



Enabling Grids for E-scienceE

Grid Concepts

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- **Introduction to**
 - e-Science
 - e-Research
 - Grids
 - e-Infrastructure
- **Grid concepts**
- **Grids - Where are we now?**

‘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

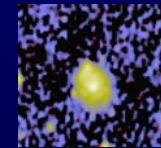
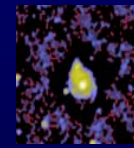
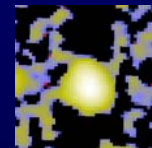
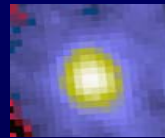
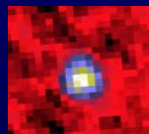
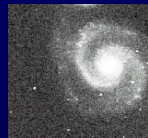
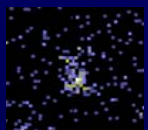
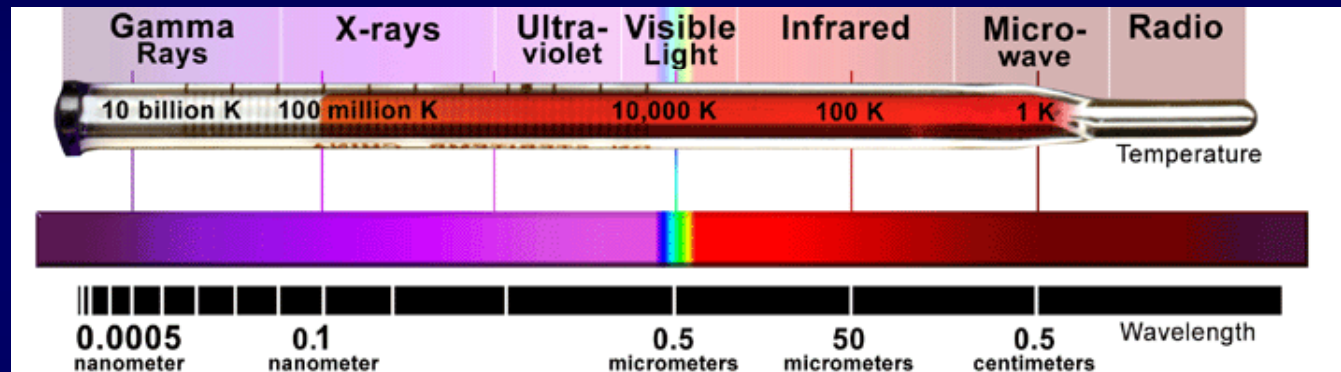
*‘e-Science is about global collaboration in key areas of science, and the **next generation of infrastructure** that will enable it.’*

Networks + Grids

- *Networks connect resources*
- *Grids enable “virtual computing”*

Virtual Observatories

Observations made across entire electromagnetic spectrum



ROSAT ~keV DSS Optical 2MASS 2 μ IRAS 25 μ IRAS 100 μ GB 6cm NVSS 20cm WENSS 92cm

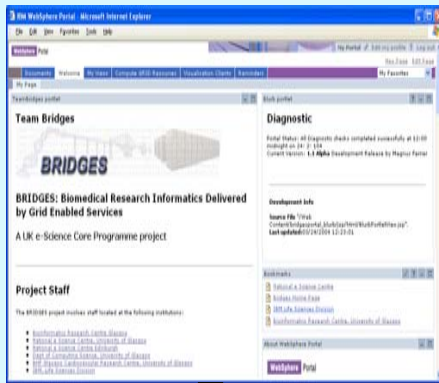
⇒ e.g. different views of a local galaxy

Need all of them to understand physics fully

Databases are located throughout the world

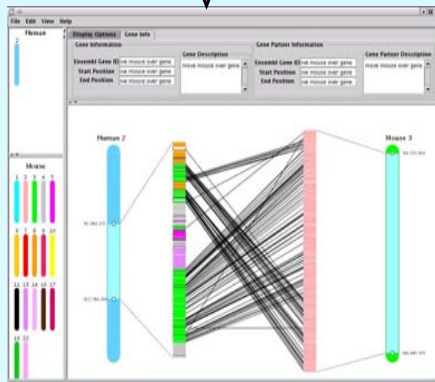
Biomedical Research Informatics Delivered by Grid Enabled Services

