



# The UK National Crystallography Service Grid Facility

Mike Hursthouse and Simon J. Coles

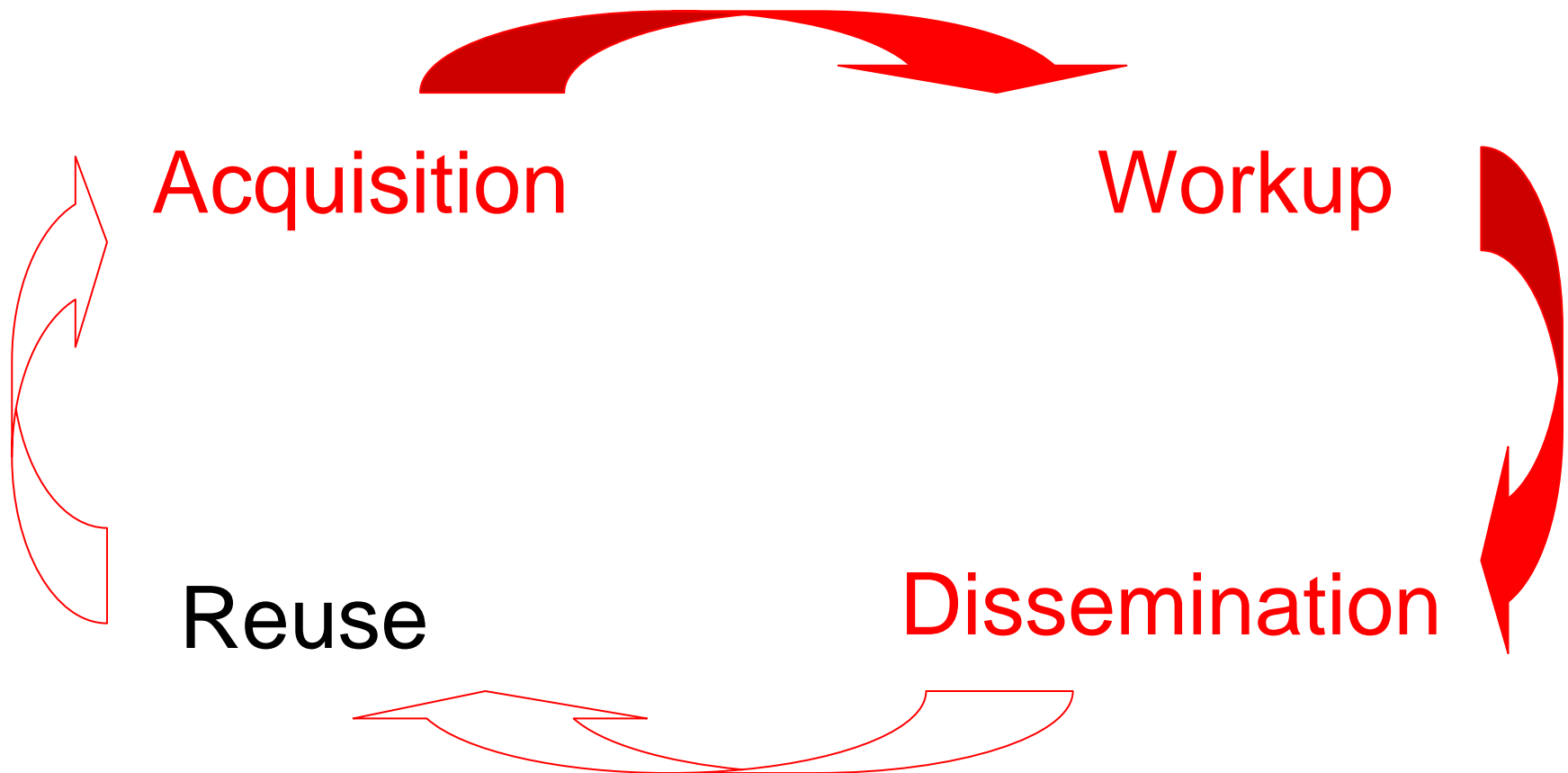
School of Chemistry

University of Southampton

*NSF Crystal Grid Raw Data  
Management Workshop*

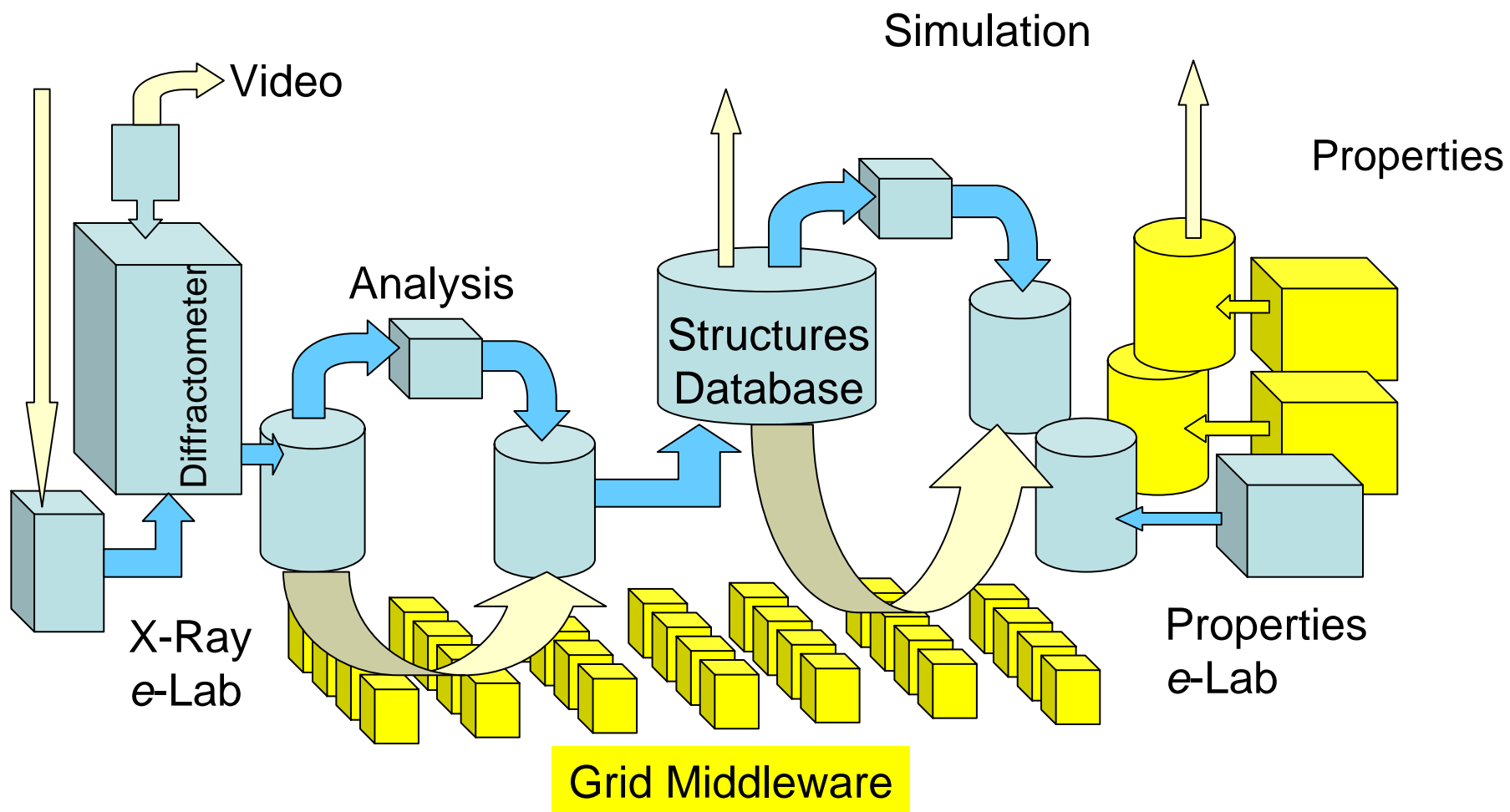


# The 'data' cycle





# E-Science environment



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# The 'Pipeline'



- 1) Application for an allocation
- 2) Secure access to NCS Grid resources
- 3) Sample submission
- 4) Monitoring sample status
- 5) Data collection
- 6) HKL data download
- 7) Raw Data Archival



# NCS Grid Service



- Security policy and procedure
- Apply to use the Service
- Submit sample details
- Monitor sample status

EPSRC CHEMISTRY PROGRAM  
National Crystallography Service  
NCS Grid Portal

**EPSRC**  
Engineering and Physical Sciences  
Research Council

**Welcome**

Welcome to the NCS Grid Service Portal. This is your base to access all of the Grid-enabled services offered by the NCS.

**NCS Grid Access**

Access to the NCS facilities via the Grid offers its users a fast and convenient method of requesting Service Allocations, submitting sample data and visualising up to the minute sample status.

The NCS Grid Access pages detail the user requirements for grid access and provides information regarding the available services, instructions on their usage and step-by-step tutorials where required.

[NCS Grid Access](#)

**2005-2006 NCS Allocation Request**

Applications for 2005-2006 NCS Allocations are currently being accepted. Please note that in order to complete the online form you will need to provide:

- A Scientific Programme outlining the objectives of your research project, the need for X-ray diffraction support and identifying the extent and scope of any funding you receive to support this research.
