NGS

National Grid Service

UK National Grid Service

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NGS IF08 – Manchester 4-5th November

www.ngs.ac.uk/innovationforum

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History of NGS

- Full production since September 2004
- Phase 2 started in October 2006
- New hardware at four core sites in September 2007

- Work in progress to transition NGS to a SLA defined service

The NGS Core, Partners & Affiliates, June 2008

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Science & Technology Facilities Council
Rutherford Appleton Laboratory

HPCx
CAPABILITY COMPUTING

BeSC
Belfast e-Science Centre

MANCHESTER 1824

CARDIFF UNIVERSITY

LANCASTER UNIVERSITY

University of Westminster

University of Southampton

University of Glasgow

KEELE UNIVERSITY

Imperial College London

University of BRISTOL

The University of Reading

UNIVERSITY OF BIRMINGHAM

New Members in the pipeline

- NW-Grid
  - NW England regional grid, Manchester, Liverpool, Lancaster and Daresbury Lab.
- HECToR
  - UK National Supercomputer
- Brunel University
  - GridPP, Tier2
- Durham University
  - GridPP, Tier2
- Liverpool University
  - GridPP, Tier2
- Royal Holloway
  - GridPP, Tier2
- EDINA and MIMAS
  - National Data Centres

- Aberystwyth
- Aston
- Daresbury
  - CATS hybrid cluster
- Hull
- Plymouth
- RAL
  - Visualization Cluster
- WRGrid
  - NE England regional grid, Sheffield, York and Leeds
- DIAMOND
  - National Synchrotron resource

Types of Member Site

- Core
  - Dedicated compute and/or data focused hardware purchased through the project
- Partner
  - Regularly tested installation of NGS defined interfaces
  - Supporting the NGS users Virtual Organisation
  - Complete a service level description (SLD)
- Affiliate
  - Regularly tested installation of NGS defined interfaces
  - 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
  - Methods to use collected externally available resources

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Applications

- Many applications installed on the NGS!
- Standard compilers on all core sites
- Other applications include:
  - Abaqus
  - Amber
  - Siesta
  - Gaussian
  - Octave
  - Gadget
  - Fasta
  - NAMD
  - LAMMPS
  - BLAST
  - R
  - ROOT
  - GAMESS
  - DOCK
  - DL_POLY
- And more…..

User access to the NGS

- Directly submit jobs using an installation of the Globus Toolkit on user workstation
- GSI-SSH terminal to connect to the resource broker or a site
  - Web applet or easy install stand alone application
- Applications repository for web-based access running applications
- P-GRADE portal for workflow
- Application Hosting Environment for MPI across the WAN
- gLite UI system

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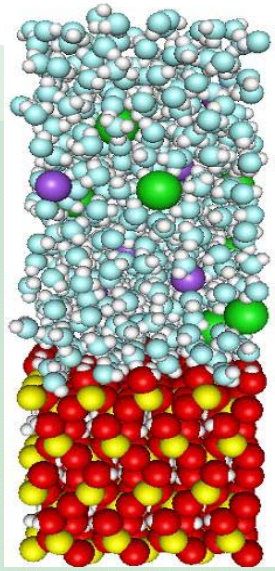
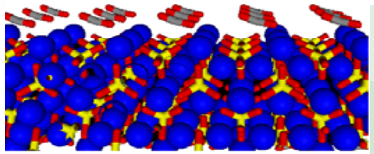
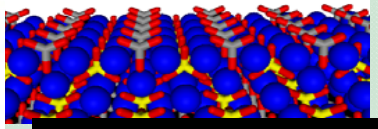
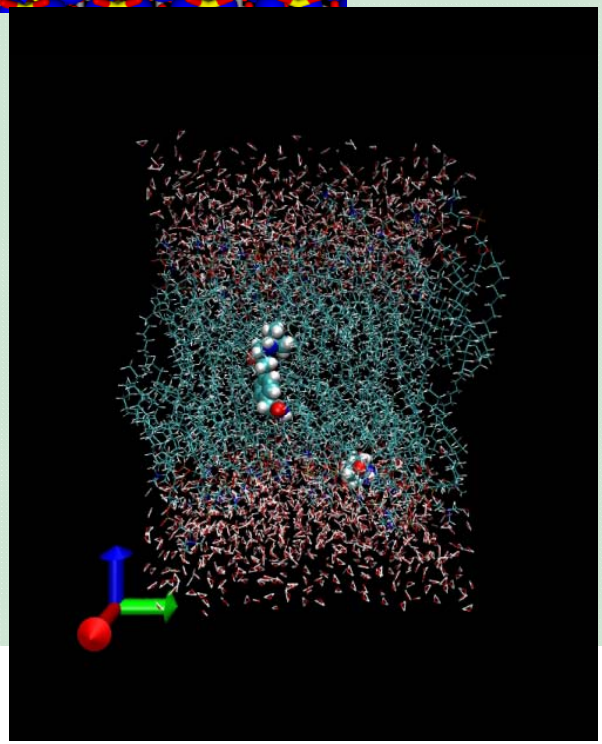
Examples