VO Authorisation

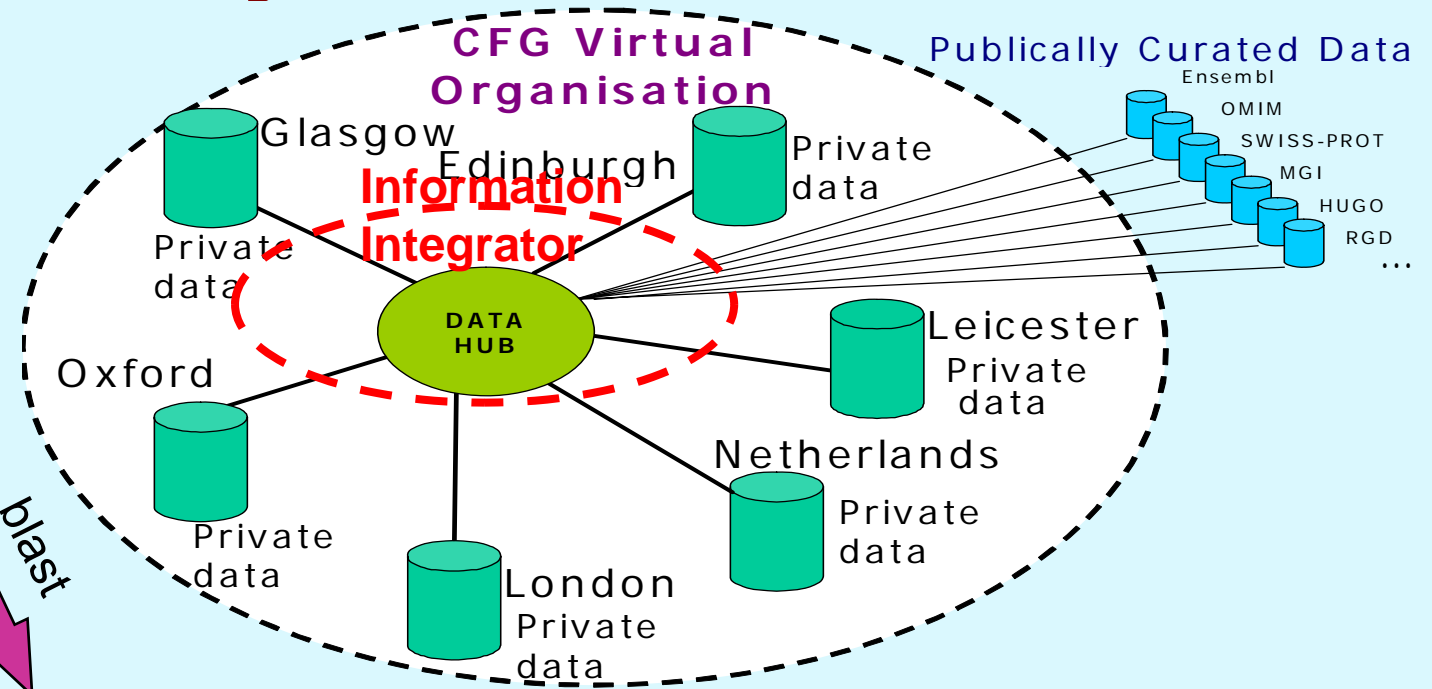


Synteny
Grid
Service

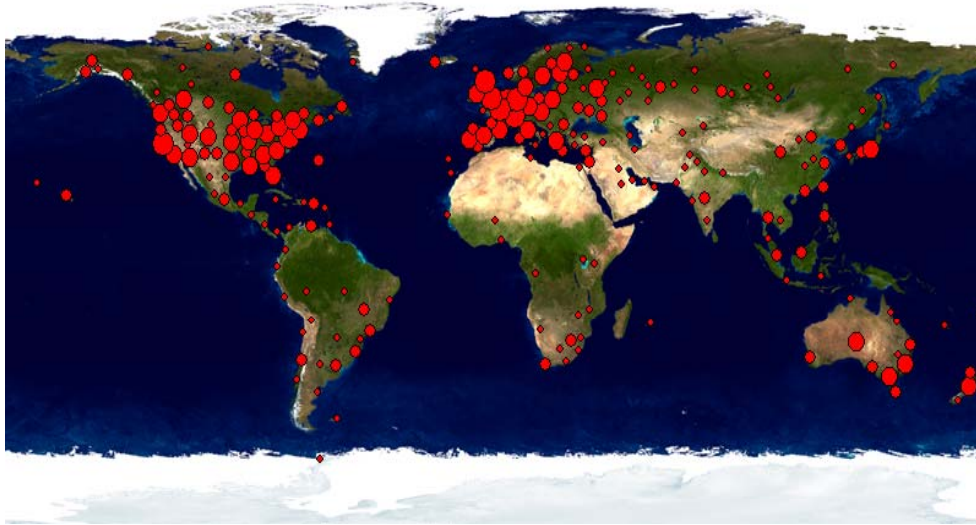
blast



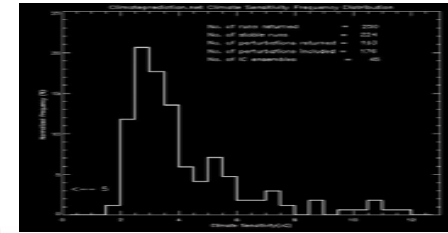
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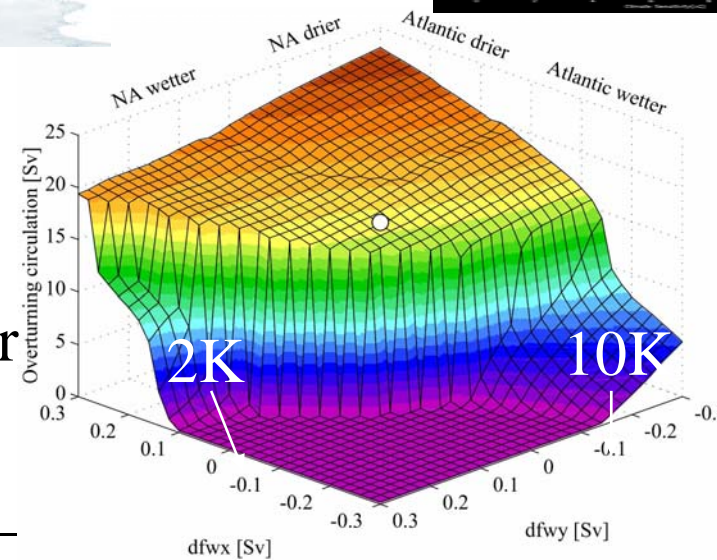
climateprediction.net and GENIE



