

Building a Sustainable European Grid Service Lessons Learned from National Experience

Neil Geddes
Director, UK National Grid Service

EPSRC

JISC

The logo for the Science & Technology Facilities Council, featuring a stylized sun or starburst icon inside a circle.

Science & Technology
Facilities Council

1. Me
2. The of the UK National Grid Service
 - A brief history of time
 - The Vision of the NGS
 - The NGS today
 - Broader UK e-Infrastructures
 - Final thoughts

I am not going to tell you anything that you do not already know !

- Director of UK Science and Technology Facilities Council (STFC) e-Science Centre
 - 100 staff at RAL and DL
 - Library ... data storage ... computing
 - LHC T1, EGEE, projects biology and materials science, NGS ...
- Principal Investigator for the UK National Grid Service
- Previously E-Science Director and the UK Particle Physics and Astronomy Research Council
 - Member of wLCG Overview Board and Collaboration Board
- This talk (mostly) as Director of the NGS

A Brief History of Time

- 2001 - UK e-Science Grid: e-Science Centres
 - GridPP, EDG and others start
- 2003 - Initial grid service ITT
 - 4 independent clusters to investigate provision of a grid service
- April 2004 - NGS pre-production service
 - EGEE, GridPP-2
- August 2004 – GOSC proposed
 - Coordinating NGS and providing central services
- September 2004 - NGS production service / GOSC
- April 2006 – NGS/GOSC phase 1 review
- May 2006 - NGS phase-2 approved
 - More integrated programme
 - EGEE-2 starts in April
- October 2006 – NGS phase-2

The Mission of the NGS

To provide coherent electronic access for UK researchers to all computational and data based resources and facilities required to carry out their research, independent of resource or researcher location

The Vision of the NGS

- National infrastructure services which allow researchers to:
 - systematically create, process, preserve and publish digital information;
 - easily navigate through the available resources;
 - be confident in the quality of the services available;
 - tie into international efforts
- To achieve this, the NGS will
 - Lead the deployment of a common grid infrastructure
 - Promote common open standards
 - Through the NGS Partnership programme, integrate services to access a growing number, scale and variety of resources
- A production Service

ScotGRID



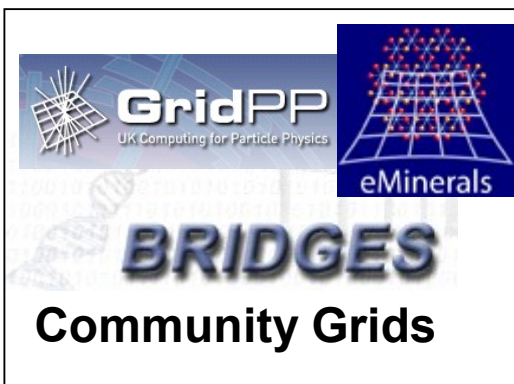
Regional and
Campus grids



HRCx + **HECtoR**

UK e-Infrastructure

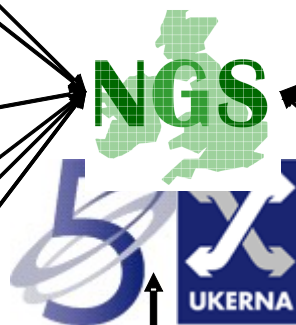
Users get common access, tools, information,
Nationally supported services, through NGS



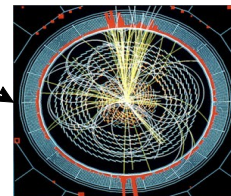
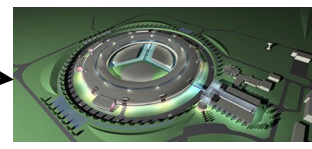
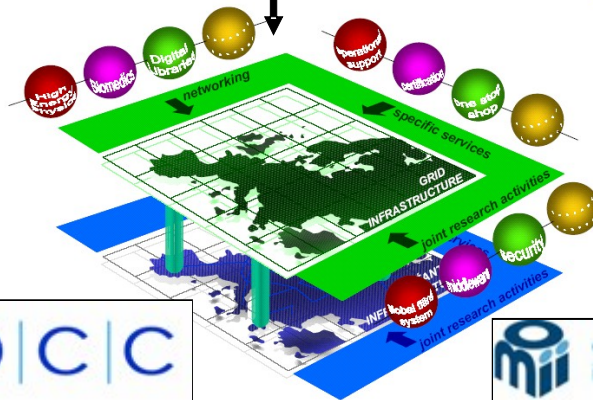
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MIMAS

