



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



<http://www.ngs.ac.uk>

UK e-Infrastructure

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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



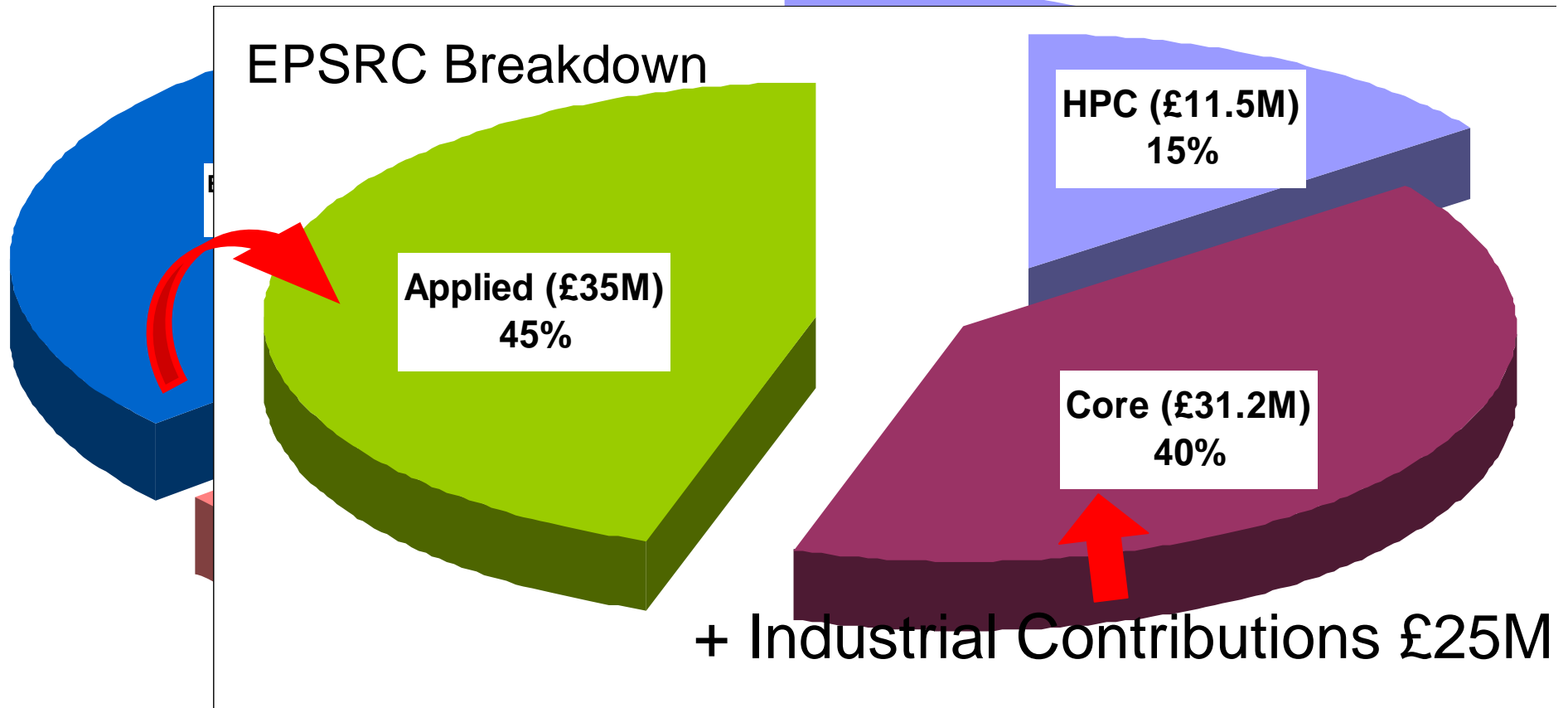
- The UK e-science programme
- The National Grid Service
- GOSC – Grid Operations Support Centre
 - UK e-Science Certification Authority (CA)
- OMII-UK – Open Middleware Infrastructure Institute
- JISC - Joint Information Systems Committee



UK e-Science Budget (2001-2006)



Total: £213M+ £100M via JISC

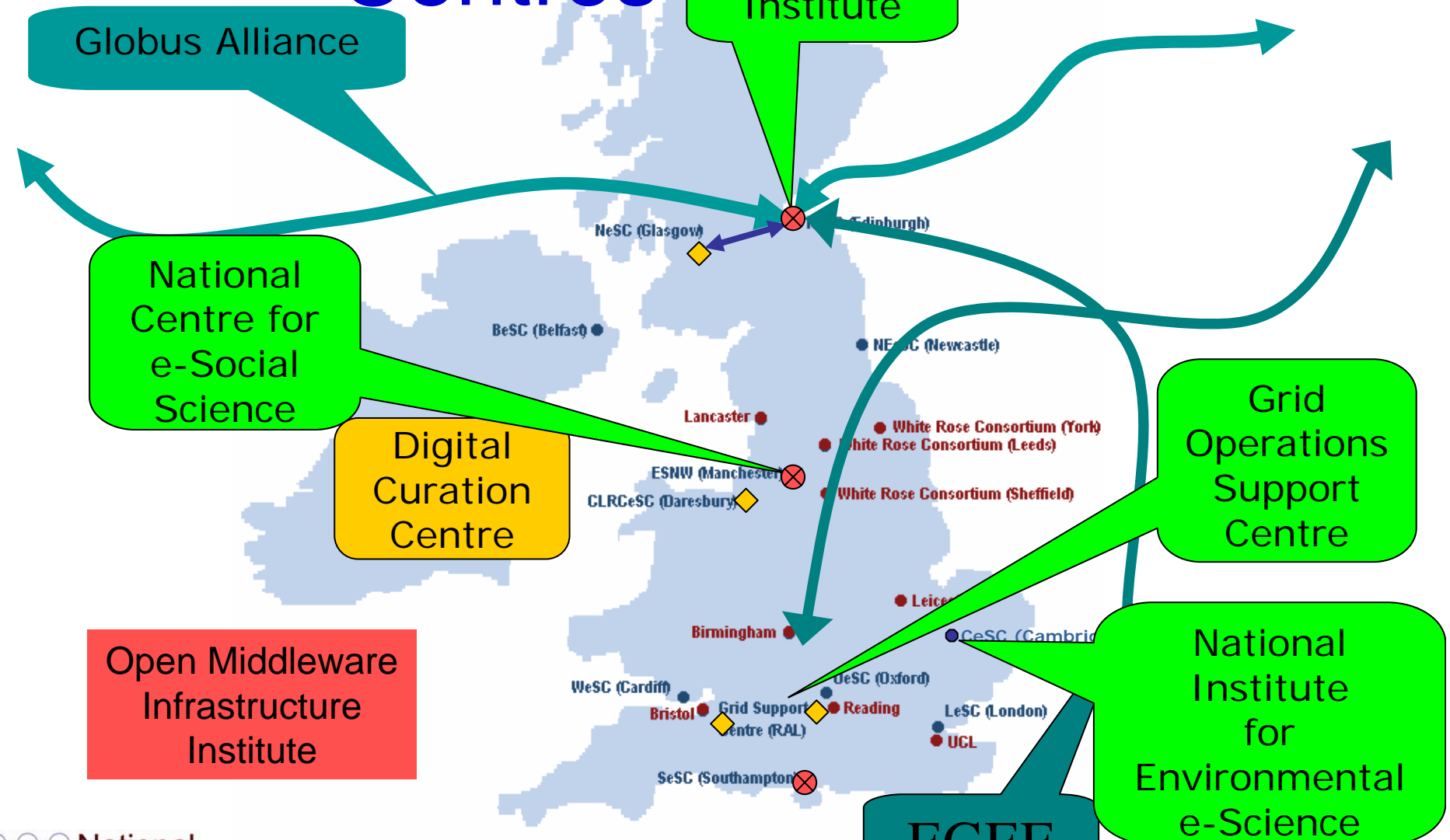


Source: Science Budget 2003/4 – 2005/6, DTI(OST)

