http://www.grid-support.ac.uk

http://www.ngs.ac.uk

UK e-Infrastructure

Mike Mineter
mjm@nesc.ac.uk

http://www.nesc.ac.uk/

http://www.pparc.ac.uk/

http://www.eu-egee.org/

Acknowledgements

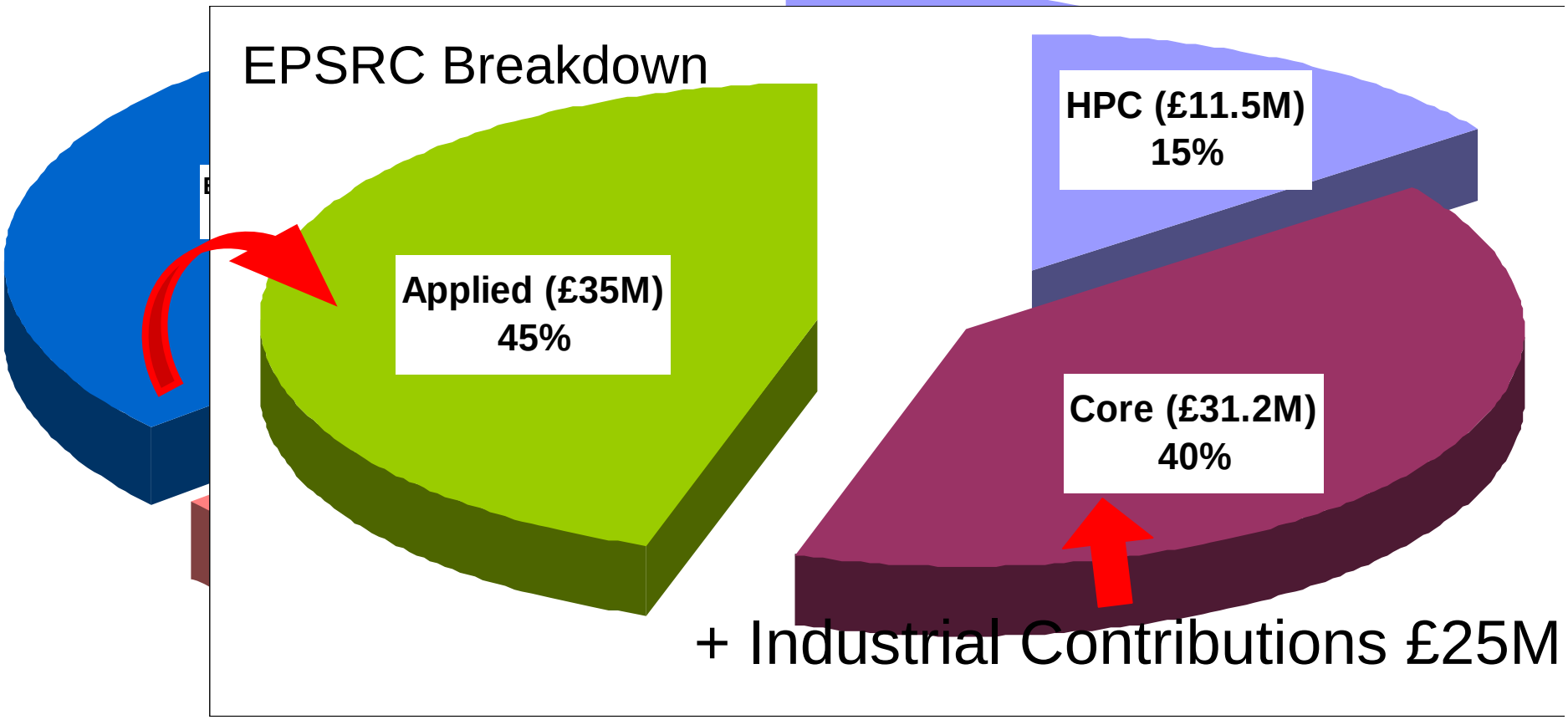
- For slides and information:
- NGS and GOSC - Stephen Pickles, Technical Director of GOSC
- OMII – Steven Newhouse
- JISC – Ann Borda, Sarah Porter, Sara Hassan, Shirley Wood
- Data centres – Peter Burnhill
- Integrative Biology

Overview

- The UK e-science programme
- The National Grid Service
- GOSC – Grid Operations Support Centre
  - UK e-Science Certification Authority (CA)
- OMII-UK – Open Middleware Infrastructure Institute
- JISC - Joint Information Systems Committee

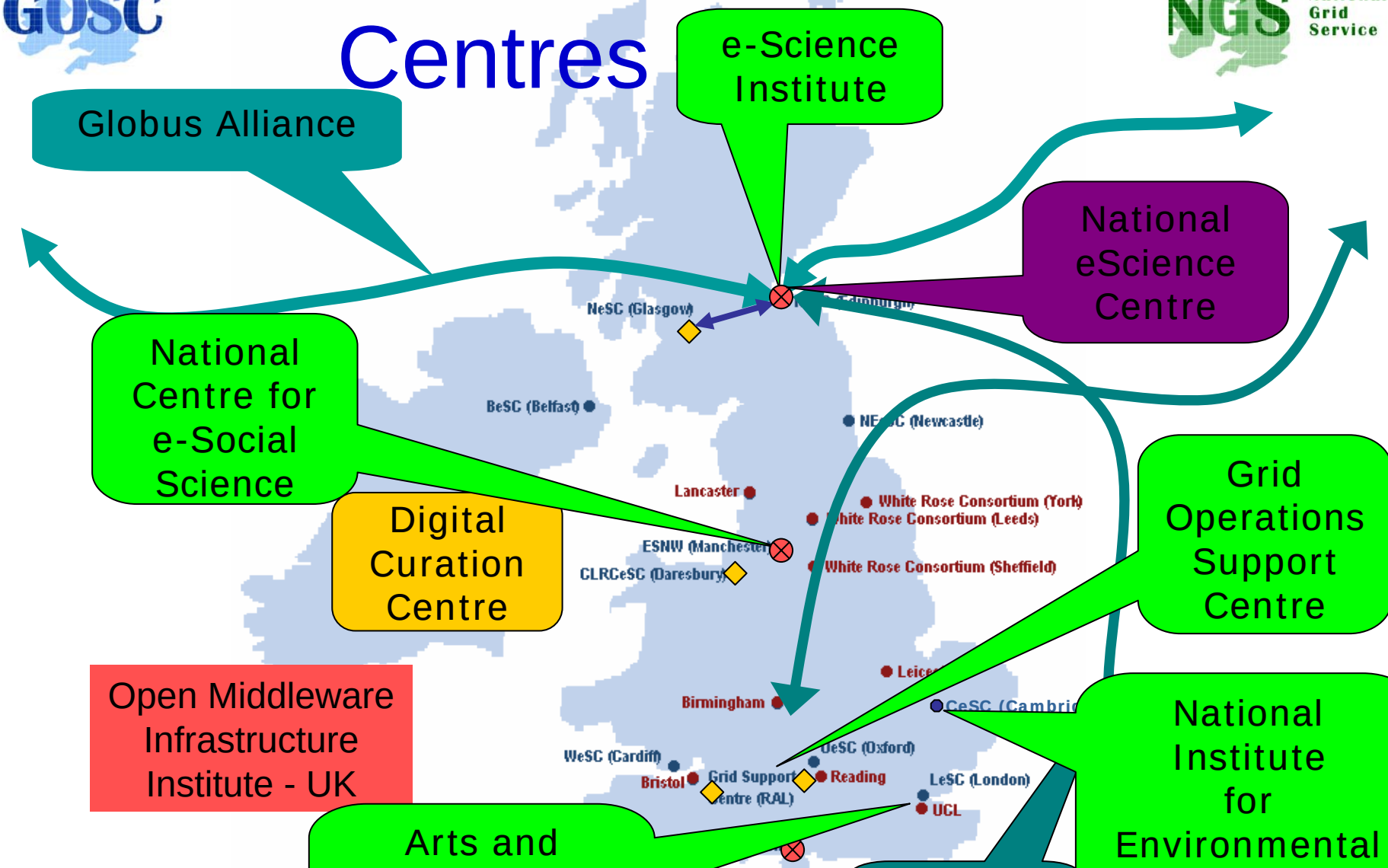
UK e-Science Budget (2001-2006)

Total: £213M + £100M via JISC



Source: Science Budget 2003/4 – 2005/6, DTI(OST)