- A short report summarising the contribution that any previous NCS Allocations have had on your research.
- A list of publications or similar output arising from such NCS Allocation involvement.

[Allocation Webform](#)

**Submission of Sample Details**

As part of the Grid initiative the NCS will soon be accepting sample submission details via a simple webform. This will be implemented at the start of the 2005-2006 Allocation year.

[Sample Details](#)

**Sample Status Database**

Secure access to the NCS status database. To apply for an NCS security token please see 'NCS Grid Access'.

[Sample Status](#)

Contact Details:  
If you require further assistance or wish to contact the service for any reason contact details can be found on the Service web page: [National Crystallography Service Webpage](#).

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# 1) Application




EPSRC Chemistry Program National Crystallography Service - Allocation Request - Mozilla Firefox

http://152.78.198.214/~pw/allocation\_details.php

Departmental Seminars | EPSRC Chemistry Pr... | EPSRC Chemistry Pr... | Southampton X-Ray ...

 EPSRC CHEMISTRY PROGRAM  
National Crystallography Service  
Application for a 2005-2006 Service Allocation



**Instructions**

Please complete the form in **FULL**. Unless stated **EACH** section is required.

**Your Details**

**Title / Salutation**  **\*Given Name**  **Family Name**

**\*Department**   
**\*Institution**   
**Address 1 (Optional)**   
**Address 2 (Optional)**   
**\*City / Town**   
**\*County**   
**\*Postcode**   
**\*Country**

**Telephone Number**   
**Fax Number**   
**E-mail**

**Project Title**

Done

Start | Pegasus Mail | Command Prompt | WinGX v1.70.0... | 05src0093r | EPSRC Chemistr... | EPSRC Chemis...