The e-Science Centres

GOSC

NGS National Grid Service



<http://www.nesc.ac.uk/centres/>





The National Grid Service



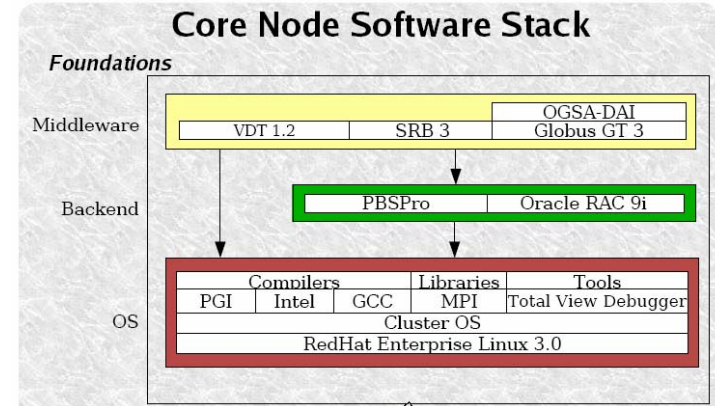
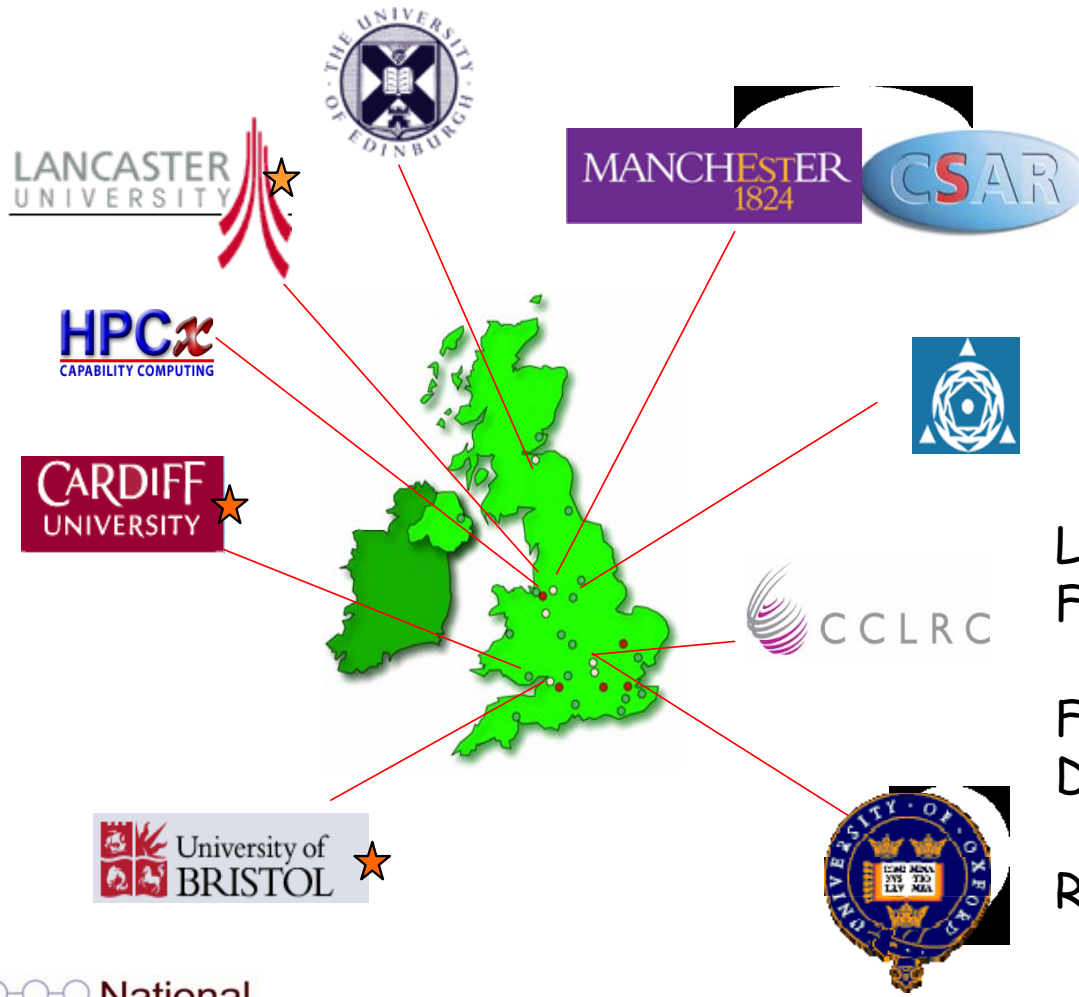
The National Grid Service



- 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

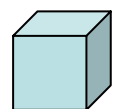
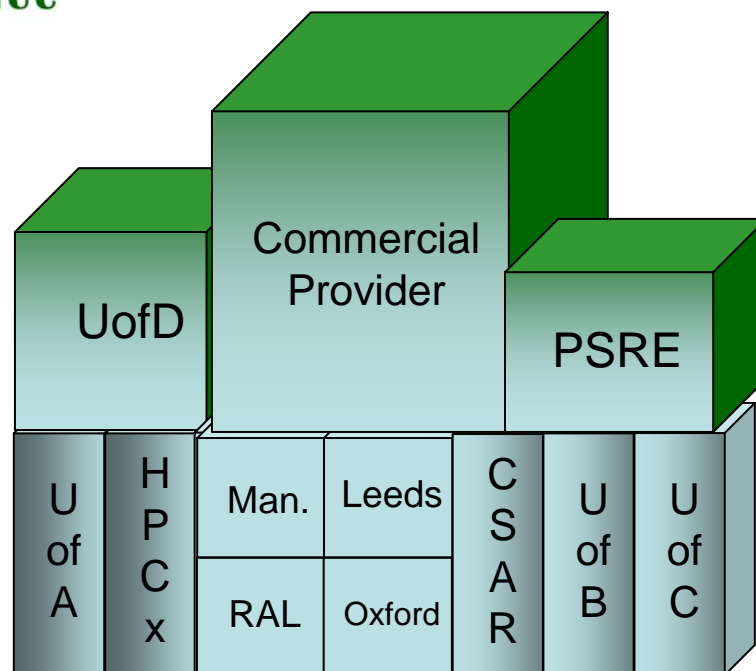


UK e-Infrastructure

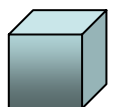




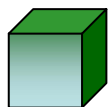
**National
Grid
Service**



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.)