The e-Science Centres



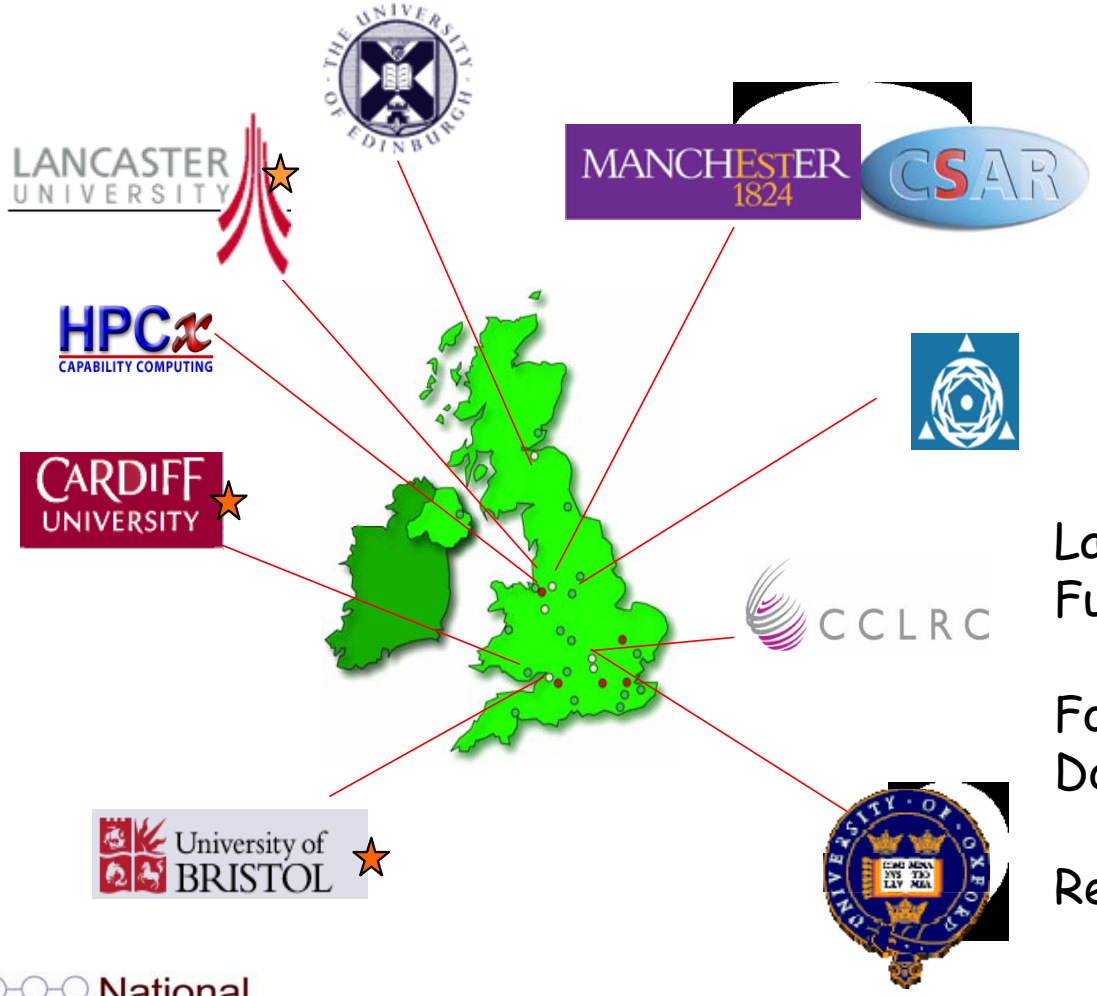
htt entres/

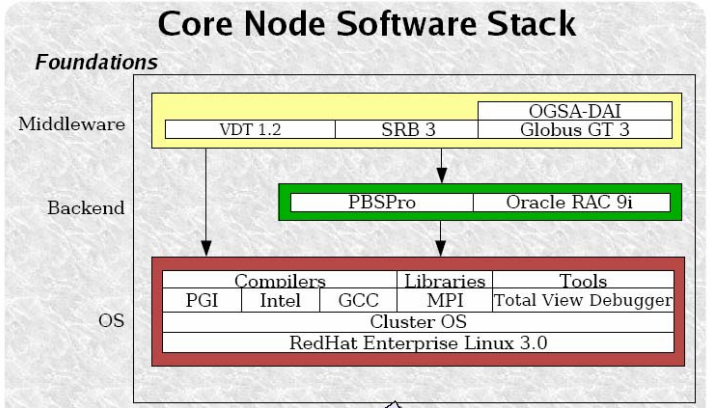
The National Grid Service

The National Grid Service

- The core UK grid, resulting from the UK's e-Science programme.
- Production use of computational and data grid resources.
- Supported by JISC, and is run by the Grid Operations Support Centre (GOSC).

The National Grid Service



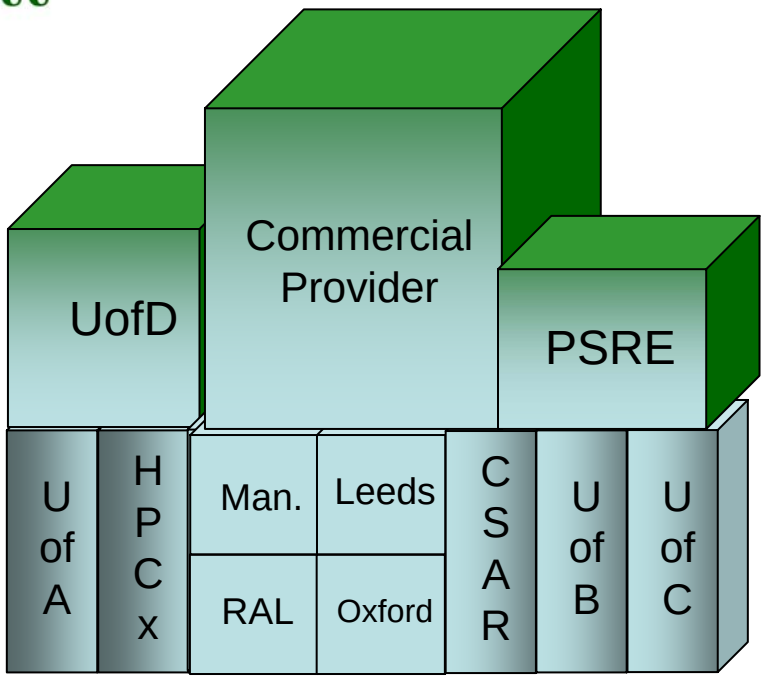


Launched April 2004
Full production - September 2004

Focus on deployment/operations
Do not do development

Responsive to users needs

National Grid Service



NGS Core Nodes: Host core services, coordinate integration, deployment and support
+free to access resources for all VOs. Monitored interfaces + services

NGS Partner Sites: Integrated with NGS, some services/resources available for all VOs
Monitored interfaces + services

NGS Affiliated Sites: Integrated with NGS, support for some VO's
Monitored interfaces (+security etc.)

NGS Overview: User view

- Resources
  - 4 Core clusters
  - UK's National HPC services
  - A range of partner contributions
    - clusters, shared mem. portals, data …
    - Partners and affiliates
- Access
  - Support UK academic researchers
  - All partners support common user base + whoever they want
  - Free at the point of use
  - Light weight peer review for limited "free" resources
    - Partners can provide larger commitments as required
- Central help desk
  - www.grid-support.ac.uk

NGS Overview: Organisational view

- Management
  - GOSC Board
    - Strategic direction
  - Technical Board
    - Technical coordination and policy
- Grid Operations Support Centre
  - Manages the NGS
  - Operates the UK CA + over 30 RA's
  - Operates central helpdesk
  - Minimum software stack
  - Policies and procedures
  - Manage and monitor partners

New partners

Over the last year, three new full partners have joined the NGS:

- Bristol, Cardiff and Lancaster
- Further details of resources can be found on the NGS web site: www.ngs.ac.uk.

- Resources committed to the NGS for a period of at least 12 months.

NGS: Gaining Access

NGS nodes

- data nodes at RAL and Manchester
- compute nodes at Oxford and Leeds
- partner nodes at Bristol, Cardiff and Lancaster

- all access is through digital X.509 certificates
  - from UK e-Science CA
  - or recognized peer

National HPC services

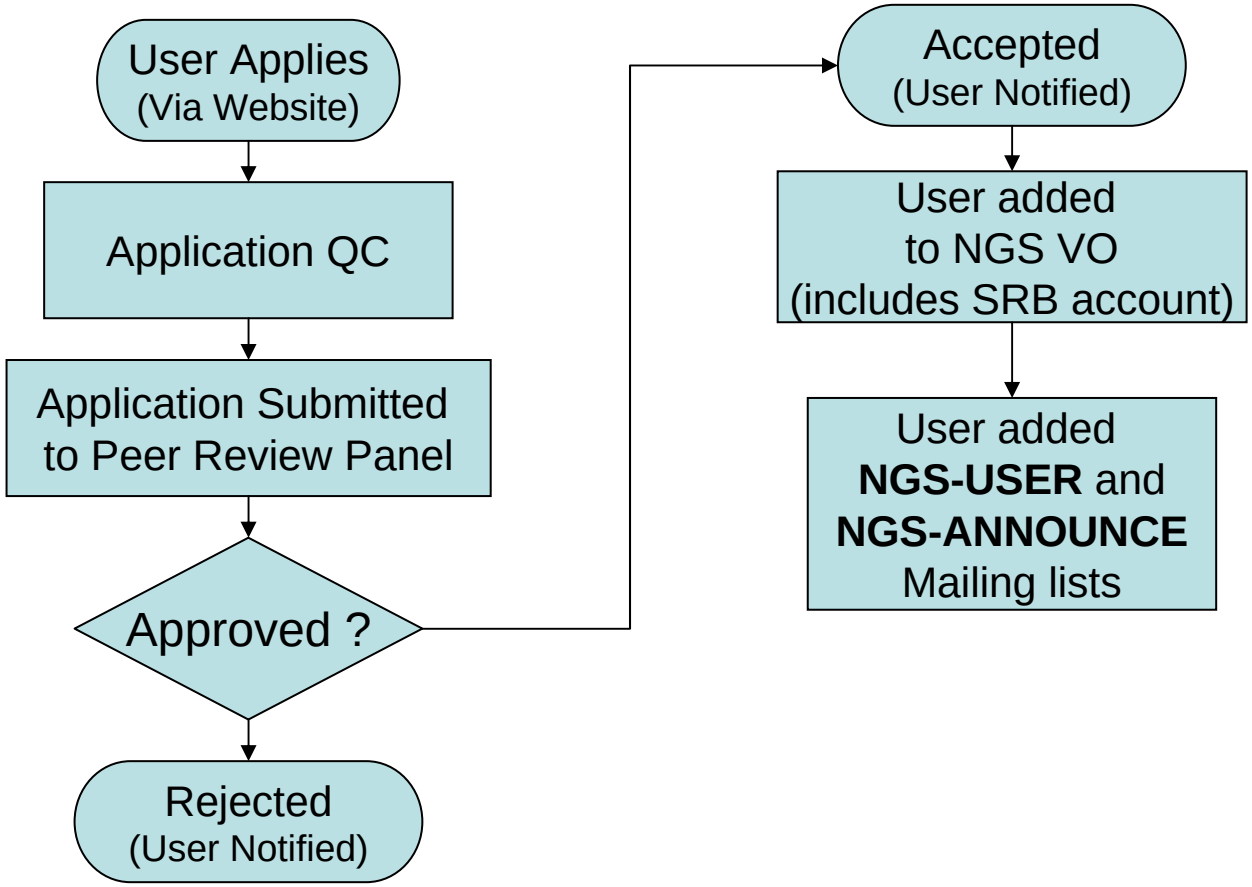
- HPCx

- CSAR

- Must apply separately to research councils

- Digital certificate and conventional (username/ password) access supported

User Registration (Process)



Projects and VOs

- Just need access to compute and data resources for users in your project?
  - Currently, mainly applications from individuals
  - project-based applications being dealt with case-by-case, as procedures are established – for these, talk to GOSC!
- Want to host your data on NGS?
  - consider SRB, Oracle, or OGSA-DAI
  - NGS maintains infrastructure
  - you populate and manage data
- Want to use NGS resources to provision services, portals for a community of users?
- Want researchers to access your data?

