



“Providing 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”



www.ngs.ac.uk

What is the UK National Grid Service?

By joining the NGS, UK academics have access to much more computing power than offered by their local clusters. The NGS works by joining together computing resources at many institutions and making them available to NGS users.

The NGS currently consists of four core sites, five partner sites and three affiliates:



NGS Core Sites

Science and Technology Facilities Council – Rutherford Appleton Laboratory (RAL)

White Rose Grid at the University of Leeds

The University of Manchester

University of Oxford

Partner Sites

Cardiff University

University of Glasgow

Lancaster University

Queen's University Belfast

University of Westminster

HPCx

Affiliate Sites

University of Edinburgh

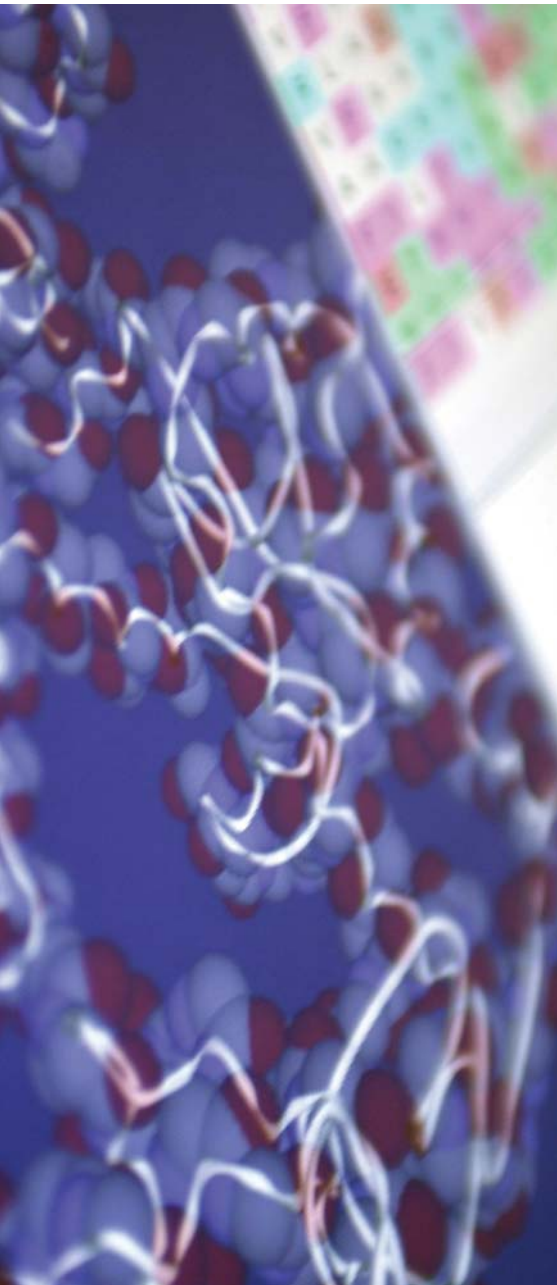
Keele University

National e-Science Centre (NeSC)

Imperial College London

University of Southampton

For further information on the benefits of your institution joining the NGS please see our website - www.ngs.ac.uk/guide/



What we offer users

In addition to **free** access to computer clusters, the NGS also offers the following:

Access to Services

As a NGS user you will have access to a large number of services including -

GSI-SSH Terminal - used as either a standalone Java application or an applet on the NGS website, the GSI-SSH terminal allows users (including those using Windows) to log onto the NGS nodes using their certificate but without needing access to the Globus commands.

Applications Repository - the NGS applications repository allows users to run jobs on the NGS through a web application. Templates of commonly run jobs are sorted on there which users may modify for their own ends.

Resource Broker - the resource broker allows users to submit a job without having to choose where to run it. The resource broker selects the best resource dependent on your job requirements and the current load on each machine.

Storage Resource Broker (SRB) - the storage resource broker enables data to be stored in various physical locations but retrievable under the same file-name. There are various interfaces to the SRB on the NGS.