UK e-Infrastructure



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



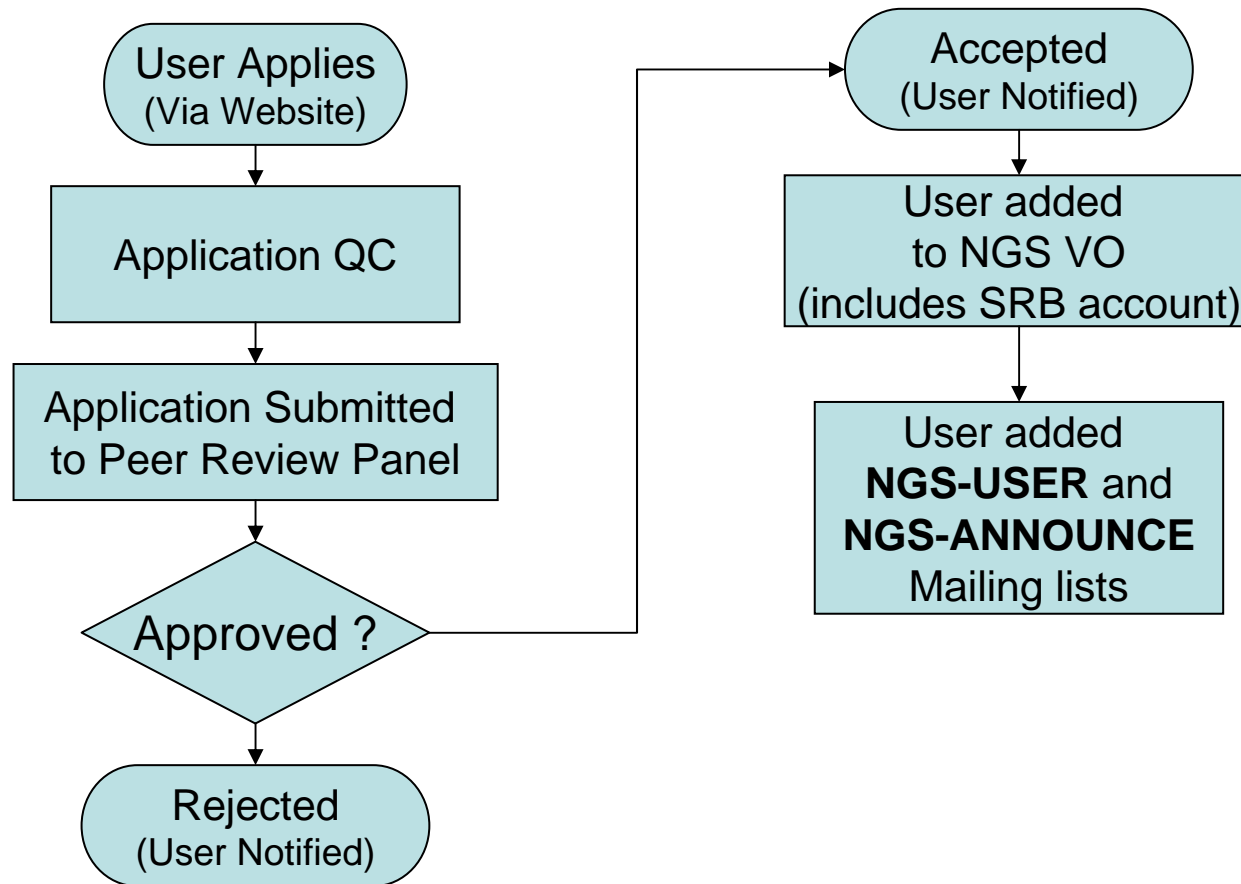
- CSAR



- 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



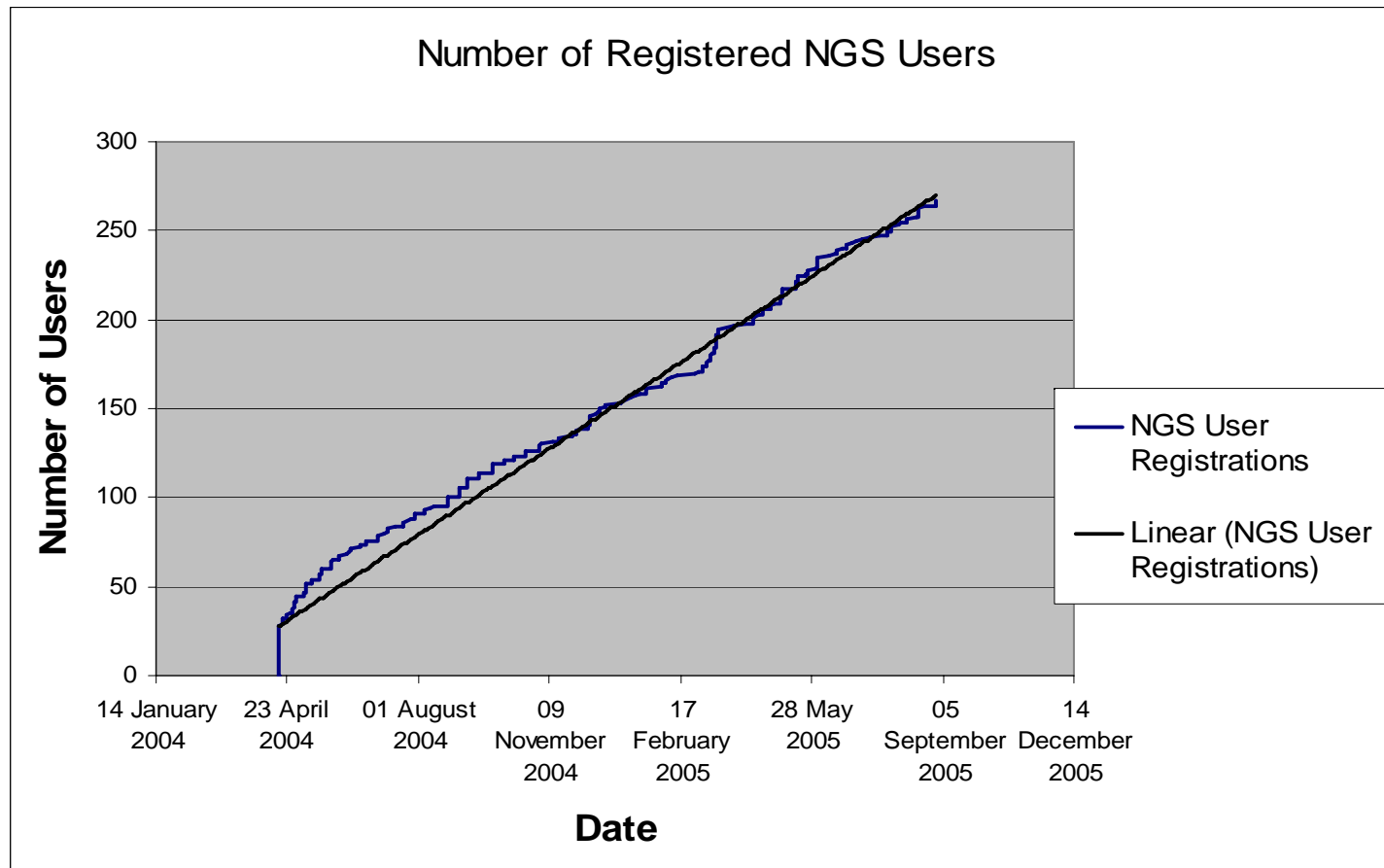
How Do I Get A Certificate?