EPSRC Chemistry Program National Crystallography Service - Allocation Request - Mozilla Firefox

http://152.78.198.214/~pw/allocation\_details.php

Departmental Seminars | EPSRC Chemistry Pr... | EPSRC Chemistry Pr... | Southampton X-Ray ...

**Allocation Details**

**Allocation Requested Per Annum:** Indicate the number of data collections and/or structure determinations required (enter 0 if appropriate).  
50 Data collection(s)  
0 Full structure determination(s)

**Facilities available locally to the applicant in the area of service requested:**

**Reason(s) why the local facilities are inadequate:**

**Have you previously been awarded a National Crystallography Service Allocation?** Yes  No   
(if yes you will be asked to provide documentary details on the following page)

**Have any publications arisen as a result of previous National Crystallography Service Allocations?** Yes  No   
(if yes you will be asked to provide documentary details on the following page)

**Proceed to Research Details**

**Before proceeding any further please ensure that this page is completed in full.**  
The required fields of this page will be checked before moving on to the next page where you will be requested to provide your case for support and optionally details of any previous NCS Allocations and associated publications.

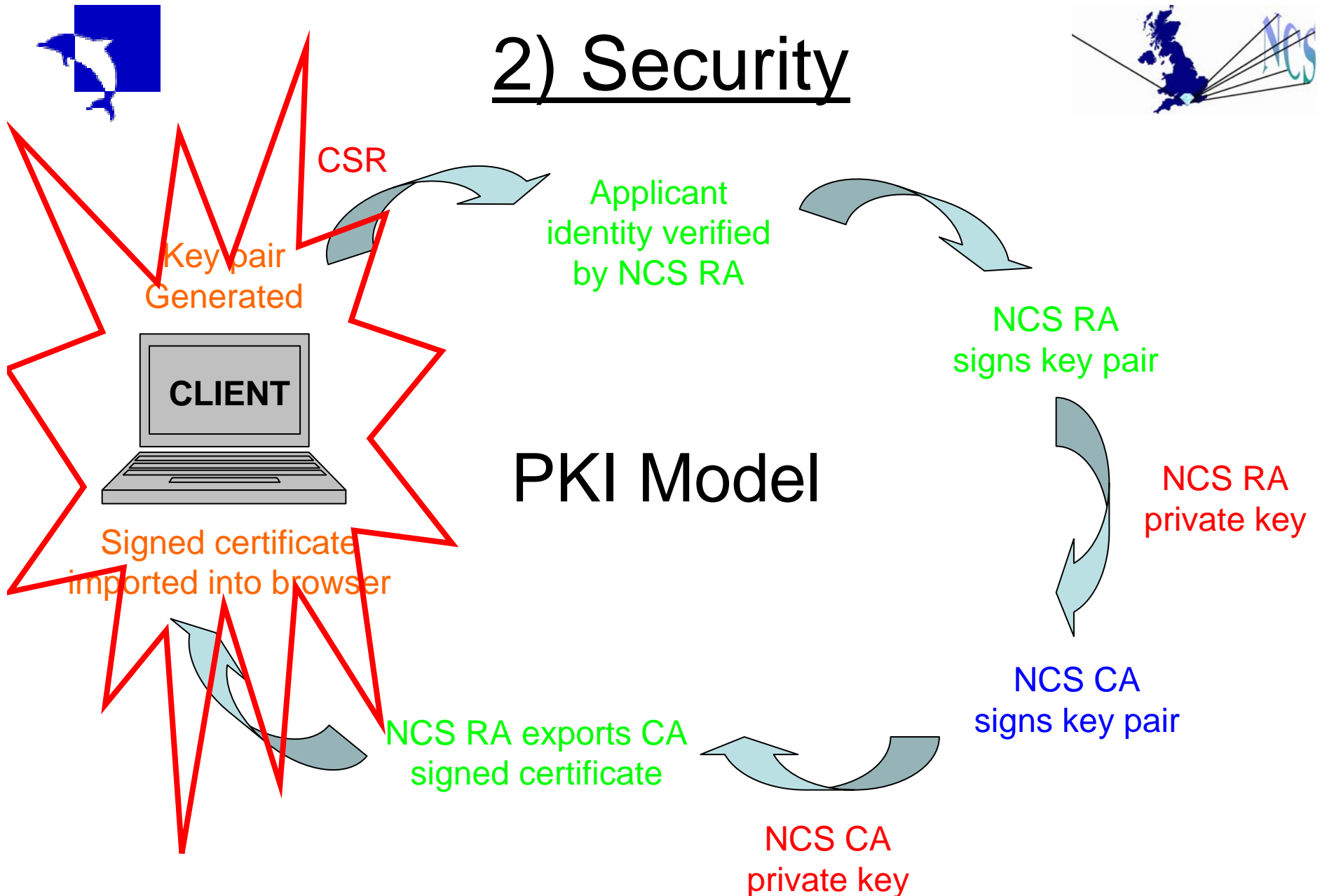
**Contact Details:**  
If you require further assistance or wish to contact the service for any reason contact details can be found on the Service web page: [National Crystallography Service Webpage](#).

