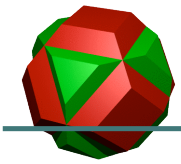

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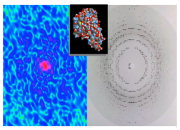
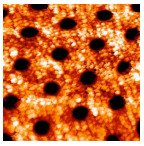
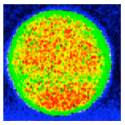
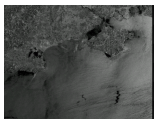
Experiments on the Grid









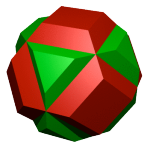
The UK National Crystallography Grid Service

Jeremy Frey

CombeChem Project

School of Chemistry

University of Southampton, UK



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Plan

- UK e-Science & The Comb-e-Chem Project
- Security!
- The National Crystallography Grid Service
  - Architecture
  - Demo
  - Data Grid
- The future

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UK e-Science programme

Support for collaborative research

Grid Infra-structure

Computational Grid
- compute on demand

Data Grid
-flow of data

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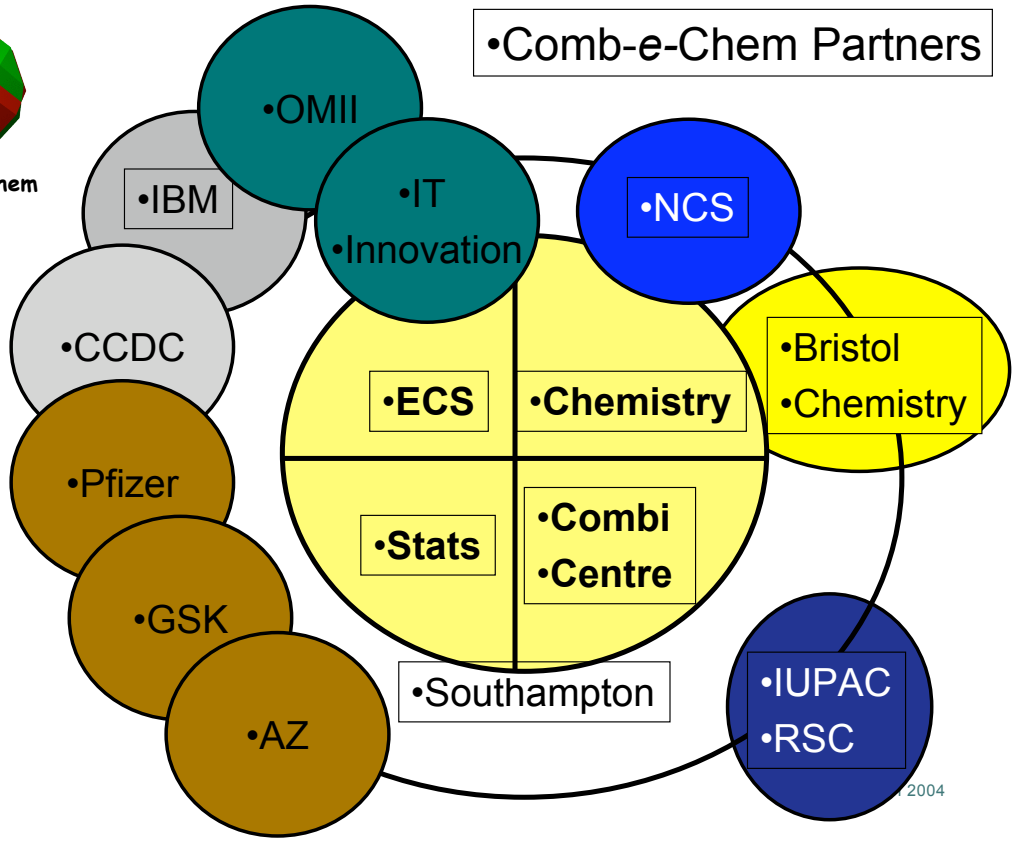

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People

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- **Chemistry (Southampton & Bristol**)
  - Mike Hursthouse, Chris Frampton, Jon Essex, Jeremy Frey, Guy Orpen, Stephan Christensen, Thomas Gelbrich, Sam Peppe, Hongchen Fu, Graham Tizard, Suzanna Ward, Lefteris Danos, Jamie Robinson, Kieron Talyor, Chris Woods, Rob Gledhill
- **National Crystallography Service (NCS)**
  - Simon Coles, Mark Light, Ann Bingham, Peter Horton
- **Electronics and Computer Science (Southampton)**
  - Dave De Roure, Luck Moreau, Mike Luck, Hugo Mills, Graham Smith, Simon Miles, Nicky Harding, Gareth Hughes, Nick Humphries, monica schraefel, Terry Payne
- **It-Innovation (Southampton)**
  - Mike Surridge, Ken Meacham, Steve Taylor, Daren Marvin
- **Statistics (Southampton)**
  - Alan Welsh, Sue Lewis, Ralph Manson, Dave Woods
- **Rutherford Appleton Laboratory**, Atlas Data Centre
- **IBM** – Colin Bird, Syd Chapman

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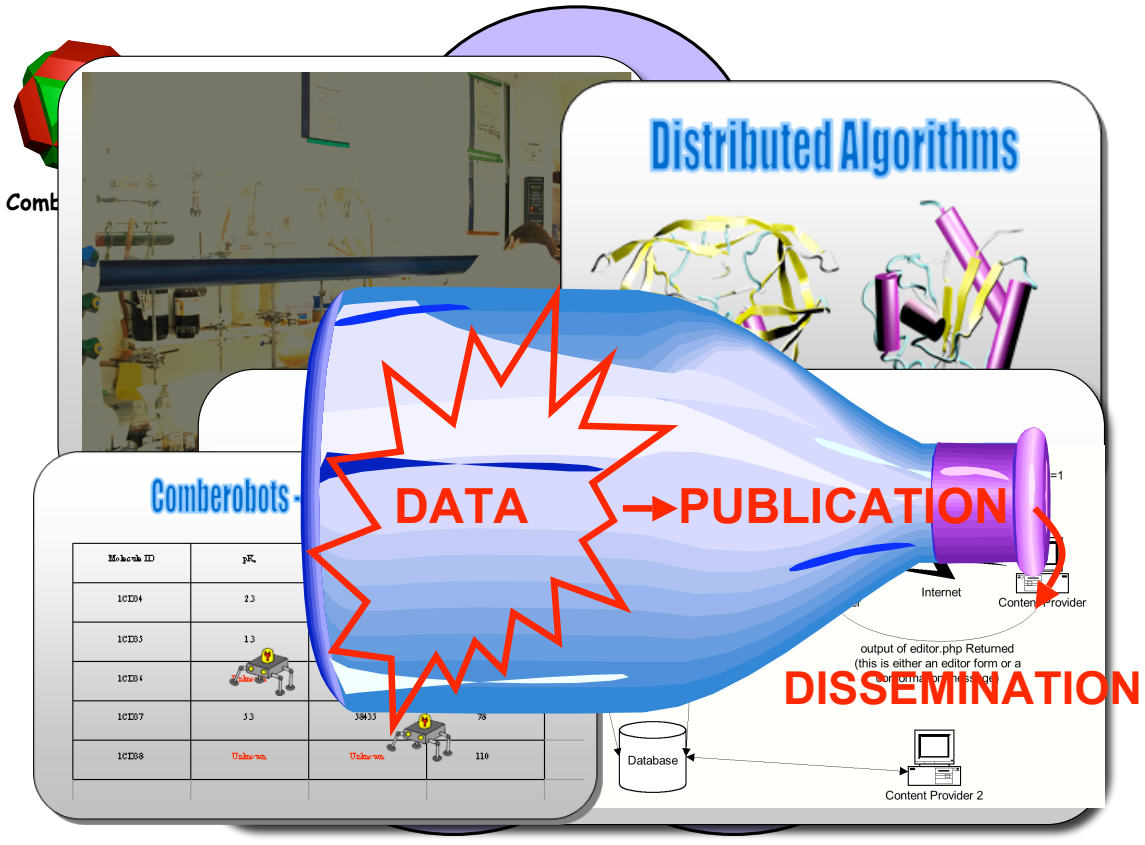

