



# e-Science for STFC Facilities

The STFC is one of Europe's largest multidisciplinary research organisations supporting scientists and engineers world-wide. It operates world-class large-scale research facilities, provides strategic advice to the government on their development and manages international research projects in support of a broad cross-section of the UK research community.

This article describes the current work to integrate e-Science capabilities into the large-scale research facilities operated by the STFC.



ISIS and DLS Facilities at RAL

## The Facilities

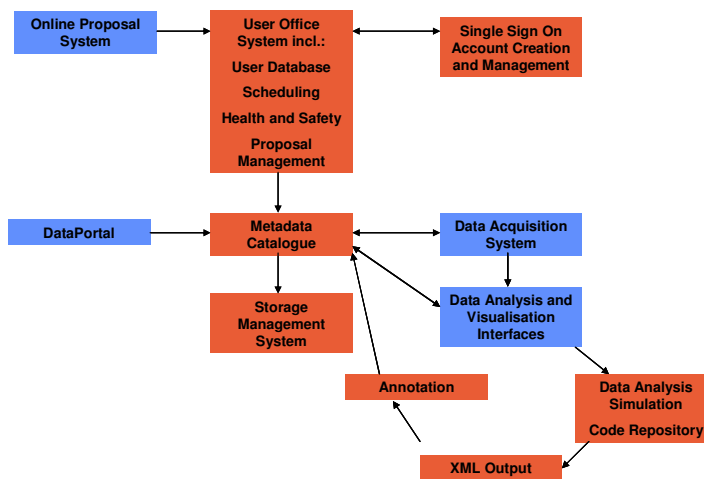
The STFC has started a work program to integrate key e-Science services within the following large scale research facilities:

• ISIS is the world's leading pulsed neutron & muon source situated at the STFC Rutherford Appleton Laboratory (RAL). It supports an international community of around 1600 scientists who use neutrons and muons for research in physics, chemistry, materials science, geology, engineering and biology.

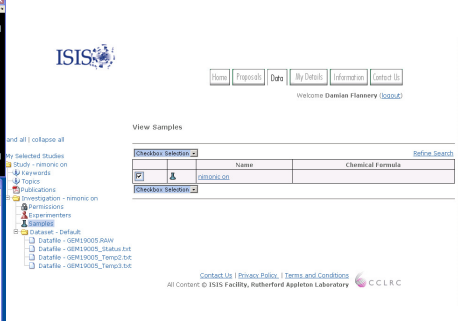
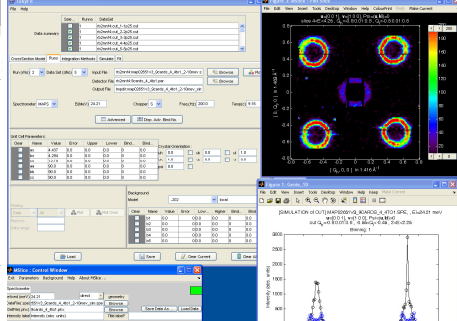
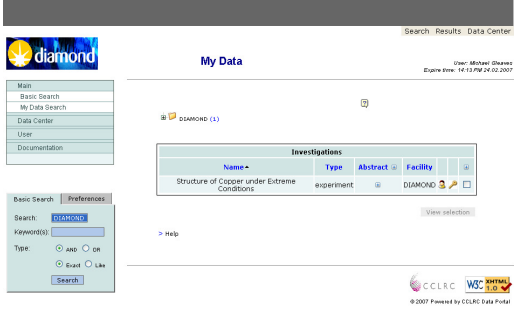
• Diamond Light Source (DLS) is a new third generation synchrotron currently being built at the Harwell site in Oxfordshire. Synchrotrons produce ultra-bright light which is made up of a combination of ultraviolet light and x-rays. This is used to investigate the internal structure of materials, having a number of different

applications including: biomedical science, medical research, environmental science, agriculture, mineral exploration, material science and forensics.

• Central Laser Facility (CLF) work involves development and application of advanced, world-leading laser facilities. These are used for ultra-fast time-resolved infrared spectroscopy and to provide high repetition rate ultra-high intensity laser irradiation (petawatt). The facilities enable a broad base of rapidly expanding areas of research to be investigated with applications in inertial confinement fusion, astrophysics simulations, bioscience, accelerator science and molecular physics.



e-Infrastructure for Research Facilities



## Data Portal for DLS

### Aims of the Project

The e-Science Centre was founded with the distinct aim to 'Grid enable' the facilities. This was defined as developing, deploying and running e-Services for experimental, computing and data facilities, to further the Science carried out at these facilities. E-Science is aiming to achieve this goal by:

- Working collaboratively with Facilities and their users
- Creating a powerful, long lasting scientific knowledge resource for UK academia.
- Enabling users to get rapid access to their current and past data, related experiments, publications etc., leading to improved analysis through more complete information.
- Providing an integrated Infrastructure for Data Management and Advanced Analysis

### Joint Achievements

In order to produce a Facilities infrastructures on common core components agreement with the facilities have been reached on:-

- Production of CSMD a common metadata format.

## Interactive interface for Toby Fit

- ICAT will be used as metadata catalogue
- NeXus data format will be used for all future data
- Using the same underlying Proposal system
- Single Sign On between all facilities and services - one user id for all
- SRB and Petabyte DataStore for data location management and long-term storage.
- Using SCARF for advanced Data Analysis
- Oracle databases for operational use, largely maintained and operated by the Scientific Database Group

### Supporting Services & Tools

The functionalities of the e-Infrastructure are supported by a variety of Services within the STFC e-Science Centre, these are at present: Scientific Database Services, SRB Services, Petabyte DataStore, SCARF, National Grid Service, North West Grid, UK Certificate Authority.

The facilities work is also based on software tools developed within the e-Science centre e.g.

## ISIS back catalogue

AgentX, My Condor Submit (MCS), Remote My Condor Submit (RMCS), Information Catalogue (ICAT) and Data Portal

### The Future for e-Science Facilities.

Globally, we are currently going through a golden age for big science. There are increasing numbers of large scientific projects like Diamond, ISIS and CLF being built. Also, there are also other new facilities on the horizon for example 4GLS; the UK Muon and Neutrino factory; and European Square Kilometres Array.

e-Science has an important role in providing computing infrastructure that allows the scientist to use the facility more efficiently. By providing new ways to store, manage and analyse the incredible amounts of data that these these facilities will create. e-Science will allow the scientist to concentrate on doing better science.

The e-Science Facilities projects are at a development stage and initial versions of the e-Science infrastructures are currently being deployed at DLS, ISIS and CLF for feedback from the scientific community.