Done

Start | Pegasus Mail | Command Pr... | WinGX v1.7... | 05src0093r | EPSRC Chem... | EPSRC Che... | Microsoft Po... | NCS Grid Scr... | 15:49

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## 2) Security





# 2) Security

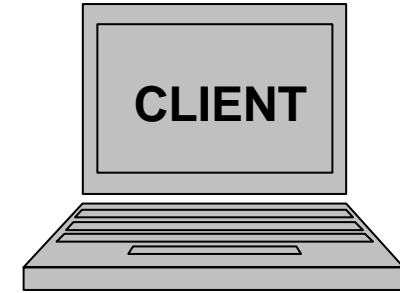


## 'User friendly' NCS registration procedure!

Applicant identity  
independently  
verified by NCS

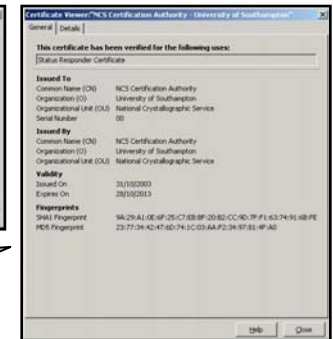
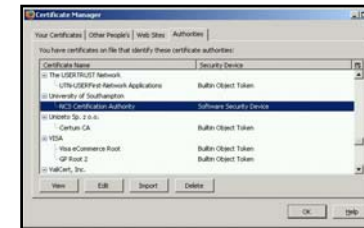
Panel award  
access to NCS

Signed certificate  
imported into browser



NCSA signs  
key pair

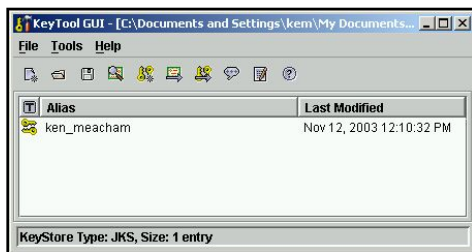
NCSA exports  
signed certificate



Passcode &  
signed PFX

CSR

NCSA  
private key



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# 3) Sample Submission



EPSRC CHEMISTRY PROGRAM  
National Crystallography Service  
Sample Submission Form

Thank you for submitting the details of your sample.

A brief summary of the details you have just submitted is given below. For your convenience this has also been e-mailed to the address you supplied (s.j.coles@soton.ac.uk).

Name: Dr Simon Coles  
Project title: Very cool crystallography  
Your reference: SCRAP  
Service requested: Data collection only

Please ensure that your sample(s) are packaged appropriately and that your reference "SCRAP" is clearly visible. The Service is fully equipped to deal with material which is air sensitive and/or solvent dependant, details can be found on the Service webpage: [Shipping of Sensitive Samples](#)

Please print this page and use the packaging and shipping labels below to simplify and speed-up the process.

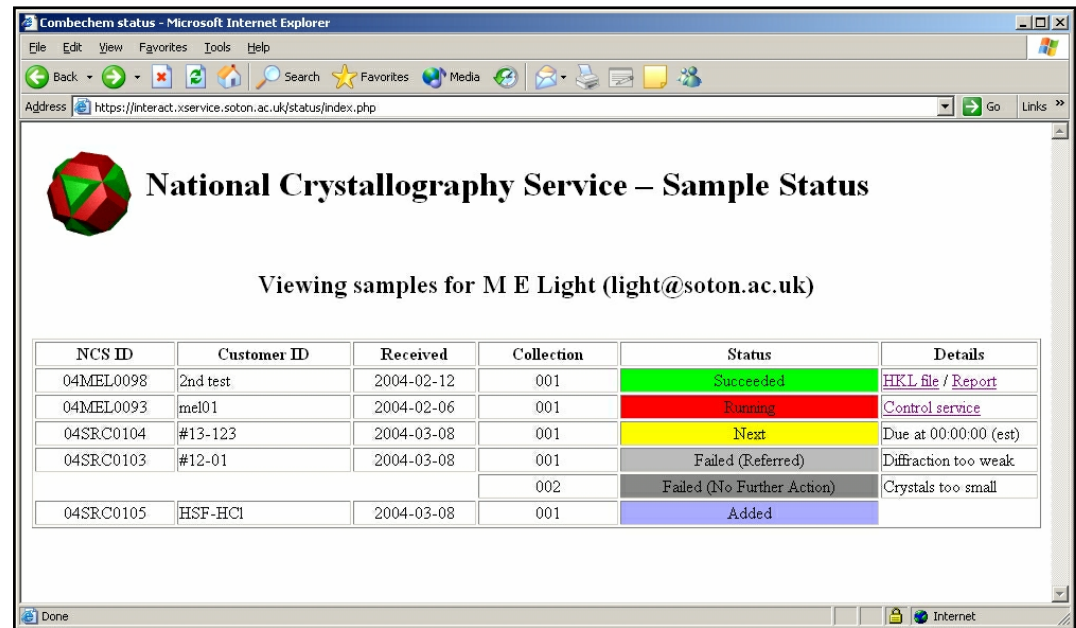
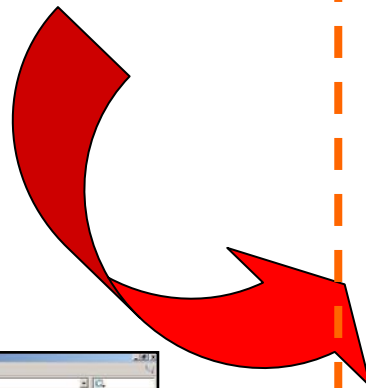
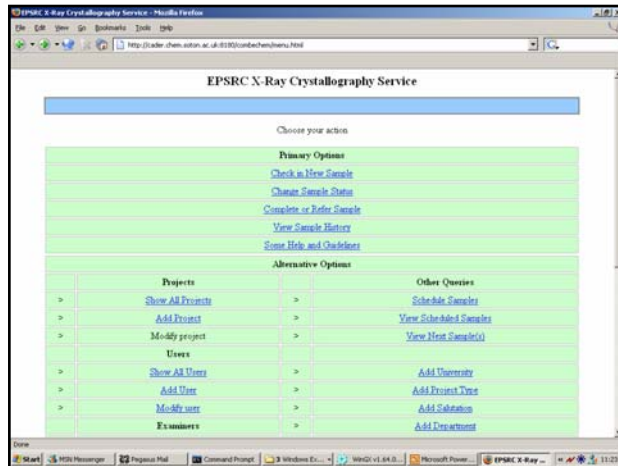
Delivery address:

Mrs Ann Bingham  
EPSRC National Crystallography Service  
School of Chemistry  
University of Southampton  
Highfield  
Southampton  
SO17 1BJ

Sample details:



# 4) Status monitoring



NCS

CLIENT

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## 5) Data Collection



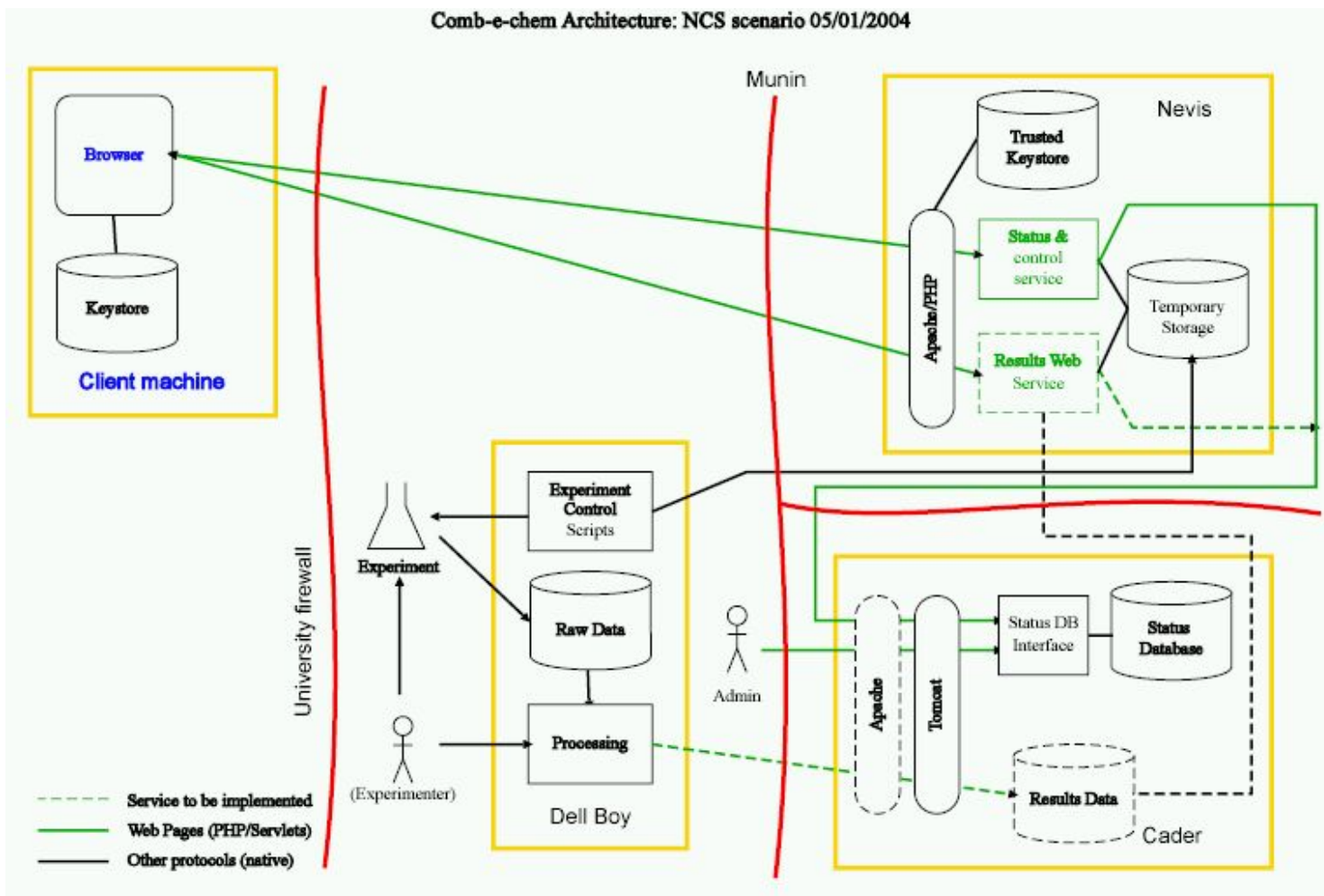
- Decision making
  - Does the crystal diffract?
  - Best parameters for unit cell determination?
  - Can a unit cell be indexed and is it sensible?
  - What are the best parameters for the data collection?
- Bruker-Nonius 'COLLECT' libraries linked in Python using tkinter
- Invoke 'DENZO' & 'SCALEPACK' externally through command line defaults