- Largest climate model ensemble
- >45,000 users, >1,000,000 model years

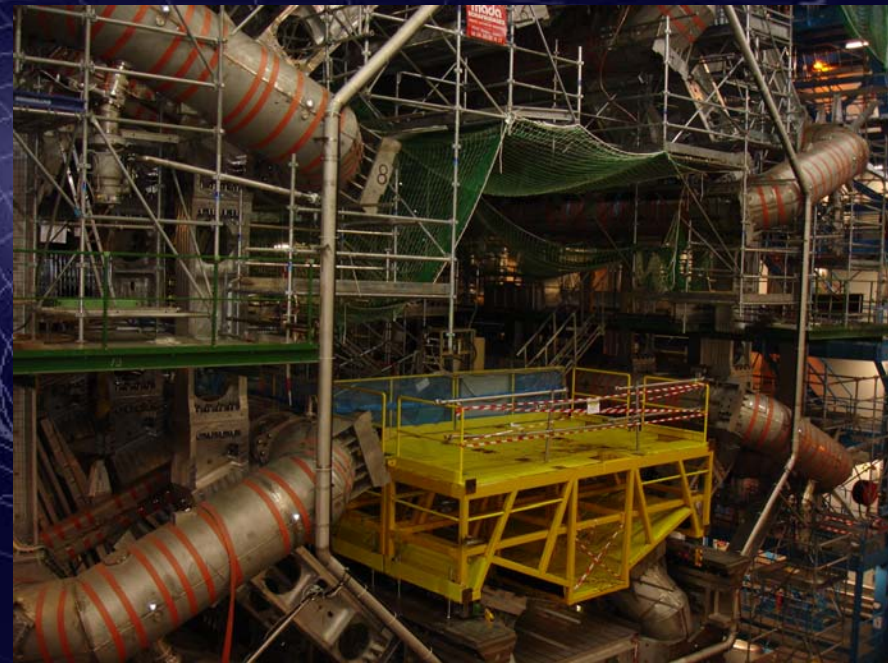


Response of Atlantic
circulation to freshwater
forcing



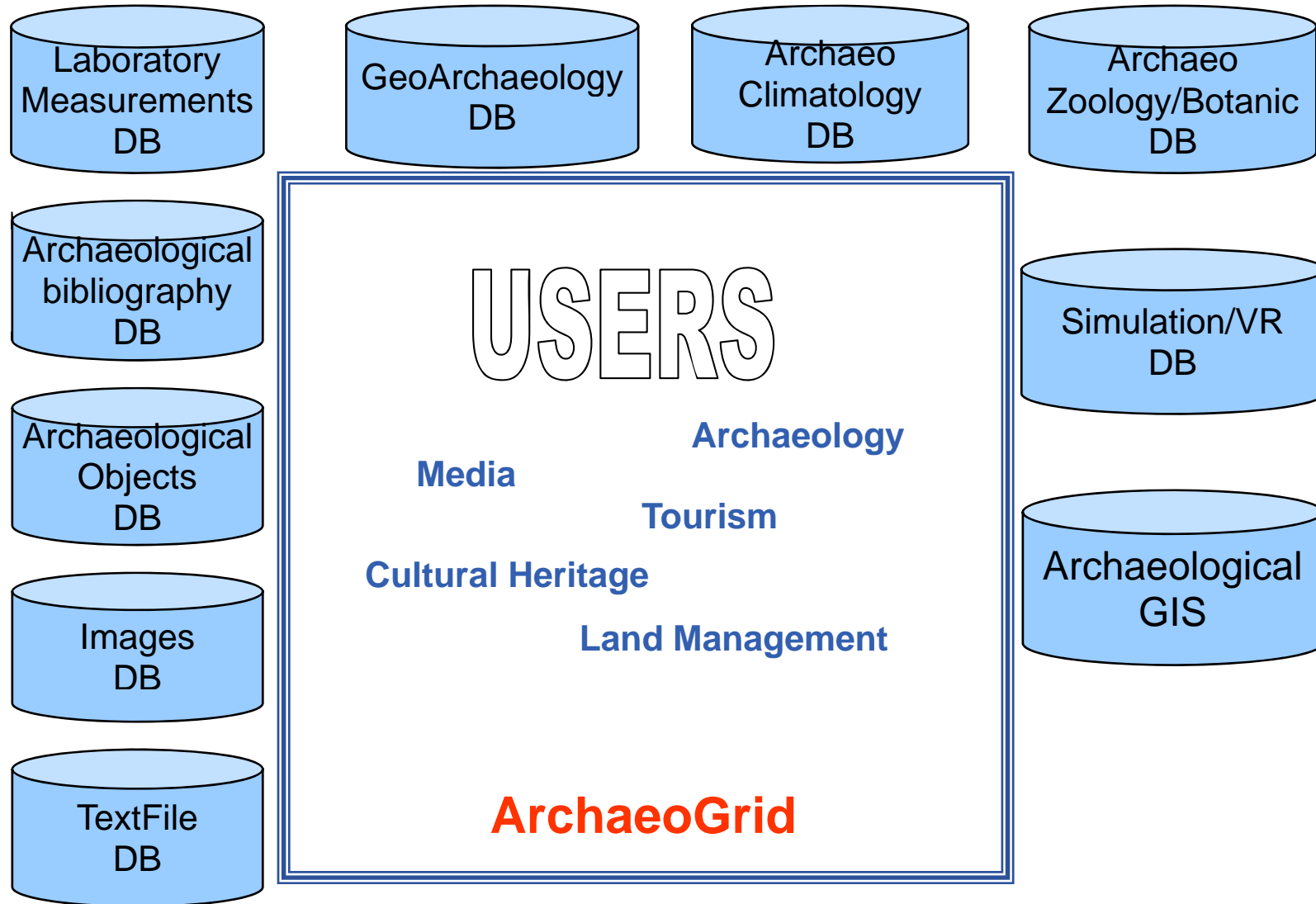
PP ARC

UK Grid for Particle Physics



GridPP www.gridpp.ac.uk

ATLAS detectors, 2/3/06



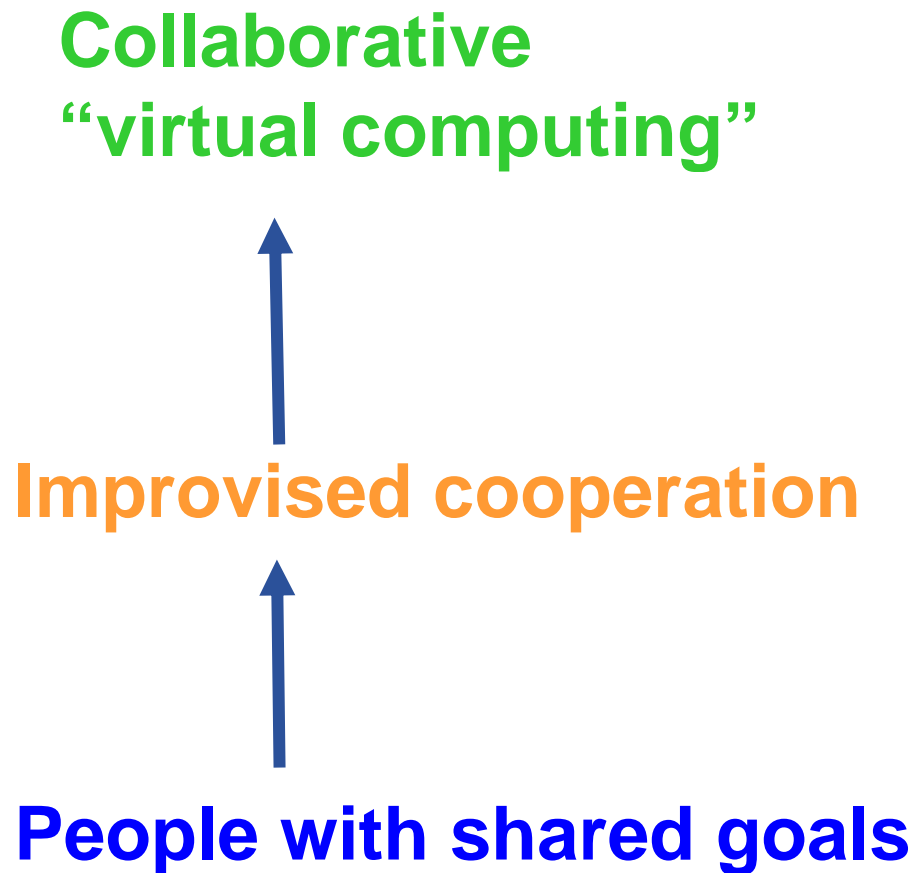
<http://www.accessgrid.org/>

Cameras



Microphones

- **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
- **Began with focus in the “big sciences” hence initiatives are often badged as “e-science”**
- **Relevance of “e-science technologies” to new user communities (social science, arts, humanities...) led to the term “e-research”**



Sharing data, computers, software
Enabled by Grids:

