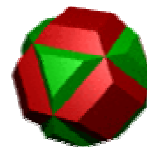# NCS Grid Service

Ken Meacham, Mike Surridge, Steve Taylor, Simon Coles, Mark Light, Ann Bingham,
Mike Hursthouse, Sam Peppe, Jeremy Frey, Graham Smith, Hugo Mills
Comb-e-chem Project, University of Southampton.

National Crystallography Service

The EPSRC funded National Crystallography Service (NCS) is a facility available to the entire UK academic Chemistry community. The EPSRC funds a team of experts and 'state of the art' instrumentation, based in Southampton University School of Chemistry, to provide this service. This is an exceptionally important service as crystal structure determination is easily the most information rich method of characterisation of a compound and many research papers cannot be published without confirmation of identity by crystal structure analysis.

The NCS has a broad base of users covering a whole range of chemical applications and whose structural expertise can range from none / novice to expert crystallographers. This service therefore provides support to those that have no facilities, whilst also complimenting the less powerful instrumentation available to most experts. The NCS has approximately 150 subscribers who submit >1000 samples per annum. This, coupled with providing a departmental service and maintaining the crystallography research group interests, is approximately an order of magnitude higher throughput than the average crystallography laboratory.

The NCS is currently at the forefront of pioneering the fully automated crystal structure determination experiment. This involves both hardware and software developments, such as robotic sample changing, intelligent computation of a data collection strategy & automated data processing and workup. This is the only way that we can possibly keep pace with the increasing demand for a high throughput of samples and is of course much cheaper and more reliable than employing humans, as robots can operate 24 hours a day without (too much) complaint!

NCS on the Grid

One way to automate the experiment is to get the remote user to drive it themselves!

The NCS is perfectly suited to hosting an interactive Grid service for a number of reasons:

- The submitter of a sample will have a more detailed knowledge and understanding of it and hence be able to purposefully contribute to the experiment
- The users of the service are distributed across the UK, yet need to collaborate closely with NCS staff
- NCS staff are overrun with 'demanding' samples and the ability of a user to manage their routine samples greatly relieves this pressure
- High throughput demands effective sample management and tracking, especially when a user has multiple samples in the system
- A user can monitor 'out of hours' experiments to ensure they complete successfully and that most effective use of 'instrument time' is made

Comb-e-Chem Trust Network
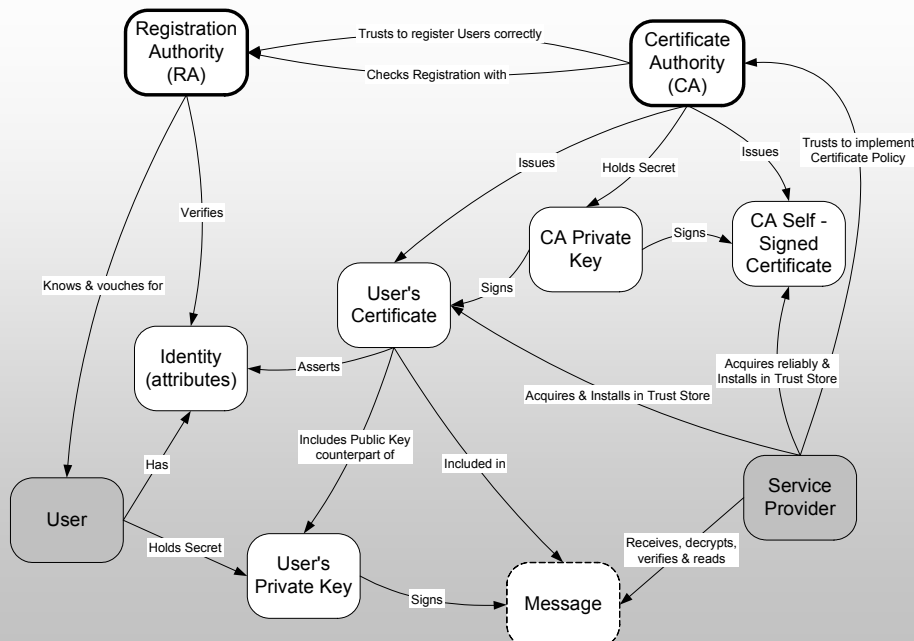
Security

Security is crucial to the successful operation of the NCS Grid Service, both in terms of the authentication of users and, and in maintaining the integrity of their data.

For NCS, we have set up a well-defined trust network, with its own CA and RA. Only users with a valid NCS certificate may access the Grid Service.

