



UK National Grid Service, a
production grid infrastructure for a
heterogeneous provider and user
community

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Overview

- Our Mission and Goals
- Services and Resource Providers
- Supporting User Communities

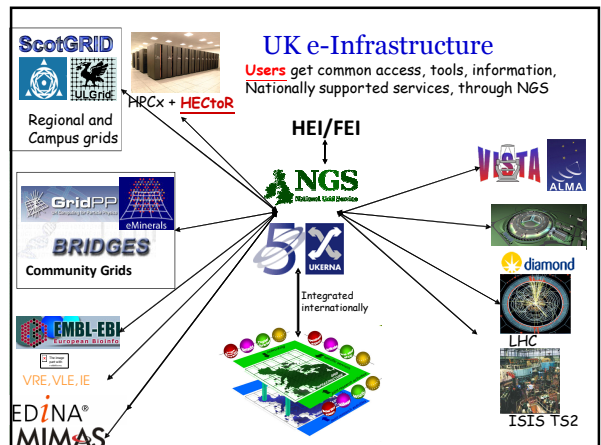


NGS Mission and Goal

To enable 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.

Goal:

- To enable a production quality e-infrastructure
 - Expand towards all Higher Education Institutes and UK based research institutions
 - Continue to support cutting edge research
- To deliver core services and support
 - Research computing groups within universities and research organisations to help them support users
 - Highlight Collaborative research in key communities
- Integrate with international infrastructures following user community demand





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How do we do this?

- Moving towards a standards based infrastructure
 - Independent of any external single middleware
 - Community specific interfaces deployed where necessary
 - Demonstration of benefits of using the same interface locally, regionally, nationally and internationally
- Policies and best practice framework for the operation, inter-operation and sharing of research computing services across the UK.
 - Repository of relevant user and system documentation.
 - Quality review of member services
- National help desk and support centre,
- Operation of the underlying core services
- Targeted training and outreach



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All institutions

- To have all UK HEI as members
- We
 - Must aim to be as broad a church as possible
 - Must collate requirements from research computing at the institutional level
 - Cannot be dominated by the requirements of a single community
 - Cannot aim to drive a single solution onto resource providers



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Issues

- Resources within institutions;
 - Are heavily used by user communities that have little or no interest in externally provided resources and e-infrastructure
 - New user communities increasingly have 'different' data problems requiring shared filesystems, secure data requirements, legal obligations
 - Are frequently upgraded therefore have commercially contracted support agreements for specific operating systems.
 - Have service managers who have to run their services ensuring cost recovery of utilization for hardware, staff and running costs
 - Want to see benefit to participating in grids, measured and audited exchange of resources, "I'll allow resource **EXCHANGE** with university X, not pure donation"
 - Are driven by local green IT considerations



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Campus Grids and the NGS

- Significant number of research intensive institutions are building their own campus grid
 - c.f A number of research led institutions have a similar computational capacity individually to an average EGEE Tier 1
- Mostly some form of Condor based system
 - Either Computing Services based desktop systems, Cardiff looking at rolling out 8k node system
 - Or Condor-G based metascheduling for the whole institution
 - OMII-UK GridBSsystems
- For HTC want to see their own assets fully utilised before using externals



Organisational Membership

- Personnel
 - Appointment of an institutional Campus Champion
 - Liaison between HEI/research organisation and NGS



Campus Champions

- The first level of NGS membership, they are;
 - A source of information regarding NGS resources and services
 - A source of user accounts on their campus
 - A conduit for the campus e-infrastructure needs, requirements and challenges
 - A host for an NGS training event giving visibility to the institutions commitment
 - The direct access to the outreach and training group in the NGS



Organisational Membership

- Personnel
 - Appointment of an institutional Campus Champion
 - Liaison between HEI/research organisation and NGS
- Resource Exchanging
 - Regularly tested installation of NGS defined interfaces as described in the NGS Sits Level Services Document
 - Partner
 - Supporting access by a significant body of NGS users
 - Publish a service level description (SLD) detailing the services offered
 - Affiliate
 - Maintains control over permitted users



What does the NGS offer?

