

The UK National Grid Service

Grids, NGS and Campus Grids

Dr Andrew Richards (STFC)
OGF20 Manchester

Outline

- NGS Background
 - History
 - Current Resources
 - User base
- Integration / Interoperation
 - GridPP, EGEE, LCG, Teragrid, others...
 - National Resources / Infrastructures
 - Campus Grids

The NGS

A Production Quality Grid
(Background...)

A Brief History of Time

- 2001 - UK e-Science Grid
 - GridPP 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 started in April
- October 2006 – NGS phase-2

The Mission of the NGS

The Mission of the National Grid Service

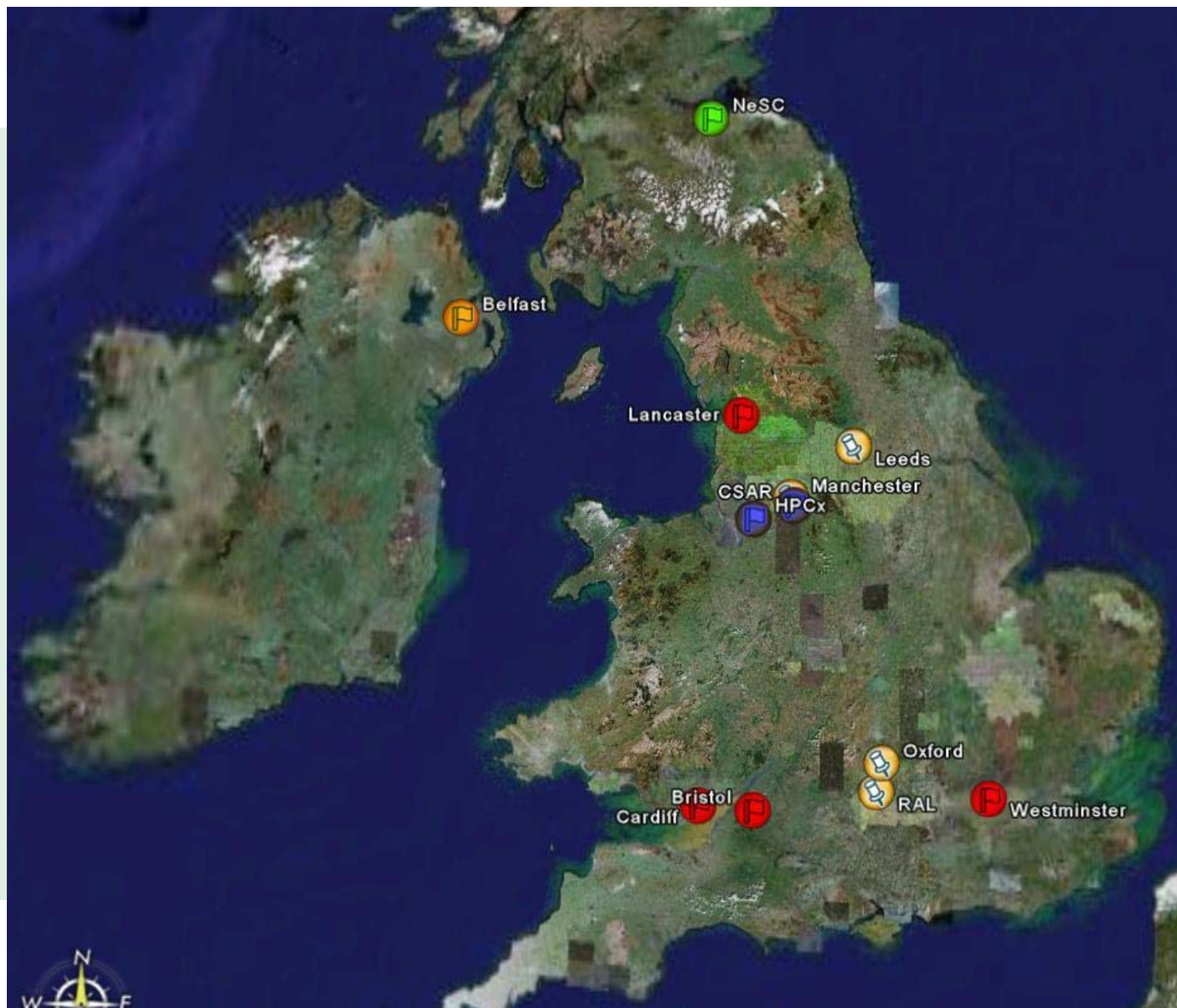
- To provide coherent electronic access for UK researchers to all computational and data based resources and facilities required to carry out their research, independent of resource or researcher location

Key Themes

- Provide the users what they need with as low an additional barrier as possible.
 - As if by magic give them access to much more.
- “Content”
 - Services – data, computation, ...
- NGS will only grow if the content grows
 - Not the job of 1 person or organisation
 - Job of everyone