Plans

Small set of fixed plans

NCS

Variable plans, written by chemist (difficult!)

Synthetic Chemistry

Ad-hoc, implied by process execution

Phys Chem data analysis

Continuum of plan types

Experiments on the Grid

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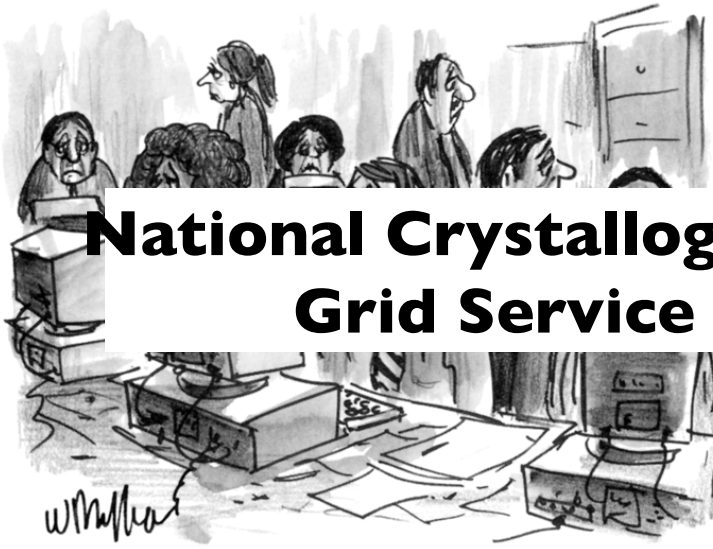

National Crystallography Grid Service

Are we simply building a rod to beat selves n?

Is the user out there?

No, the computers are up, We're down

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Grid Service – Why?

- 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 busy 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

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Security and trust for experiments and data

"On the Internet, nobody knows you're a dog."

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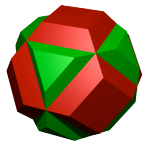
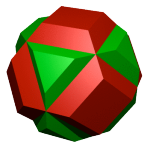


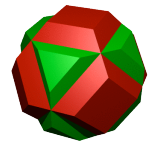
Security

- Security is crucial to the successful operation of the NCS Grid Service,
  - authentication of users
  - maintaining the integrity of their data.
- For NCS, we have set up a well-defined trust network, with its own CA and RA.
- All data transfer is encrypted,
  - A user is authorised to access only their own data, or monitor their own experiments.
  - the user's credentials are mapped to the appropriate authorisation or datasets.

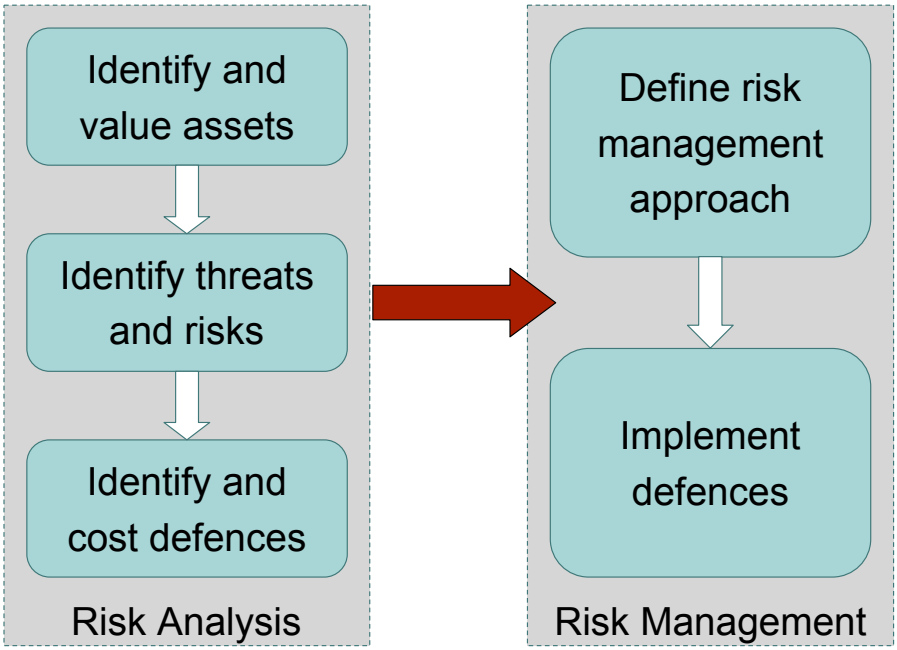


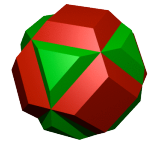
Security Overview

- Security risk management
- Security technology development
  - process-based authorisation extensions
  - WS-Security message processing
- Security implementation
  - operating policies and public key infrastructure



Asset-Based Security





Application to NCS Service

- Assets:
  - campus system and network integrity (M/H)
  - sample tracking data (M)
  - experimental result data (L/M)
  - grid service integrity (L/M)
- Risks:
  - system attacks from outside campus (H)
  - systems attacks from inside campus (H)
  - compromise of remote user credentials (H)
  - internal user error (M)

Public Key Infrastructure

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- Requirements:
  - be able to authenticate “singleton” remote users
  - be easy to operate by Chemists
  - be secure enough for academic users & Industry?
- Analysis of existing NCS authentication:
  - uses personal knowledge of user community
  - uses contextual information (e.g. EPSRC project codes)
  - lightweight for both NCS and their customers
- Public key infrastructure developments:
  - Comb-e-Chem certification policy agreed
  - procedures developed for NCS to certify remote users
  - operational responsibility transferred to Chemistry