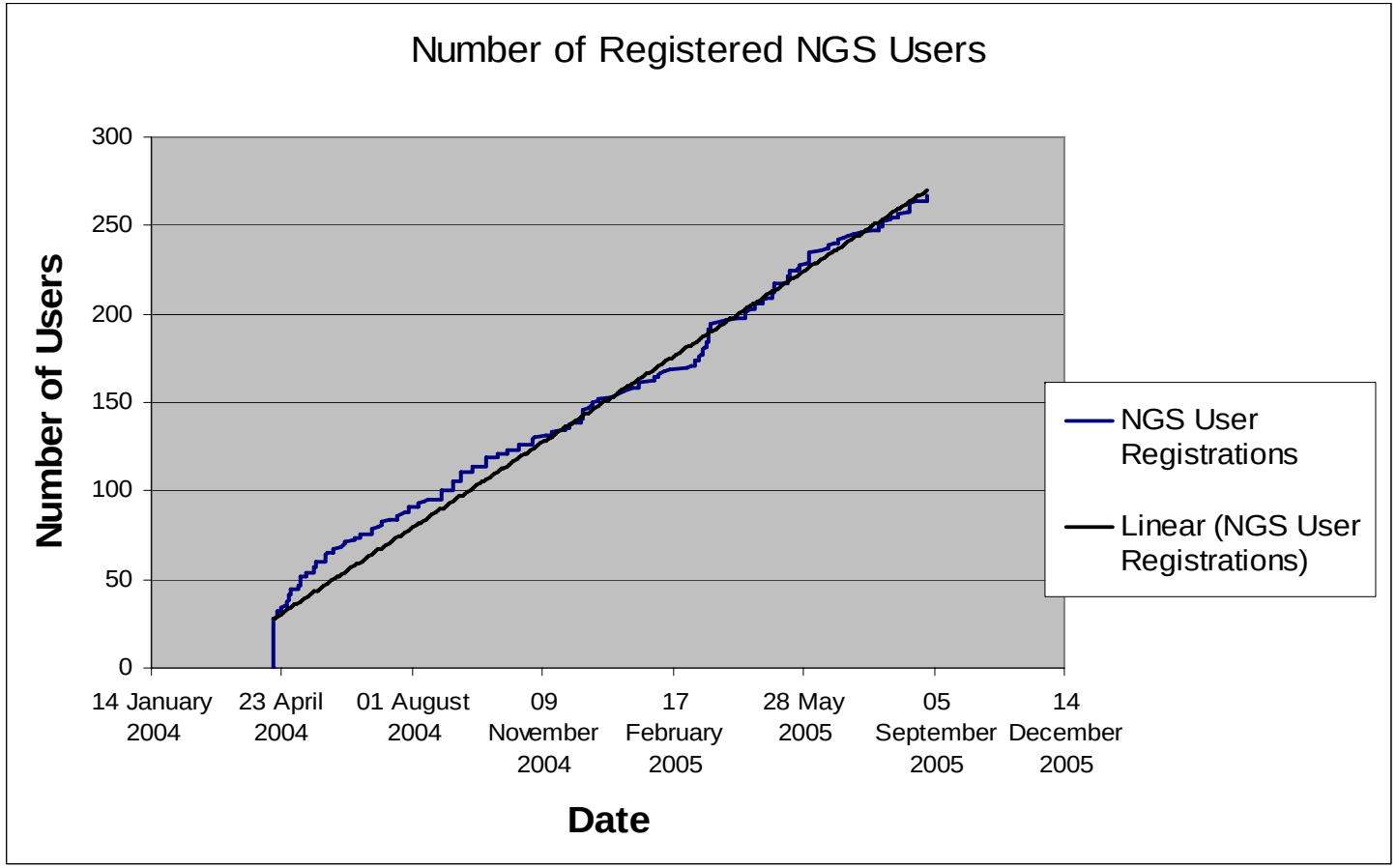
Why Join?

- Users increasingly want resources as services and not as complicated bits of kit
  - common interfaces across a range of facilities
- Funders of regional and national facilities want common interfaces to lower barriers to access
- By joining you leverage the national expertise in running these services
  - technical advice and support
  - security procedures and incident response
  - tools to help monitor and patch
  - Get it at lower cost by joining the NGS
- Members get a say in the technical decisions about the NGS

How Do I Get A Certificate?

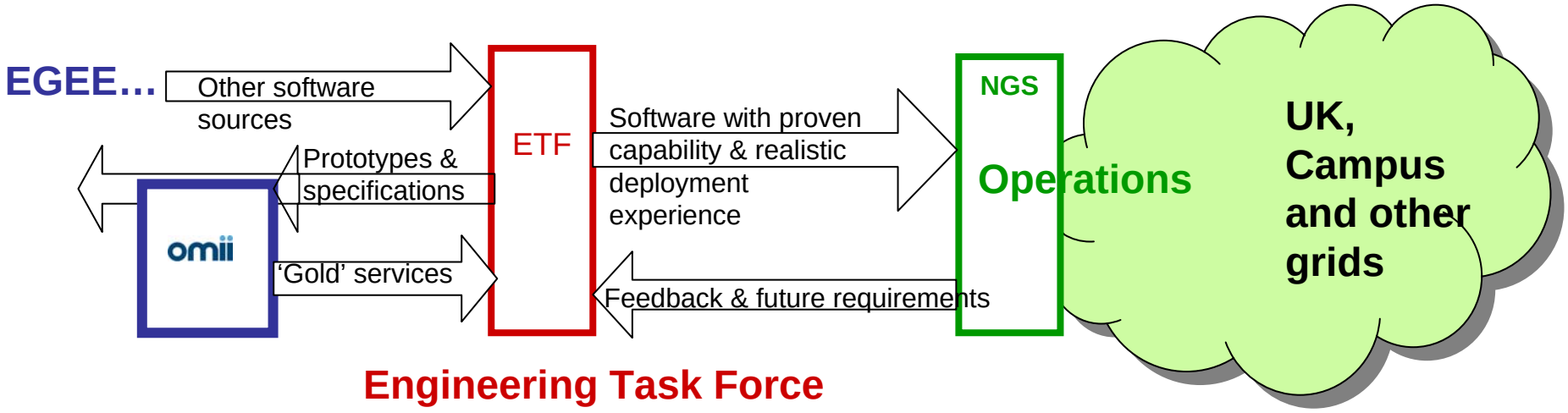
- You need a valid UK certificate before applying for an NGS account:
  - https://ca.grid-support.ac.uk, the UK Certificate Authority.
  - You will probably need to provide non-electronic proof of identity to your local representative of the CA.
    - For example: show your passport.
    - See http://www.grid-support.ac.uk/archive/ca/ralist.htm.
  - Always keep this certificate secure.
    - E.g. DO NOT LEAVE IT ON ANY NGS CORE NODE !
    - Do store it on a USB drive, that you keep safe!!

NGS Users


Number of Registered NGS Users
Number of Users
300
250
200
150
100
50
0
14 January 2004
23 April 2004
01 August 2004
09 November 2004
17 February 2005
28 May 2005
05 September 2005
14 December 2005
Date
NGS User Registrations
Linear (NGS User Registrations)

NGS: Managing middleware evolution

- Important to coordinate and integrate with deployment and operations work in EGEE and similar projects.
- Engineering Task Force makes recommendations for deployment on NGS.