# 5) Data Collection



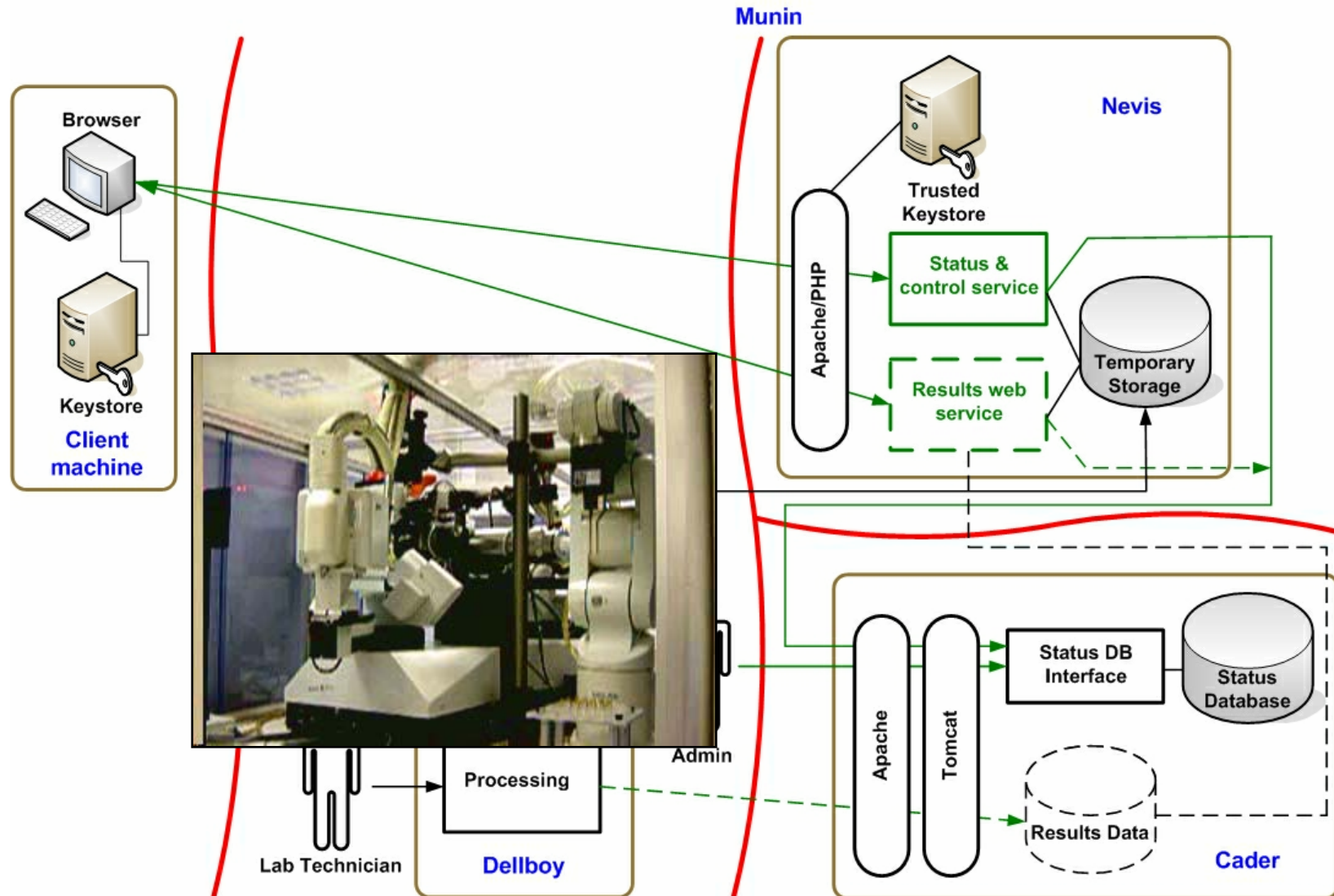
## Automated experiment steering service: Architecture