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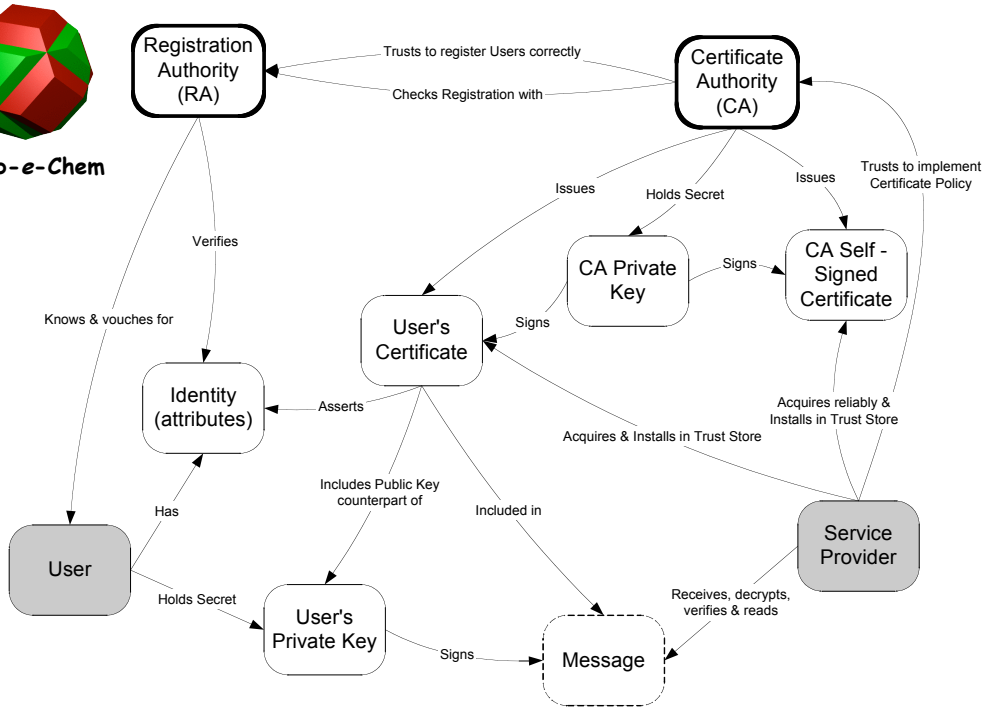

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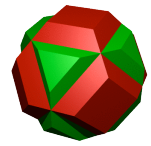
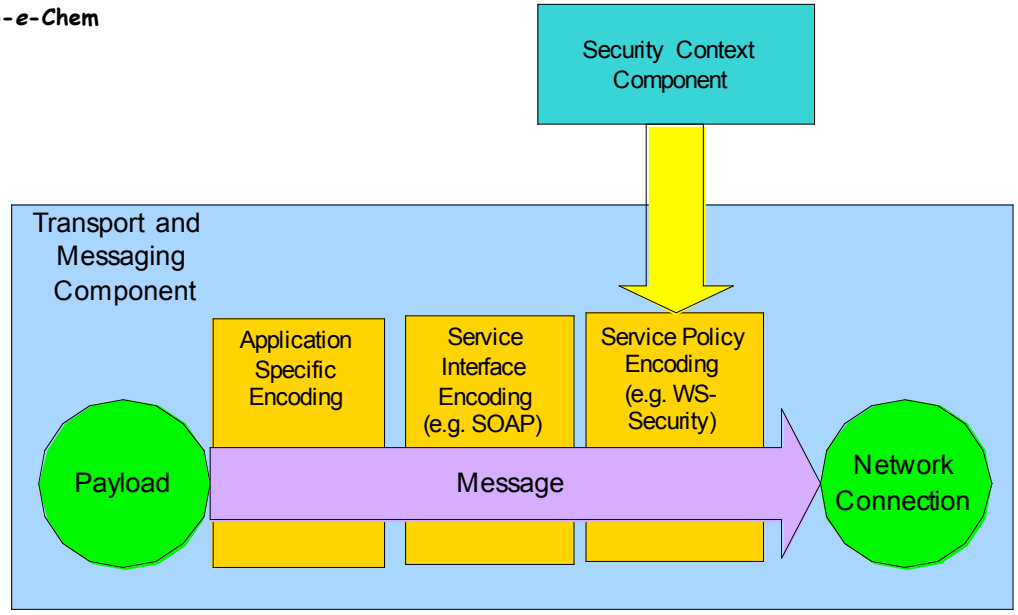
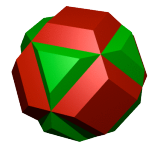
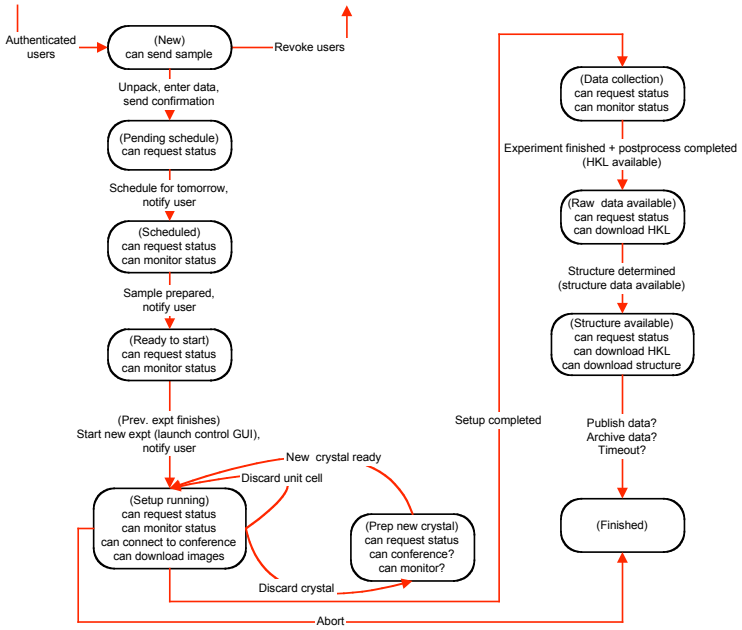