LIBRARY
HS1LIB



Integrated
internationally



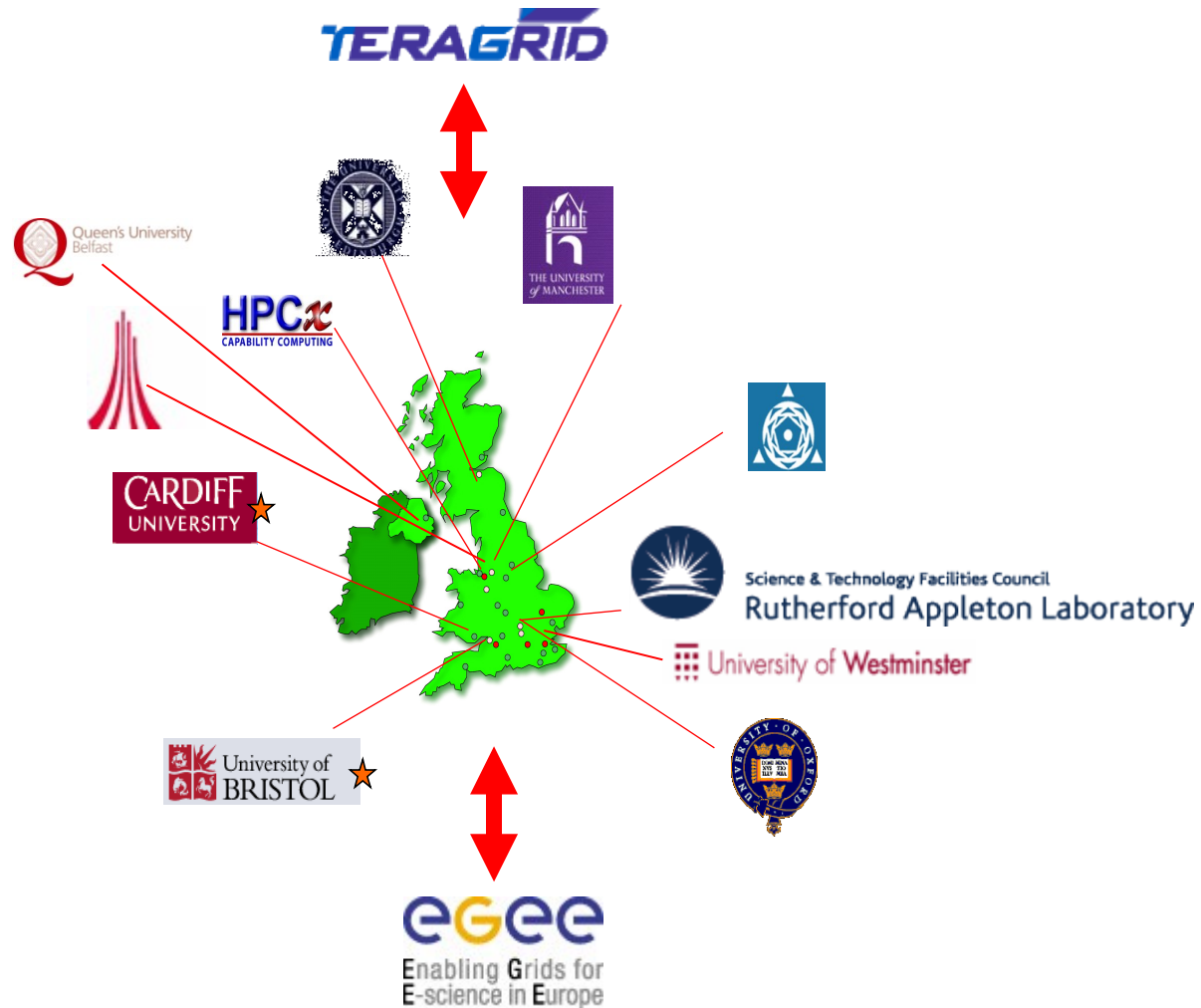
LHC



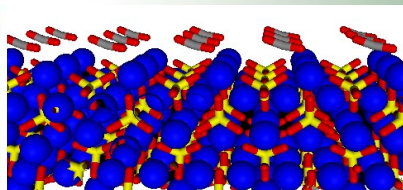
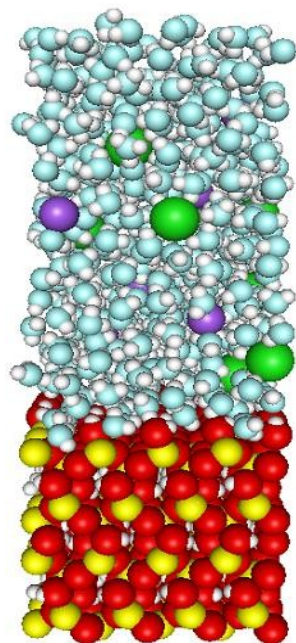
ISIS TS2