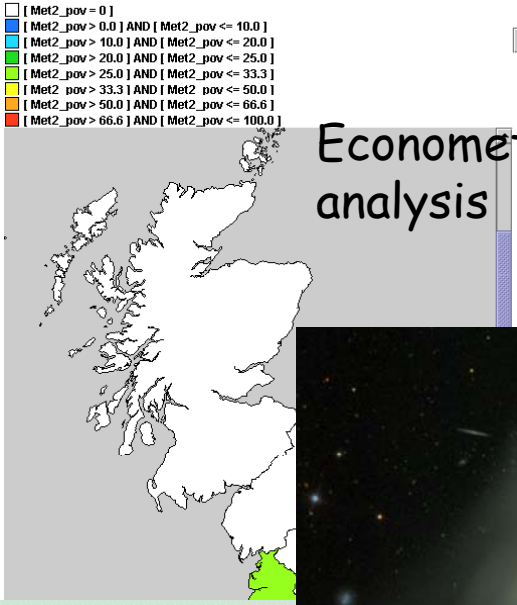


Molecular Dynamics

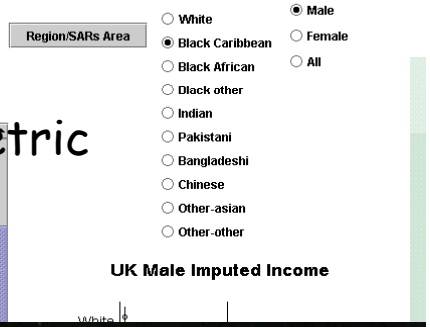




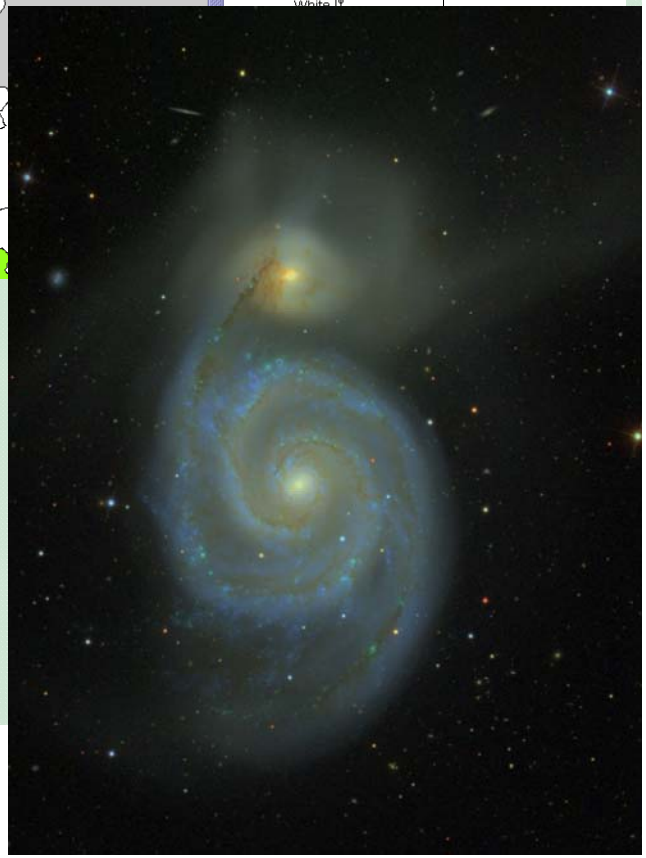
Protein - drug interactions



Econometric analysis



Astrophysics data storage and analysis



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NGS Future

2009-2014

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Service Delivery

- The following services are classed as the core components needed to support grid/e-infrastructure related research within the UK.
  - This service list is not fixed and can be increased or decreased dependant on specific service demand or changing service requirements of the NGS project partners.
  - The list of core services provided will be reviewed every 6 months to ensure developing customer requirements are met.

- Service Management
- Outreach
- Training
- UK CA
- Support service
- Auxiliary Services e.g. MyProxy, VOMS, Accounting Exchange Service, Monitoring
- Operational Security
- OPN
- International engagement/interface

Project Work-packages

1. Project Management
   - Day to day project management to oversee transition from project to service.
2. Service Delivery
   - Oversee ongoing service management.
3. Transition to SLA
   - To define and SLA that meets the service requirements of the JISC and facilitates cross funding body work and the ability to define and meet specific requirements with other such funding bodies.
4. Accounting and charging models
   - Implement a national accounting exchange framework to facilitate exchange of accounting data between institutes and enable institutes to charge for resource usage.
   - Explore charge models, and mechanisms for charging, that an institute may adopt to facilitate provisioning services on a charged for basis
5. Partner support and development
   - Provide support (buddying) to HEI's to assist with installation and becoming an NGS partner resource.
   - Development of tools to meet HEI requirements to assist with joining NGS
   - Increase participation in NGS Operations forums to facilitate community support across HEI's

Commissioned Services

- Additional services and resources above and beyond those of the core ‘business as usual’ services
  - Through either direct funding from the NGS or other funding sources.
    - N.b. Some additional service could be free e.g. provision of lightpaths at no cost to NGS/resources as ja.net provisioned to provide
  - During the transition phase of NGS-3 some of these services will initially be funded from the NGS grant and transitioned to separate partner/commissioned services which are sustained in line with user requirements through direct funding or appropriate cost recovery/charge models.
- Examples:
  - Compute services (free and charged for)
  - Data Storage
  - Visualisation
  - Specialist training facilities
  - CSE type support
  - Light Path connections
  - Etc.

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Next steps

- Broad discussion with stakeholders
  - Users, HPC-SIG, Campusgrid-SIG, GridPP…
- Include key people in proposal development
  - DB, PELC …
- Develop ideas/proposal through September
- Proposal to JISC late October
  - And to EPSRC too
- Input from GridPP...