- 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

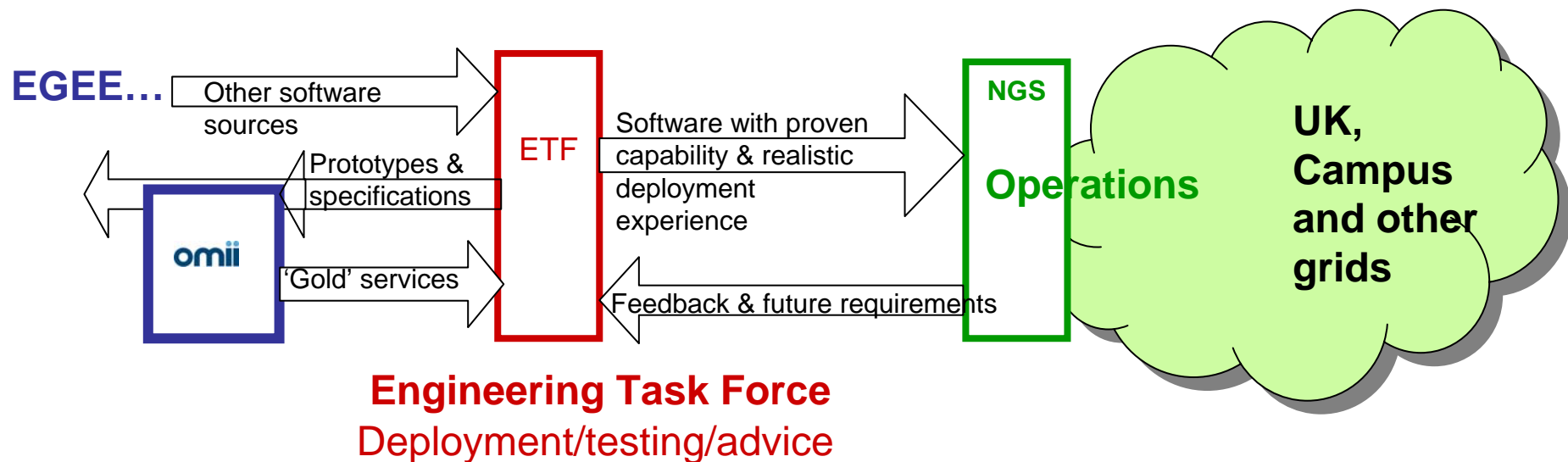




NGS: Managing middleware evolution



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





NGS software



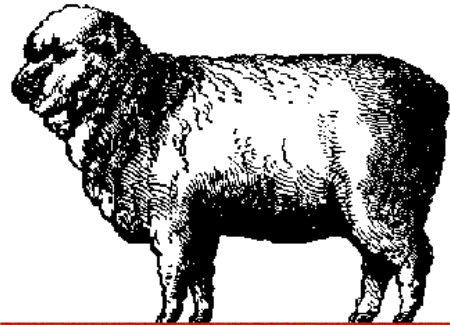
- Computation services based on **Globus Toolkit 2**
 - Use compute nodes for sequential or parallel jobs, primarily from batch queues
 - Can run multiple jobs concurrently
- Data services:
 - **Storage Resource Broker**:
 - Primarily for file storage and access
 - Virtual filesystem with replicated 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

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 A NUTSHELL

A Desktop Quick Reference

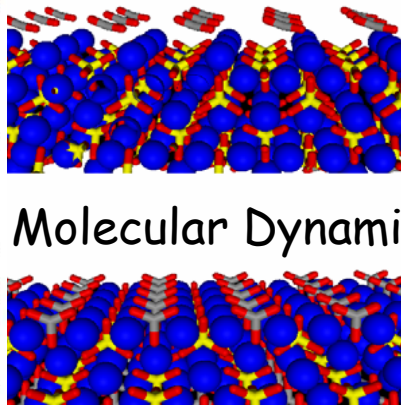
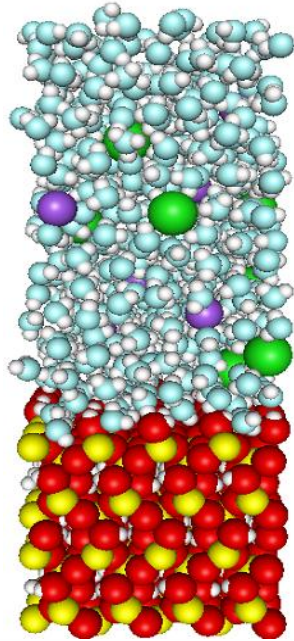
With apologies to
O'REILLY®

Neil Chue Hong

- 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,...

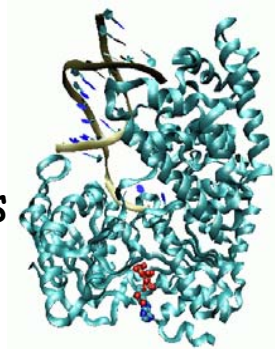
Slide from Neil Chue Hong

Applications: 1

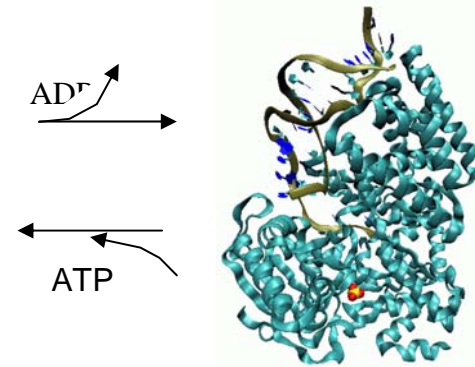


Molecular Dynamics

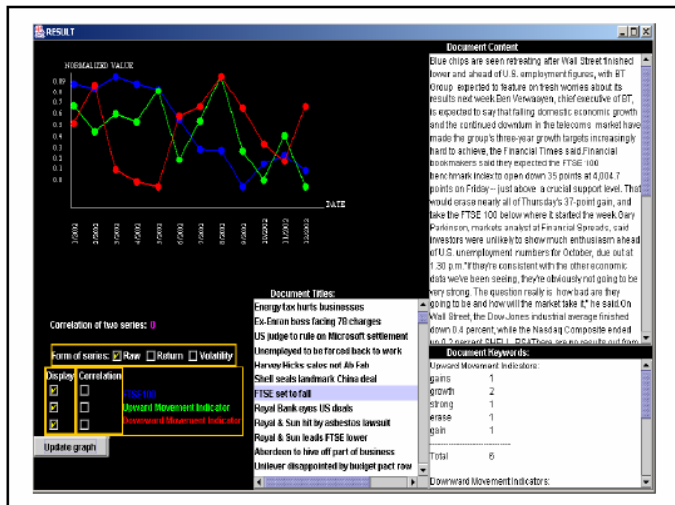
substrate complex



product complex



Lattice Boltzmann
Text mining



Calculating drug affinities

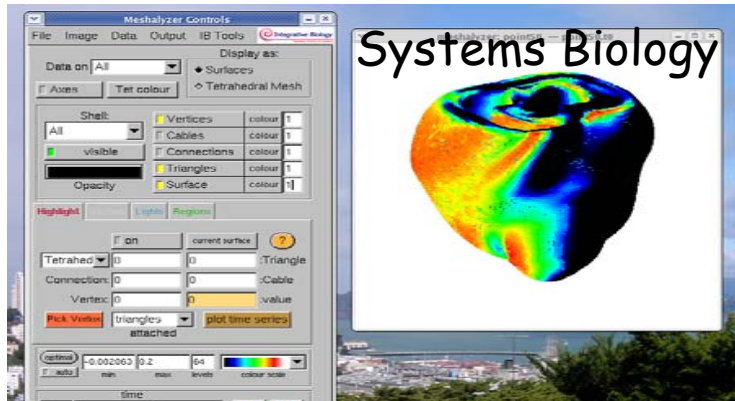
Thermodynamic integration is ideally suited for a HPC Grid

