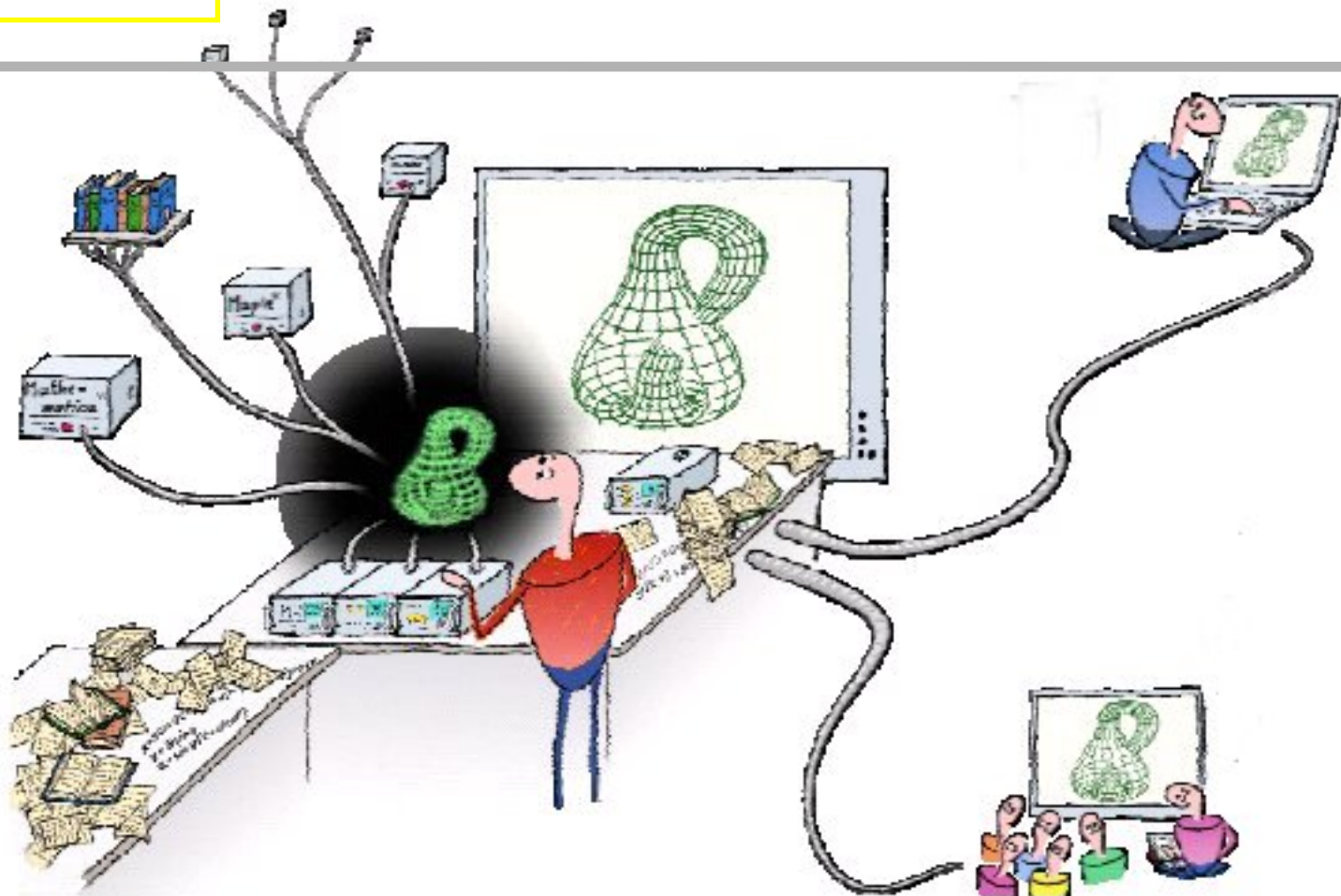




Australian Research Council
**MOLECULAR + MATERIALS
STRUCTURE NETWORK**

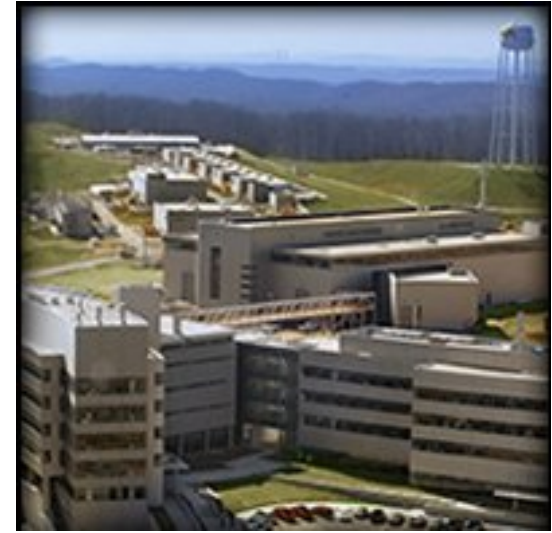
APAC07; DeRCAP. October 11 2007.