National, regional
International: EGEE grid

Email
File exchange
ssh access to run programs

Enabled by networks:
national, regional and
International: GEANT

Grids: a foundation for e-Research

- enabling a whole-system approach

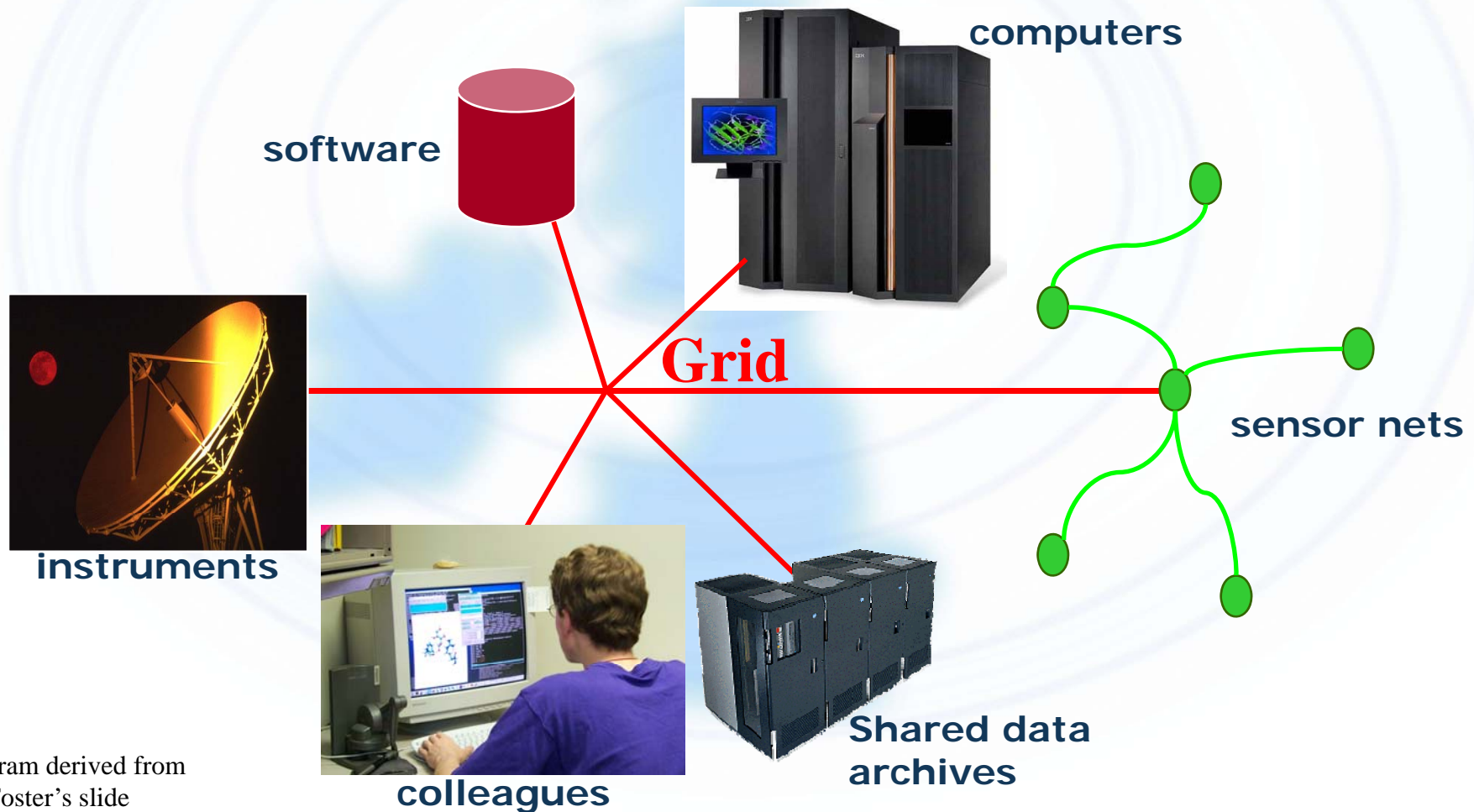
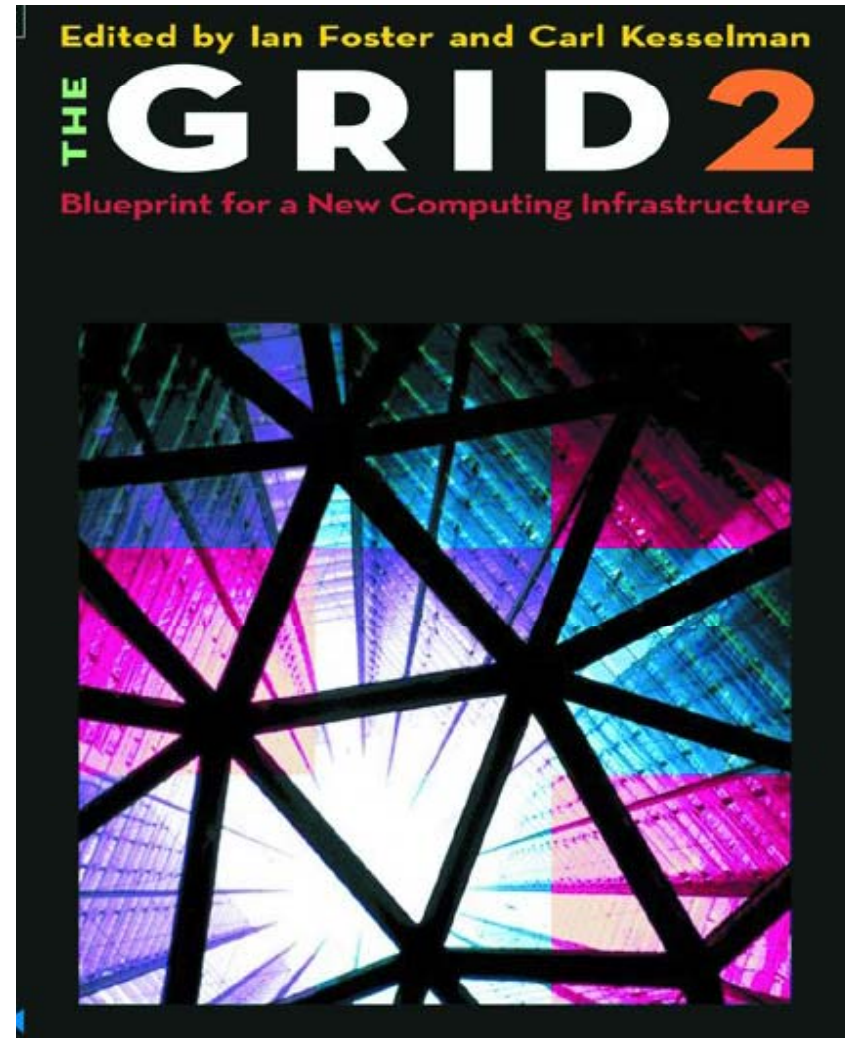
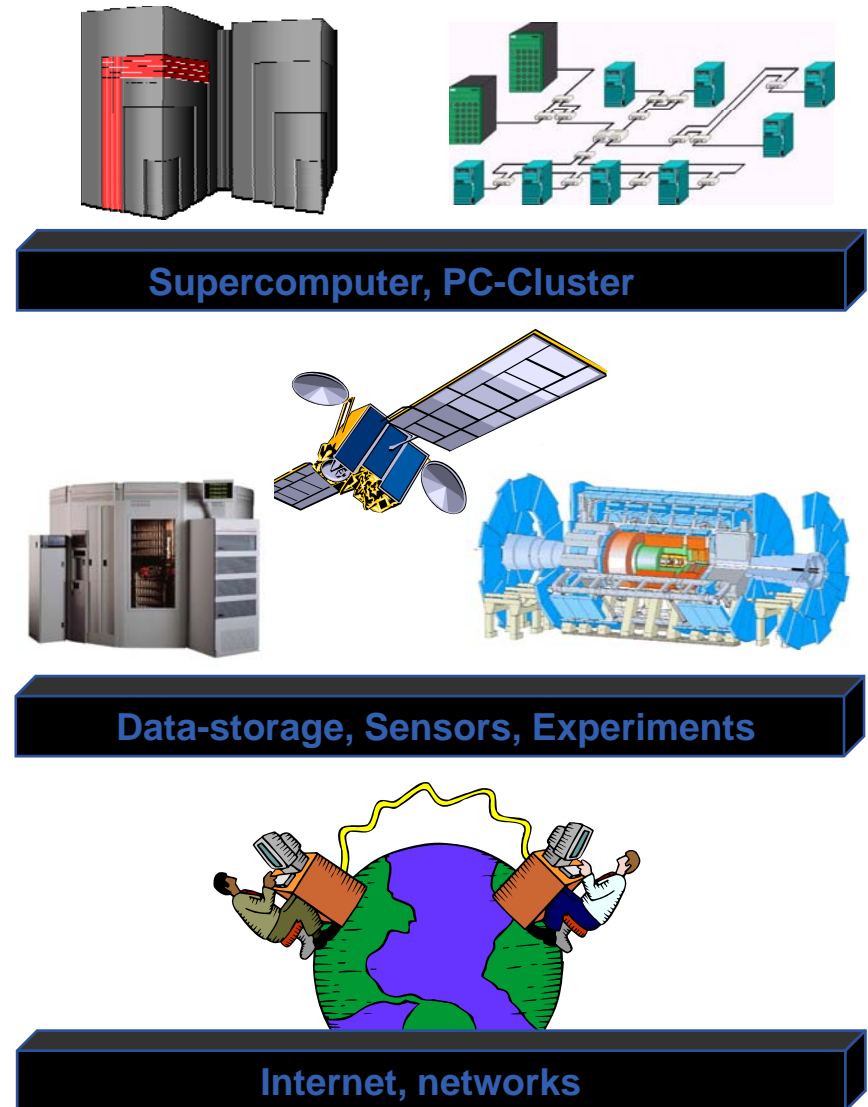
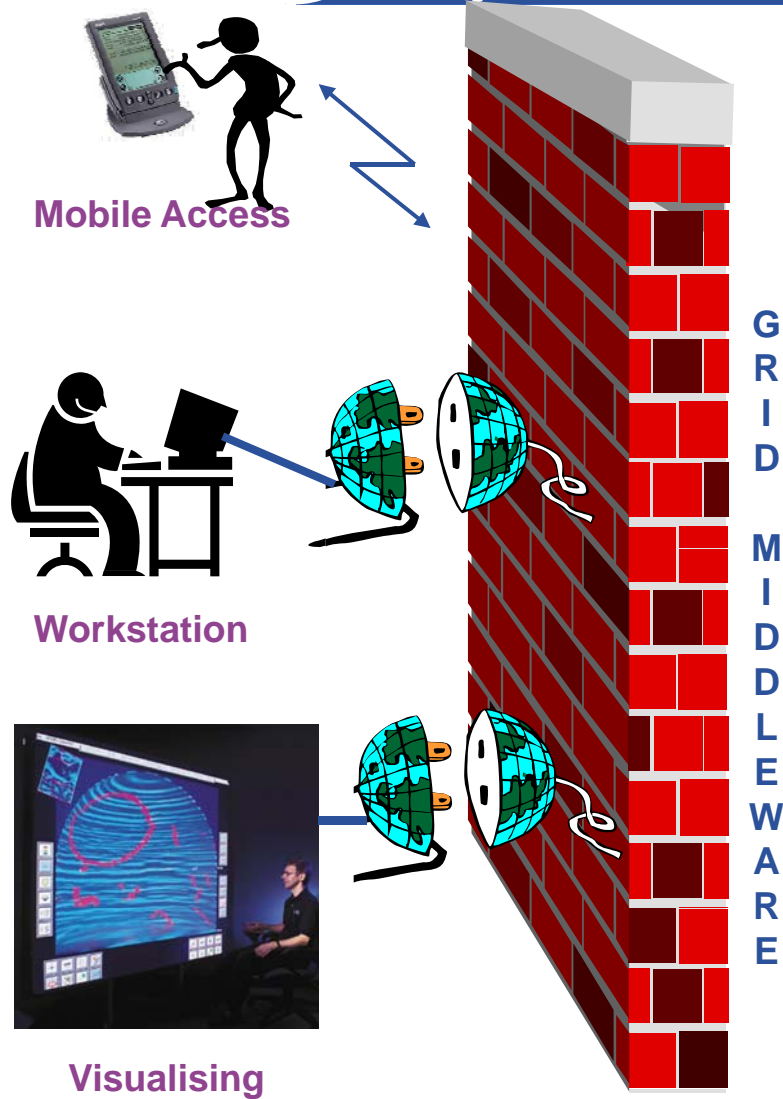


Diagram derived from
Ian Foster's slide

- 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,...