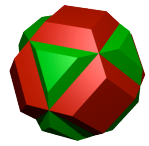
WS-Security Processor





Process-Based Authorisation





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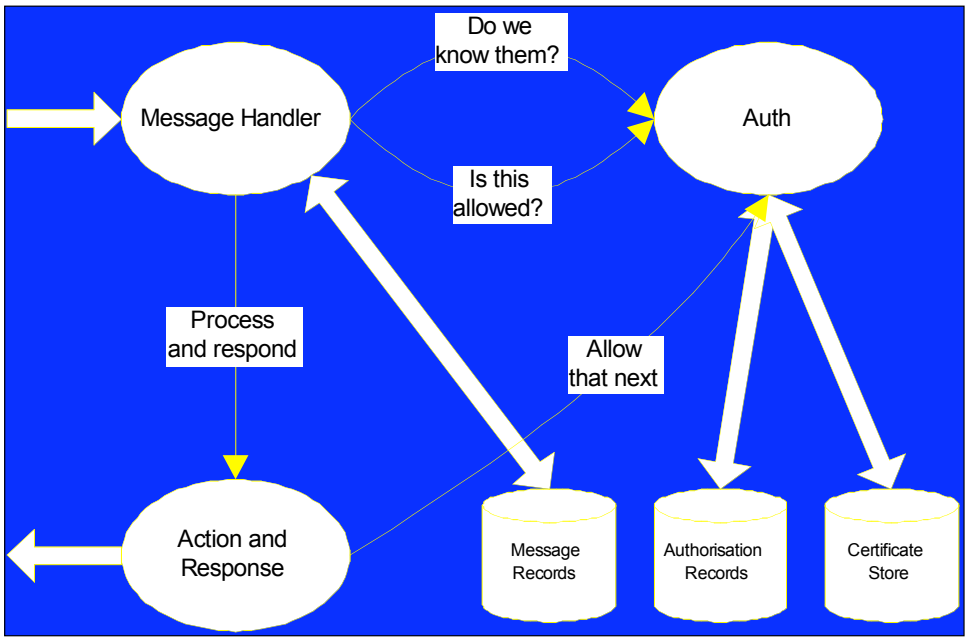
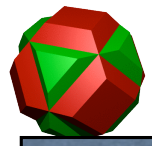
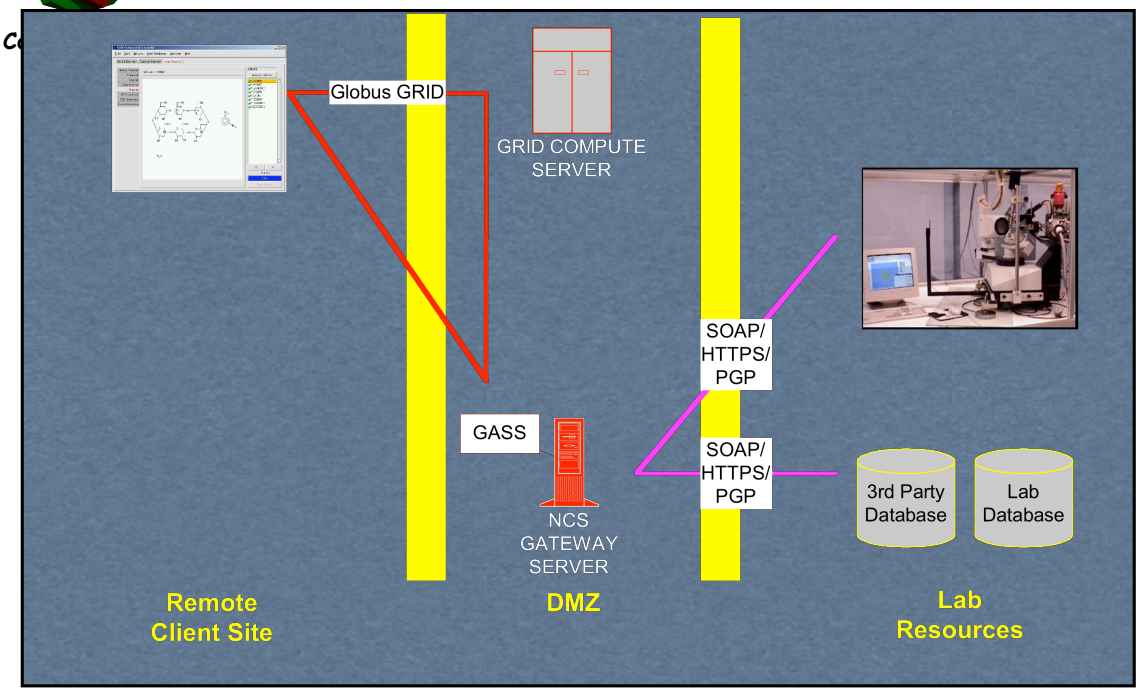
Implementation

