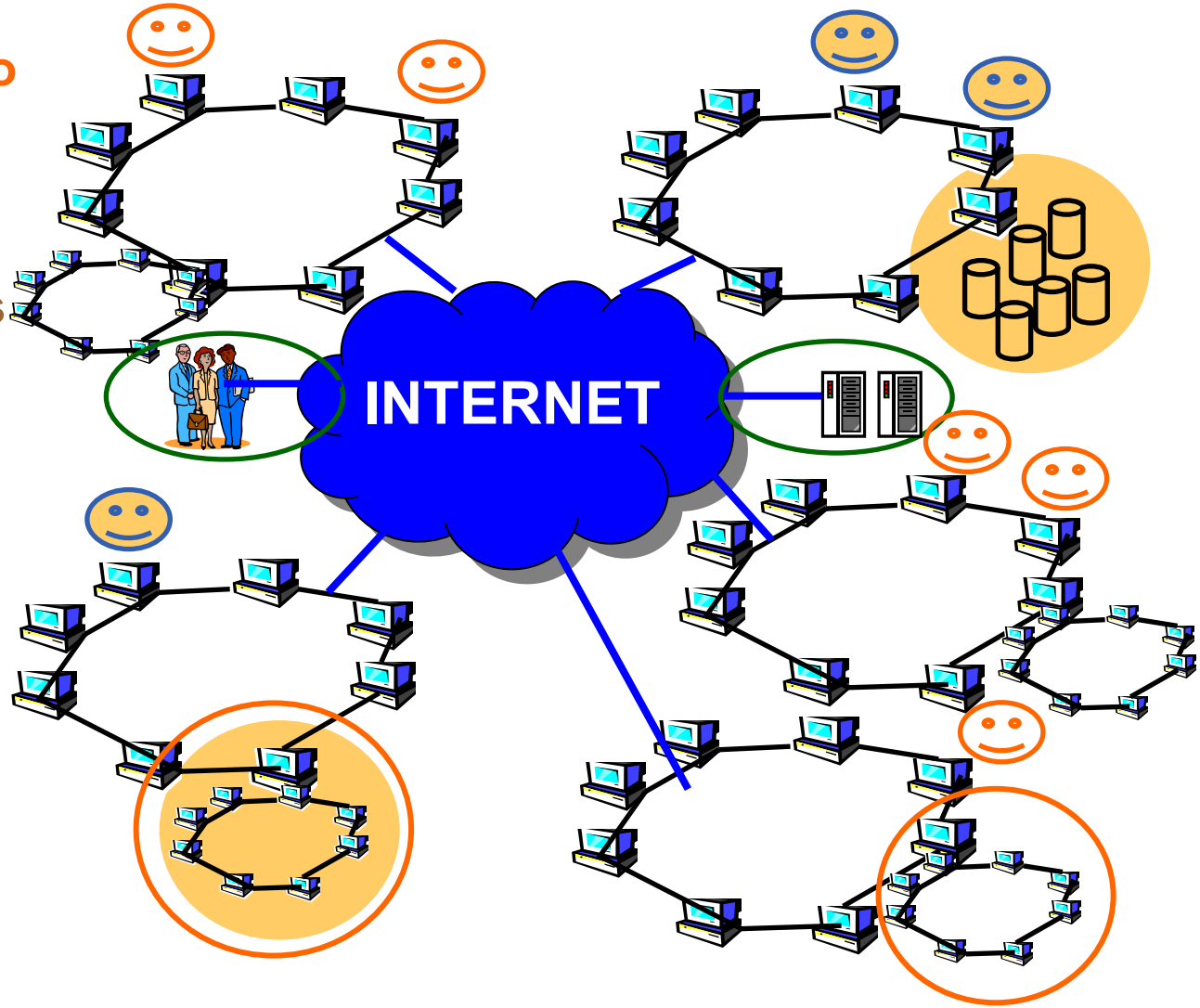
Grid concepts

Virtual organisations and grids

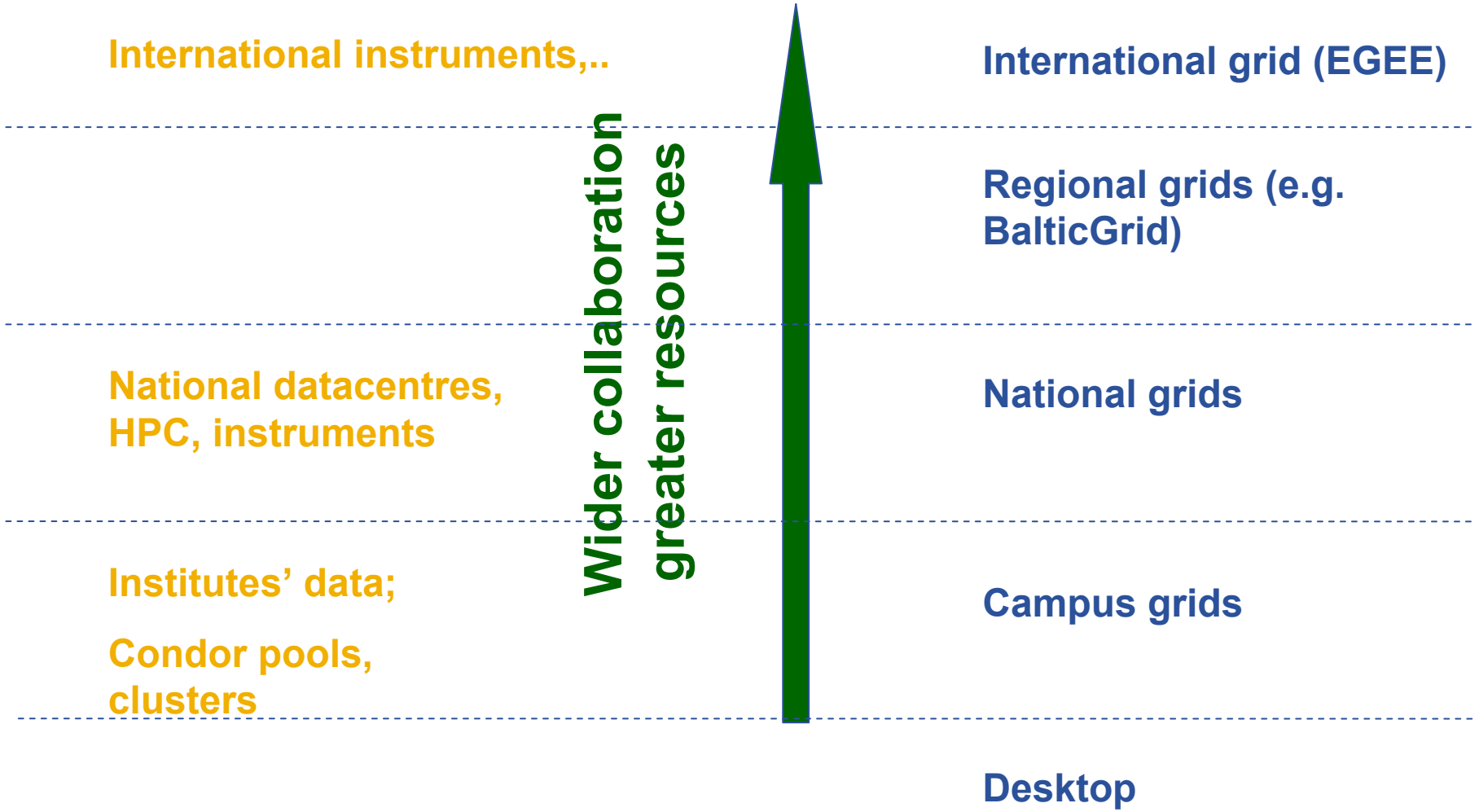
- **What is a Virtual Organisation?**
  - People in different organisations seeking to cooperate and share resources across their organisational boundaries
  - E.g. A research collaboration
- **Each grid is an infrastructure enabling one or more "virtual organisations" to share and access resources**
- **Each resource is exposed to the grid through an abstraction that masks heterogeneity, e.g.**
  - Multiple diverse computational platforms
  - Multiple data resources
- **Resources are owned by VO (in EGEE – some grids have central provision also). Negotiations lead to VOs sharing resources**

Typical current grid

- **Virtual organisations negotiate with sites to agree access to resources**
- **Grid middleware runs on each shared resource to provide**
  - Data services
  - Computation services
  - Single sign-on
- **Distributed services (both people and middleware) enable the grid**