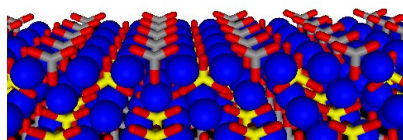
The NGS Today



Applications: 1

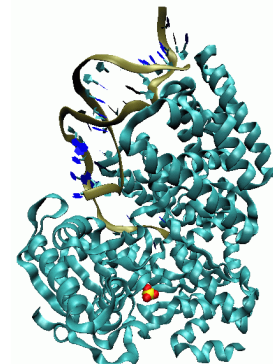
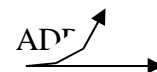
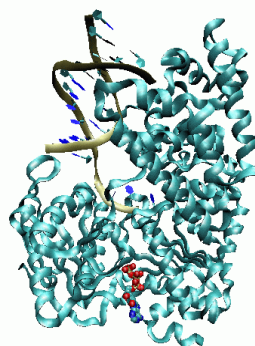


Molecular Dynamics



substrate complex

product complex



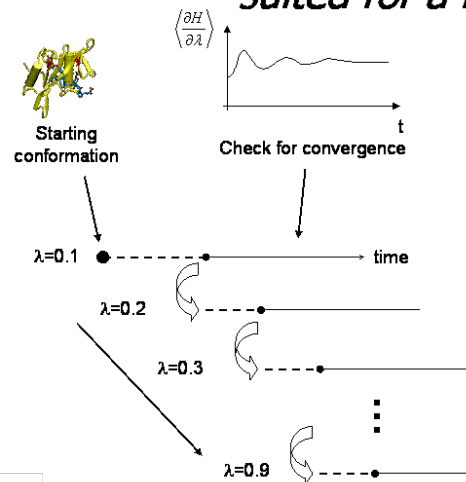
Lattice
Boltzmann
Text mining

Thermodynamic integration is ideally suited for a HPC Grid

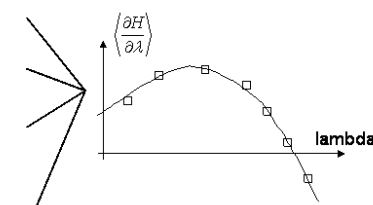
Calculating drug affinities



Use steering to launch, spawn and terminate λ - jobs



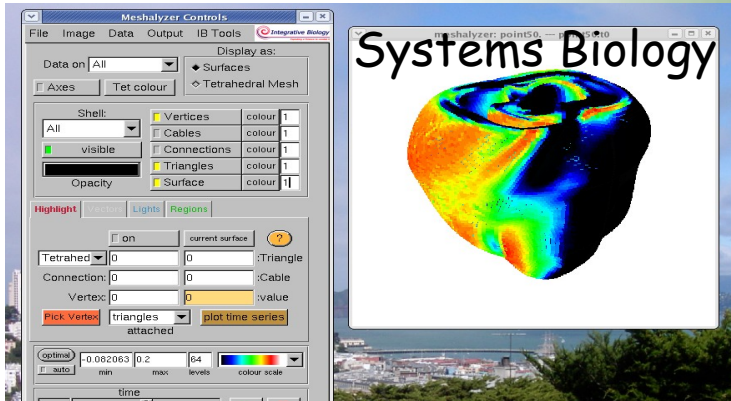