Engineering Task Force
Deployment/testing/advice

NGS software

- Computation services based on Globus Toolkit 2
  - Use compute nodes for sequential or parallel jobs, primarily from batch queues
  - Can run multiple jobs concurrently
- Data services:
  - Storage Resource Broker:
    - Primarily for file storage and access
    - Virtual filesystem with replicated files
  - "OGSA-DAI": Data Access and Integration
    - Grid-enabling databases (relational, XML)
  - NGS Oracle service
  - GridFTP for efficient file transfer
- Authorisation and Authentication using GSI
- Portal to support collaboration and ease use

Data services on NGS

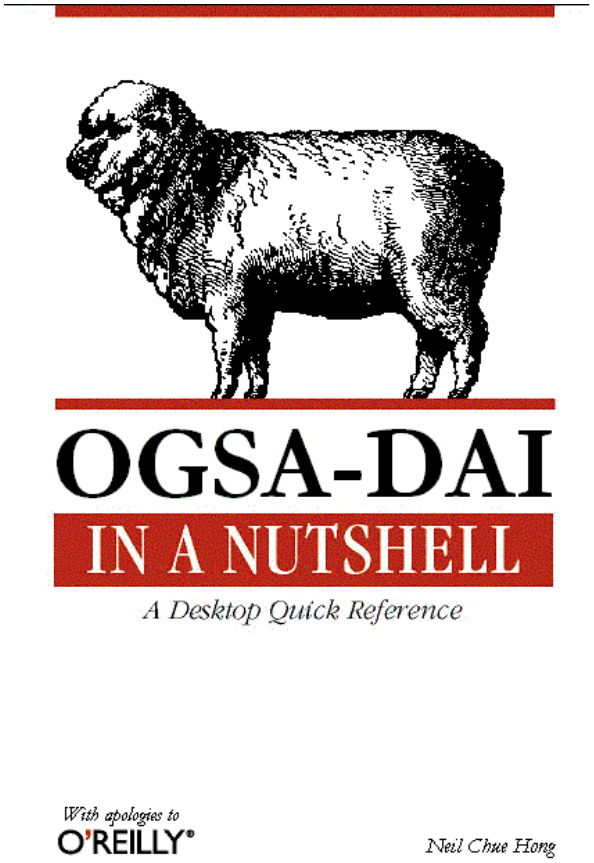
Simple data files

- Middleware supporting
  - **Replica files**
  - **Logical filenames**
  - **Catalogue**: maps logical name to physical storage device/file
  - **Virtual filesystems**, POSIX-like I/O
- **Storage Resource Broker**
  - **(3.3.1 since December 2005)**

Structured data

  - RDBMS, XML databases
  - Often pre-existing
  - Do NOT want to replicate
- Require *extendable* middleware tools to support
  - Move computation near to data
  - Underpin integration and federation
- **OGSA –DAI**
  - DAI: Data access and integration

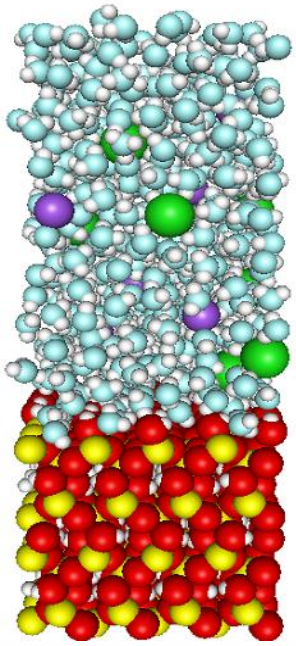
OGSA-DAI In One Slide

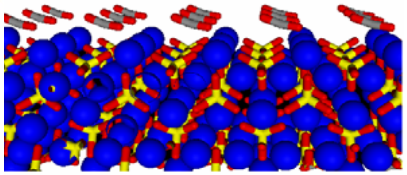


- An *extensible framework* for data access and integration.
- Expose heterogeneous data resources to a grid through web services.
- Interact with data resources:
  - Queries and updates.
  - Data transformation / compression
  - Data delivery.
- Customise for you project using
  - Additional Activities
  - Client Toolkit APIs
  - Data Resource handlers
- A base for higher-level services
  - federation, mining, visualisation,…