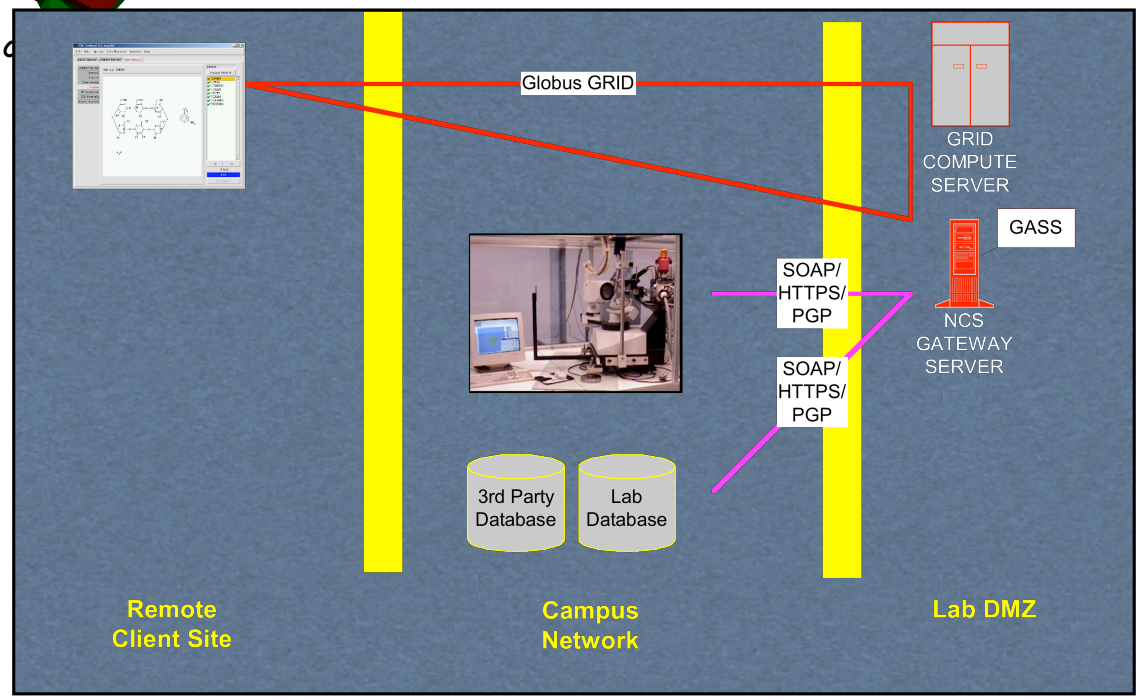




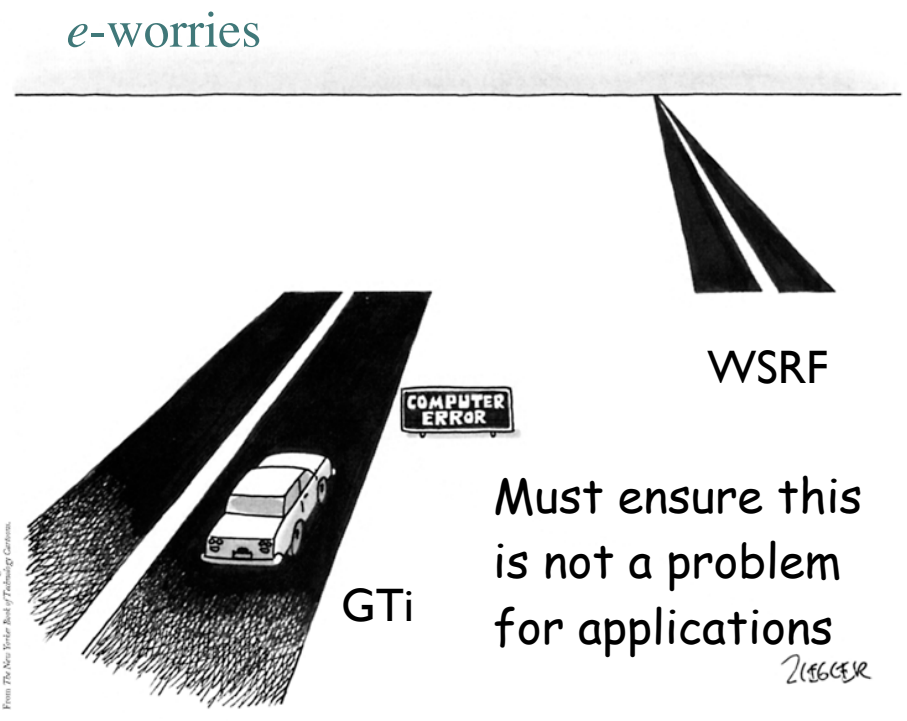
ECSES Architecture



Firewall Management Issues

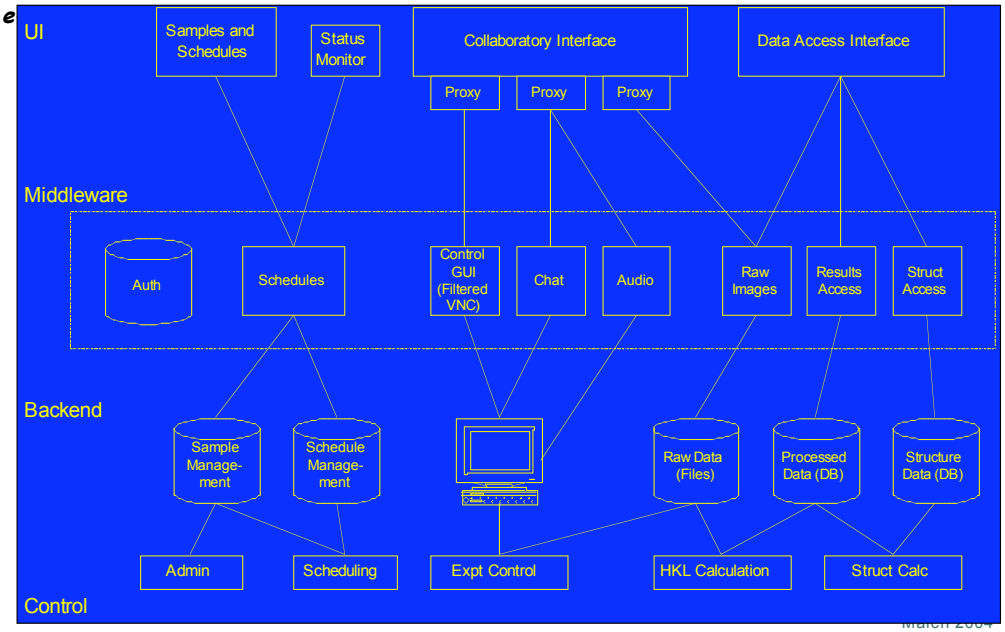


Comb-e-Che



NCS Lab Service

Comb-e



NCS Grid Service Architecture

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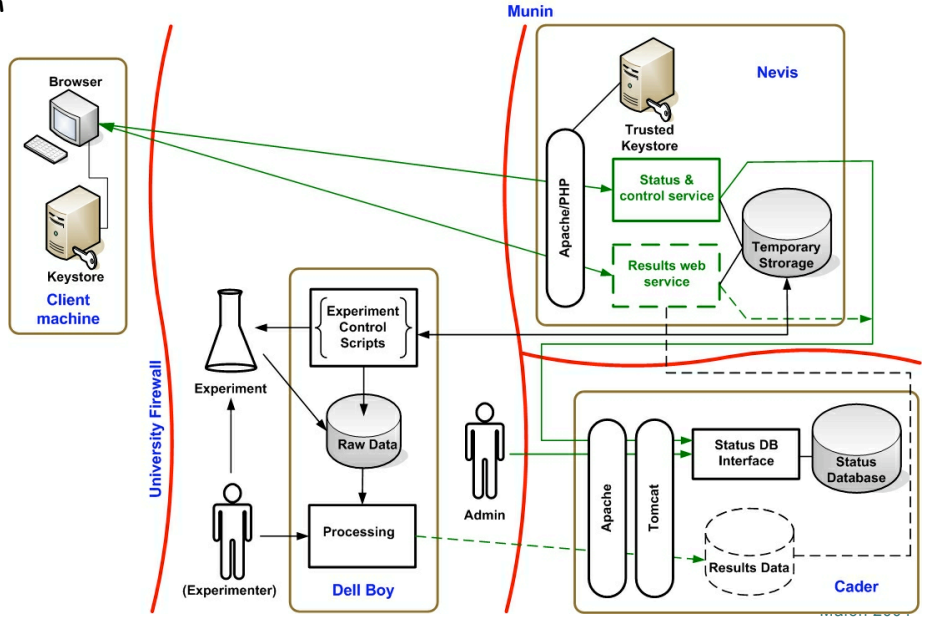

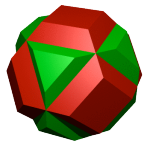

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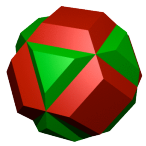
NCS - How it works

- The Status Service determines the client's Distinguished Name (DN) from their NCS certificate
  - queries the Sample Database
  - list of all samples submitted by the client
  - they may only see their own samples.
- client's browser, shows the status of each sample.
  - 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.



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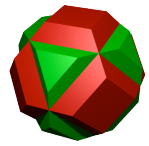
Experiment Control Services

- The Control Service provides the client with a portal to their running X-ray diffraction experiment
  - opportunity to observe the experiment in progress, and to steer it if they wish.
- The display is continuously updated,
  - reflects the current state of the experiment
  - 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.



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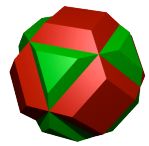
Experimental Steering

- 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!).



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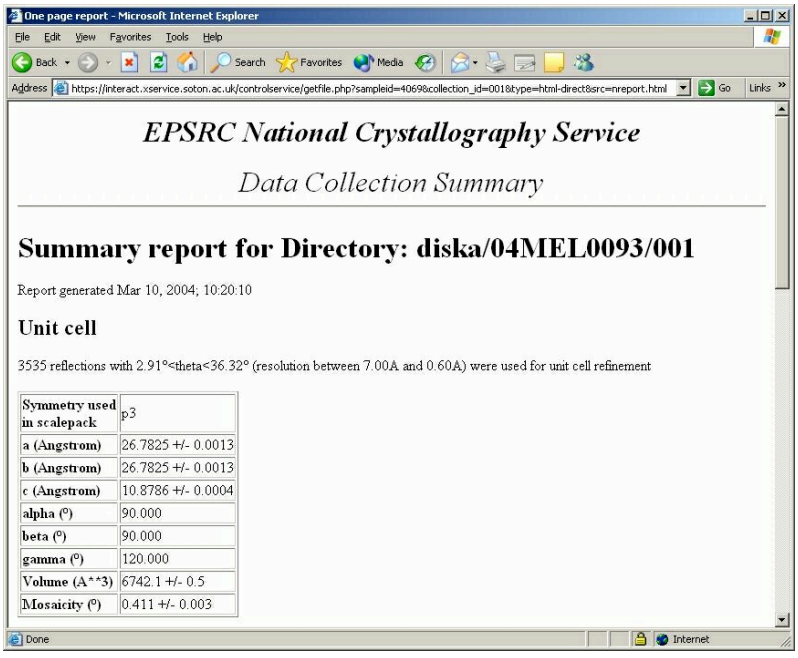
Once the experiment has completed, a summary of the results is automatically published and linked to the Sample Status page.