All data transfer is encrypted, and each user is authorised to access only their own data, or monitor their own experiments. This is achieved by mapping the user's credentials to the appropriate authorisation or datasets.
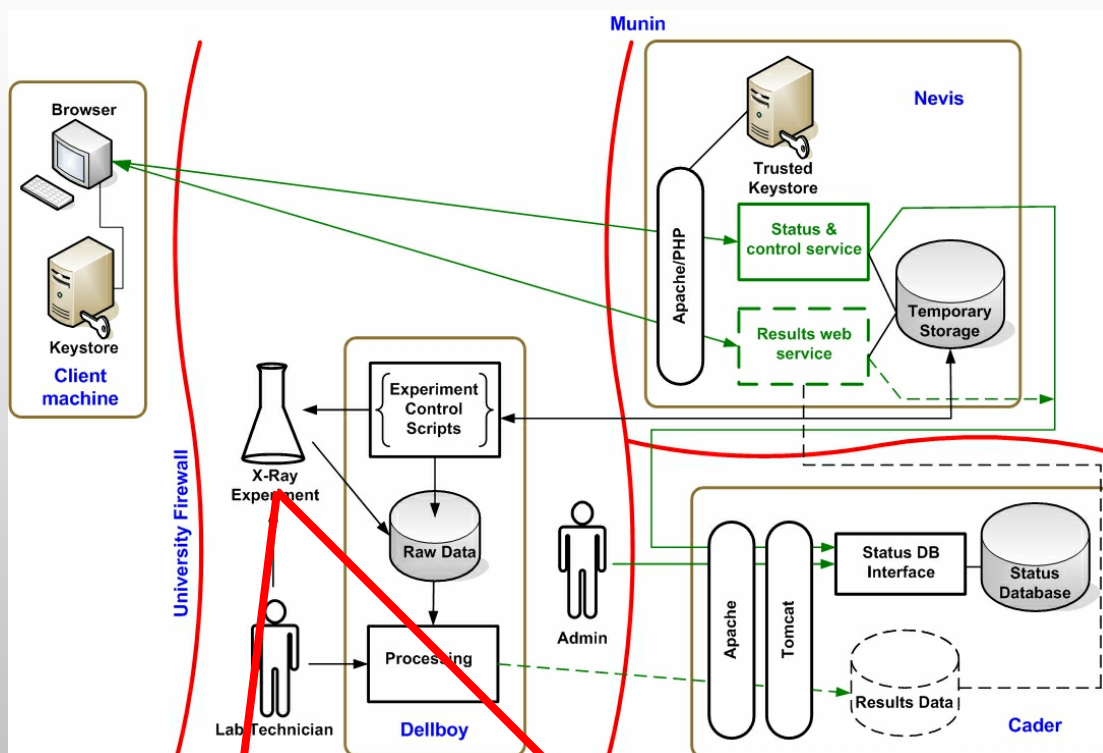
NCS Grid Service
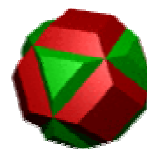
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Architecture
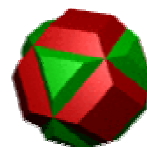

X-ray Diffractometer

Sample Changing Robot

NCS Grid Service

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Sample Status Service

National Crystallography Service – Sample Status

Viewing samples for M E Light (light@soton.ac.uk)

NCS ID	Customer ID	Received	Collection	Status	Details
04MEL0098	2nd test	2004-02-12	001	Succeeded	HKL file / Report
04MEL0093	mel01	2004-02-06	001	Running	Control service
04SRC0104	#13-123	2004-03-08	001	Next	Due at 00:00:00 (est)
04SRC0103	#12-01	2004-03-08	001	Failed (Referred)	Diffraction too weak
			002	Failed (No Further Action)	Crystals too small
04SRC0105	HSF-HCl	2004-03-08	001	Added	

Client sample list

User-defined sample IDs

Sample may have multiple collections

Current states of each sample (collection)

Further details and available links

Results Data

EPSRC National Crystallography Service

Data Collection Summary

Summary report for Directory: diska/04MEL0093/001

Report generated Mar 10, 2004; 10:20:10

Unit cell

3535 reflections with 2.91°<theta<36.32° (resolution between 7.00A and 0.60A) were used for unit cell refinement

Symmetry used in scalepack	p3
a (Angstrom)	26.7825 +/- 0.0013
b (Angstrom)	26.7825 +/- 0.0013
c (Angstrom)	10.8786 +/- 0.0004
alpha (°)	90.000
beta (°)	90.000
gamma (°)	120.000
Volume (A**3)	6742.1 +/- 0.5
Mosaicity (°)	0.411 +/- 0.003

Once the experiment has completed, a summary of the results is automatically published and linked to the Sample Status page.