MyProxy Upload Tool - this is a common method of accessing services such as the applications repository, which allows users to store a proxy certificate on a remote server.

Oracle 10g - the Oracle databases on the NGS offer the ability to store large amounts of data with the ability to perform computationally intensive queries.

Grimoires - offers a single point of reference for service providers and consumers, providing an extended UDDI registry for service discovery. In essence, this allows those publishing services in the registry to attach searchable, domain-specific metadata to service entries.

GridSAM - provides a Web Service for submitting and monitoring jobs managed by a variety of Distributed Resource Managers (DRM).

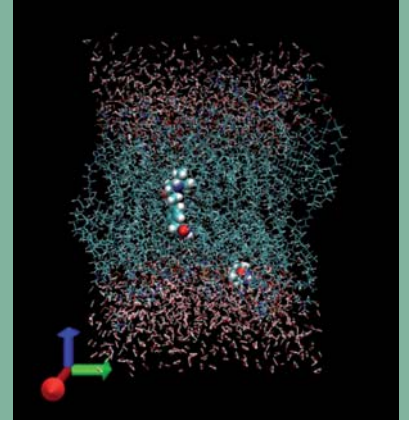
NGS Helpdesk

No matter if you are just starting out with Grid computing or if you are an experienced Grid user, the NGS helpdesk is there to help. Operated by staff experienced in the use of Grid computing, they can be reached by email or telephone at support@grid-support.ac.uk or 01235 446822.

Training

The NGS, in conjunction with the National e-Science Centre's Training, Outreach and Education team, organise a number of training events through out the year for Grid users of all levels. Details of training courses can be found on their website at www.nesc.ac.uk/training/events

Simulations performed on the NGS show drugs permeating through a membrane - water is represented by the red and white lines and the membrane by turquoise lines. There are two drugs permeating through the membrane. Dr B.Cheney, University of Southampton.



Software

Nodes within the NGS run the main compilers Intel, GNU and Java. In addition many libraries and packages are installed such as:

- Siesta
- Gaussian
- ncbiBlast
- DL_POLY
- Gromacs
- Fftw
- Amber
- NAMD
- VASP
- Oracle Client
- R
- SABRE
- And many others...

If there is an application you would like to see installed on the NGS, please contact the helpdesk with details of the application and why you wish to use it. Suggestions for further additions are always welcome.



The spiral galaxy, Messier 81, which is 12 million light years from earth.

Grid Computing in Action

Whether you are a chemist or bioinformatician, a quantum physicist or a social scientist, the NGS can help you. Since starting in October 2004, the NGS has helped over 600 researchers, scientists and developers advance their research.

Membrane Permeation

Researchers at the University of Southampton investigating the thermodynamic and kinetic properties of small molecule membrane permeation approached the NGS for assistance with their computationally intensive scientific challenge. The traditional approach depended on all-atom classical molecular dynamics (MD) simulations of a drug permeating through a membrane. The MD simulations require many millions of time-steps and would take several years on a modern desktop computer for each drug studied.

The researchers grid-enabled their modifications of the legacy molecular dynamics software package CHARMM, and collaborated with researchers at the University of Manchester and University College London to host their application on the NGS in the Application Hosting Environment.

By using the NGS, the simulation time was cut from years per drug to about 2 weeks, allowing drug research to move forward much faster than would have otherwise been possible.

