

HPCX SLD	
Version 0.2	28 Jul. 04



## HPCx on the UK National Grid Service (NGS)

### Aim

To make available resources and supercomputing services as described below via the UK National Grid Service to the UK academia.

### Facilities

Approx 1600 IBM Power-4 CPUS. Organised as a cluster of multiple 32 CPU systems, with fast interconnects. Two major upgrades of the facility are planned during the lifetime of this service. The current hardware configuration is documented at <http://www.hpcx.ac.uk/services>

### Service Provider

The HPCx Consortium, namely UoE HPCX Ltd, is led by the [University of Edinburgh](#), with the [Council for the Central Laboratory for the Research Councils](#) (CCLRC) and [IBM](#). The project is funded by [EPSRC](#). The core service is provided by EPCC at the University of Edinburgh and CSED at the CLRC Daresbury Laboratories.

### Inclusions

1. The following Grid middleware for the support of the UK Level 2 Grid is installed:
  - a. Globus Toolkit 2.4.3 including GridFTP with MDS reporting to the UK e-Science MDS maintained at the Grid Support Centre and later (when established) at the Grid Operation Centre.
  - b. Loadleveler jobmanager.
  - c. SRB client (to be confirmed).
2. The following software for developing and running programs is mounted:
  - a. IBM AIX compiler suite (C/C++/F90 includes OpenMP support)
  - b. IBM Parallel Operating Environment (POE) includes IBM MPI and LAPI.
3. The list of application packages available on HPCx is detailed at the following location <http://www.hpcx.ac.uk/research> divided up by research community. This includes the following packages:
  - a. H2MOL
  - b. PRMAT
  - c. AMBER
  - d. PMEMD
  - e. CHARMm
  - f. DL\_POLY
  - g. GAMESS-UK
  - h. GAUSSIAN

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- i. NAMD
- j. NWChem
- k. CFX
- l. NEWT
- m. POLCOMS
- n. AIMPRO
- o. CASTEP
- p. CRYSTAL

See the individual pages for details of support and licensing.

4. Digital certificates management: accept certificates issued by the UK e-Science Certificate Authority and those CAs with which the UK e-Science has agreements. The Certificate Revocation List is updated on a regular basis.
5. Information: An *Introduction* document for users of the system; the Web pages describing local arrangements are available at <http://www.hpcx.ac.uk/>.
6. An administrative web-site <https://www.hpcx.ac.uk> providing the following:
  - a. User registration
  - b. Resource management and on-demand usage statistics.
  - c. Requests for gridmap file changes
  - d. Requests for password reset
7. Provision of *permanent* backed up home disk space
8. Provision of *permanent* non backed up work disk space
9. Provision of *temporary* non backed up disk space for users' files.
10. Provision of tape archive storage accessed through IBM's Tivoli Storage manager.
11. Fault reporting and tracking system.
12. Helpdesk system for user support [helpdesk@hpcx.ac.uk](mailto:helpdesk@hpcx.ac.uk).
13. Training courses are available to users see <http://www.hpcx.ac.uk/support/training>.
14. A series of technical reports are available at <http://www.hpcx.ac.uk/research/hpc>.
15. Loadleveler Batch job control: Note the majority of the resource is ONLY available for access from the batch queues.

## Exclusions

1. The Operating regime of this service is defined by a contract between UoE HPCX Ltd and EPSRC. This contract takes precedence over any information presented in this document.
2. Users of HPCx must be members of research projects, which have been awarded a grant of HPCx resources by one of the relevant research councils. The project PI or their nominated representatives must therefore approve all user accounts on this service. Instructions for applying for user accounts on HPCx can be obtained here: [http://www.hpcx.ac.uk/projects/new\\_users](http://www.hpcx.ac.uk/projects/new_users)
3. HPCx resources are allocated via research grants.
4. Users are required to agree to the HPCx conditions of use <http://www.hpcx.ac.uk/services/policies/tandc.html>
5. HPCx is not exclusively for use via the Grid. This system provides interactive access via the standard IBM version of ssh rather than via GSI-SSH.
6. Only the Login/Job-submission nodes are directly connected to the Internet. Grid applications that need to make socket connection to/from running applications will need to use port forwarding. A port-forwarding tool was developed for the

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teragyroid project and is available on HPCx. No special procedures are required for data retrieval as the file systems are common to all nodes.

## Service Level

### *Quality*

1. GITS results are published regularly and their results monitored to identify problems.
2. Test results published on the NGS Web site,

### *Availability*

3. HPCx will be available at all times subject to: essential planned maintenance to hardware or software, unplanned outages and failures out of hours to be dealt with ASAP.

### *Reliability*

4. The reliability of the service is monitored and figures are made available for inspection on the HPCx web site. We aim for the system to be serviceable for at least 99% of the time.

Detailed information about service policies is available at the following web page

<http://www.hpcx.ac.uk/services/policies>.

## **Helpdesk service levels**

Certain minimum standards of performance have been set for the Helpdesk by HPCx's funding bodies. They include:

- To resolve 97% of all queries within three working days;
- To resolve 97% of all administrative queries within two working days;
- To resolve 75% of all queries within one working day.

Excluded from these measurements are queries classified as *in-depth*. These include:

- technical queries which require more than one person-day of full-time work to resolve;
- queries which require further communication with the user, when the user does not immediately respond;
- queries which have to be referred to a third party, when that third party does not immediately respond.

Details of how we measure up to these standards will be posted on the website.

## Compliance

1. Availability statistics are published on the HPCx Web pages.

## Operational Framework

1. Faults should be reported to the Helpdesk via email: [helpdesk@hpcx.ac.uk](mailto:helpdesk@hpcx.ac.uk)
2. Change Control

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New releases of Globus software will be agreed in advance with other sites at the NGS Team meetings. Users are informed prior to upgrading taking place via HPCx User mailings.

## Definitions

1. *NGS web site* – [www.ngs.ac.uk](http://www.ngs.ac.uk).
2. *Globus* – a toolkit providing a set of services to enable grid applications and the underlying grid infrastructure to inter-operate.
3. *GridFTP* – an FTP service with extensions to meet requirements of grid environments
4. *GSIssh* – a version of ssh (secure shell) that uses the Globus Security Infrastructure (GSI) for authentication with X509 certificates.
5. *MDS – Monitoring and Discovery Service*: a way of querying a grid service about its configuration and status.
6. *SRB – Storage Resource Broker*: a client-server middleware that provides a uniform interface for connecting to heterogeneous data resources over a network and accessing replicated data sets.
7. *UoE HPCX Ltd* is a wholly owned subsidiary of the University of Edinburgh set up for the provision of High Performance Computing services.