NCS Grid Service

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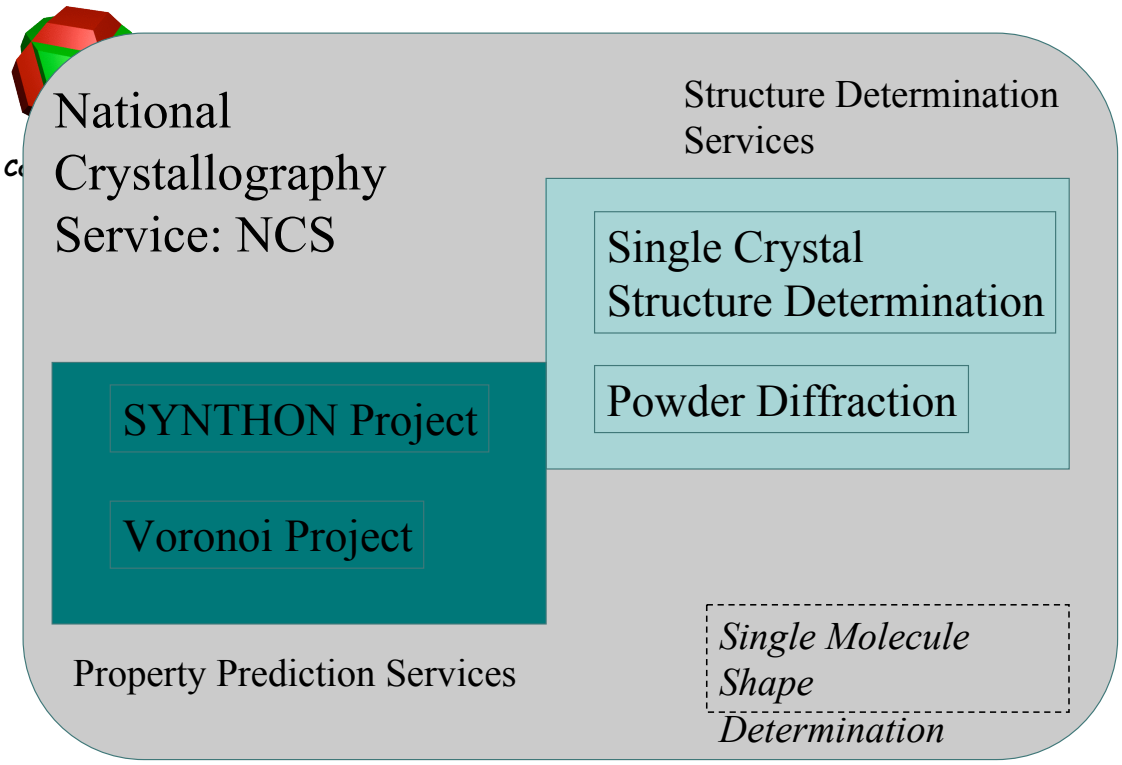

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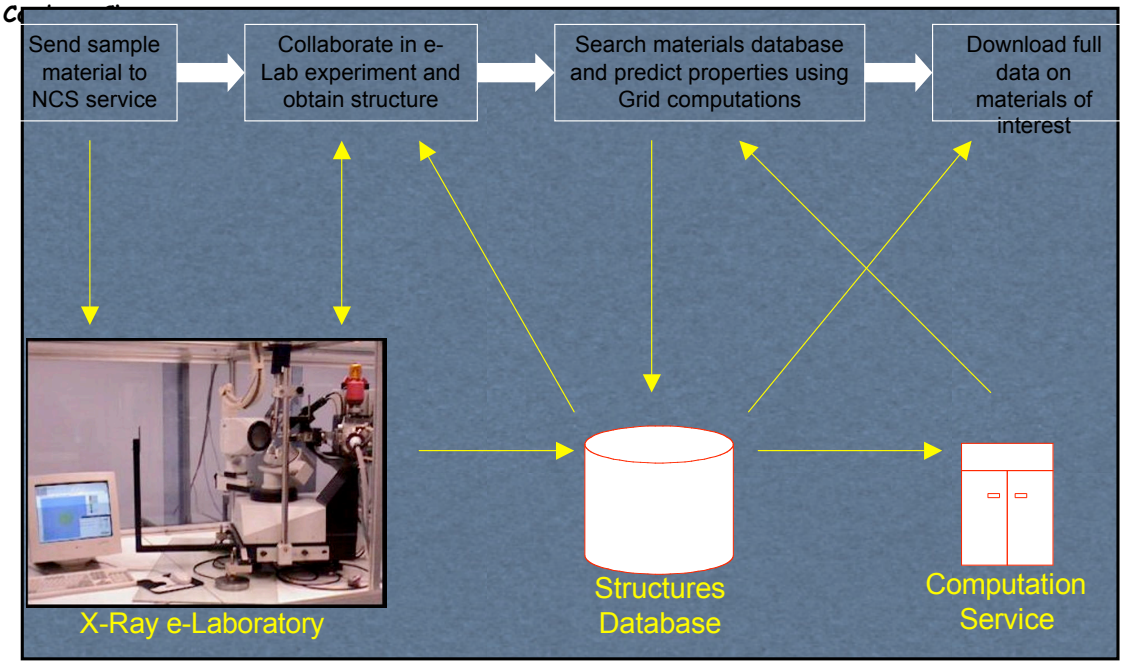
NCS WORKFLOW