NGS & Partners, 2007



Core Services

- UK Certification Authority (+ RA Network)
- Helpdesk / User Support
- Documentation
- Training (*NeSC www.nesc.ac.uk)
- Website(s), Wiki
- MyProxy (National Service + Java Client Upload tools)
- Portal (NGS Application Repository)
- INCA / GITS Monitoring
- BDII
- SRB
- User Accounting System
 - Registration, Accounting, Policing
- Advanced Reservation
- gLite Resource Broker / UI
- GOCDB
- GSISSH Term
- *GRIMOIRES (UDDI) **

Resources available to users

NGS core nodes

- Linux IA32 clusters
- data nodes at RAL and Manchester
 - each 15 TB, 40 processors
- 128p compute nodes at Oxford and Leeds
- ***PHASE 2 NOW BEING INSTALLED!***
- free at point of use
- apply through NGS web site
 - ~500 registered users
- accept conditions of use
- light-weight peer review
 - 1-2 weeks
- access is through digital X.509 certificates
 - from UK e-Science CA
 - or recognized peer

National HPC services

- HPCx
- HeCToR (expected 2007)

Must apply separately to Research Councils

NGS partner sites

- Compute nodes at Bristol and Cardiff, Lancaster, Westminster
 - Access as per NGS core nodes
- Belfast

NGS affiliates

- NeSC
- User access at discretion of affiliate

NGS-2 Core Hardware



Compute Nodes

- 48 nodes with Dual Socket Dual Core AMD Opteron 280 processors, 8GB memory 2x80GB disks, Myrinet 2000
- 8 nodes with Quad Socket Dual Core AMD Opteron 280 processors, 32GB memory 2x80GB disks, Myrinet 2000

Storage

- 8 storage nodes Dual Socket Dual Core AMD Opteron 280 processors, 8GB memory 2x80GB disks, Myrinet 2000, Fibre HBA
- 5 x 12 TB Infotrend Storage Arrays
- Qlogic 5200 SANbox

Initial BenchMarks

- Initial testing using HPL (top 500 gigaflops tester) on 240 Cores gives 934Gflops (81% peak). The full system should have 256 Cores available but some nodes have hardware problems

ScotGRID



Regional and
Campus grids



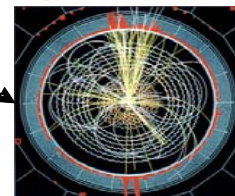
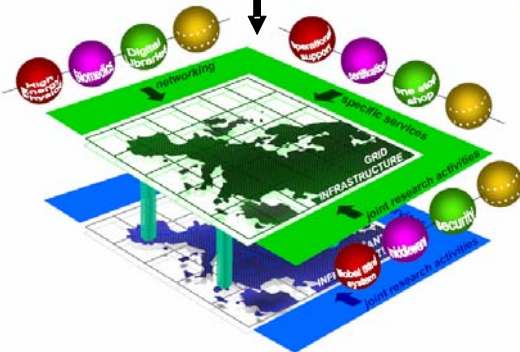
HPCx + HECtoR

UK e-Infrastructure

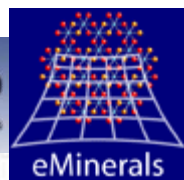
Users get common access, tools, information,
Nationally supported services, through NGS



Integrated
internationally



ISIS TS2



BRIDGES

Community Grids



JISC

VRE, VLE, IE

EDINA[®]
MIMAS

Access Mechanisms

X509 based access, part of Shibboleth developments

- Direct GSISSH login
- Globus tools
- Portals
- Resource Brokers / UI machines
- AHE (Application Hosting Environment)
- GridSAM
-*your own application...*

NGS Applications Repository (https://portal.ngs.ac.uk)



Pluto Portal Driver - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://localhost:8080/pluto/portal/JSFMyFacesportlet/_rp_JSFMyFacesportlet_row1_col1

Getting Started Latest Headlines

Microsoft Outlook Web Access NGS Portal 3.0 Alpha NGS - Certification Authority ... Pluto Portal Driver

Test Admin dave JSFMyFacesPortletDemo JSFMyFacesPortletDemo MixedJSF_NormPortlets chapter04Portlets JSFPortletDemo

JSFMyFacesPortletDemo

view | max | min | nor

Start | Credentials | Browse + Load Jobs | Upload/Download Tool | Job Categories | Browse Host | Admin | Info/TODO

ActiveJob: Detail | Execute Host | Description | Ams | Env | File Systems | Stage File/Dir | JSDL | Submit

User: AUTHENTICATED_USER Active Job: Own:JobProfile name Save SaveAsNew New

Browse and Load The 'Active Job' From NGS And Personal Repositories

① In Job Category: (Create/Edit JobCategories) All

② With Status: all

③ Search / List Job Profiles: NGS Personal

Results Found: (6)

Description	Name	Exe	Modified	Status (Check)	Load
View jp1	jp1	/bin/hostname	Dec 14, 2006	UNSUBMITTED	load
View jp1	jp1	/bin/hostname	Dec 19, 2006	UNSUBMITTED	load
View daveTestLSF	daveTestLSF	/bin/cat	Dec 19, 2006	COMPLETED	load
View daveTestLSF2	daveTestLSF2	/bin/cat	Dec 19, 2006	UNSUBMITTED	load
View mpiDemo	mpiDemo	/home/ngs0153/mpi_test	Dec 21, 2006	COMPLETED	load
View mpiDemo	mpiDemo	/home/ngs0153/mpi_test	Dec 21, 2006	UNSUBMITTED	load