**DeRCAP: A Molecular and Materials Structure
Determination Perspective**



Advanced Photon Source (APS)



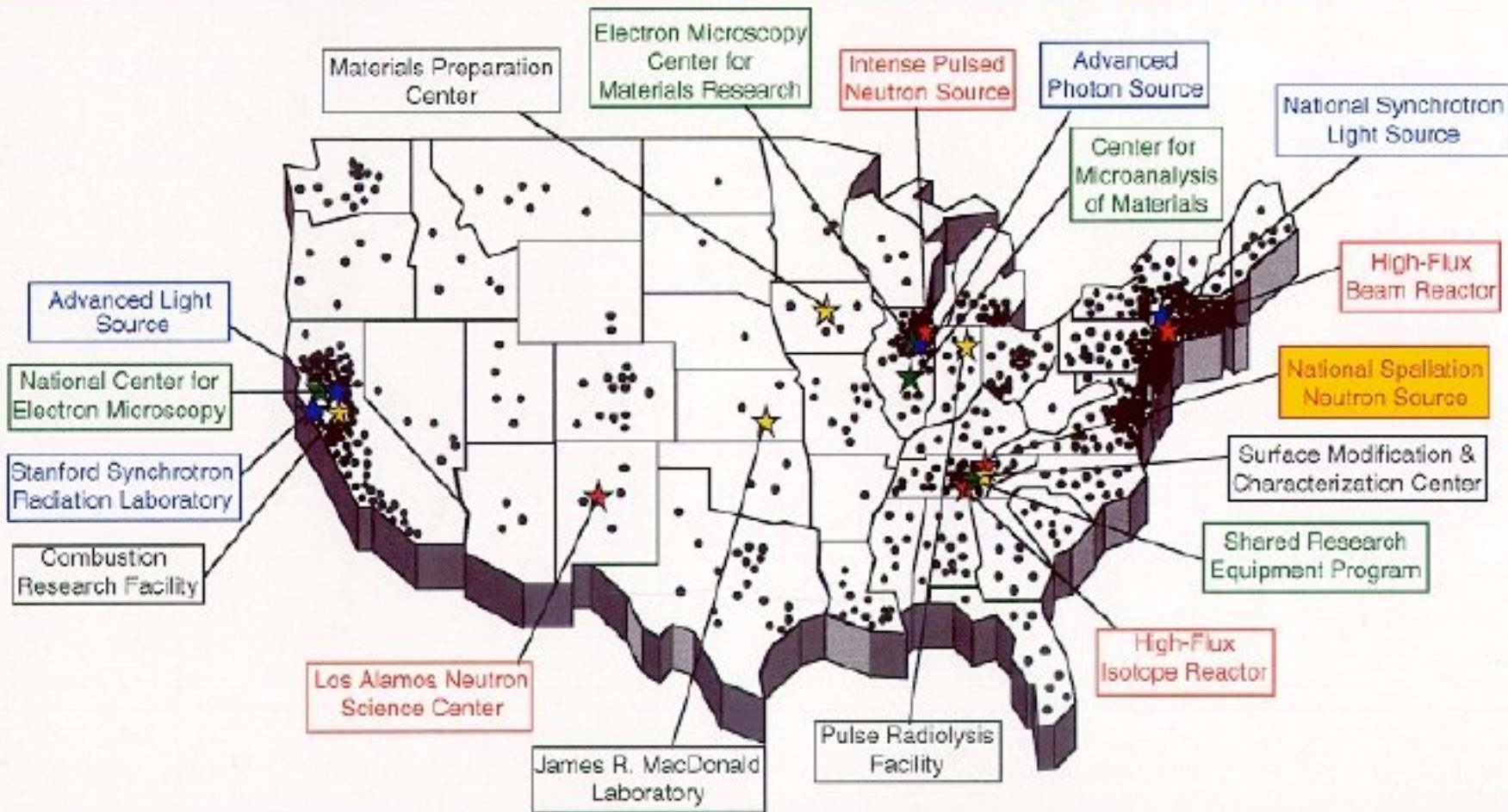
Spallation Neutron Source (SNS)