- **A shared resource**
 - That enables science, research, engineering, medicine, industry, ...
 - It will improve UK / European / ... productivity
 - Lisbon Accord 2000
 - E-Science Vision SR2000 – John Taylor
 - Commitment by UK government
 - Sections 2.23-2.25
 - Always there
 - c.f. telephones, transport, power, internet

Science & innovation investment framework 2004 - 2014

July 2004



department for
education and skills



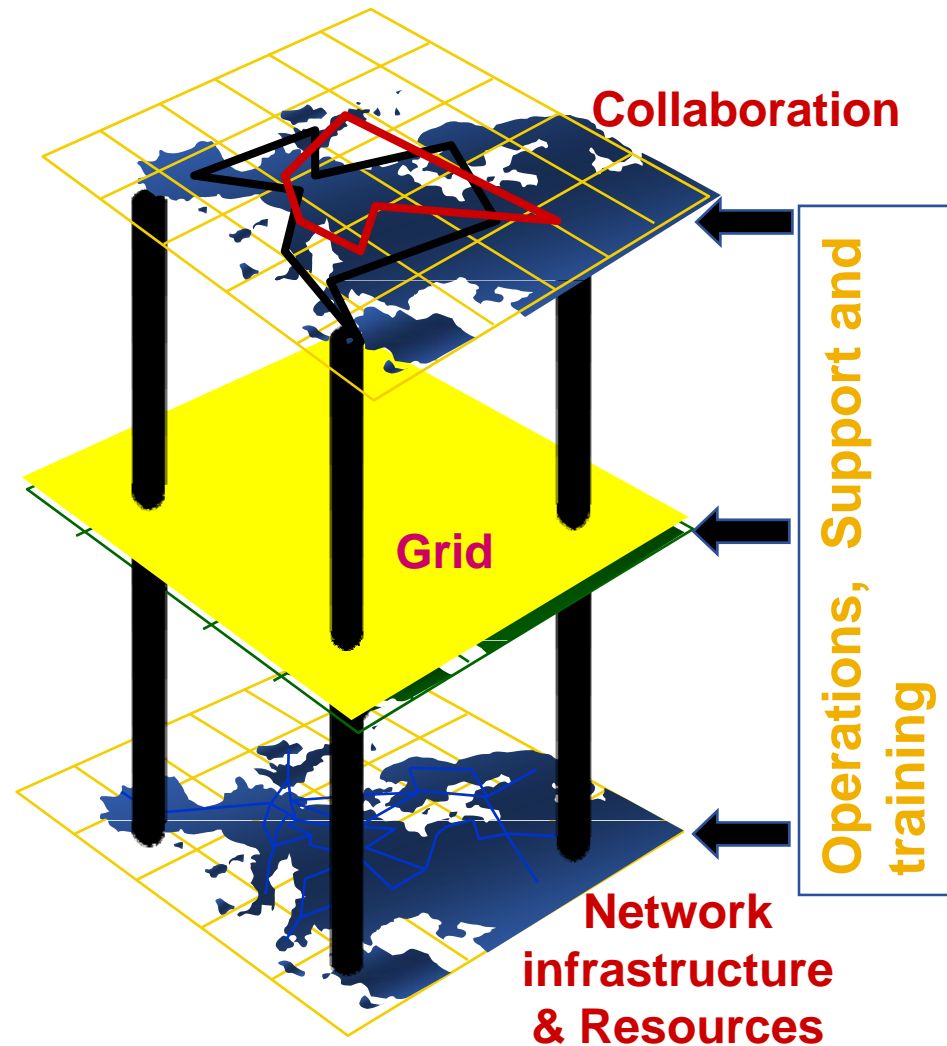
Gordon Brown
Chancellor of the
Exchequer

Charles Clarke
Secretary of State for
Education and Skills

Patricia Hewitt
Secretary of State for
Trade and Industry

What is e-Infrastructure?

- **Grids:** permit resource sharing across administrative domains
- **Networks:** permit communication across geographical distance
- **Supporting organisations**
 - Operations for grids, networks
- **Resources**
 - Computers
 - Digital libraries
 - Research data
 - Instruments
- **Middleware**
 - Authentication, Authorisation
 - Registries, search engines
 - Toolkits, environments
 - E.g. for collaboration



- **Digital technology – exponential growth - e.g. bandwidth**
- **Opportunities for e-Infrastructure to support faster, better, different research**
 - Sharing expertise
 - Support for cooperation and communication
 - Sharing computation services
 - E.g. to serve occasional peaks of high demand for computation (especially trivially parallelisable ones)
 - Sharing data
 - New sensors and instruments
 - Databases
- **Based on an infrastructure that requires and enables multidisciplinary research**
 - Requires: IT + domain specialists
 - Enables: New interdisciplinary research

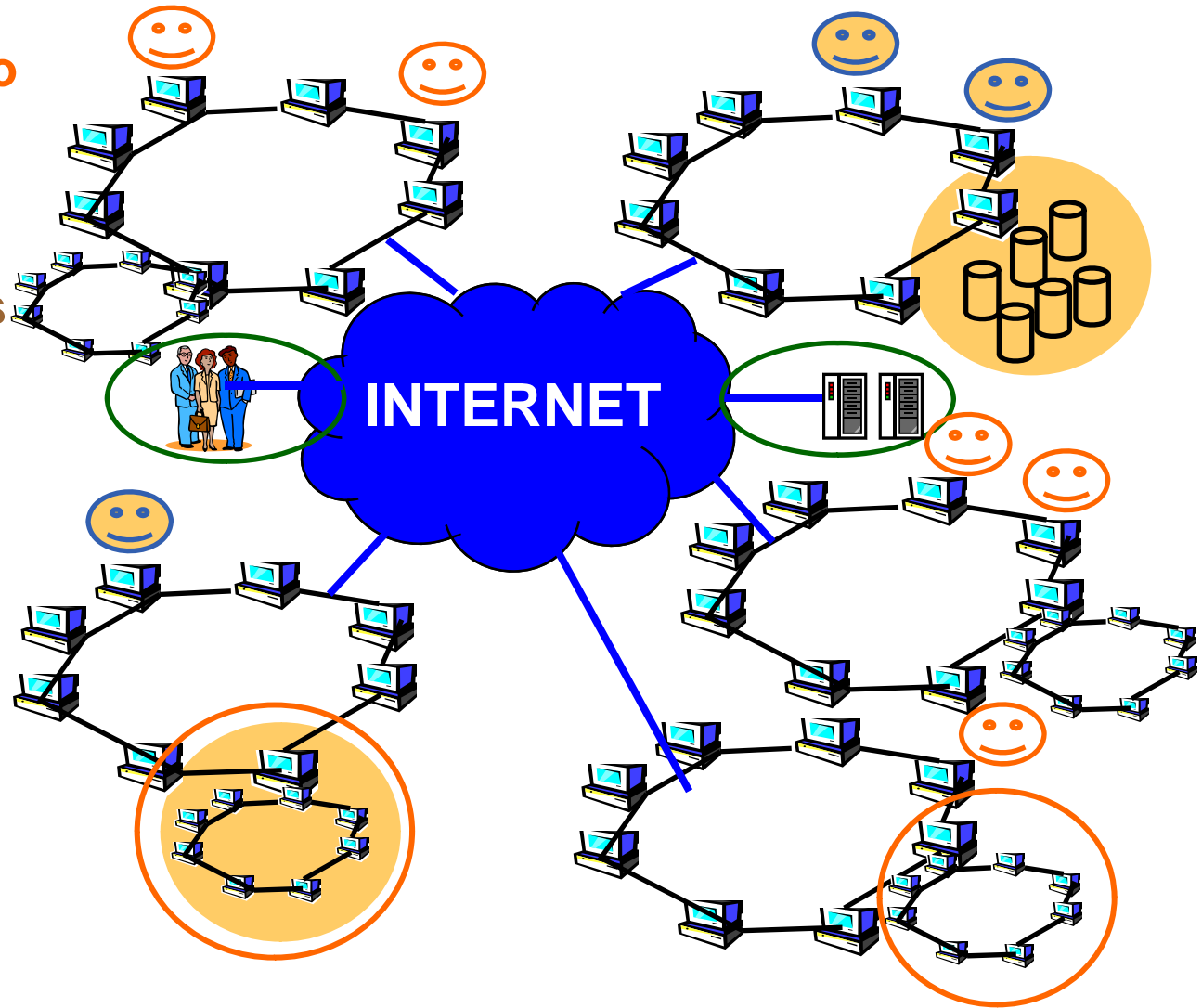
- **The term “Grid” has become popular!**
 - Sometimes in Industry : “Grids” = clusters
 - Motivations: better use of resources; scope for commercial services
 - Also used to refer to the harvesting of donated, unused compute cycles
 - (SETI@home, Climateprediction.net)
 - These are e-Infrastructure but are not “grids” from the e-Research viewpoint!
- **Grid computing: virtual computing across administrative domains**

- **“e-science” and “e-research”**
 - Collaborative
 - Sharing resources
 - Often data, often compute intensive
- **Grids**
 - Permit resources in different administrative domains to be viewed as if one computer
 - Single sign-on
- **e-Infrastructure**
 - Networks + grids + resources + operations, support, training
 - Sustainable services that underpin e-science, commerce.....