Done

Pluto Portal Driver - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://localhost:8080/pluto/portal/JSFMyFacesportlet/_rp_JSFMyFacesportlet_row1_col1

Getting Started Latest Headlines

Microsoft Outlook Web Access NGS Portal 3.0 Alpha NGS - Certification Authority ... Pluto Portal Driver

MixedJSF_NormPortlets chapter04Portlets JSFPortletDemo

ActiveJob: Detail | Execute Host | Description | Ams | Env | File Systems | Stage File/Dir | JSDL | Submit

User: AUTHENTICATED_USER Active Job: Own:JobProfile name Save SaveAsNew New

JSDL Job Description

The Job Submission Description Language (JSDL) is an XML Schema language designed to describe compute jobs in XML independent of middleware. The XML document shown is constructed (graphically) via the portal interface and is validated according to the JSDL Schema (and JSDL POSIX extensions where required) which ensures its correctness.

The XML document can be copied and saved for: archiving, sharing, uploading, for use in other Grids with different middleware. (Use the portal as a graphical JSDL editor).

Please note, the portal fields JobType + JobManager + Port are (currently) not parsed when uploading JSDL. These fields require manual update via the portal if you upload JSDL.

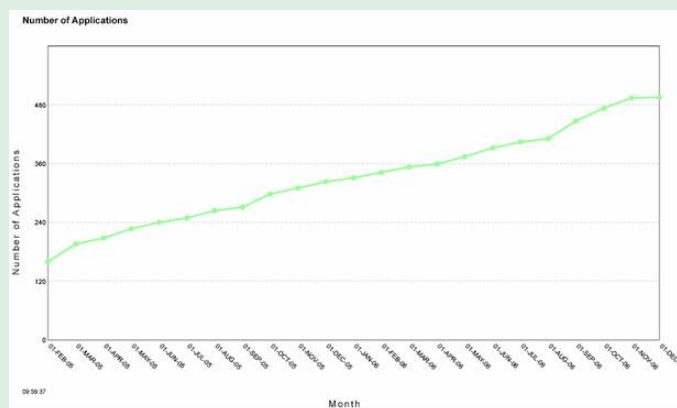
Upload (paste-in) a new JSDL document to re-initialize the Active JobProfile: View Upload/parse

```
<?xml version='1.0' encoding='UTF-8'>
<jSDL:JobDefinition xmlns:jSDL="http://schemas.ggf.org/jSDL/2005/11/jSDL">
  <jSDL:JobDescription>
    <jSDL:JobIdentification>
      <jSDL:JobName>JobProfile name</jSDL:JobName>
    </jSDL:JobIdentification>
    <jSDL:Application>
      <jSDL:ApplicationVersion>1.0</jSDL:ApplicationVersion>
    </jSDL:Application>
    <jSDL:POSIXApplication xmlns:jSDL="http://schemas.ggf.org/jSDL/2005/11/jSDL-posix">
      <jSDL:Output>stdOut.txt</jSDL:Output>
      <jSDL:Error>stdErr.txt</jSDL:Error>
      <jSDL:ProcessCountLimit>1</jSDL:ProcessCountLimit>
    </jSDL:POSIXApplication>
    <jSDL:Application>
      <jSDL:Resource>
        <jSDL:FileSystem name="WORKINGDIR">