The many scales of grids



Empowering VO's

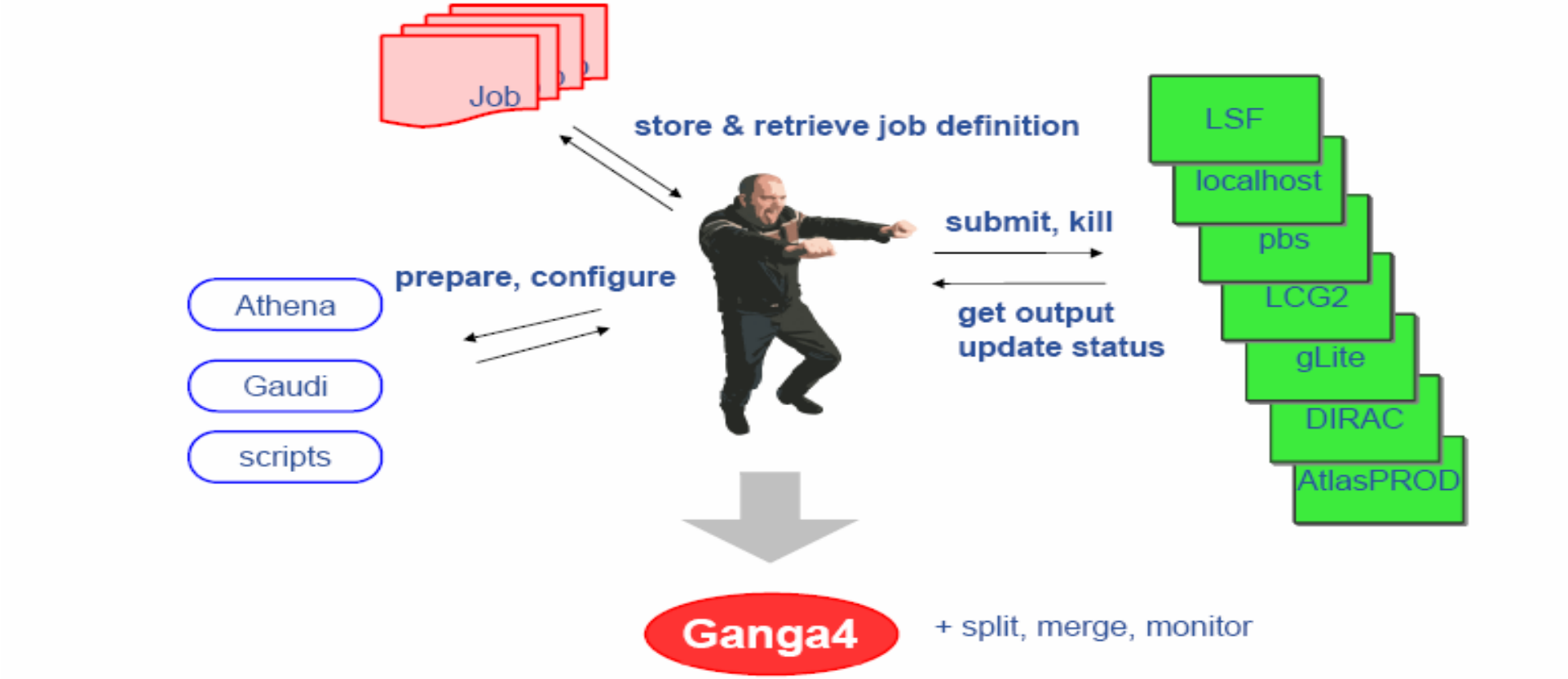
Where computer science meets the application communities!

VO-specific developments:

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

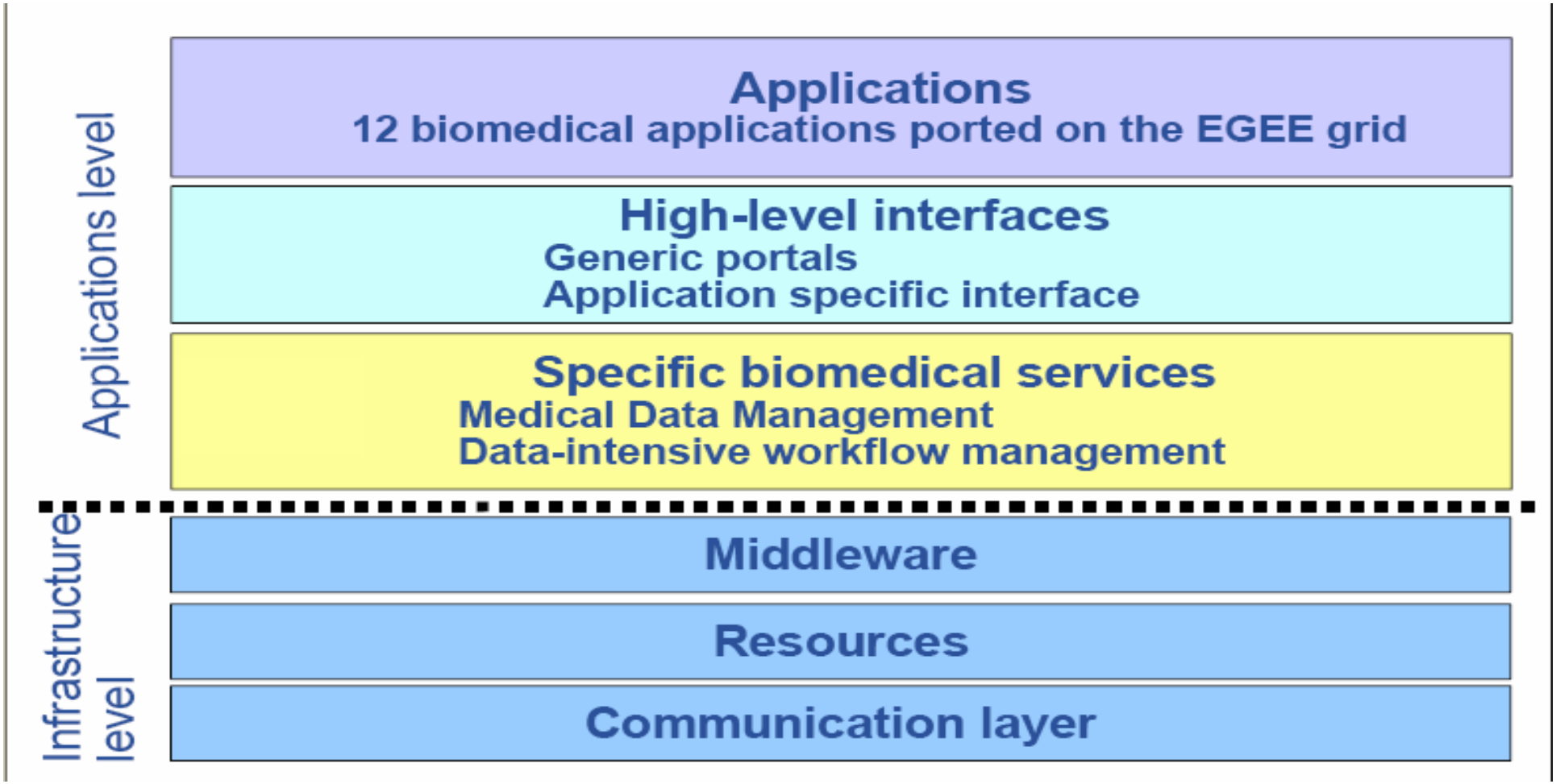
Production grids provide these services.