Data Grid

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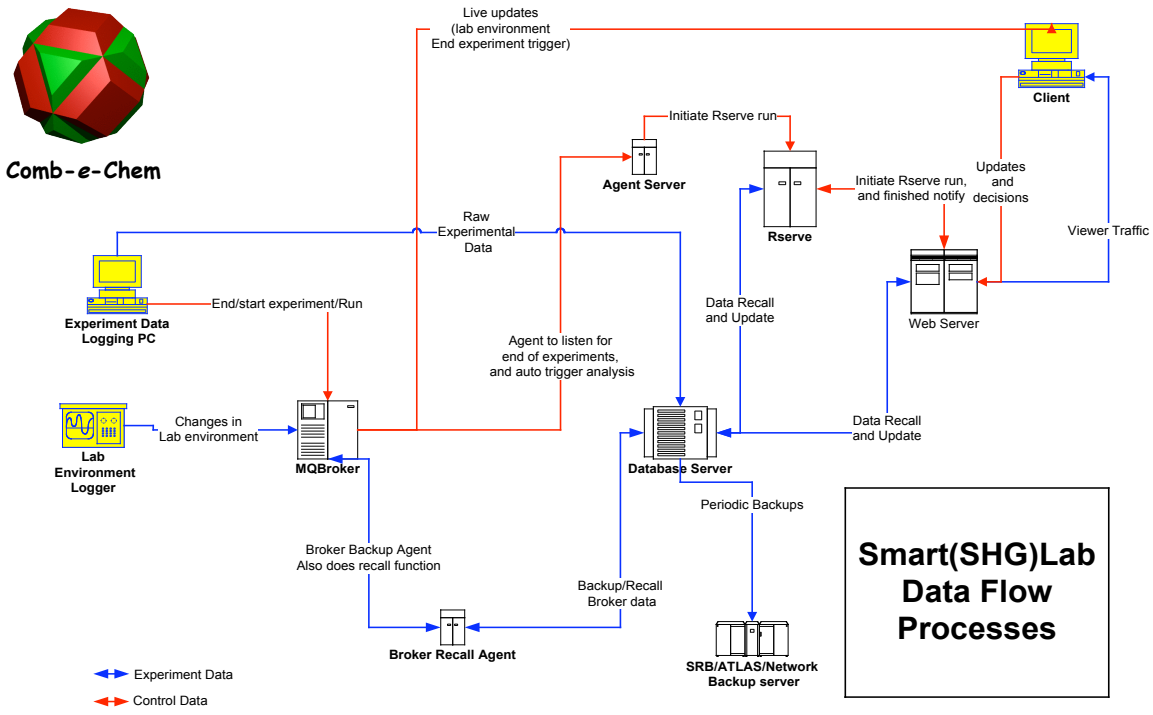
- Issues of interaction with existing databases
- Graphical front ends currently make for complex query architecture over a grid
- This is being addressed and will employ a workflow system with full provenance



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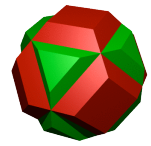
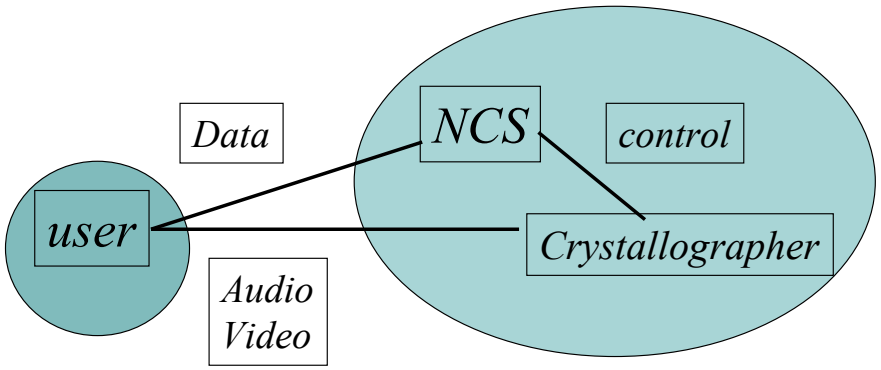
Increased Remote Control?

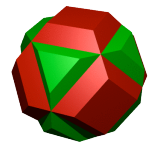
- Remote control of equipment
  - Interaction with people & equipment
- Safety Critical Systems
  - External & Internal control of systems can lead to safety conflicts
  - Safety critical software (avoid at this stage)



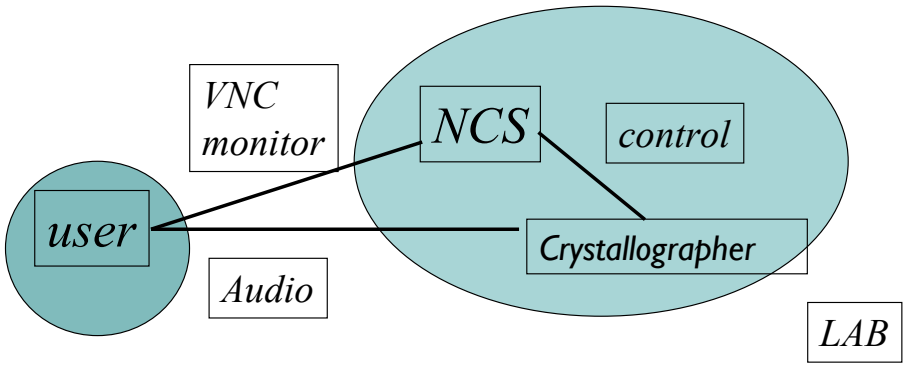
User – Crystallographer Interactions



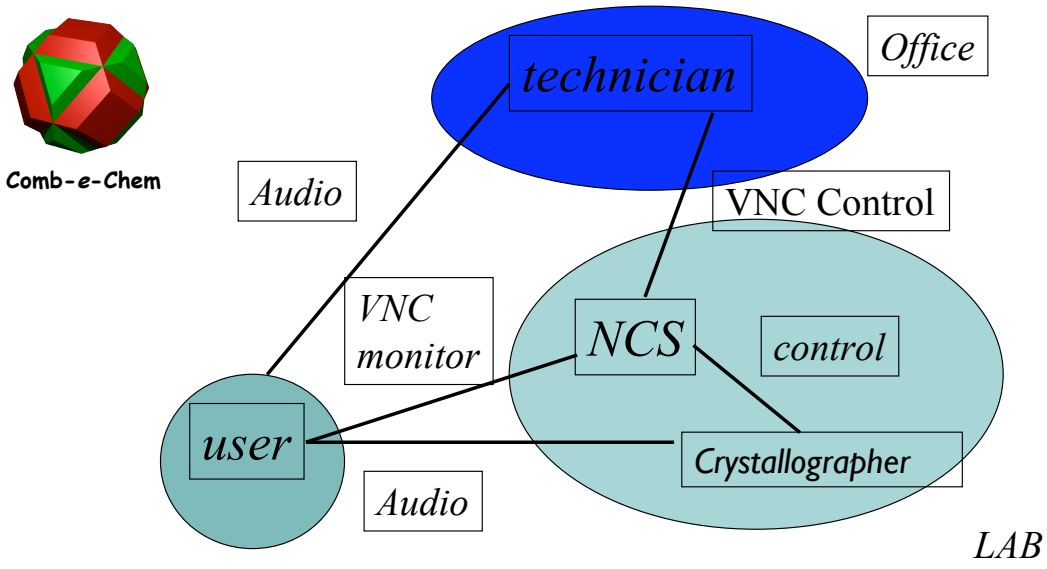
Video – *fun but useful with limited bandwidth*