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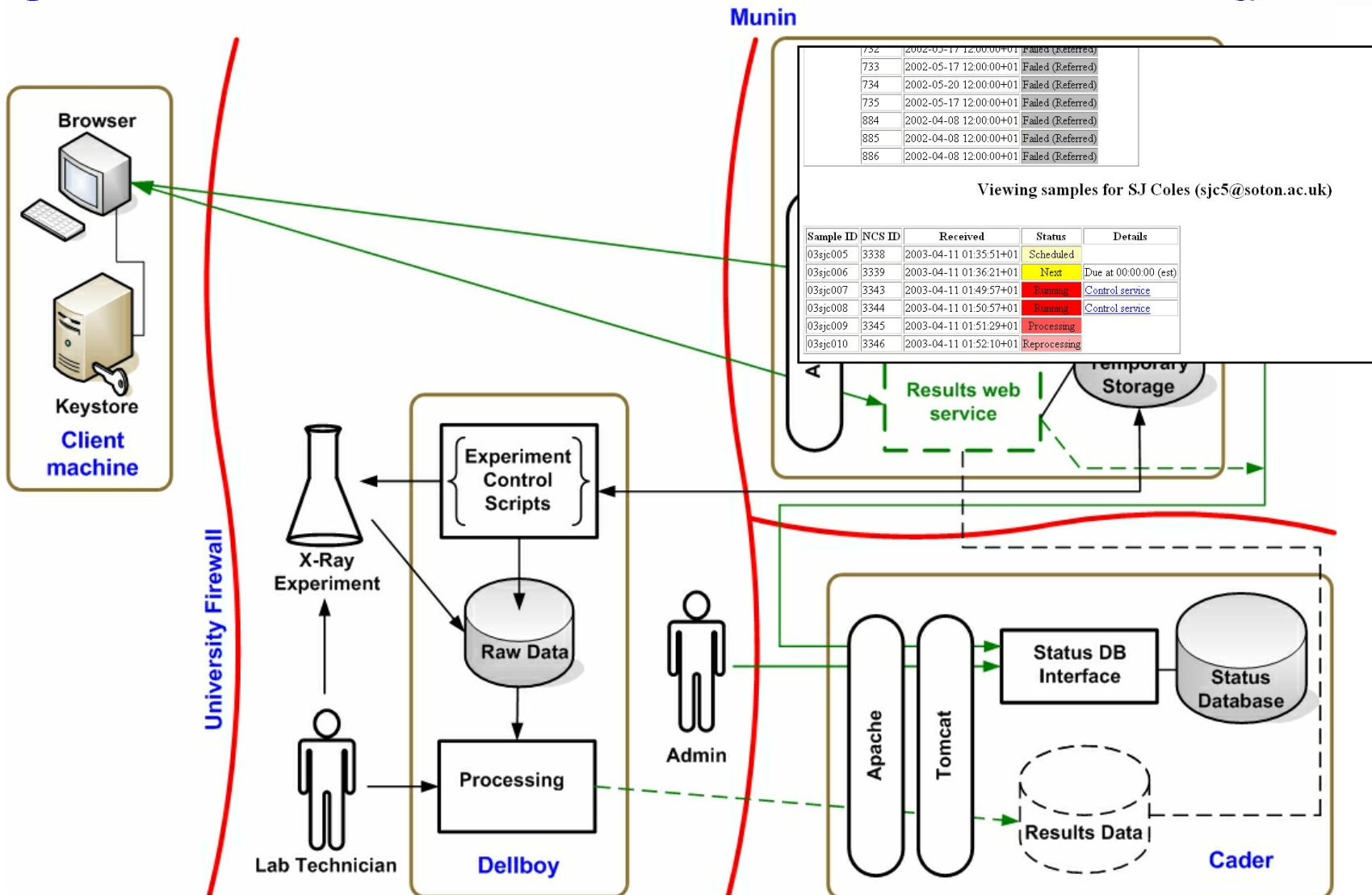