Example of higher-level service -1: GANGA



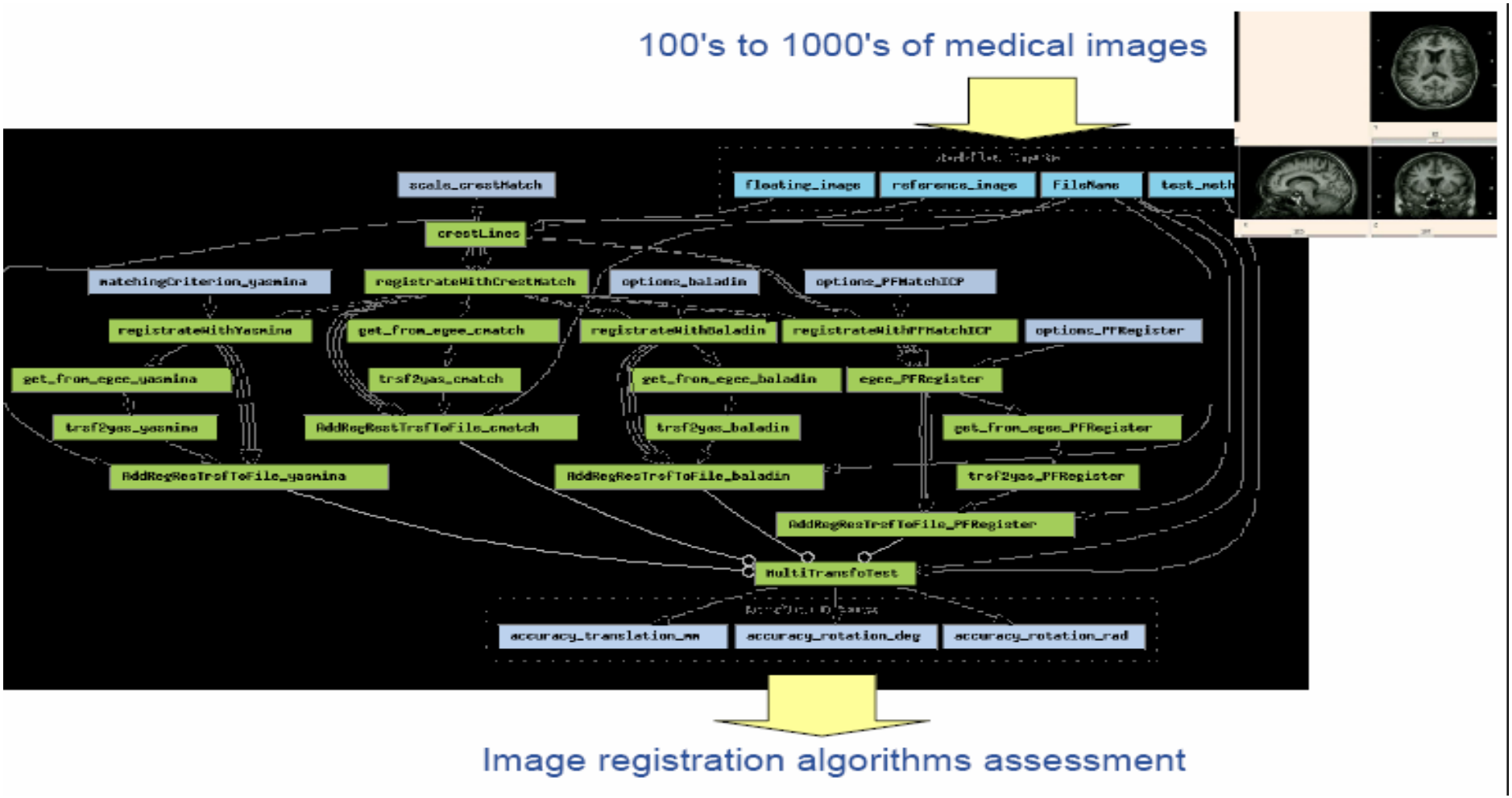
- **Ganga is a lightweight user tool**
  ganga.web.cern.ch/
- **But also: Ganga is a developer framework**