Use steering to launch, spawn and terminate λ -jobs

Combine and calculate integral

Run each independent job on the Grid

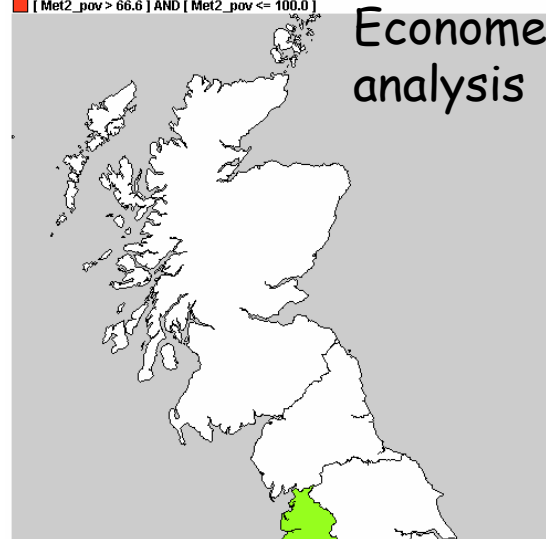
Applications



Systems Biology

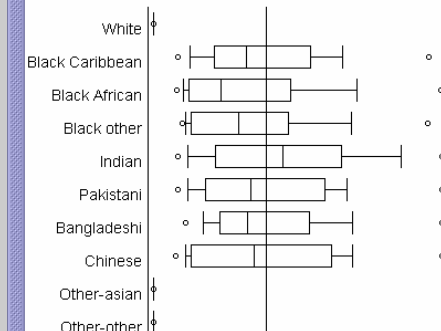
- [Met2_pov = 0]
- [Met2_pov > 0.0] AND [Met2_pov <= 10.0]
- [Met2_pov > 10.0] AND [Met2_pov <= 20.0]
- [Met2_pov > 20.0] AND [Met2_pov <= 25.0]
- [Met2_pov > 25.0] AND [Met2_pov <= 33.3]
- [Met2_pov > 33.3] AND [Met2_pov <= 50.0]
- [Met2_pov > 50.0] AND [Met2_pov <= 66.6]
- [Met2_pov > 66.6] AND [Met2_pov <= 100.0]

Econometric analysis



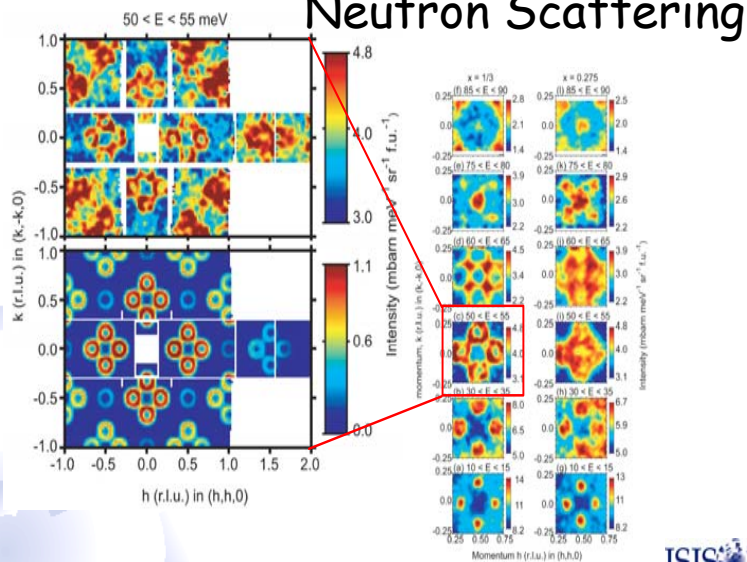
- Region/SARs Area
- White
 - Black Caribbean
 - Black African
 - Black other
 - Indian
 - Pakistani
 - Bangladeshi
 - Chinese
 - Other-asian
 - Other-other