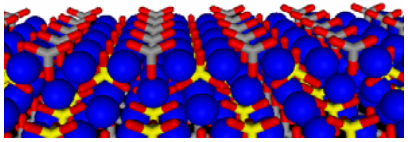
Slide from Neil Chue Hong

Applications: 1

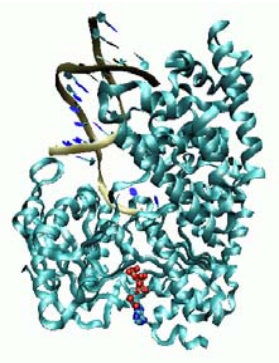


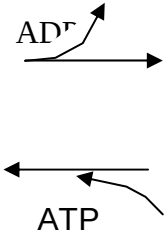


Molecular Dynamics

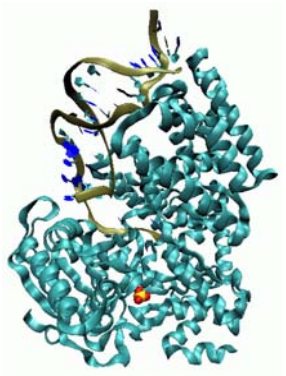


substrate complex



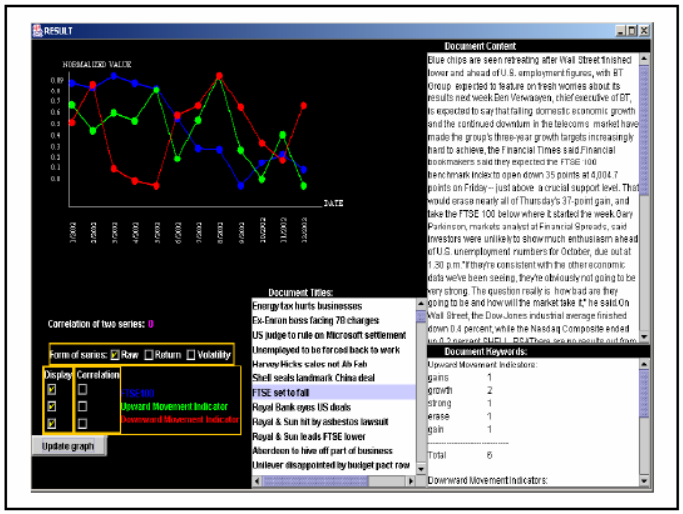


product complex

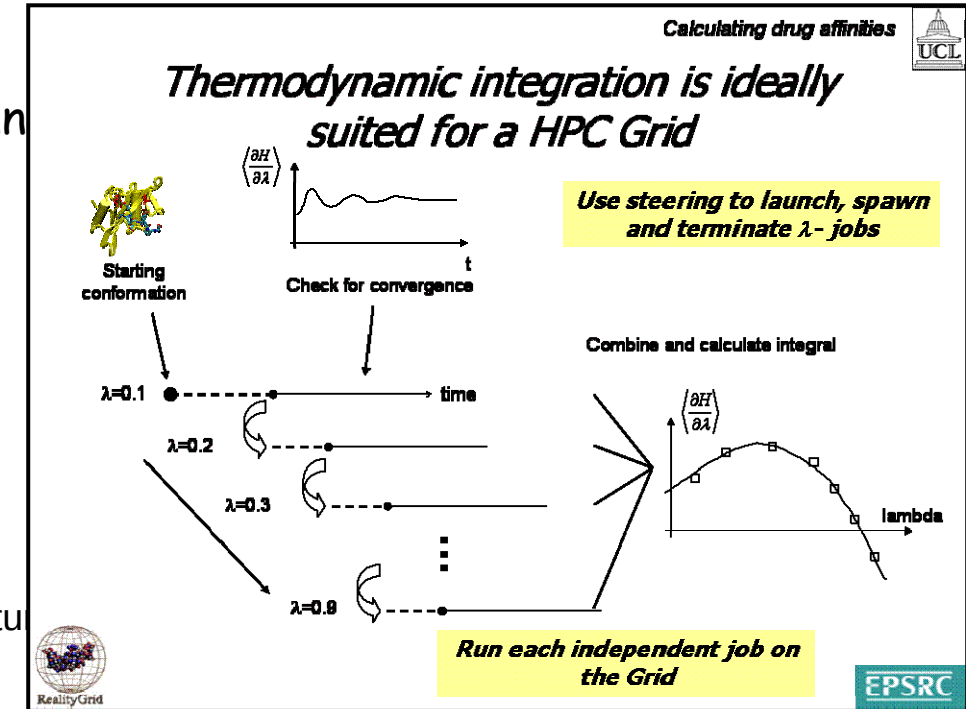


Lattice Boltzmann

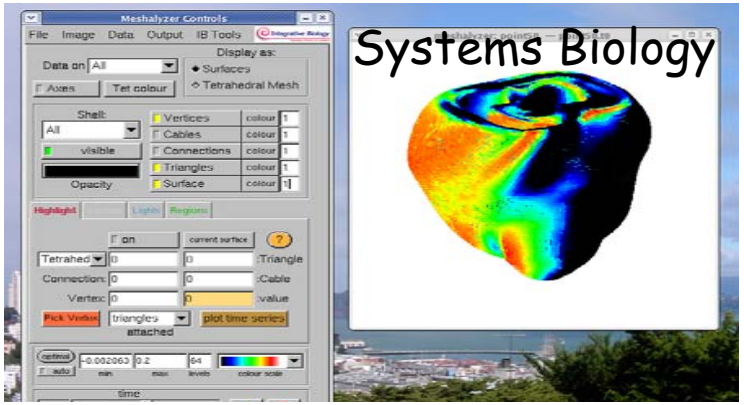
Text mining



UK e-Infrastructu

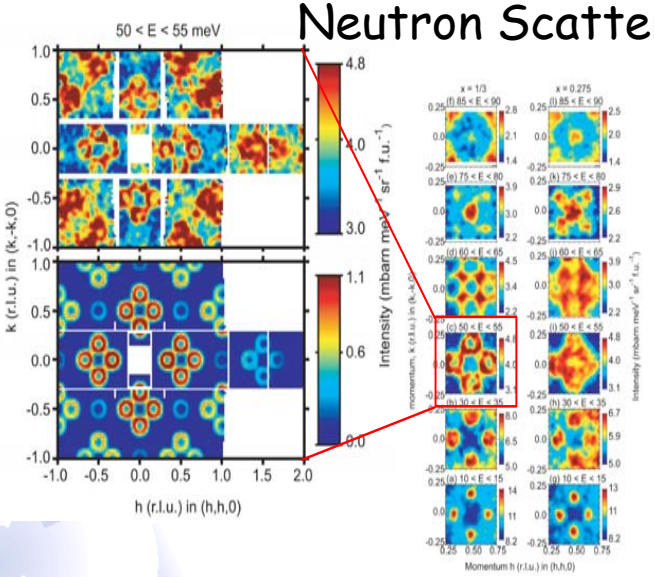


Applications

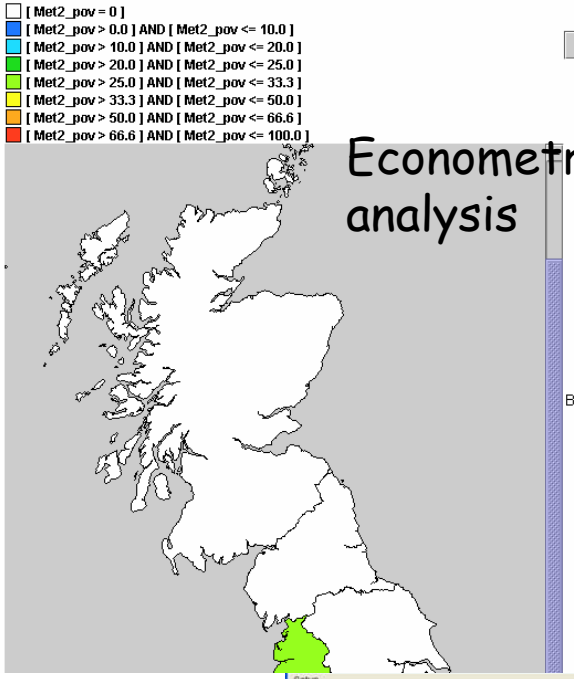


Example: $La_{2-x}Sr_xNiO_4$

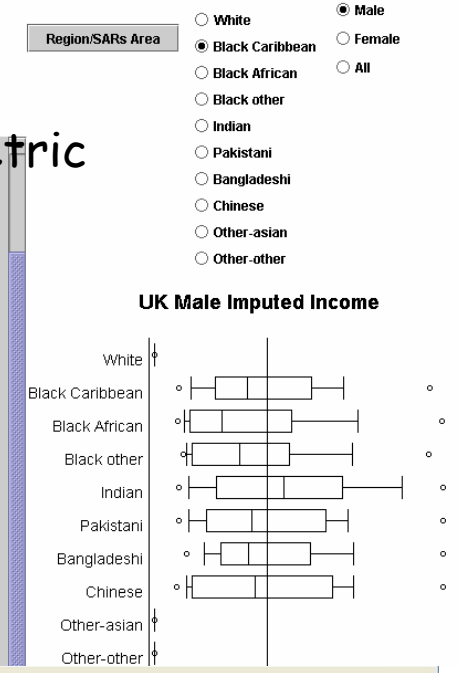
Neutron Scattering



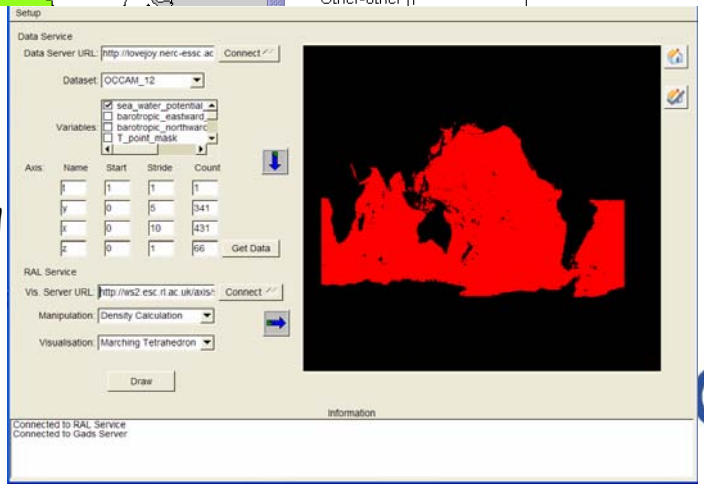
H. Woo et al, Phys Rev B 72 064437 (2005)