Example – Biomedical applications

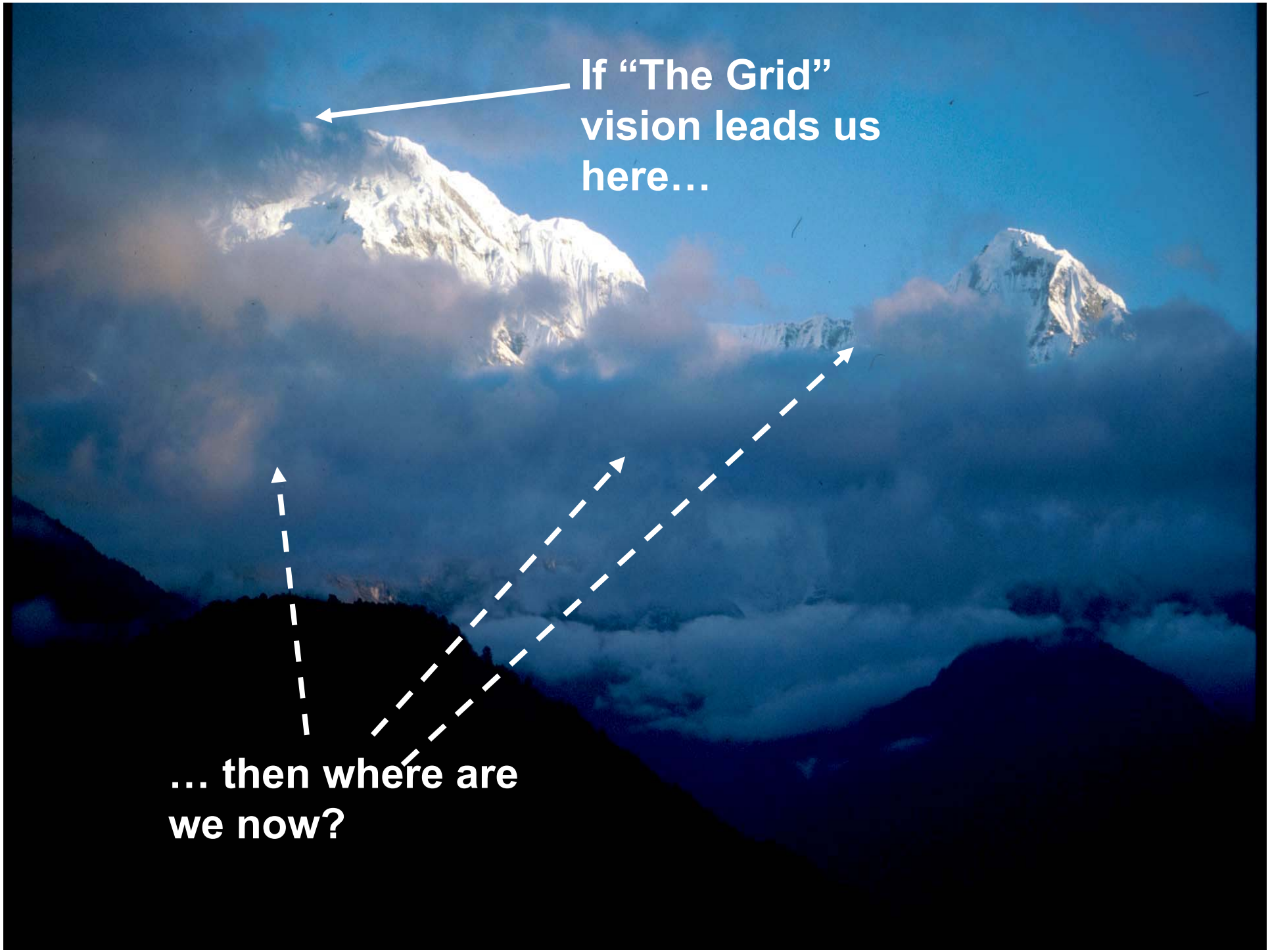


Biomedical community and the Grid, EGEE User Forum, March 1st 2006, I. Magnin

Example of Workflow



Biomedical community and the Grid, EGEE User Forum, March 1st 2006, I. Magnin


If “The Grid” vision leads us here…
… then where are we now?

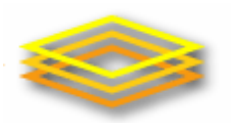
Grids: where are we now?

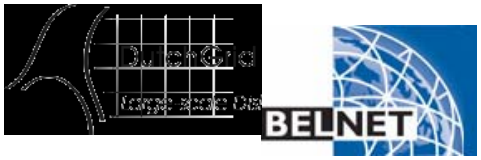
- **Many key concepts identified and known**
- **Many grid projects have tested, and benefit from, these**
  - Empowering collaborations
  - Resource-sharing
- **Major efforts now on establishing:**
  - **Production Grids *for multiple VO's***
    - "Production" = Reliable, sustainable, with commitments to quality of service
    - Each has
      - *One stack of middleware that serves many research communities*
      - *Establishing operational procedures and organisation*
    - Challenge for EGEE-II: federate these!
  - **Standards** (a slow process)
    - e.g. Open (formerly Global) Grid Forum, http://www.gridforum.org/
    - Extending web services…. Friday afternoon!
  - **Broadening range of research communities**
    - arts and humanities, social science …