UK Male Imputed Income

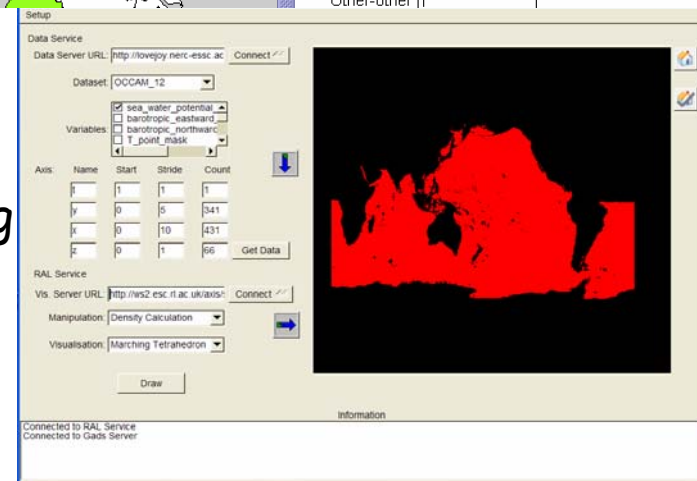


Example: $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$

Neutron Scattering



Climate modelling



Infrastructure



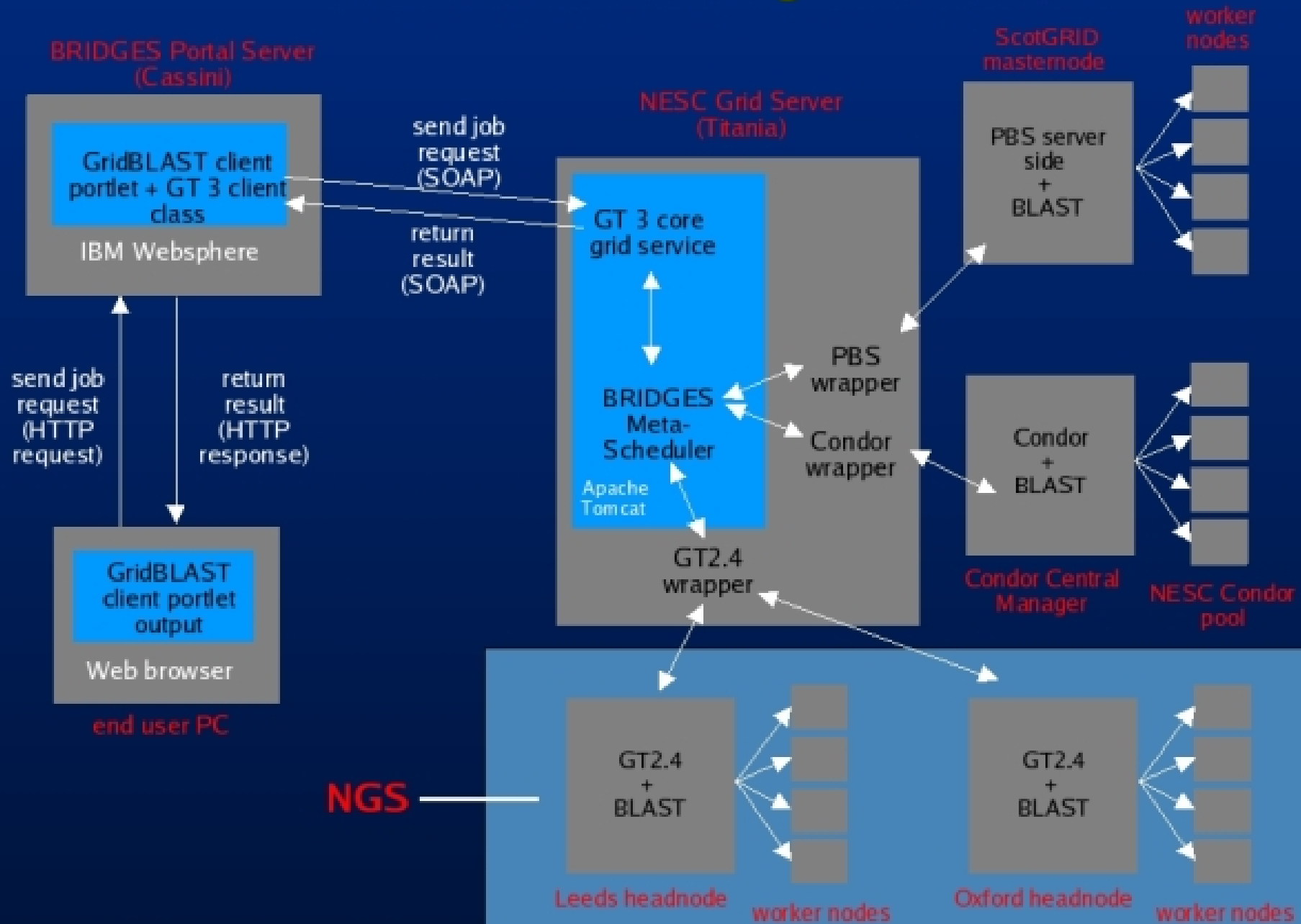
Applications: 2



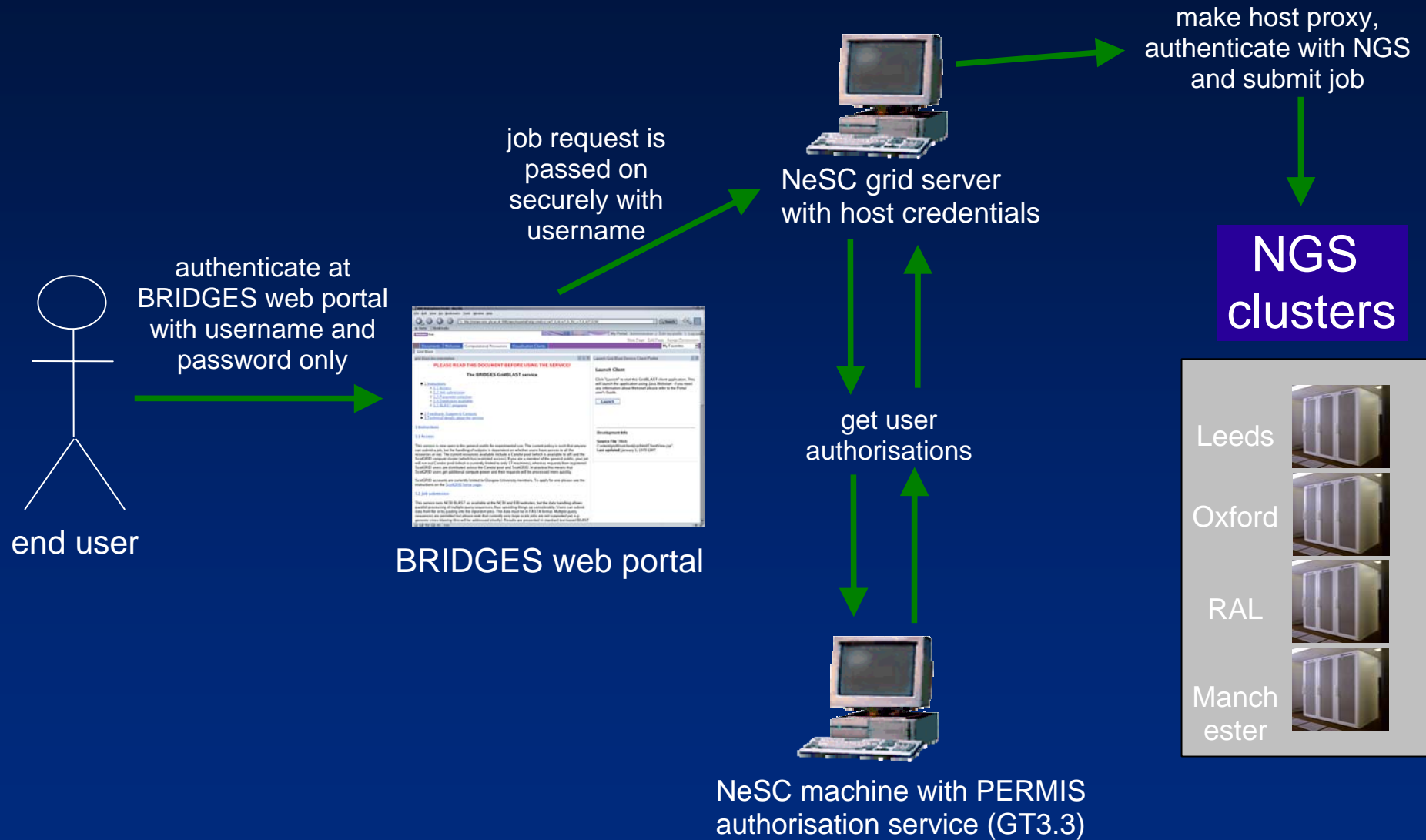
Other Applications:

- 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 activities
 - 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