Econometric analysis



Climate modelling



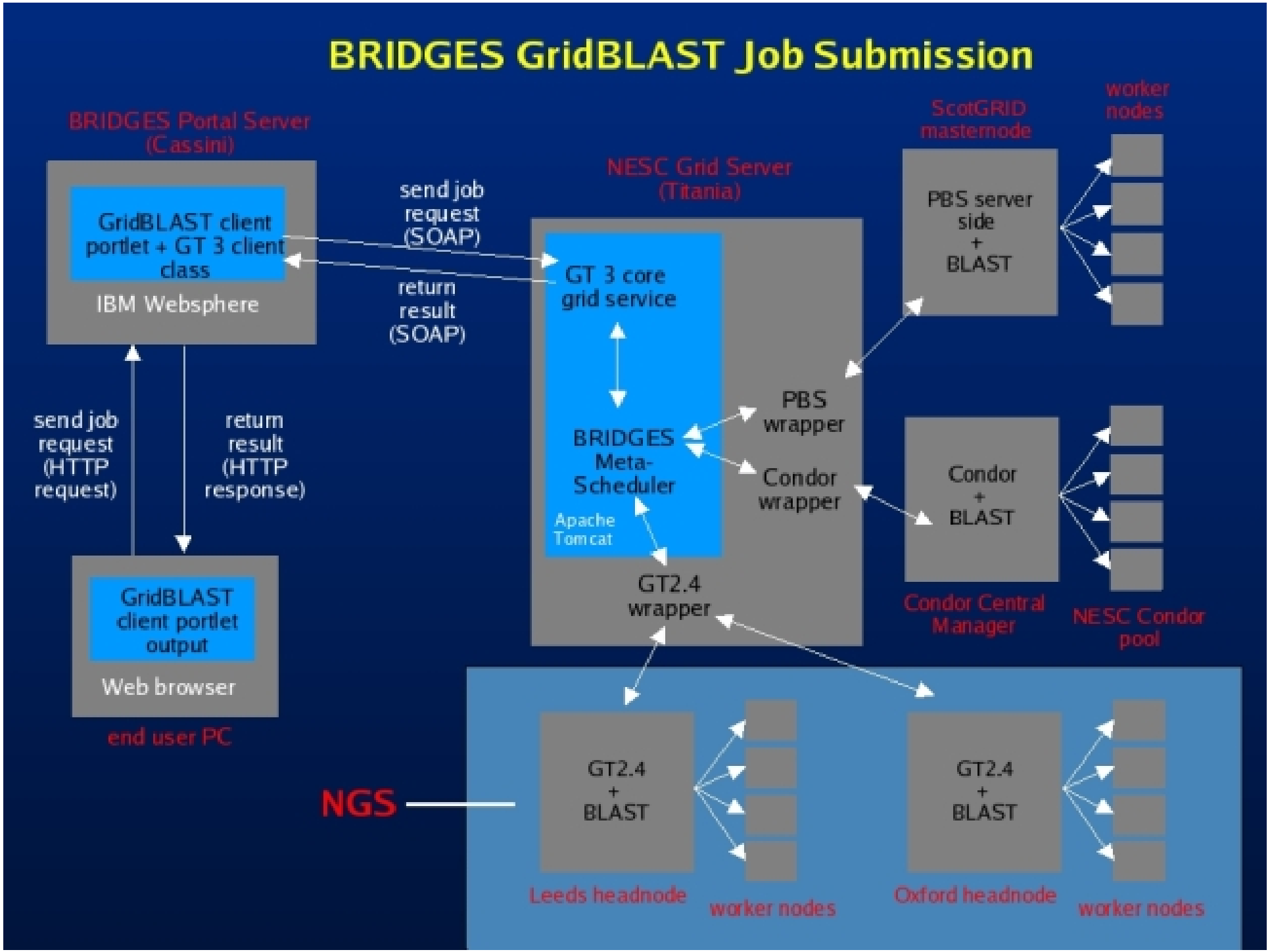
Infrastructure

Applications: 2

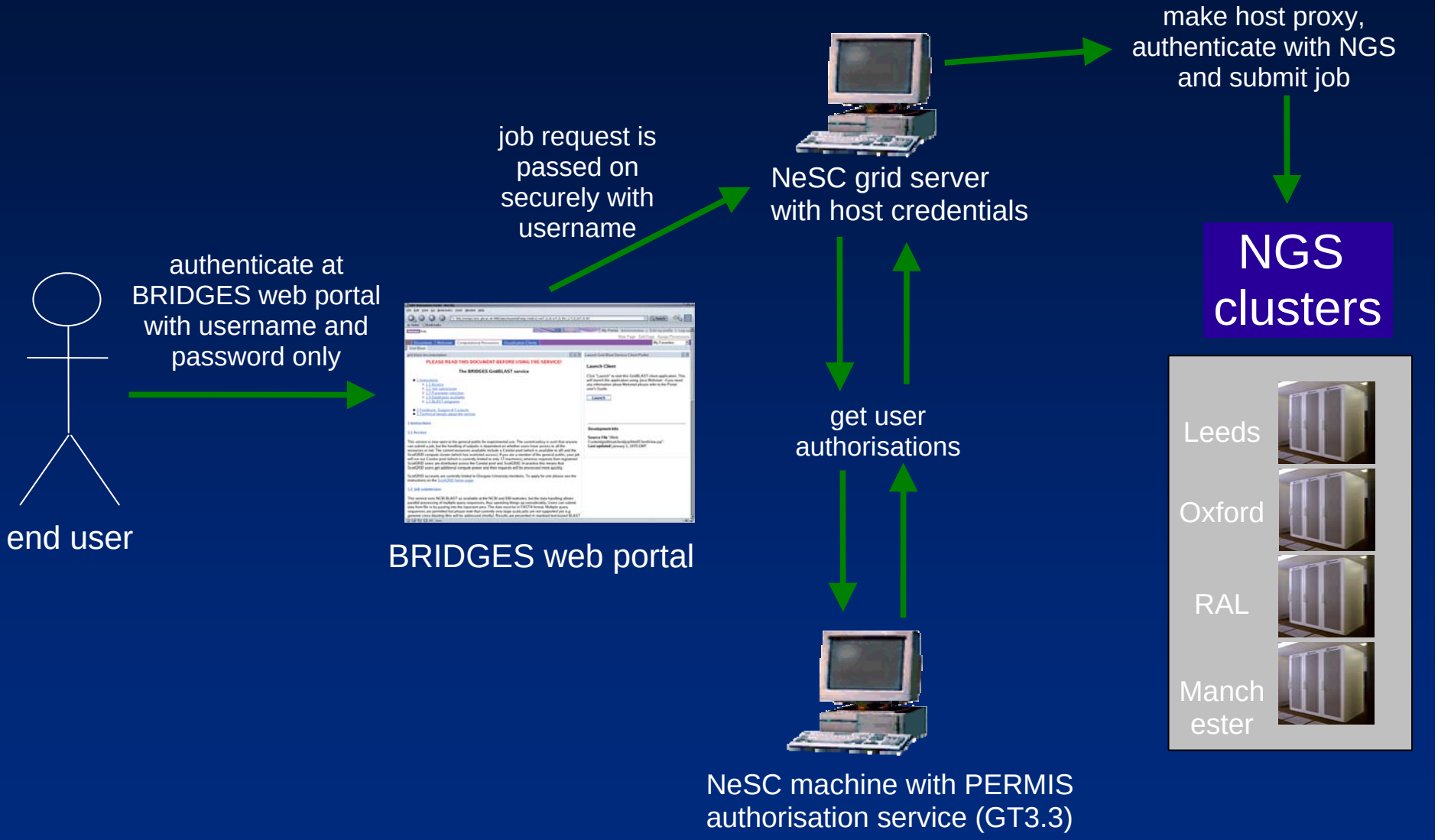
Other Applications:

- nano-particles
- protein folding
- ab-initio protein structure prediction
- radiation transport (radiotherapy)
- IXI (medical imaging)
- Biological membranes
- Micromagnetics
- Archaeology
- Text mining
- Lattice QCD (analysis)
- Astronomy (VO services)

- Many, but not all, applications cover traditional computational sciences
  - Both user and pre-installed software
- Several data focused activites
- Common features are
  - Distributed data and/or collaborators
- Not just pre-existing large collaborations
  - Explicitly encourage new users
  - Common infrastructure/interfaces

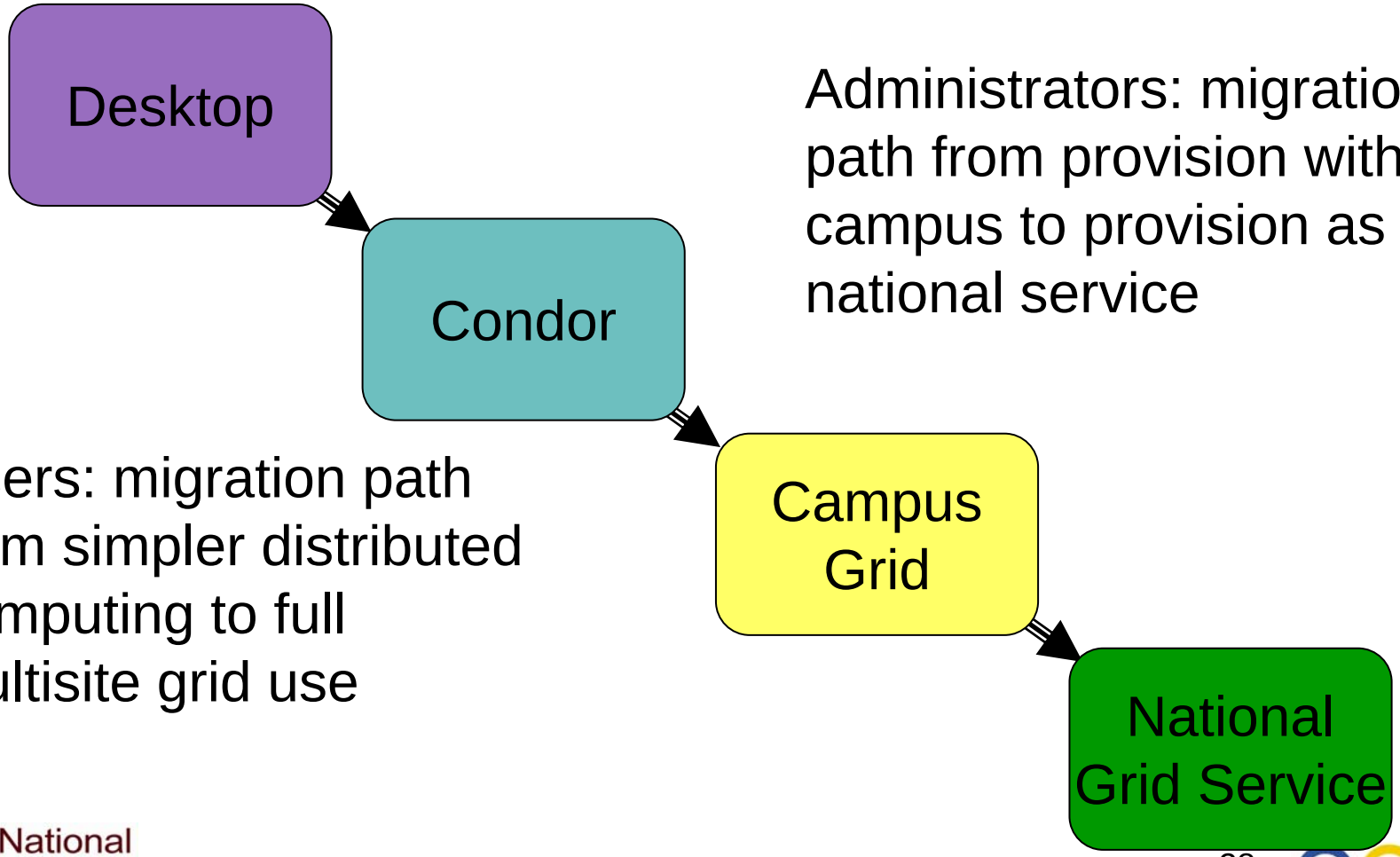

BRIDGES GridBLAST Job Submission
BRIDGES Portal Server (Cassini)
GridBLAST client portlet + GT 3 client class
IBM Websphere
send job request (SOAP)
return result (SOAP)
NESC Grid Server (Titania)
GT 3 core grid service
BRIDGES Meta-Scheduler
Apache Tomcat
PBS wrapper
Condor wrapper
GT2.4 wrapper
ScotGRID masternode
PBS server side + BLAST
worker nodes
Condor + BLAST
Condor Central Manager
NESC Condor pool
send job request (HTTP request)
return result (HTTP response)
GridBLAST client portlet output
Web browser
end user PC
NGS
GT2.4 + BLAST
Leeds headnode
worker nodes
GT2.4 + BLAST
Oxford headnode
worker nodes

Security in BRIDGES – summary



Slide by Micha Bayer, NeSC

Migration paths



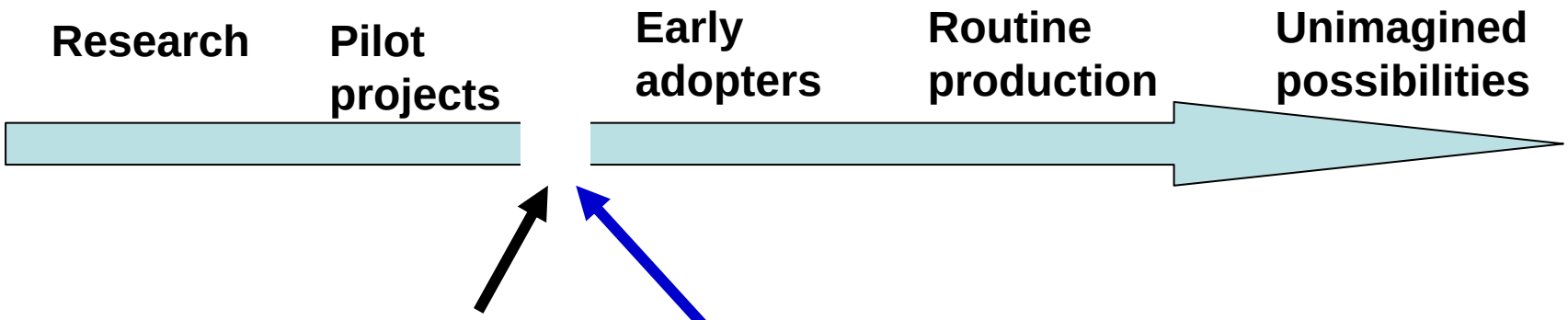
Administrators: migration path from provision within campus to provision as national service

Users: migration path from simpler distributed computing to full multisite grid use

Based on slide by Jonathan Giddy, Welsh e-Science Centre

OMII-UK: Open Middleware Infrastructure Institute

Building e-Research



Researchers are not funded to provide production quality software for others to use

OMII-UK exists to help bridge this gap!

Open Middleware Infrastructure Institute

To be a leading provider of reliable interoperable and open-source Grid middleware components services and tools to support advanced Grid enabled solutions in academia and industry.