- Compute services
 - Access to more and different resources
 - Different ways of running jobs e.g. multi site MPI
- Data services
 - Access to data storage
 - Support and advice
 - New ways of accessing data
- Access Services
 - User facing services providing methods to use available resources
- Central Support services
 - Individual services needed to support user access, control and management



NGS Site Level Services Document

- Description of the different solutions to service requirements challenges
- A set of different modules describing a particular function, each with a number of solutions which are grouped together as profiles
- Supported interfaces are community driven, we will not/cannot dictate what we make available.
- For example we are currently supporting the following computational interfaces:
VDT gLiteGlobus 4 GridSAM



NGS Recommended Profile

- User Authentication and Authorisation: x509 (VDT)
- Information System: GLUE (VDT)
- Compute resource Service: Pre-WS GRAM (VDT)
- Data Transfer Tools: GridFTP (VDT)
- Storage Management, Database Hosting & User Data access Services: Clients (SRB, SRM, OGSA-DAI)
- User Interface Service: GSISSH (VDT)



NGS EGEE/GridPP Node

- User Authentication and Authorisation: x509 (gLite)
- Information System: GLUE (gLite)
- Compute resource Services: Pre-WS GRAM (gLite)
- Data Transfer Tools: GridFTP (gLite)
- Storage Management, Database Hosting & User Data access Services: Client & Server (SRM)



NGS Data services

- Database (Oracle & MySQL)
 - Supports both user communities and NGS core services
 - STFC and University of Manchester
- Storage Resource Broker
 - Share, replicate and access data with colleagues more efficiently
 - Distributed metadata capable storage system
- Filesystem access to disk storage
 - SCP, GSI-SCP, AFS (on the way)
- Service based methods to access structured data using OMII-UK OGSA-DAI
- All integrated with the NGS user authentication and authorisation mechanisms




Specialist services

- Westminster**
 - Operates and supports P-GRADE portal and GEMLCA legacy application support services
- Belfast e-Science Centre**
 - Web Service Hosting Container Service
 - Web service containers into which projects or VOs can deploy their own Web or Grid services, using automatic deployment technology
- Oxford e-Research Centre**
 - OMII-UK GridSAM
 - OGF HPC-Basic Profile compliant Job submission
 - Promoting interoperability with international grids
 - Eucalyptus Cloud system
 - Exposing AWS compatible interfaces and functionality to NGS users
- STFC Rutherford Appleton Laboratory**
 - Visualisation using specialised cluster from within the STFC e-Science Viz group



Process for a New Service

1. User/Research community propose new service
2. Research and Development Team
 1. Deploy test service, working with community
 2. Develop appropriate service documentation
 3. Final test service deployed on further NGS sites
 4. Service ready for production deployment
3. Operations Team
 1. Deploy operational production service
4. Liaison Team
 1. Publicize the availability of the new service
 2. Training materials developed with the community and training events held



Current status of NGS

- Over 900 registered users, not including EGEE/wLCG users
- 25 member institutions
 - 11 partner resources
 - 18 affiliate resources
- Currently in discussion with 8 further institutions to add both compute and data resources



The NGS Member Institutions, Summer 2009



NGS User access to the NGS

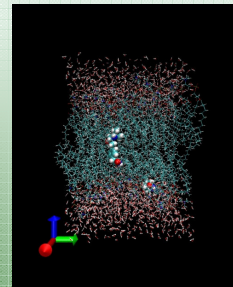
- Directly submit jobs using an installation of the Globus Toolkit, personal Condor or similar on your workstation
- GSI-SSH terminal to connect to a User Interface system or directly to an individual site
 - Web applet or easy install stand alone application
- NGS Portal/Applications repository for web-based access running applications
- P-GRADE portal for workflow
- Application Hosting Environment for MPI across the WAN
- Data system access through HERMES D&D tool, supports SRB, GridFTP, HTTP, SCP

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Simulation performed on the NGS of a drug permeating through a membrane