```

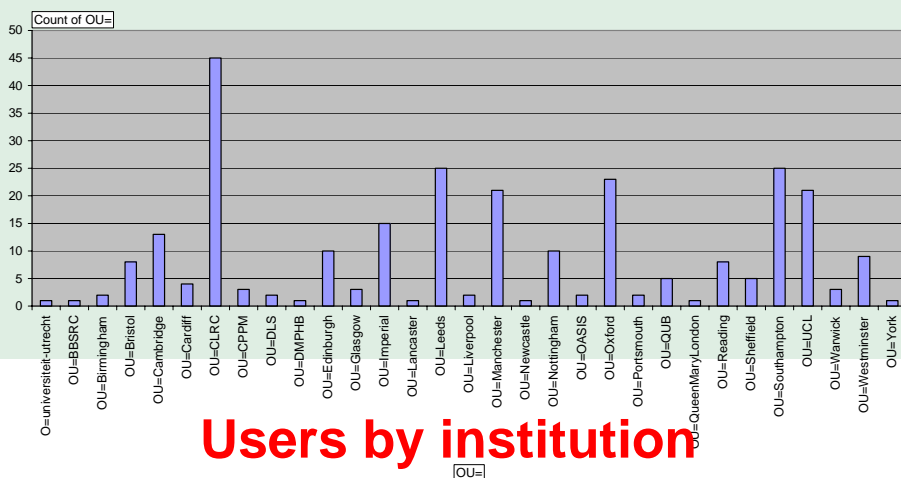
Done

Usage



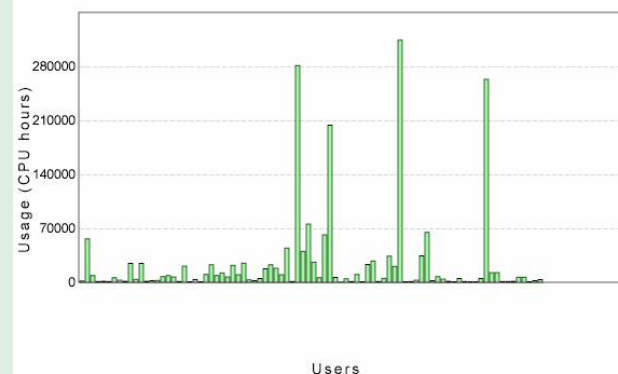
~500 users

Total

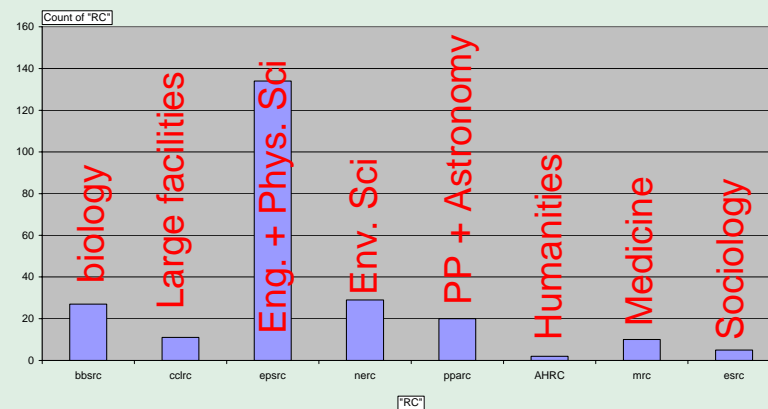


Users by institution

CPU Usage by anonymous users across 4 core sites

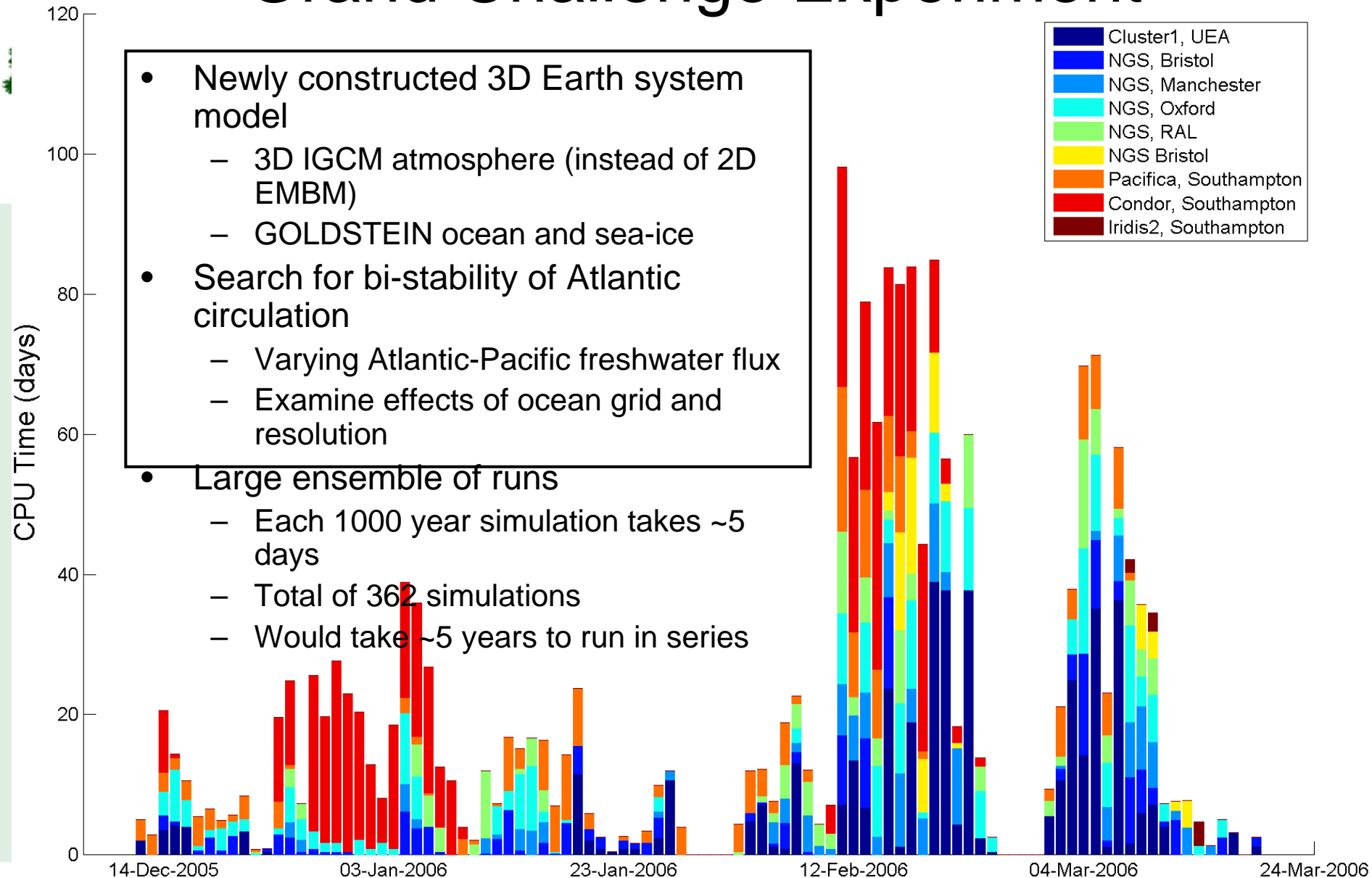


CPU time by user



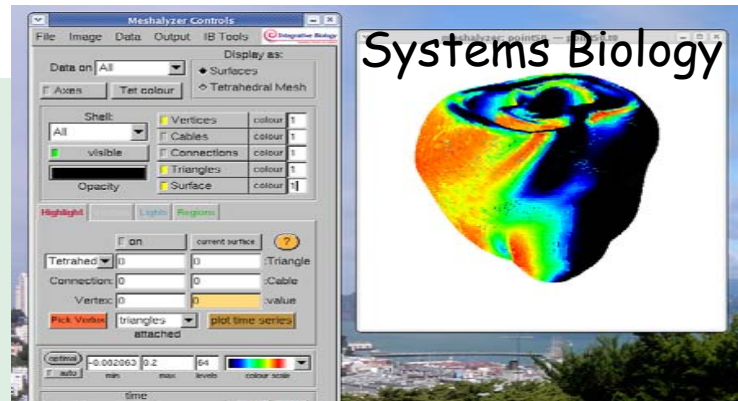
Users by discipline

Grand Challenge Experiment



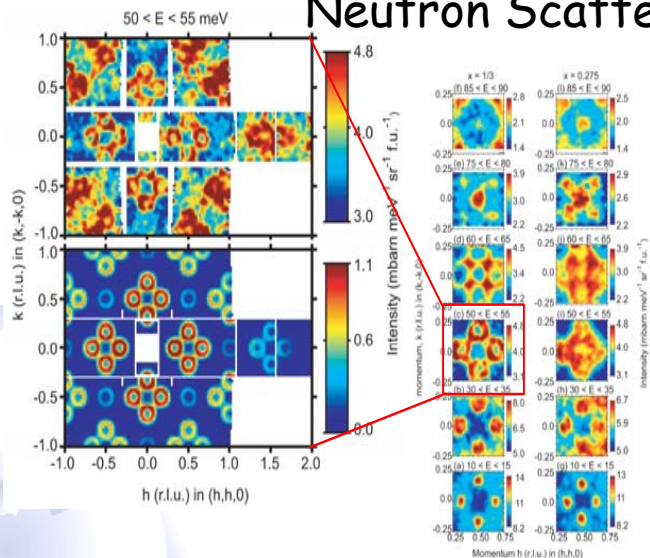
- Newly constructed 3D Earth system model
 - 3D IGCM atmosphere (instead of 2D EMBM)
 - GOLDSTEIN ocean and sea-ice
- Search for bi-stability of Atlantic circulation
 - Varying Atlantic-Pacific freshwater flux
 - Examine effects of ocean grid and resolution