How it works

The Status Service determines the client's Distinguished Name (DN) from their NCS certificate, then queries the Sample Database for a list of all samples submitted by the client (they may only see their own samples).

Samples are presented in the client's browser, showing the status of each sample (or collection). In this way, the client may regularly track the progress of their samples within the NCS system.

Once a sample enters the Running state, a link is made available to the Control Service, whereby the client may monitor the running experiment.

HKL File

The main output from the data processing is a reflections (or HKL) file. The client may use this to calculate the full crystal structure of their sample, or make use of the NCS structure calculation service.
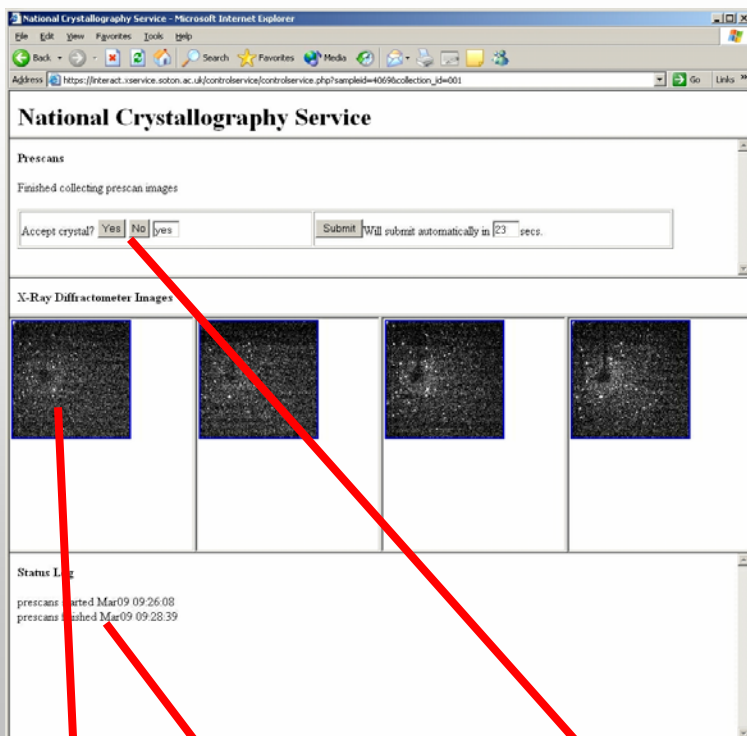
NCS Grid Service
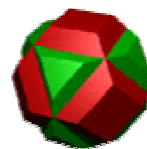
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Experiment Control Service

How it works

The Control Service provides the client with a portal to their running X-ray diffraction experiment, giving them the opportunity to observe the experiment in progress, and to steer it if they wish.

The display is continuously updated, to reflect the current state of the system as the experiment goes through its various stages (prescans, unit cell determination, full data collection and data processing).
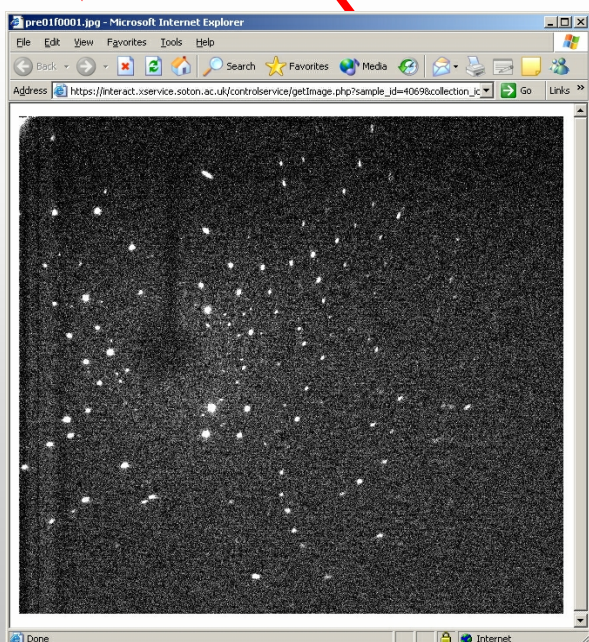
Scanned images and other raw data are collected by the diffractometer, and published via the portal, enabling the client to make informed decisions at each stage whether to continue the experiment, etc.

Parameter Adjustment

Key experiment parameter values may be adjusted.

Enlarged Scan

Full size images may be viewed, by clicking on the corresponding image thumbnail.

Experimental Steering

The client can examine the images returned for the prescan, to determine the quality of the crystal. They may then choose to reject the crystal if they wish. A timeout ensures that the experiment may continue, if the client is not present (or takes too long to decide!).

Status Log

The status of the experiment is displayed in the Status Log.