Combine and calculate integral



Run each independent job on the Grid

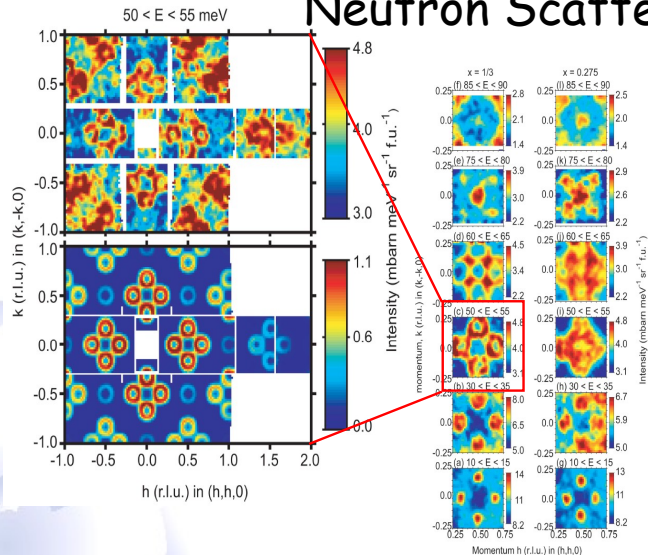


Applications: 2

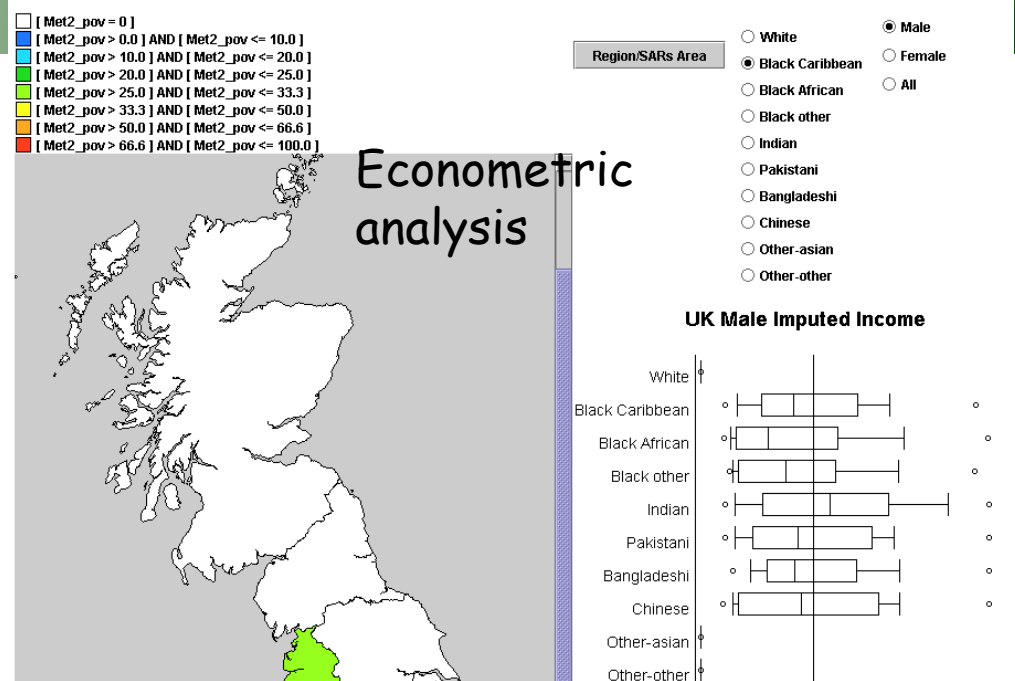


Example: $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$

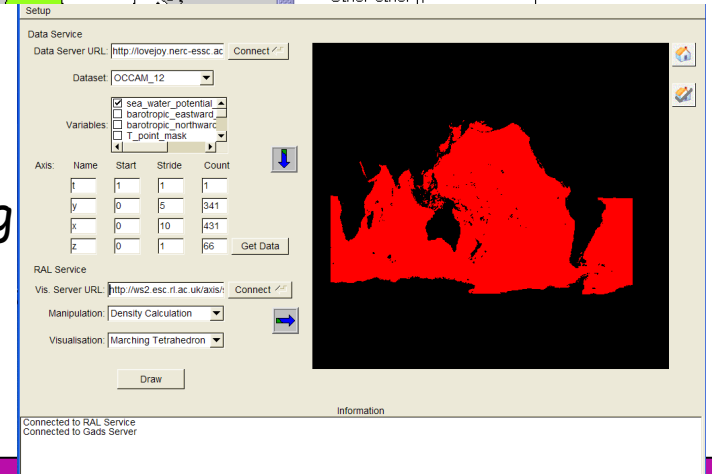
Neutron Scattering



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

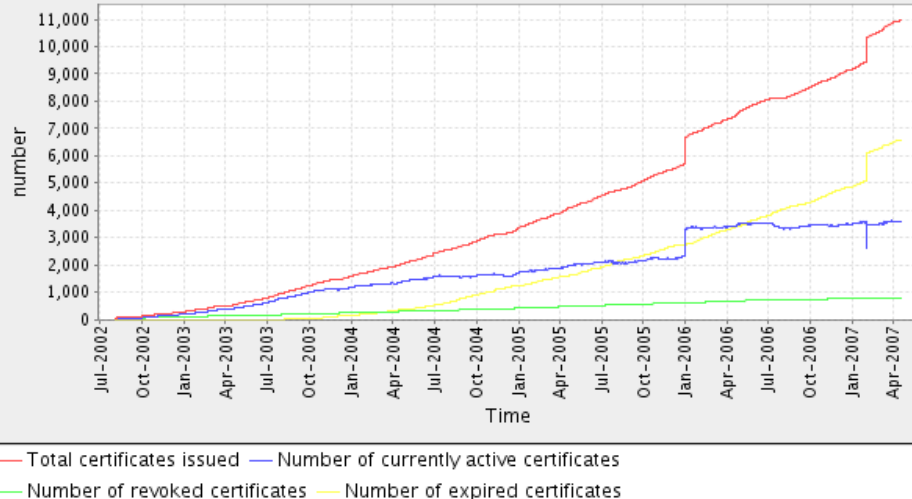


Climate modelling

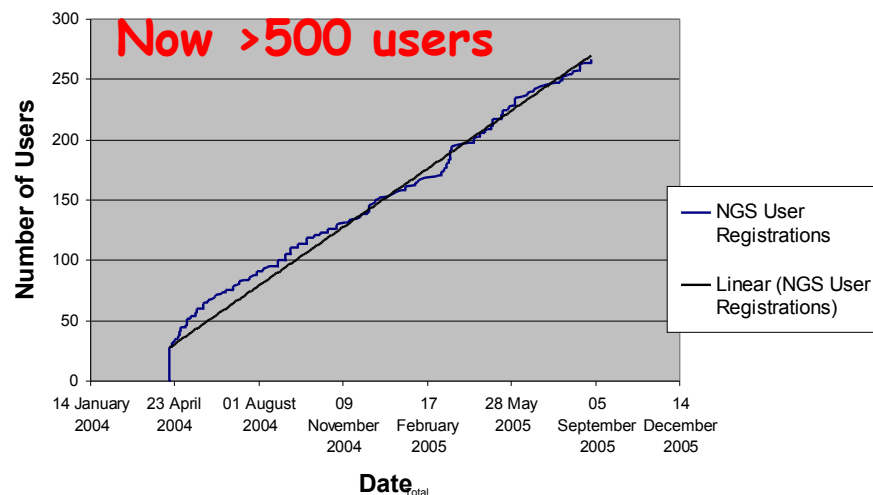


NGS Use

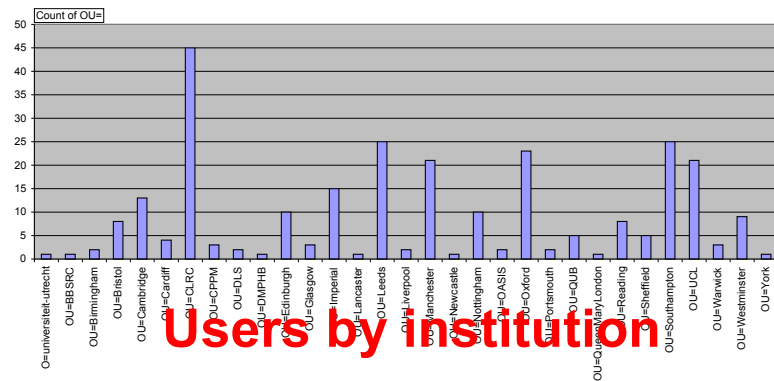
Certificates Issued by UK CA