- Large ensemble of runs
 - Each 1000 year simulation takes ~5 days
 - Total of 362 simulations
 - Would take ~5 years to run in series

Applications



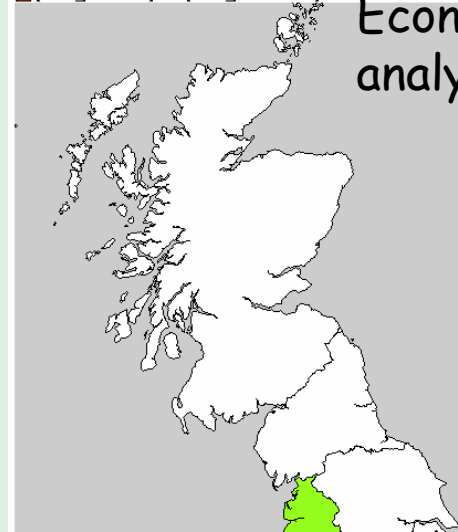
Example: $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$

Neutron Scattering



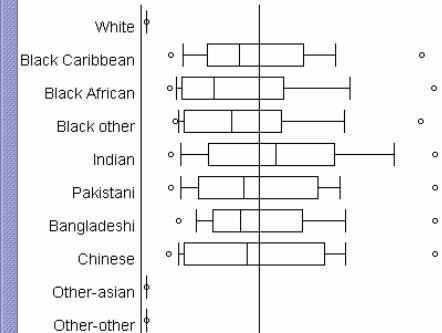
[Met2_pov = 0]
 [Met2_pov > 0.0] AND [Met2_pov <= 10.0]
 [Met2_pov > 10.0] AND [Met2_pov <= 20.0]
 [Met2_pov > 20.0] AND [Met2_pov <= 25.0]
 [Met2_pov > 25.0] AND [Met2_pov <= 33.3]
 [Met2_pov > 33.3] AND [Met2_pov <= 50.0]
 [Met2_pov > 50.0] AND [Met2_pov <= 66.6]
 [Met2_pov > 66.6] AND [Met2_pov <=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