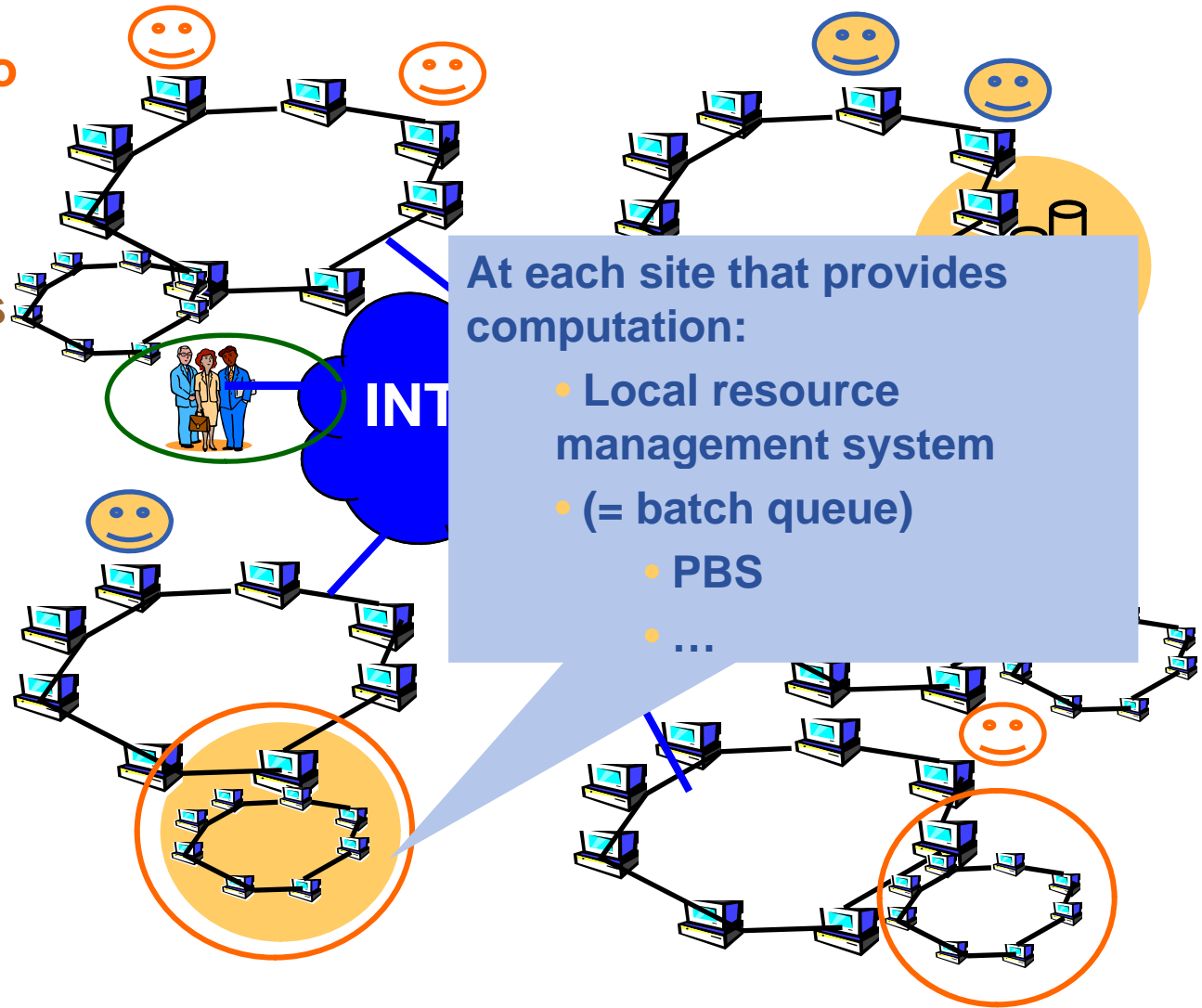
Grid concepts

- **What's 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**
- **Key concept: The ability to negotiate resource-sharing arrangements among a set of participating parties (providers and consumers) and then to use the resulting resource pool for some purpose. (Ian Foster)**

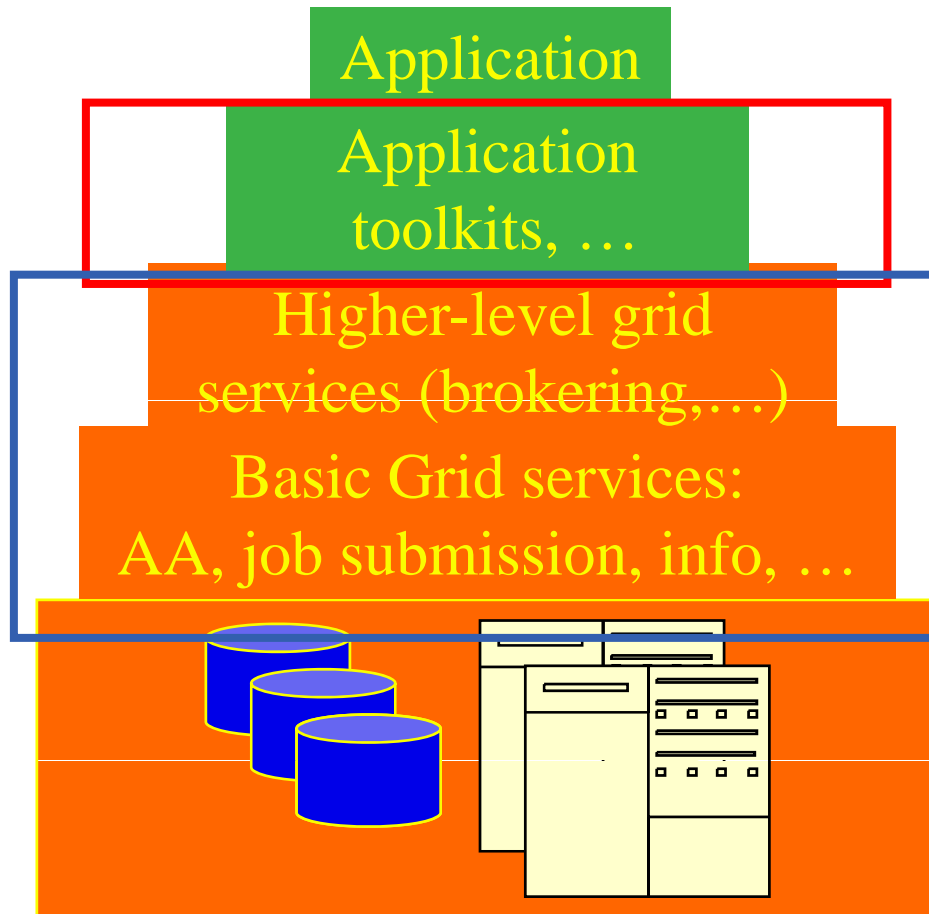
- **Virtual organisations negotiate with sites to agree access to resources**
- **Grid middleware runs on each shared resource to provide**
 - Data services
 - Computation services
 - Single sign-on
- **Distributed services (both people and middleware) enable the grid**