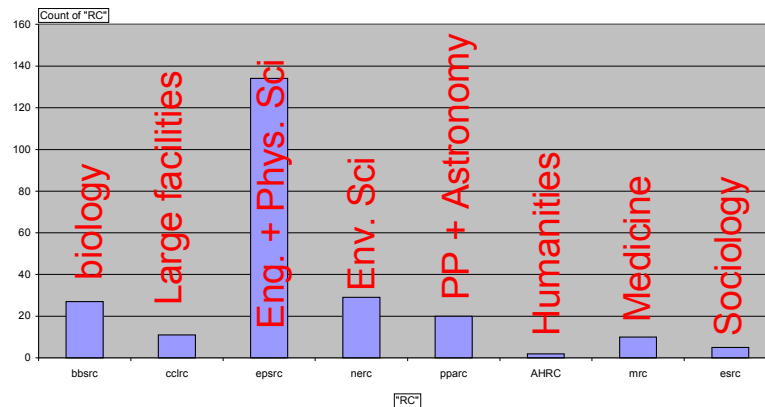
Number of Registered NGS Users



Total



Users by Institution



Users by discipline

- Most significant users come from:
 - Projects funded explicitly to include a large component of large scale distributed collaboration
 - People who do this anyway
 - NGS sites
- Others scale linearly
 - People who we talk to ?
 - They don't tell their friends ? – but they do come back
 - Its hard to get started without handholding ?
 - “joining” in is hard
 - Its's hard to break out across disciplines