Econometric analysis

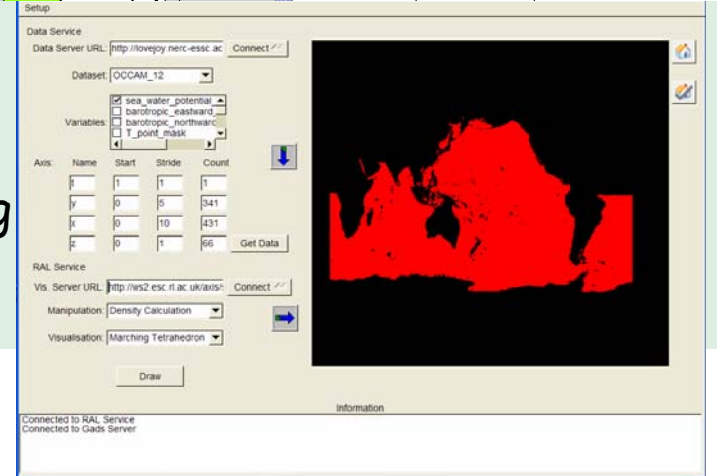


- Region/SARs Area**
- ☐ White
 - ☒ Black Caribbean
 - ☐ Black African
 - ☐ Black other
 - ☐ Indian
 - ☐ Pakistani
 - ☐ Bangladeshi
 - ☐ Chinese
 - ☐ Other-asian
 - ☐ Other-other
- ☒ Male
☐ Female
☐ All

UK Male Imputed Income

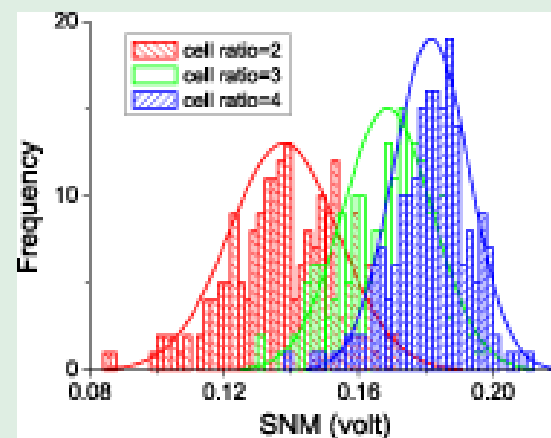
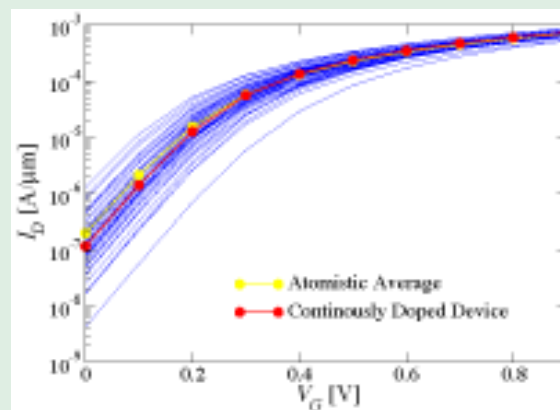
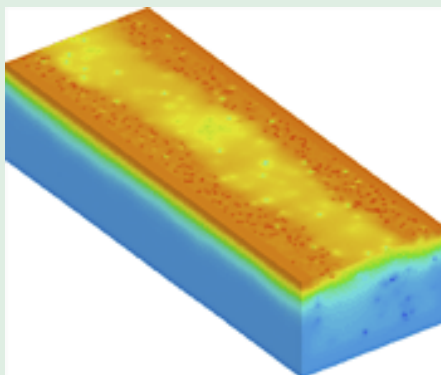


Climate modelling



nano-CMOS

- To develop a grid-based infrastructure to support the early evaluation of the impact of next-generation CMOS devices, examining in particular their increasing variability on the design of current and future electronic circuits and systems





NGS

National Grid Service

101010001000000100100
101010001000000100100

?



1010100010000001

Integration / Interoperation

Joining

- You can join the NGS as:
 - A single user
 - A VO (externally hosted, or hosted by the NGS)
 - A Project accessing NGS resources via own infrastructure and where NGS ‘sees’ only a single user e.g. BRIDGES project
 - OR as A Resource Provider
- See <http://www.ngs.ac.uk/access.html>

NGS Brands

The NGS brand should connote production quality service and support.

We can use the NGS brand to encourage sites to participate, but must spend it wisely.

- An **NGS Affiliate** is a site certified to be NGS-compatible.
- An **NGS Partner** is a site that offers significant resources or services to NGS users.