Astronomy databases

Since 2000, the Sloan Digital Sky Survey (SDSS; www.sdss.org) has been taking

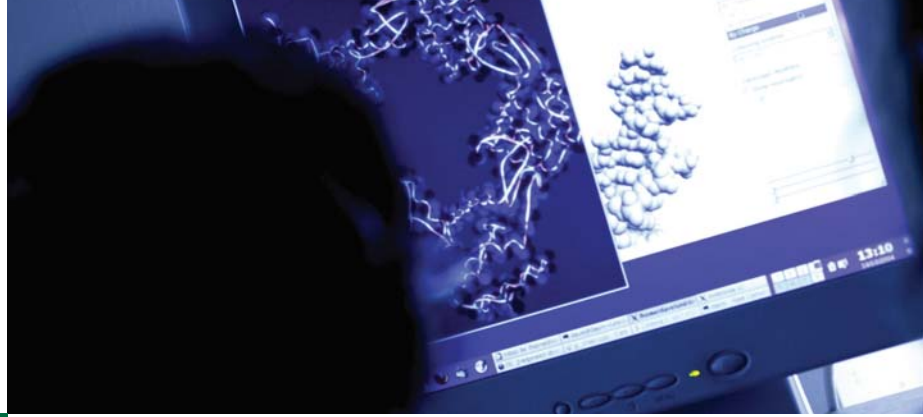
multi-colour digital images of the northern sky. To date, nearly 300 million celestial objects have been detected over the last seven years. The data has been used to support research on all areas of astronomy and cosmology, from asteroids to the large scale structure of the Universe.

All this data however presents difficulties with both storage and access for the users so researchers at the University of Portsmouth turned to the NGS for assistance. A PhD student from the SDSS project investigated the use of Oracle databases hosted on the NGS to store the data.

To date almost 2 Terabytes of SDSS data has been successfully transferred to the NGS Oracle database in Manchester with a separate Microsoft SQL database at Portsmouth holding another 2 Terabytes of similar data. Joint queries on the two databases have been successfully run.

With such diverse resources, the team at the University of Portsmouth has been experimenting with grid data management software such as OGSA-DAI and OGSA-DQP. They've been exploring its performance with jointly accessing SDSS data both on the NGS and Portsmouth.

Accessing distributed, diverse astronomy databases easily is a key requirement of future astronomy projects. The next generation of astronomy surveys include the Large Synoptic Survey Telescope which will produce petabytes of raw image data.



White Rose
university consortium
Universities of Leeds, Sheffield & York

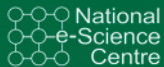


Science & Technology
Facilities Council



Engineering and Physical Sciences
Research Council

oerc



National
e-Science
Centre

JISC



MANCHESTER
1824
The University of Manchester

How to join

The first step in becoming a NGS user is to apply for a digital certificate issued by a trusted Certificate Authority to prove your identity. You can apply for a digital certificate at www.ngs.ac.uk by clicking on "Apply for Access" on the home page and following the easy instructions. You will then need to visit your local Registration Authority (RA) operator with some photographic identification such as a passport. An email will be sent informing you of your local RA operators.

Once you have your digital certificate you can go to the NGS website and fill in the simple application form, stating your research case for using the NGS. This application then undergoes a light-weight peer review process which lasts a maximum of 1-2 weeks. After that period you will, if your application is successful, receive a welcome email with your account details and informing you what to do next.

Further Information

You can find further information about the NGS on its website at www.ngs.ac.uk. The website contains documentation and online tutorials for self-guided learning.

Contacts

The NGS is keen to hear from potential users, partners and affiliates. If you would like more information on any part of the NGS then please contact:

NGS Support Centre
Email support@grid-support.ac.uk
Tel - +44 (0) 1235 446 822

NGS
e-Science Centre
STFC Rutherford Appleton Laboratory
Harwell Science and Innovation Campus
Didcot, Oxfordshire. OX11 0QX
UK

Keep in touch with the NGS

Mailing lists

If you would like to be kept up to date with news from the NGS then join our mailing list to receive fortnightly news updates including events and training opportunities.

<http://www.jiscmail.ac.uk/lists/NGS-NEWS.html>

If you are a user of NGS resources then join our status mailing list to be kept up to date with service news and updates.

<http://www.jiscmail.ac.uk/lists/NGS-STATUS.html>

Newsletter

The NGS produces a quarterly newsletter containing a large variety of news about the NGS including user case studies, NGS site news, application updates and conference reports. The latest edition of NGS News can be found on our website in the Outreach section.