Challenges

- 1 Shared vision, shared infrastructure

ScotGRID



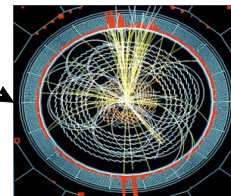
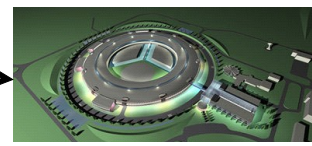
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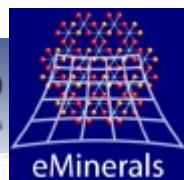
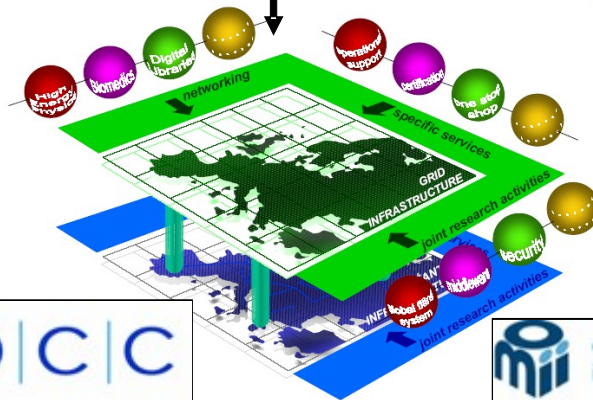


ISIS TS2

NGS



Integrated
internationally



BRIDGES

Community Grids



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Challenges

1. Shared vision, shared infrastructure
3. Compromise and collaboration

Many Stakeholders and Actors

- Parallel infrastructures
 - NGS, e-minerals, EGEE, GridPP ...
 - Distrust of generic services
- Middleware development
 - OMII, GLite, Globus...
- Sysadmins, developers, users...
- If some one else's requirements are different, it doesn't make them invalid
 - Struggle for resources
 - Lack of confidence in the future

Challenges

1. Shared vision, shared infrastructure
3. Compromise and collaboration
5. Responsibility

What is a “European Grid Service” ?

- What are trying to sustain?
 - Grid computing for the LHC ?
 - Grid computing for someone else ?
 - Data infrastructure/interoperability ?
 - Middleware ?
 - Progress towards
 - Pressure to change ?
 - U-Tube and Google ?
- Need to be specific about what we are and are not doing
 - And who is paying for it
 - Recovering from the grid hype



NGS

National Grid Service

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Timing – The Hype Cycle



- Need ensures sustainability
 - Not everyone needs everything
- Make it clear what you do for who
 - Funding agencies
 - Efficient use of resources
 - Support for excellence and focusing on core business
 - Infrastructure often spans organisations
 - Users
 - Added benefits and tools
 - more work
 - Service providers
 - Added benefits and support network
 - more work

NGS sustainability workshop

- Recent workshop on NGS sustainability highlighted 4 areas
 - Services
 - User focus
 - Support for collaboration
 - Centre of expertise and evangelism

- Complex palette of resources and needs
 - Paid for services
 - Commercial services
 - Shared resources
- NGS role
 - Incubate and support interfaces
 - Central/common services
 - Common market
 - Gateway to commercial services
 - UK gateway to European/US Grid Infrastructure
- Specific work theme through 2007
 - Understand the needs and requirements

Concluding Thoughts

- **Governments and Funding agencies need to drive the development of an agreed and shared vision for the future, engaging key stakeholders.**
 - Strong strategic commitment from, and coordination between, funding agencies and key user communities remains an important driver for the current infrastructure development.
 - Key stakeholders have to agree what infrastructure they want (and how they expect it to be funded)
 - Strategic policy steer associated with some sustained core funding
- **Joining the broad infrastructure, as a user or provider, must become easier, justifiable and self sustaining.**
 - Stringent requirements on performance and availability may only be relevant to a small subset of the infrastructure
- **Work with, and for, key users**
 - User focused services
 - Application led with an infrastructure requirement
 - Balance high profile winners and “something for everyone”