NGS Compatibility

Resource providers join the NGS by

- Running compatible middleware
 - as defined by NGS Minimum Software Stack (three levels of conformance)
 - doesn't prescribe software versions
 - and verified by compliance tests
- Providing support and security contacts
- Providing site-specific information to users, through, but not limited to, the NGS web site

Two levels of membership:

1. Affiliates

- run compatible stack, integrate support arrangements
- adopt NGS security policies

2. Partners also

- make “significant resources” available to NGS users
- enforce NGS acceptable use policies
- provide accounting information
- define commitments through Service Level Descriptions
- influence NGS direction through representation on NGS Technical Board

Acceptable Use Policies

- NGS currently has its Terms and Conditions of Use that all users have to accept
 - <http://www.ngs.ac.uk/NGS-tacu.html>
- We are looking towards adopting the VO Policies of EGEE/LCG/GridPP/... (something common) for VO's that we host and support on our VOMS infrastructure, to be consistent.
- For support of external VO's, if we accept the VO, then the VO 'Manager' has to accept our TACU, but not each individual member.

ScotGRID



Regional and
Campus grids



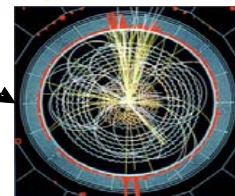
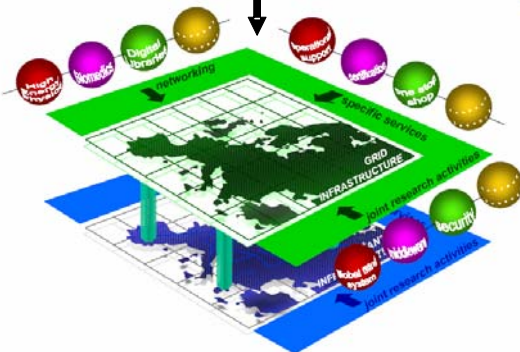
HPCx + HECtoR

UK e-Infrastructure

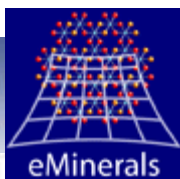
Users get common access, tools, information,
Nationally supported services, through NGS