Name: Dr Brian Cheney
Institution: University of Southampton
Research: Membrane Permeation

*Drs Brian Cheney and Jonathan Essex research membrane permeation of small molecules at the University of Southampton. They're interested in learning what physical and chemical features make a molecule a good or bad permeant, and in developing ways to quantify and estimate a molecule's permeability. We are enabled by submission onto **parallel resources not available locally***

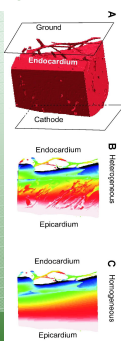


NGS Integrative Biology Project

Name: Thushka Maharaj
Institution: University of Oxford
Research: The effects of defibrillation on the heart

Thushka Maharaj is part of an international collaboration studying the effects of applying an electrical shock to both healthy and diseased hearts, in an attempt to understand exactly how defibrillation works.

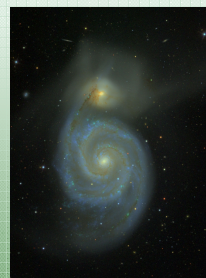
*"We use **parallel code with around a million nodes.**" explains Thushka. "But we can get 20ms of animation in 20 minutes using 32 CPUs on the NGS. And the benefits of services such as the **Storage Resource Broker** are immense - it's fantastic to be able to share data with colleagues all over the world so easily."*




NGS Using the NGS to access geographically distributed astronomy databases

Name: Helen Xiang
Institution: University of Portsmouth
Research: Astronomy databases

*Helen Xiang and Professor Robert Nicol at the University of Portsmouth have been working on Astronomy databases. They use software called **OGSA-DAlto** to **link up astronomy data** that is stored on the NGS and at Portsmouth. This way they can retrieve the data from two places with one command.*

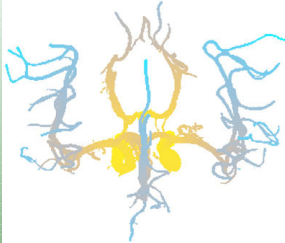





GENIUS

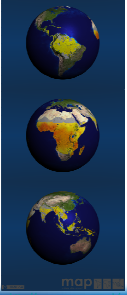


Name: Peter Coveney
Institution: UCL
Research: Model large scale patient specific cerebral blood flow in clinically relevant time frames

Yield patient-specific information which helps plan embolisation of arterio-venous malformations, aneurysms, etc. from inside the operating theatre.
 Use **MPICH-G2** for concurrent submission into NGS, TeraGrid, DEISA and LONI resources from the **AHE** tool


Institutional User communities

- Malaria Map
- Phylogenetic Analysis of DNA
- Analysis of Clinical ECG data
- Biochemistry
- Astronomy
- Chemistry
- Satellite image analysis
- Heart modelling
- Supporting direct campus to national grid integration using Condor-G and OMII-UK GridBS.

User Applications

- Many applications installed on the NGS including:
 - ABAQUS
 - Amber
 - Siesta
 - Gaussian
 - Octave
 - Gadget
 - Fasta
 - NAMD
 - LAMMPS
 - BLAST
 - R
 - ROOT
 - GAMESS
 - DOCK
 - DL_POLY
- And an extremely large number of users who build their own code and submit it



Database Users

- Surrey/Bath University
 - Large volumes of medical observational data
- University of Portsmouth/Mimas
 - Census information
- Southampton University/eScience Centre
 - Genie
 - Chemistry Triple Store
- BADC [British Atmospheric Data Council]
 - Storage of weather models used for predictions.

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Conclusions

- NGS is here to support university research computing services support their research communities by making connection of ITS enabled resources easier
- To achieve sustainability we must move beyond the current single view of 'grid' as e-infrastructure
- Connectivity using standard interfaces will include national data sources including EDINA, MIMAS, as well as experimental facilities such CLF, DIAMOND, e-Merlin, ISIS and JET
- Institutional resources must install more than one set of interfaces until a standard is defined to support various communities

**NGS**

[Thank You](#)

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