- Formed University of Southampton (2004)
  - Focus on an easy to install e-Infrastructure solution
  - Utilise existing software & standards
- Expanded with new partners in 2006
  - OGSA-DAI team at Edinburgh
  - myGrid team at Manchester

Activity

- By providing a software repository of Grid components and tools from e-science projects
- By re-engineering software, hardening it and providing support for components sourced from the community
- By a managed programme to contract the development of “missing” software components necessary in grid middleware
- By providing an integrated grid middleware release of the sourced software components

The Managed Programme:

- Integrated with the Distribution
  - OGSA-DAI (Data Access service)
  - GridSAM (Job Submission & Monitoring service)
  - Grimoires (Registry service based on UDDI)
  - GeodiseLab (Matlab & Jython environments)
  - FINS (Notification services using WS-Eventing)
- Delivering into the repository
  - BPEL (Workflow service)
  - MANGO (Managing workflows with BPEL)
  - FIRMS (Reliable messaging)

Overview

- The UK e-science programme
- The National Grid Service
- GOSC – Grid Operations Support Centre
- OMII – Open Middleware Infrastructure Institute
- **JISC – Joint Information Systems Committee**
  - **Services: NGS, Networking, Data Centres**
  - **Programmes**

JISC

Super JANET

JISC provide budget to UKERNA

JISC guide UKERNA through the JCN

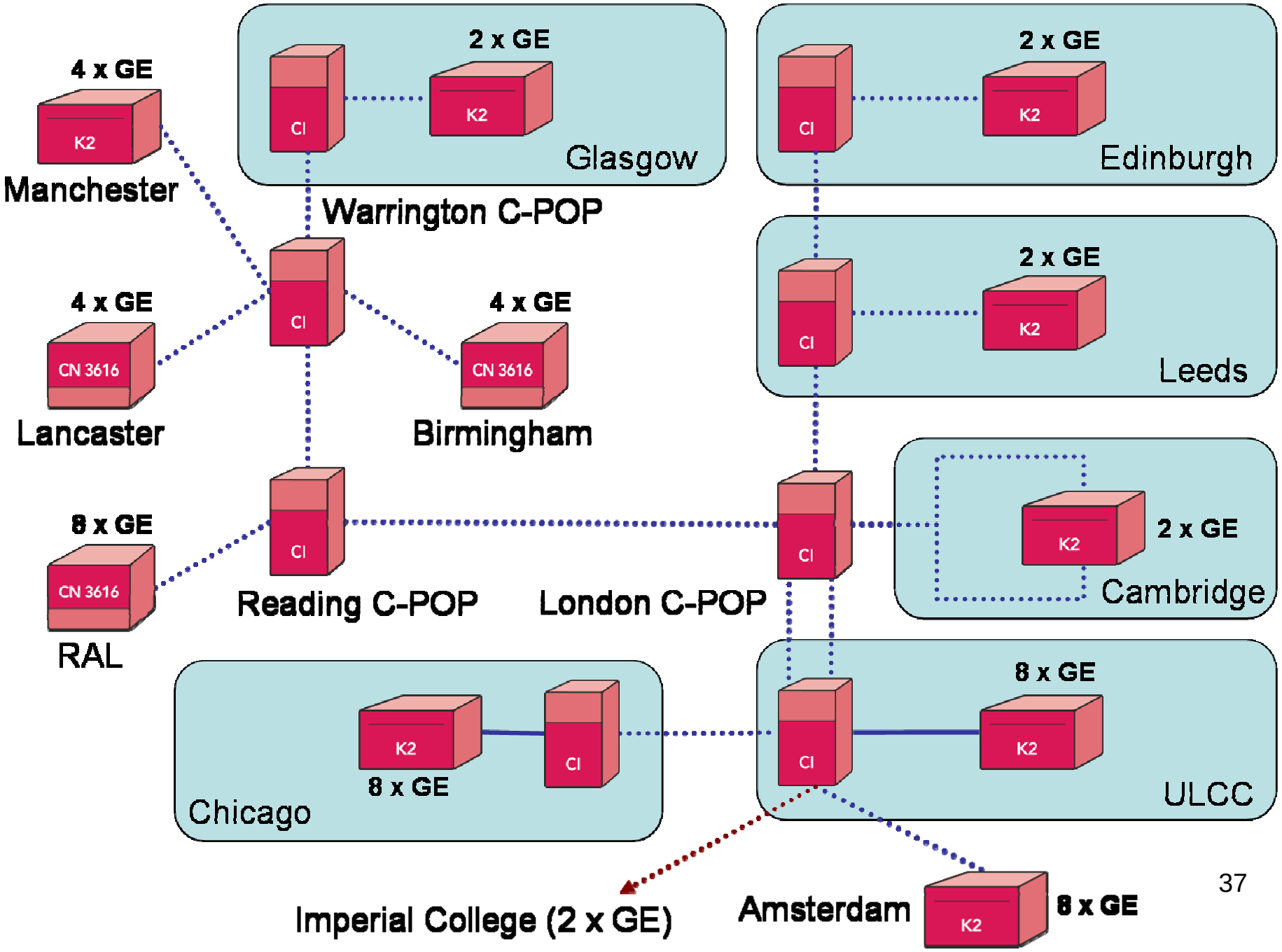
UKERNA provide and manage JANET

Present incarnation is SJ4

SJ5 en route

UKLight

- Funded by HEFCE and managed by UKERNA
- UK's first national switched circuit optical network
- Complements the SuperJanet4 production network
- National dark fibre facility for use by the photonics research community
- 10Gbit/s backbone to selected points in the UK
- Channels can be multiplexed, e.g. 4 x 2.5Gbit/s
- Connects to global optical networks via 10Gbit/s links to Chicago (StarLight) and Amsterdam (NetherLight)
- ESLEA is the first widely scoped project to exploit UKLight for a range of scientific applications


4 x GE
K2
Manchester
2 x GE
CI
K2
Glasgow
Warrington C-POP
2 x GE
CI
K2
Edinburgh
4 x GE
CN 3616
Lancaster
CI
4 x GE
CN 3616
Birmingham
2 x GE
CI
K2
Leeds
8 x GE
CN 3616
RAL
CI
Reading C-POP
London C-POP
CI
K2
2 x GE
Cambridge
K2
8 x GE
Chicago
CI
8 x GE
CI
K2
ULCC
Imperial College (2 x GE)
Amsterdam
K2
8 x GE

What are (JISC) Data Centres?

- EDINA http://www.edina.ac.uk/
  - Mulitmedia
  - Geospatial
- MIMAS http://www.mimas.ac.uk
  - Census
- What do they do?
  - Content delivery – with AA (currently ATHENS)
  - Licensing authority

- OGSA-DAI territory!
  - Access databases as services on the National Grid Service
- Amongst challenges:
  - ATHENS / Shibboleth / X.509 integration

