



THE WHITE ROSE GRID e-Science Centre

The National Grid Service

The National Grid Service is a UK grid computing service that is free at the point of use to all UK academics. The NGS aims to provide coherent access to the resources required to enable UK e-Research. The service consists of four core nodes located at the Universities of Leeds, Manchester and Oxford and STFC RAL. In addition to the core sites there are various partner sites, most of which provide either compute and data resources or other grid services. Partner sites include the Belfast e-Science centre and the Universities of Bristol, Cardiff, Lancaster and Westminster.

The NGS hosts a wide variety of services and applications and welcomes requests for new software to be installed. Similarly, we welcome approaches from groups of users or virtual organisations who wish to provide access to the NGS to their users or join the NGS as partners or affiliates.

Information on applying for access to the NGS and support for NGS resources can be found on the NGS web site or by emailing the helpdesk:

<http://www.grid-support.ac.uk/>

support@grid-support.ac.uk



The Leeds NGS Node

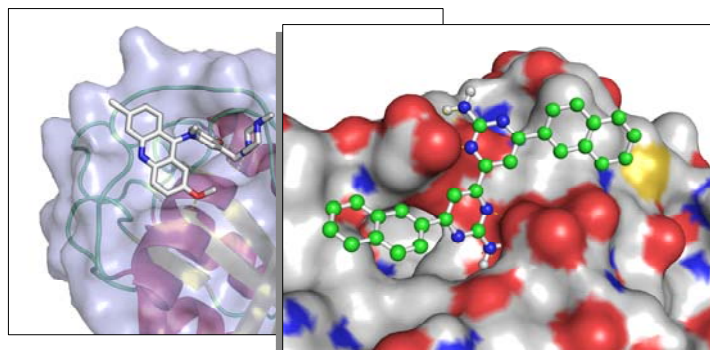
With the second phase of the National Grid Service well under way, the University of Leeds continues to host the White Rose Grid node of the NGS and provide a stable service to our users. The NGS node at Leeds consists of 256 CPU cores connected via a Myrinet 2000 interconnect for MPI communications and approximately 30TB of storage used for home areas and SRB.

The University of Leeds is also working on new services for users of the NGS. These include enabling users to host web services on the Leeds NGS node as well as the development of a grid-enabled AFS service for the whole of the NGS.

Research on the Leeds NGS Node

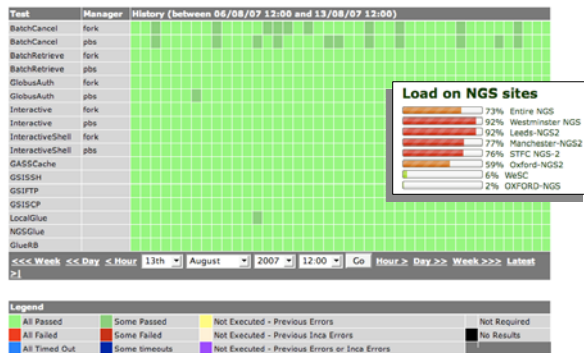
A wide variety of research is carried out on the Leeds NGS resources including modelling complex systems such as:

- Simulation of candidate drug molecules (pictured opposite)
- Modelling and Simulation for e-Social Science
- DNA deformations
- Behaviour of the HIV virus
- Biological membranes
- Quantum dynamics



Dr. Narcis Fernandez-Fuentes from the University of Leeds uses the Autodock software installed on the NGS core nodes and partner sites to virtually screen a large library of drug-like compounds against RAS. The goal is to find promising binders that will be taken forward for experimental verification and which eventually could lead to potential medical treatments of illnesses caused by mutations of this protein.

Conformance Results for Leeds



Historical results from conformance monitoring can be viewed online at <http://inca2.ngs.ac.uk/>. Current load information (inset) is available on the NGS web site: <http://www.grid-support.ac.uk/>.

Monitoring on the NGS

The White Rose Grid (through the University of Leeds) is also involved in the development and management of the NSG monitoring system. Part of the monitoring is based on Inca 2, a framework originally produced by the San Diego Supercomputer Center for Teragrid. Inca provides a flexible framework that allows the creation of custom tests to ensure that sites are conforming to the requirements set for them (see opposite).

Leeds has also produced the NGS load monitor (inset opposite), which allows users to see a summary of the current load on sites that report to the NGS federated Ganglia service. The load information automatically updates every minute without requiring users to reload the page.