Grid security and trust

- **Providers of resources (computers, databases,..) need risks to be controlled: they are asked to trust users they do not know**
  - They trust a VO
  - The VO trusts its members
- **User's need**
  - single sign-on: to be able to logon to a machine that can pass the user's identity to other resources
  - To trust owners of the resources they are using
- **Build middleware on layer providing:**
  - *Authentication:* know who wants to use resource
  - *Authorisation:* know what the user is allowed to do
  - *Security:* reduce vulnerability, e.g. from outside the firewall
  - *Non-repudiation:* knowing who did what
- **The "Grid Security Infrastructure" middleware is the basis of (most) production grids**

National grid initiatives now include…

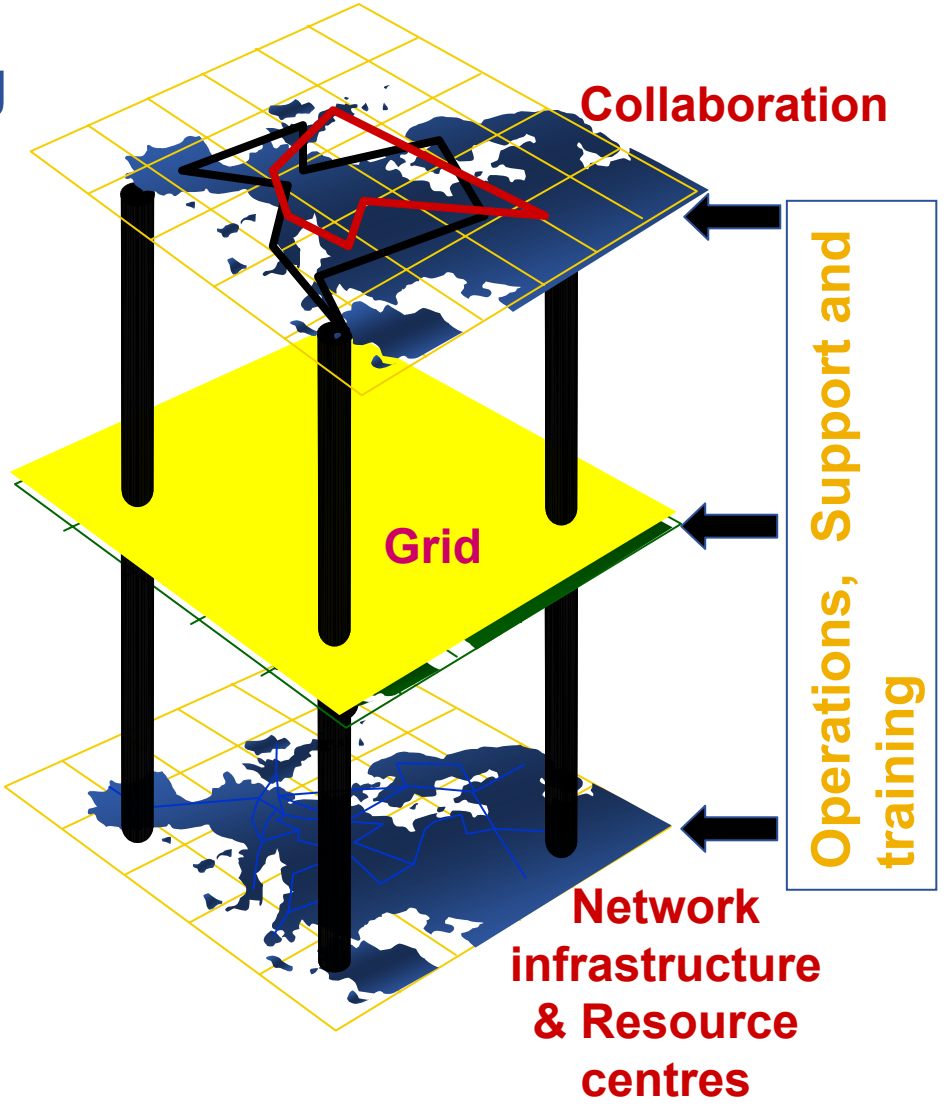




CroGrid

Summary: what is grid computing?

- **Grids: virtual computing across administrative domains**
  - Data
  - Computation
  - Collaboration
- **Orchestration of services in support of**
  - Research, diagnostics, engineering, public service,..
  - Resource utilisation and sharing



Further reading

- **Open Grid Forum** http://www.ggf.org/ **(see GGF16 for many good presentations)**
- **The Grid Cafe** www.gridcafe.org
- **Grid Today** http://www.gridtoday.com/
- **Globus Alliance** http://www.globus.org/