# 5) Data Collection



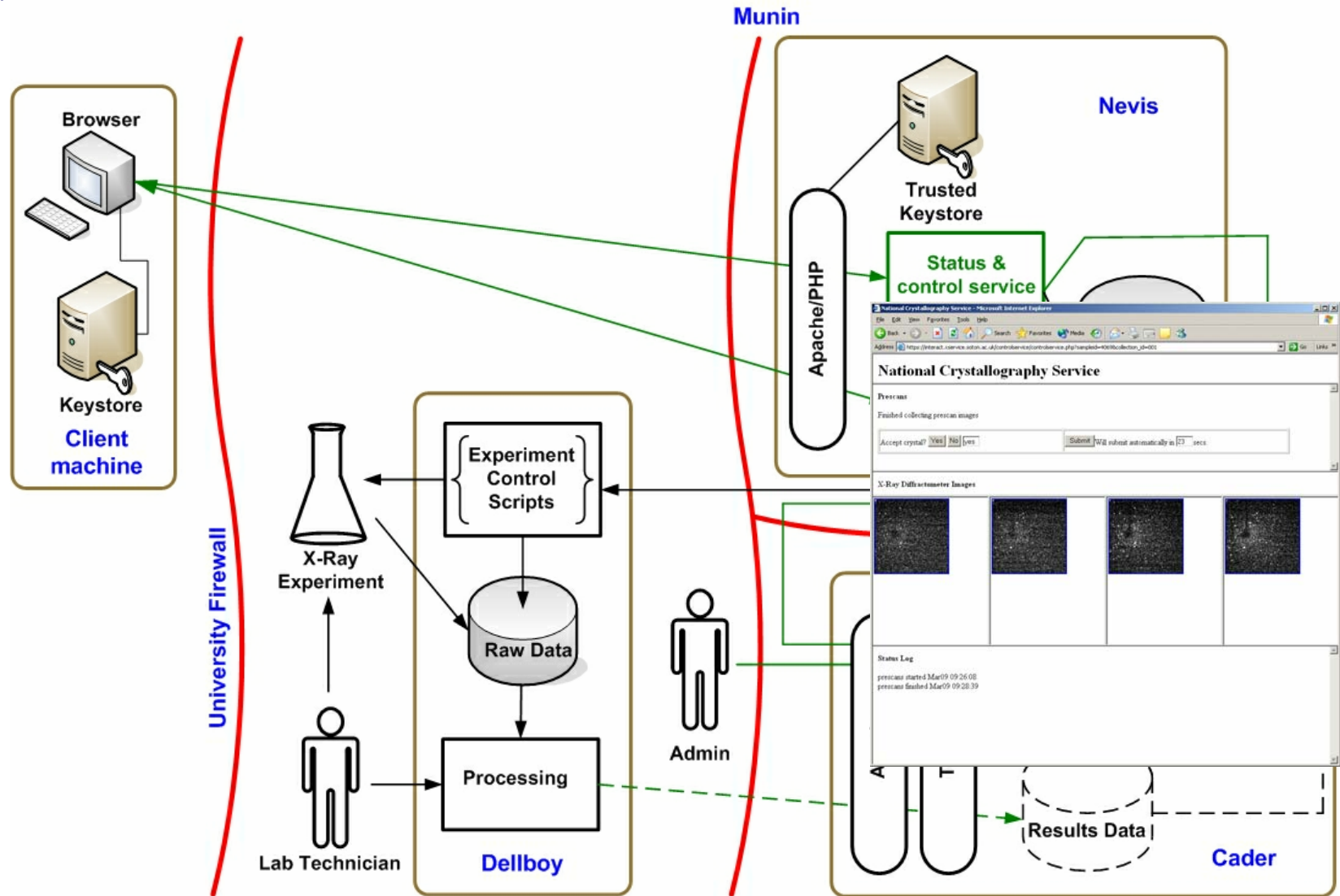


# 5) Data Collection Monitoring





# 5) Data Collection Monitoring



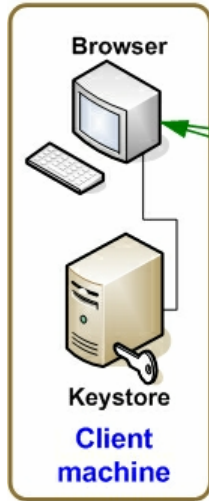
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# 6) Data Download



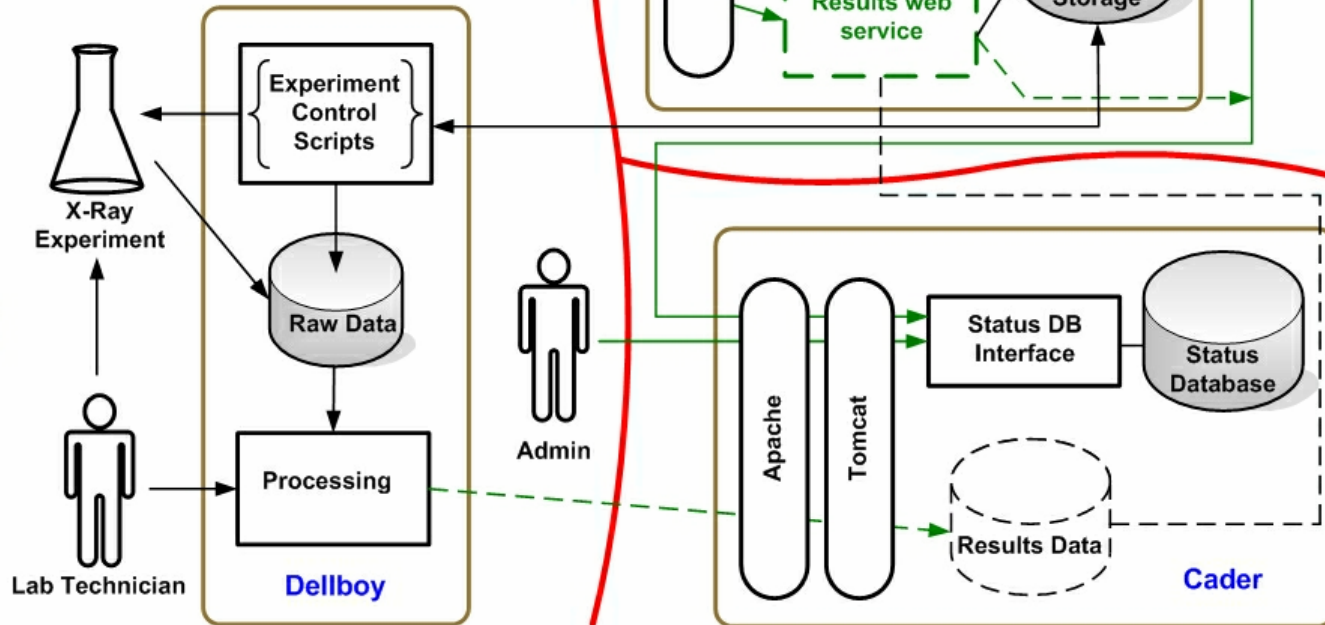
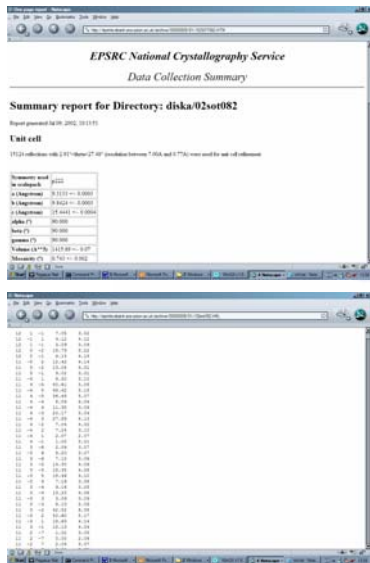
Munin



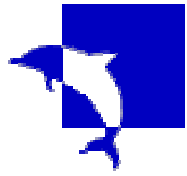
National Crystallography Service – Sample Status

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	Successful	<a href="#">HTML file</a> / <a href="#">Report</a>
04MEL0093	mel01	2004-02-06	001	Next	Due at 00:00:00 (est)
04SRC0104	#13-123	2004-03-08	001	Scheduled	
04SRC0103	#12-01	2004-03-08	001	Failed (Referred)	Diffraction too weak
			002	Failed (No Further Action)	Crystals too small
04SRC0105	HESF-HCI	2004-03-08	001	Added	



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## 7) Raw Data Archiving



### Automated Scripting of Archiving Process

- End of processing – “archive” script
- Data staged to lab server – sits for 1 month
- Data uploaded to ATLAS Data Store
- Assigned unique NCS identifier
- Script available for automated de-archiving if reprocessing needed.