- **Virtual organisations negotiate with sites to agree access to resources**
- **Grid middleware runs on each shared resource to provide**
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- **When using a PC or workstation you**
 - Login with a username and password (“Authentication”)
 - Use rights given to you (“Authorisation”)
 - Run jobs
 - Manage files: create them, read/write, list directories
- **Components are linked by a bus**
- **Operating system**
- **One admin. domain**
- **When using a Grid you**
 - Login with digital credentials – single sign-on (“Authentication”)
 - Use rights given you (“Authorisation”)
 - Run jobs
 - Manage files: create them, read/write, list directories
- **Services are linked by the Internet**
- **Middleware**
- **Many admin. domains**

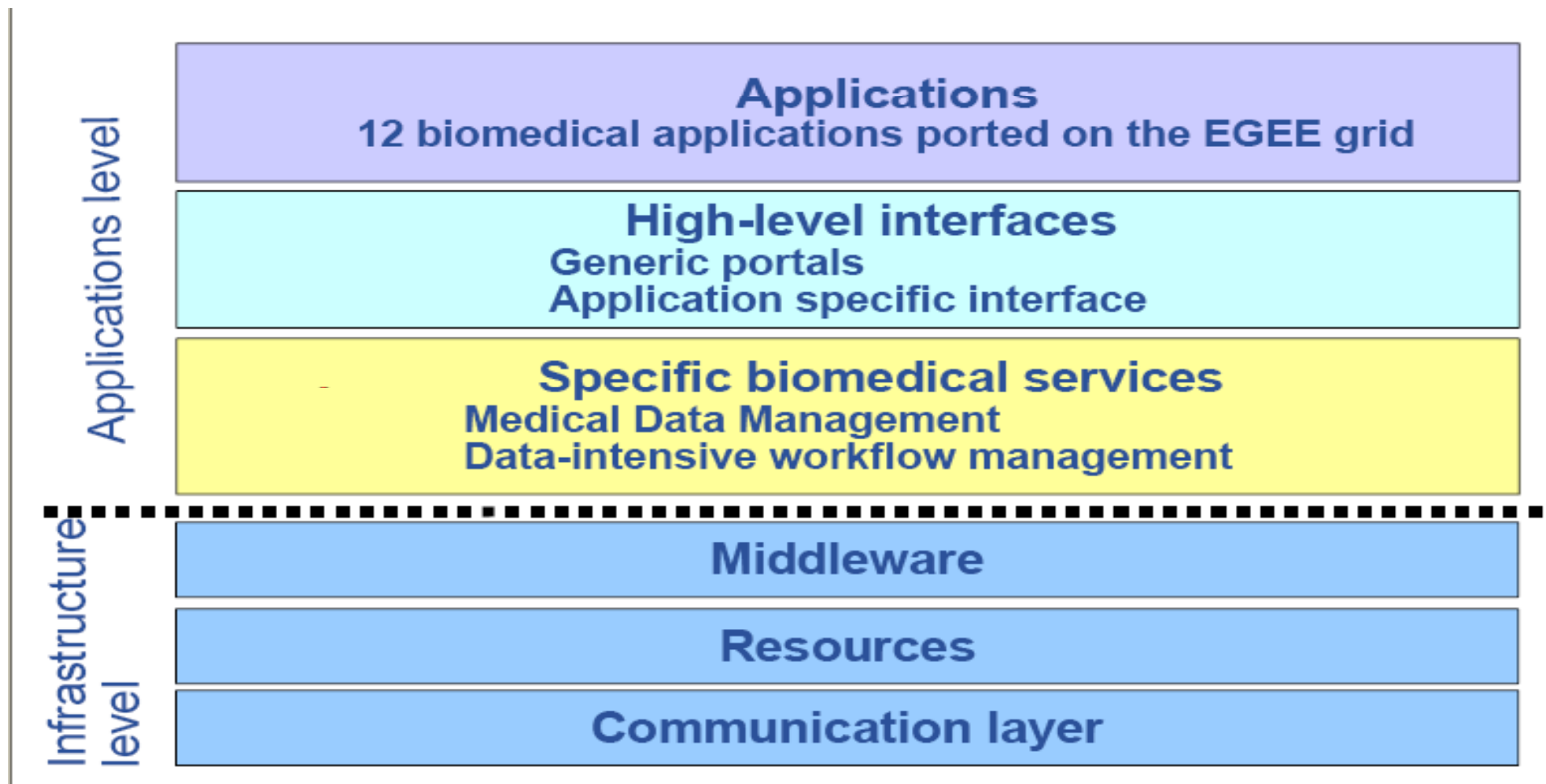


Where computer science meets the application communities!

VO-specific developments:

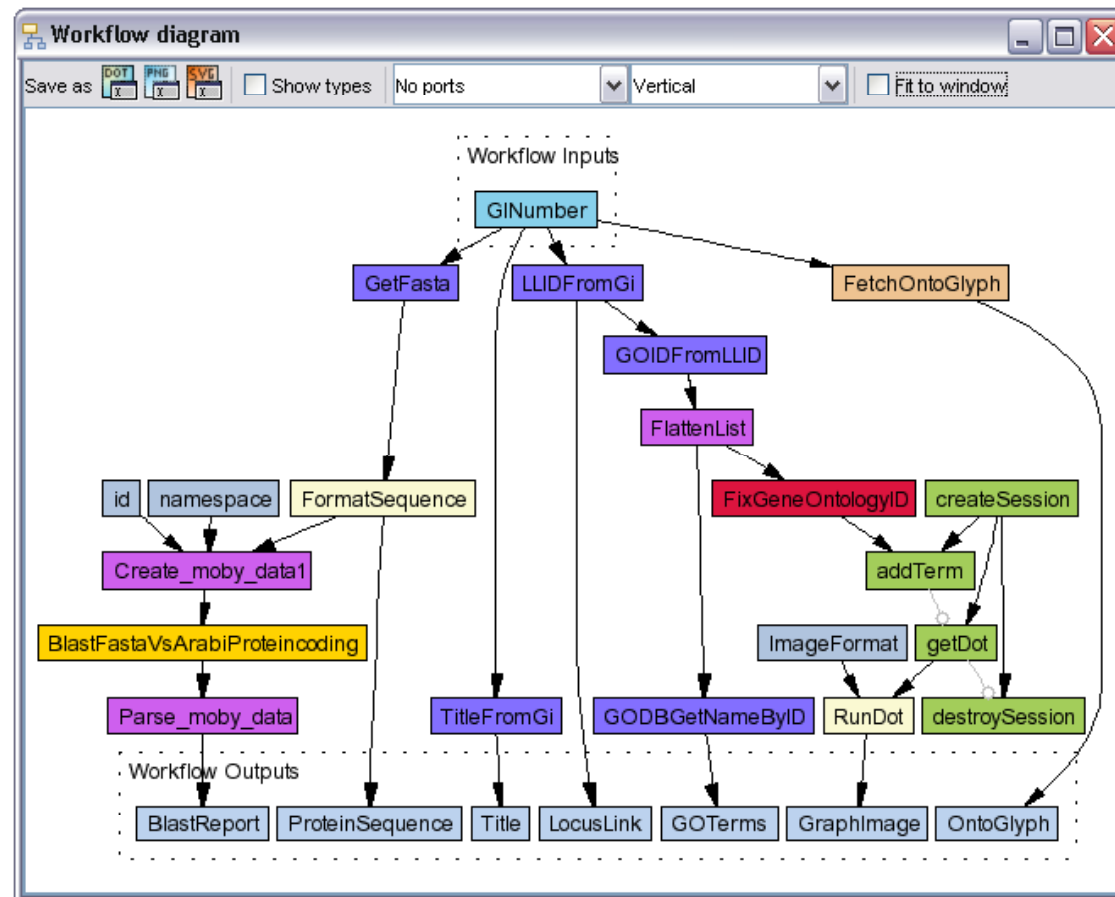
- Portals
- Virtual Research Environments
- Semantics, ontologies
- Workflow
- Registries of VO services

Production grids provide these services.



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

- 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



International instruments,..