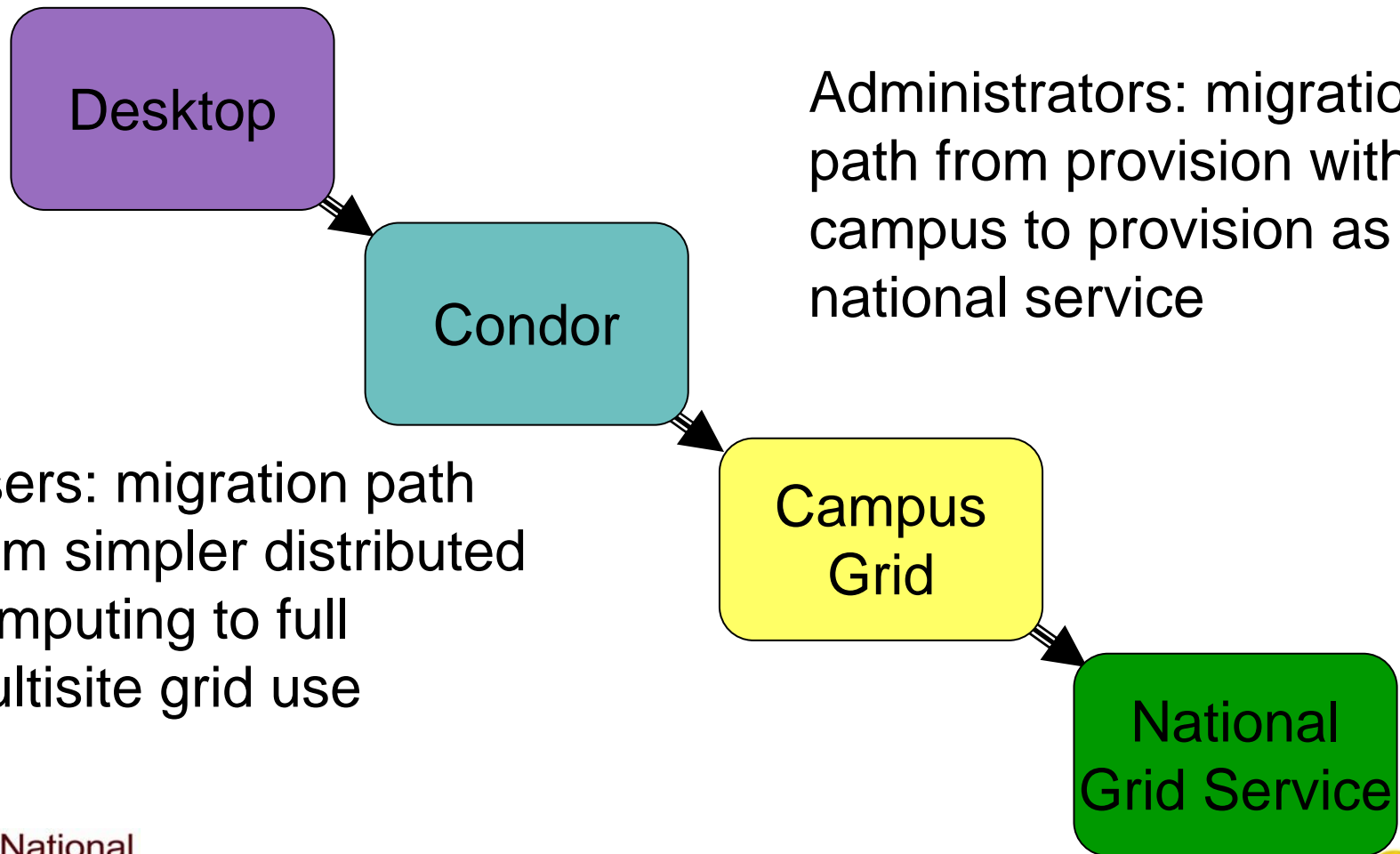
Security in BRIDGES – summary



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

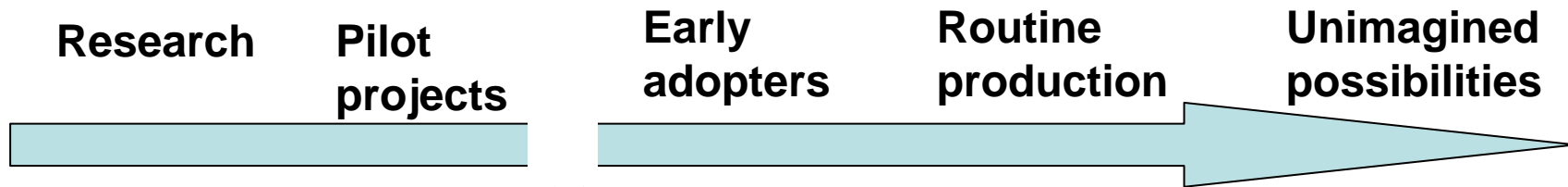




OMII-UK: Open Middleware Infrastructure Institute



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

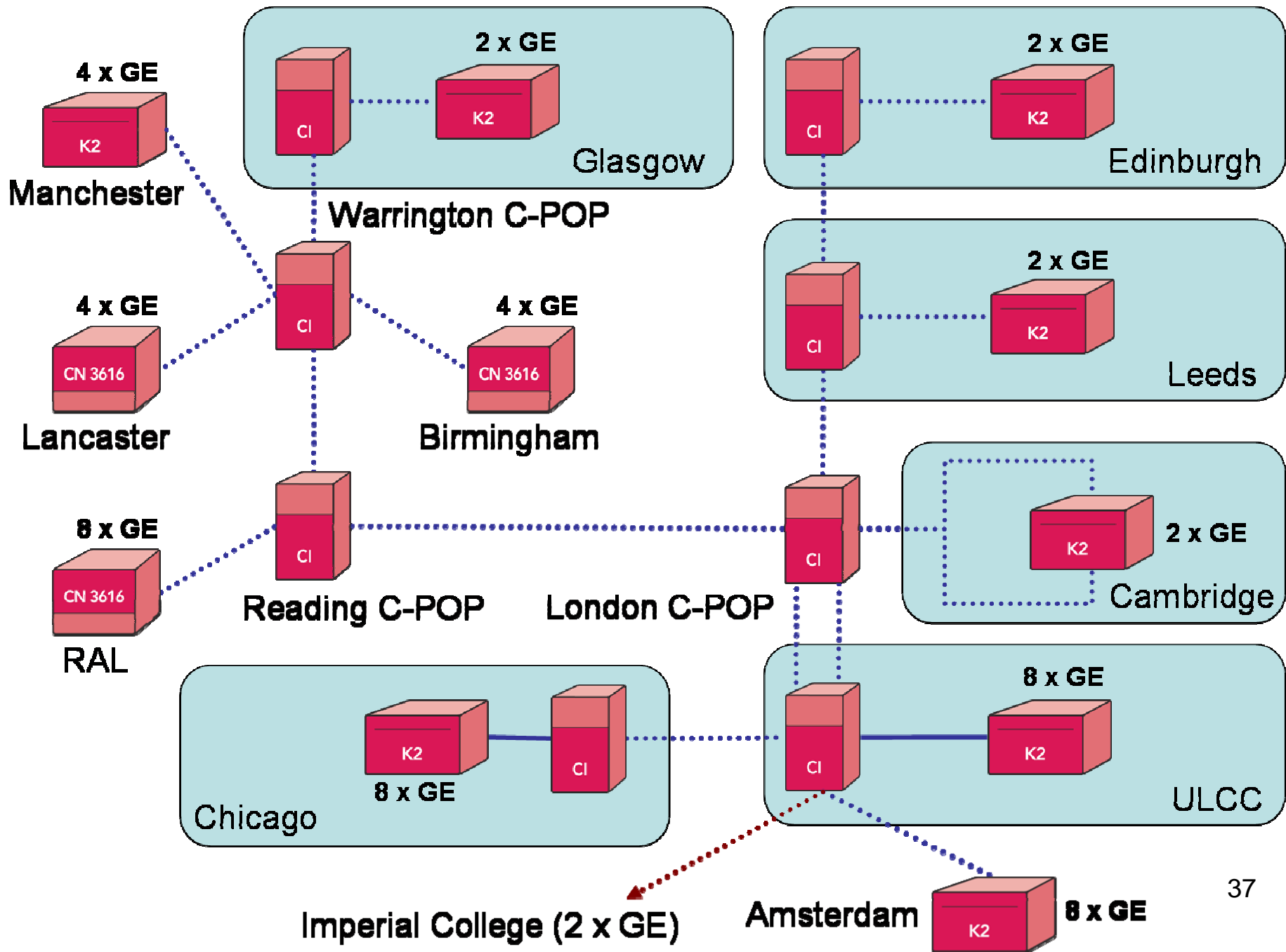
Present incarnation is SJ4

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**





What are (JISC) Data Centres?



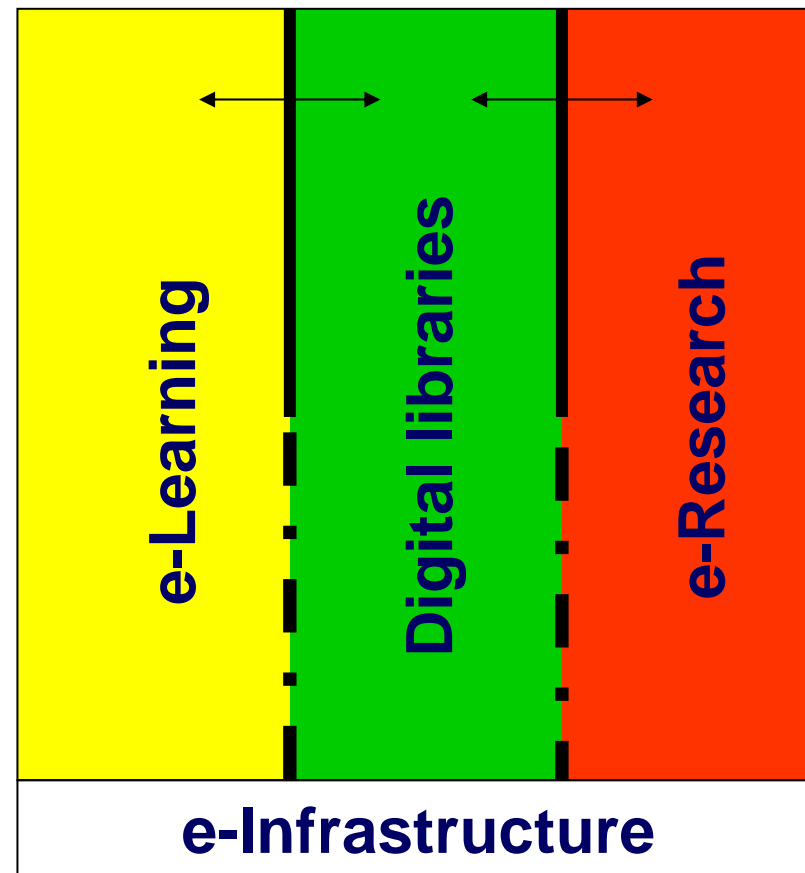
- BIDS <http://www.bids.ac.uk/>
 - Bath Information and Data Services
 - Bibliographic
- EDINA <http://www.edina.ac.uk/>
 - Multimedia
 - Geospatial
- MIMAS
<http://www.mimas.ac.uk>
 - Census
- What do they do?
 - Content delivery – with AA (currently ATHENS)
 - Licensing authority
- OGSA-DAI territory!
 - Access databases as services on the National Grid Service
- Amongst challenges:
 - ATHENS / Shibboleth / X.509 integration



JISC Programmes



- Research is only the start !