Integrated
internationally



ISIS TS2



BRIDGES

Community Grids

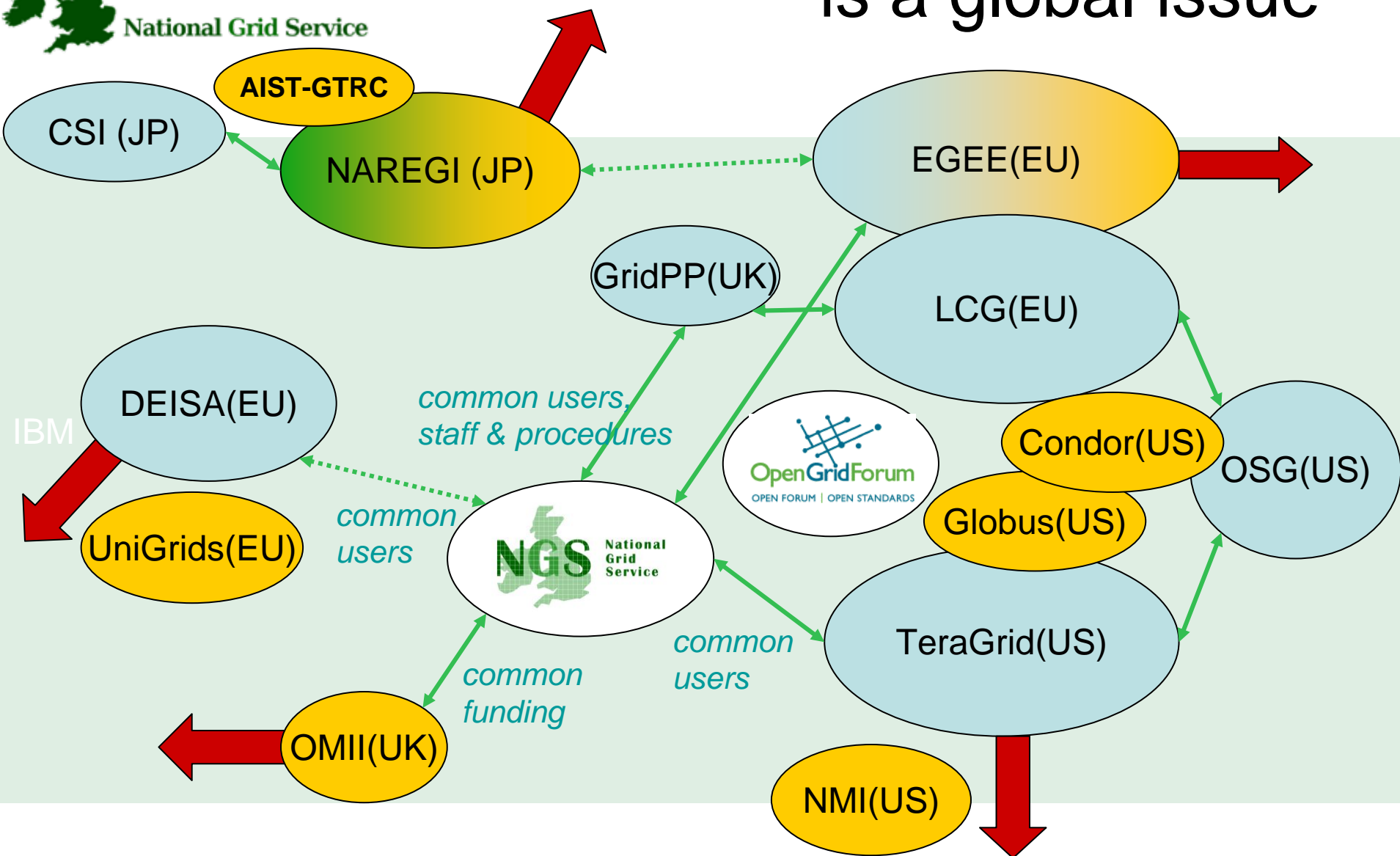


JISC

VRE, VLE, IE

EDINA[®]
MIMAS

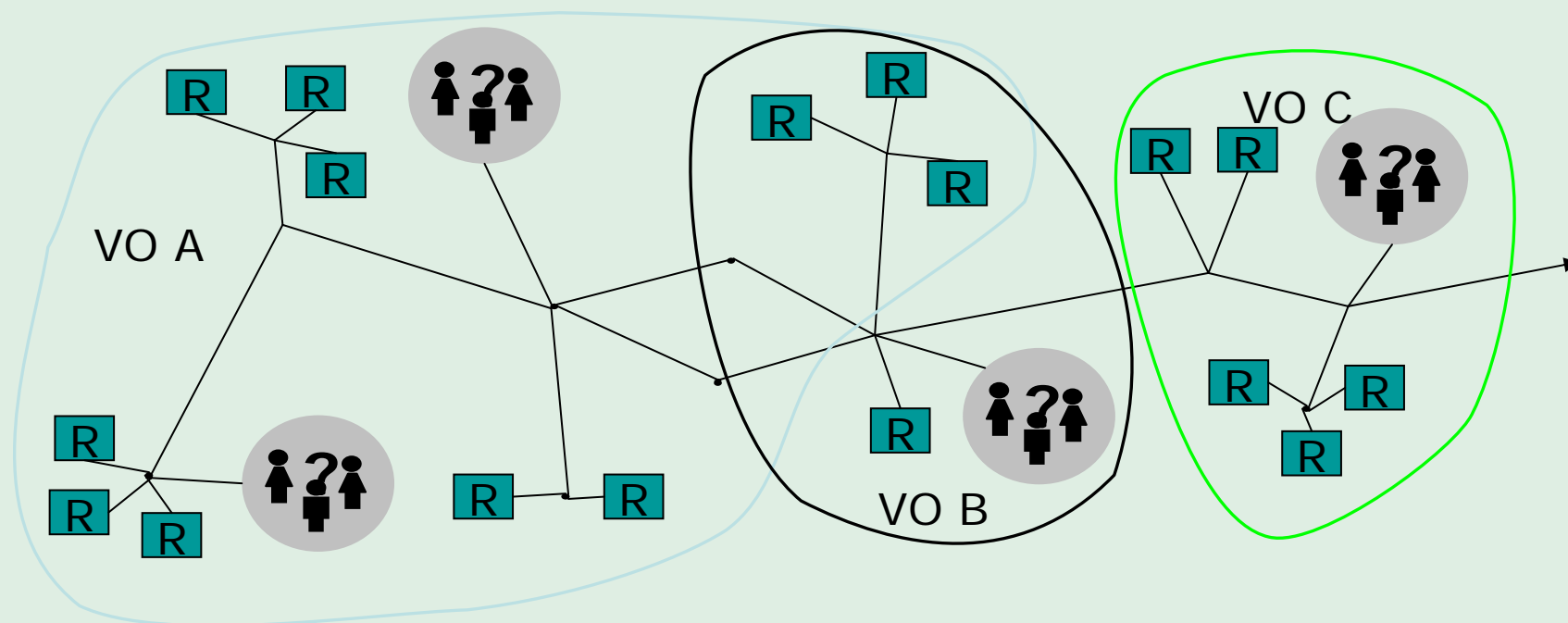
Interoperation is a global issue



Sharing and Virtual Organisations

Share (v):

- To have part; to receive a portion; to partake, enjoy, or suffer with others.



"flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources"

"...enables communities ("virtual organizations") to share geographically distributed resources as they pursue common goals -- assuming the absence of central location, central control, omniscience, existing trust relationships."

And the other bits...

- Accounting
- Management
- Charging – fEC (Full Economic Costing)
- Data
- Storage

Storage

- What do we do with all the storage?
 - What interfaces, what services, what commitments (i.e. what do we backup – what can we realistically backup?)
- What do the users want? Storage vs Data
 - Access to data facilities and/or access to long term storage
- Local provision, centralised management of service. E.g SRB – role of support centre
- Global filesystems? For all? For core?
- What can we take from EGEE or others?
- Policies? Home accounts? Long term storage?

Contact Details

Any Comments or questions or feedback on what you want is always welcome

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

Email: support@grid-support.ac.uk

NGS User Forum June 19th-20th Oxford