National datacentres,
HPC, instruments

Institutes' data;
Condor pools,
clusters

Wider collaboration
greater resources



International grid (EGEE)

National grids (e.g.
National Grid Service)

Regional grids (e.g.
Brunel/Westminster Grid
Alliance)

Campus grids

Desktop

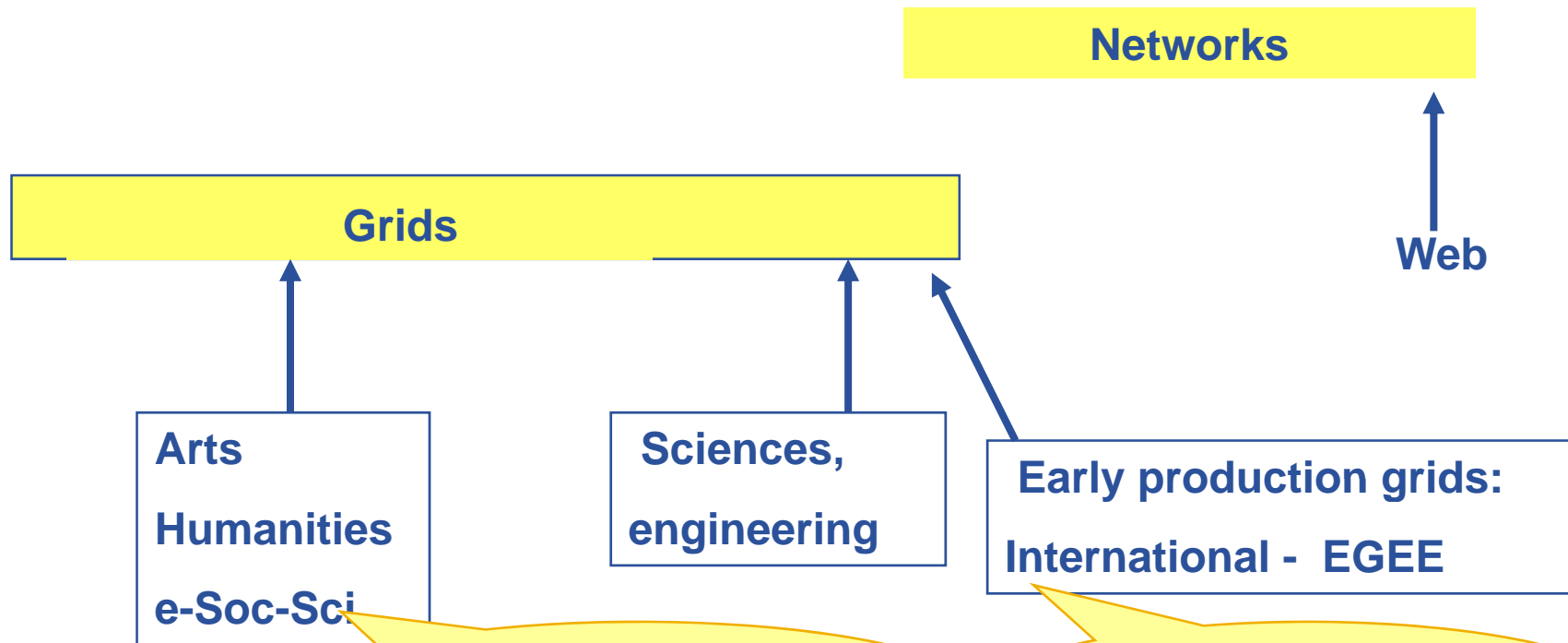


If "The Grid"
vision leads us
here...

... then where are
we now?

- Many key concepts identified and known
- Many grid projects have tested, and benefit from, these
- Major efforts now on establishing:
 - **Production Grids for multiple VO's**
 - “Production” = Reliable with commitments to quality of service
 - *In Europe, EGEE*
 - *In UK, National Grid Service*
 - *In US, Teragrid and OSG*
 - One stack of middleware that serves many research communities
 - Establishing operational procedures and organisation
 - **Standards** (a slow process)
(e.g. Open Grid Forum, <http://www.gridforum.org/>)
 - **Sustainable infrastructure**
 - Move from research funding to GEANT-like model
 - European Grid Infrastructure federating National Grid Infrastructures

Where are we now? –user’s view



Types of use:

Service-oriented, workflow, “legacy” data

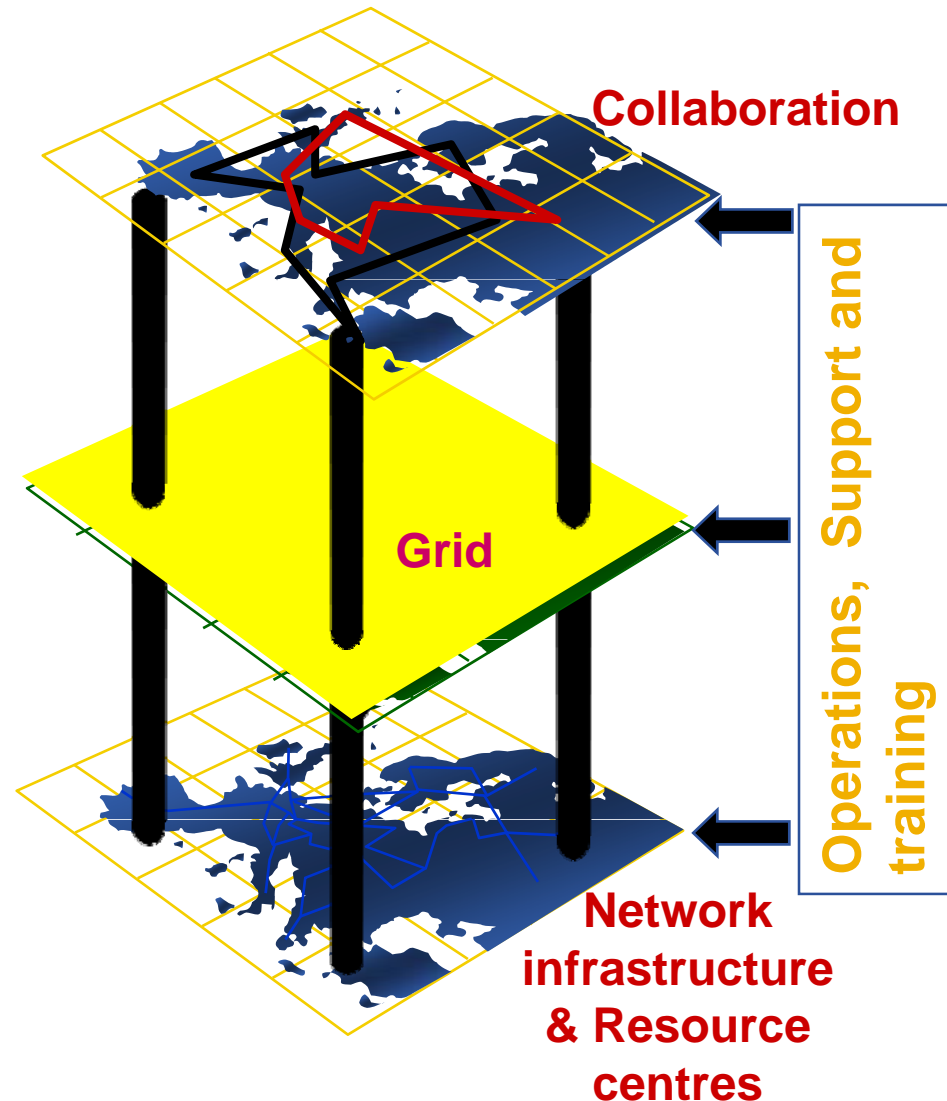
High throughput, new data

- **Standards are emerging... some near acceptance and some being discarded**
 - Standards bodies:
 - W3C <http://www.w3c.org/>
 - GGF <http://www.ggf.org/>
 - OASIS <http://www.oasis-open.org/home/index.php>
 - IETF <http://www.ietf.org/>
- **Production grids are based on de-facto standards at present**
 - Inevitably!
 - Globus Toolkit 2 especially
 - But locks a grid into one middleware stack unable to benefit from the diverse developments of new services

National grid initiatives now include...



- **Grids enable virtual computing across administrative domains**
 - Resources share authorisation and authentication
 - Resources accessed thru abstractions
- **Motivations:**
 - Collaborative research, diagnostics, engineering, public service,...
 - Resource utilisation and sharing



- **Open Grid Forum** <http://www.ggf.org/>
- **The Grid Cafe** www.gridcafe.org
- **Grid Today** <http://www.gridtoday.com/>
- **Globus Alliance** <http://www.globus.org/>
- **International Science Grid This Week**
<http://www.isgtw.org/>