JISC Programmes

- **Research is only the start !**

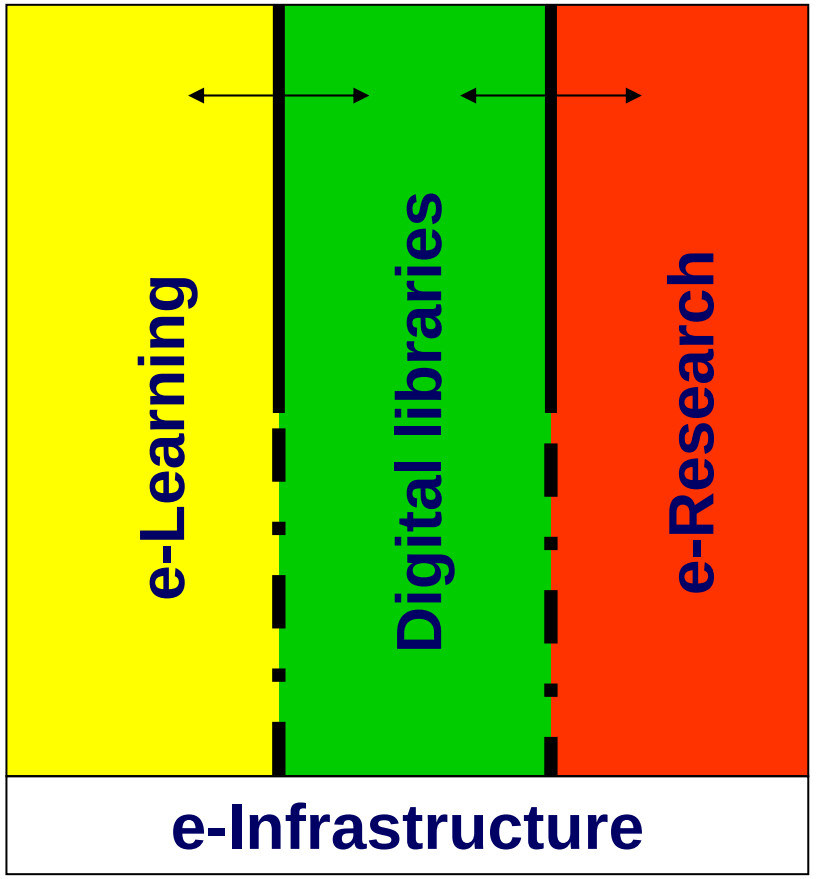


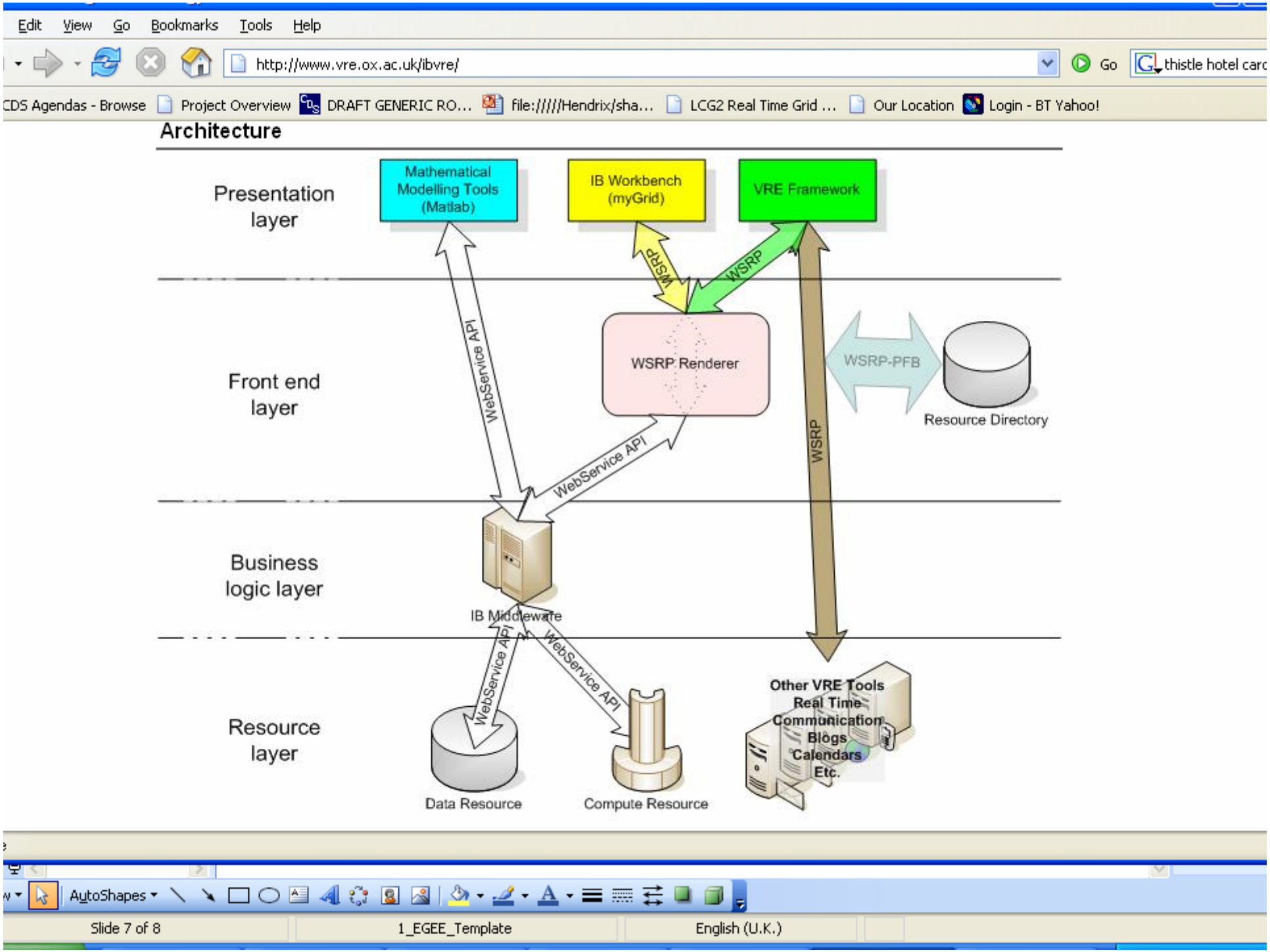
Figure derived from JISC

JISC Programmes

British Library/JISC Online Audio Usability Evaluation Workshop
Core Middleware Infrastructure
Core Middleware: Technology Development Programme
Digital Libraries in the Classroom Programme
Digital Prreservation and Records Management
Digital Repositories Programme
Digitisation Programme
Distributed e-Learning Strand
e-Learning Programme
e-Learning Tools Projects - Phase 2
Exchange for Learning (X4L) Phase 2
Exchange for Learning (X4L) Programme
Focus on Access to Institutional Resources (FAIR) Programme
JISC Framework Programme
JISC-SURF Partnering on Copyright
Network Development Programme
Portals Programme
Presentation Programme
Semantic Grid and Autonomic Computing Programme
Shared Services Programme
Supporting Digital Preservation and Asset Management in Institutions
Virtual Research Environments Programme

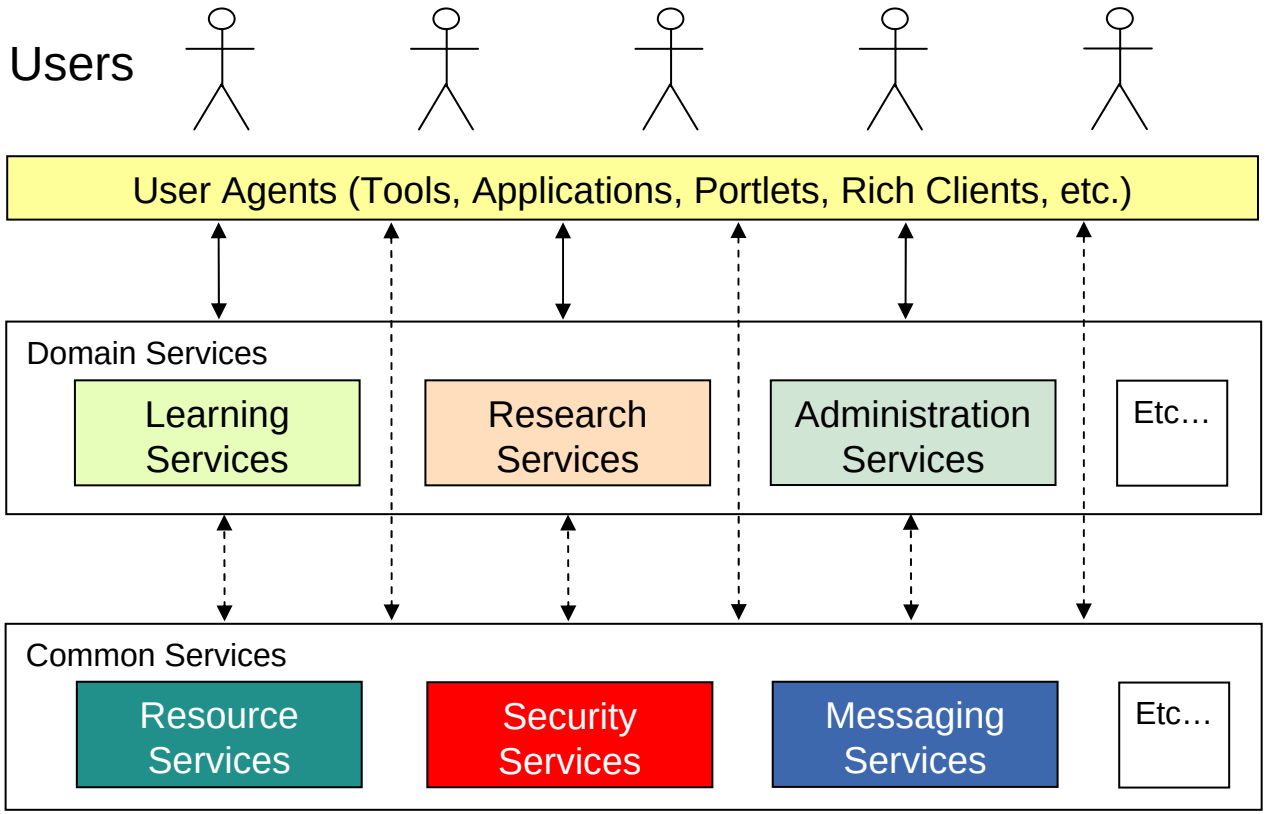
VRE development for Integrative Biology

- http://www.vre.ox.ac.uk/ibvre/
- “Whereas the existing IB Grid services have focussed on supporting the core IB experimental workflow - moving, processing and visualising data on the Grid - the IBVRE will support the research process in its widest sense i.e. activities such as identifying research areas and funding sources, building and managing projects/consortia, real-time communication, disseminating results, and provision of training to new researchers entering the field (learning and teaching support tools)”.


Edit View Go Bookmarks Tools Help
http://www.vre.ox.ac.uk/ibvre/
Go
thistle hotel carc
CDS Agendas - Browse
Project Overview
DRAFT GENERIC RO...
file:////Hendrix/sha...
LCG2 Real Time Grid ...
Our Location
Login - BT Yahoo!
Architecture
Presentation layer
Front end layer
Business logic layer
Resource layer
Mathematical Modelling Tools (Matlab)
IB Workbench (myGrid)
VRE Framework
WSRP
WSRP
WebService API
WSRP Renderer
WSRP-PFB
Resource Directory
WSRP
WebService API
IB Middleware
WebService API
WebService API
Other VRE Tools
Real Time Communication
Blogs
Calendars
Etc.
Data Resource
Compute Resource
AutoShapes
Slide 7 of 8
1_EGEE_Template
English (U.K.)

e-Frameworks Programme

- **Everyone (e-Learning, Research, Core middleware,…) are all developing services**



⇒ **The Frameworks programme is attempt to engender a coherent approach across all JISC programmes where possible**

UK e-Infrastructure providers

- The UK e-science programme
- The National Grid Service
- GOSC – Grid Operations Support Centre
- OMII – Open Middleware Infrastructure Institute
- JISC - Joint Information Systems Committee

Web Sites

- NGS
  - http://www.ngs.ac.uk
  - To see what's happening: http://ganglia.ngs.rl.ac.uk/
- GOSC
  - http://www.grid-support.ac.uk
- OMII
  - http://www.omii.ac.uk/
- CSAR
  - http://www.csar.cfs.ac.uk
- HPCx
  - http://www.hpcx.ac.uk
- Grid Operations Support Centre http://www.grid-support.ac.uk
- National e-Science Centre http://www.nesc.ac.uk
  - UK Training events http://www.nesc.ac.uk/training

- JANET http://www.ja.net/
- UKLight http://www.uklight.ac.uk
- ESLEA http://www.eslea.uklight.ac.uk