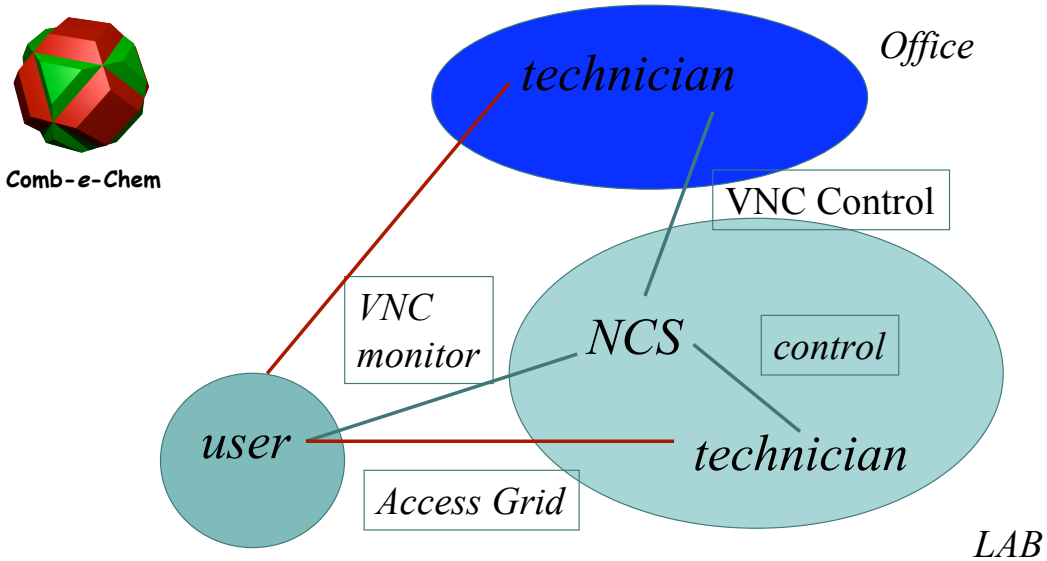
User – Crystallographer Interactions



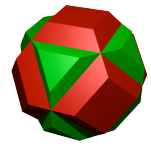
VNC *ideal for connecting existing programs – developing Web Service/SOAP VNC but how much control?*



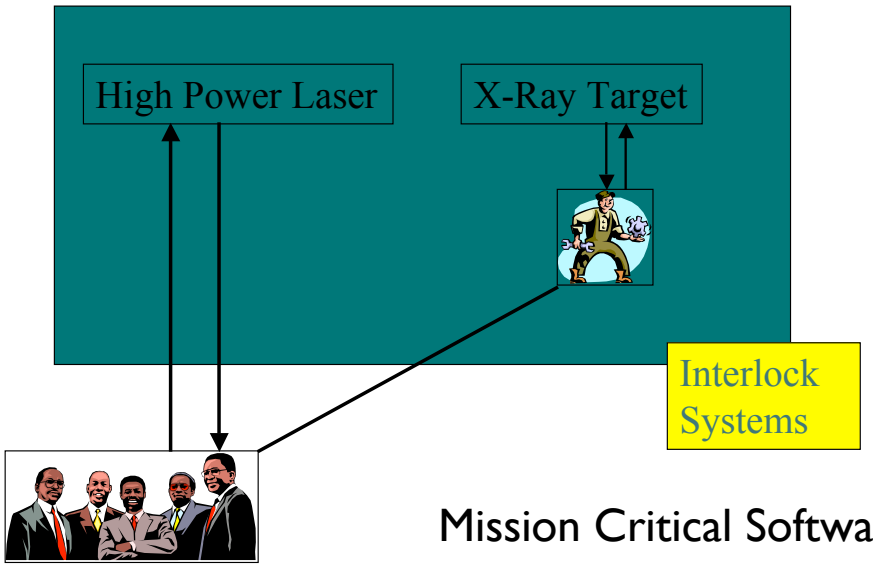
Very useful inside the service – but not suitable for deployment over the grid



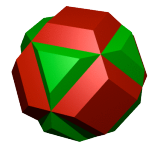
In the future will employ Access Grid techniques



Safety!



Mission Critical Software



Future

- Smart Lab front end
  - Transfer URI as well as sample giving access to the materials preparation
  - Capture of crystal selection process with user interaction.
  - More automated data analysis
  - Automatic publication (*xtl*-prints)

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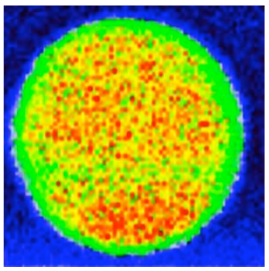
HT-Raman

- Instrument & Data Service
- Long scans – need for remote user control



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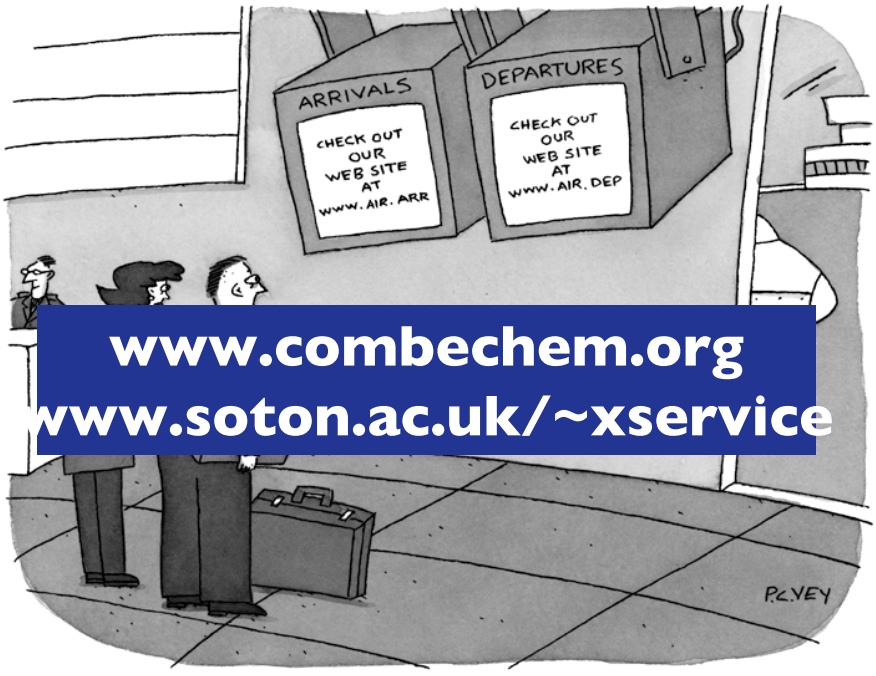
Web sites?



www.combechem.org
www.soton.ac.uk/~xservice

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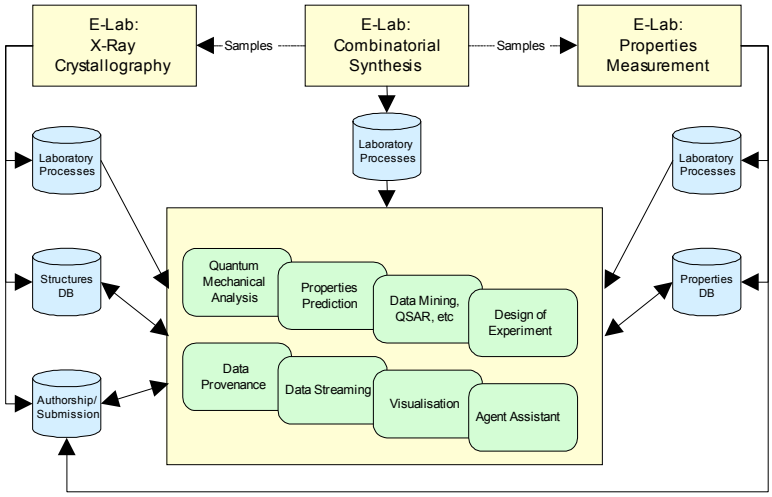
Changing the way we work



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