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 Preservation 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

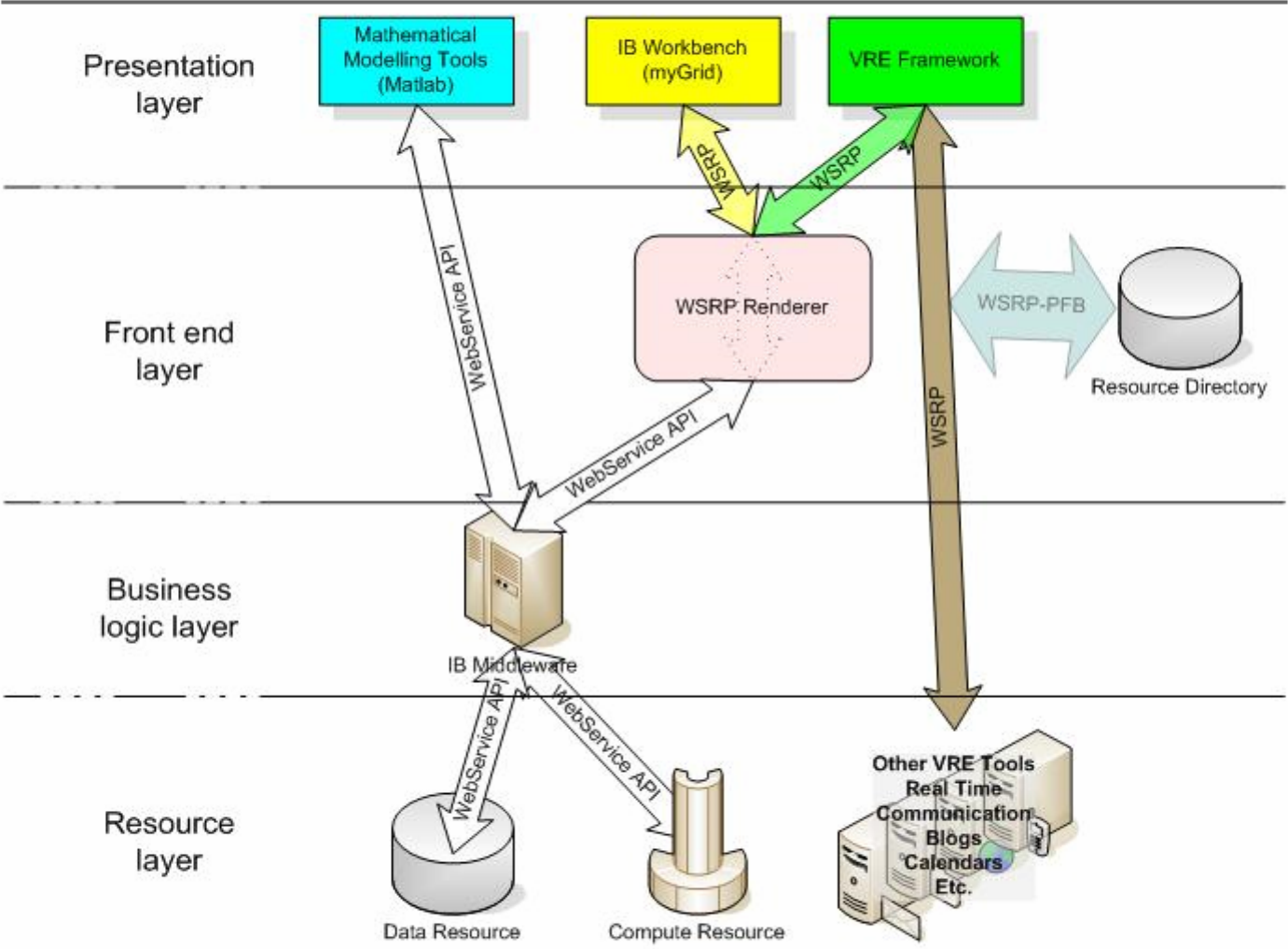


VRE development for Integrative Biology



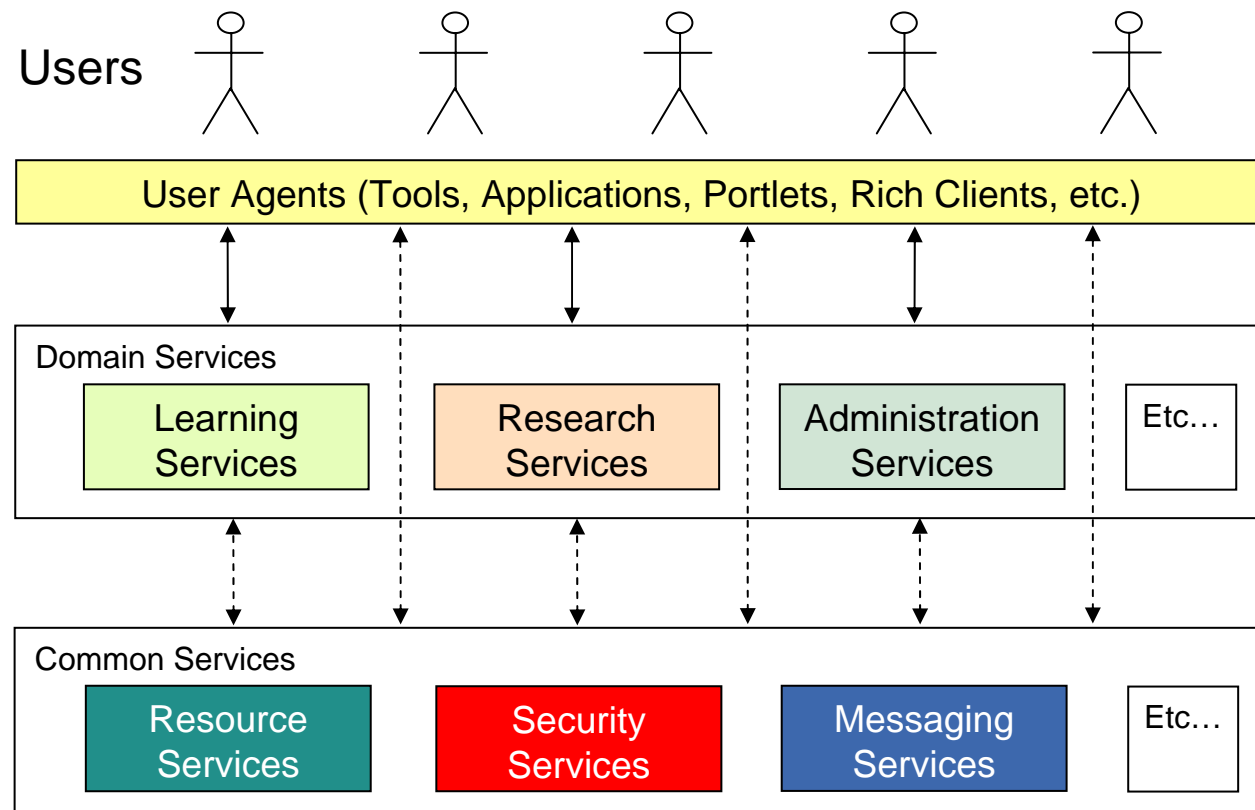
- <http://www.vre.ox.ac.uk/ibvre/>
- “Whereas the existing IB Grid services have focussed on supporting the core IB experimental workflow - moving, processing and visualising data on the Grid - the IBVRE will support the research process in its widest sense i.e. activities such as identifying research 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)”.

Architecture



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>