Stanford Synchrotron Radiation Laboratory (SSRL)



Advanced Light Source



- 4 Synchrotron Radiation Light Sources
- 5 High-Flux Neutron Sources
- 4 Electron Beam Microcharacterization Centers



Australian Synchrotron



OPAL

Shipping Data ...

- Tomography: typical high res image: 4000x2600 pix x 16bit depth = 22Mb.

Typical CT set 1500-2000 images with 6-12 micron pixels at 1x1 binning, so about 40Gb per set. Collected 10 to 20 min.

- Macromolecular Crystallography: 2000 8 Mb images or about 16 Gb collected in 3 min

“The issue as ever with the large data sets is quite simply the need move large volumes of data around ...At present, we literally travel with suitcases full of hard drives.”

The Collaboration Bandwidth 'Spectrum' ...

- **Traditional (Zero Network Bandwidth)**
 - Starts with a Site Visit
 - Telephone
 - Fax
 - Snail Mail
- **Low Bandwidth**
 - Email
 - FTP
 - Telnet
 - WWW (static)
- **Medium Bandwidth Internet**
 - Streaming audio/video
 - Screen/CPU sharing
 - Asynchronous video conferencing
- **High Bandwidth**
 - Synchronous video conferencing
 - Interactive Data Manipulation
 - Interactive Visualization
 - Interactive Instrumentation
 - Large Data Set Transfers



**SSRL-MMSN Remote Access Workshop
February 9 2006
Melbourne University Learning Laboratory**

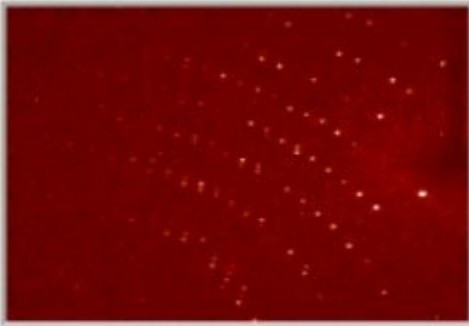
GridSphere Portal - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://iona.chem.usyd.edu.au:8095/gridphere/gridphere?col=96&gs_action=

Disable* Cookies* CSS* Forms* Images* Information* Miscellaneous* Outline* Resize* Tools* View Source* Options*

Frame Viewer




File:
frame0002.jpg

TimeStamp:
2007-04-5 11:08:00 UTC


Start

Live WebCam



Live WebCam

Live Crystal Camera



Live Crystal Camera

BIS Control

| | | |
|----------------|---------------------------------------|------------------|
| 2Theta: | <input type="text" value="30.000"/> | (-180 ... +180°) |
| Omega: | <input type="text" value="-292.000"/> | (-180 ... +180°) |
| Kappa: | <input type="text" value="0.000"/> | (-100 ... +100°) |
| Phi: | <input type="text" value="10.000"/> | (-360 ... 360°) |
| Distance (Cm): | <input type="text" value="5.000"/> | (3.2 ... 17.0cm) |

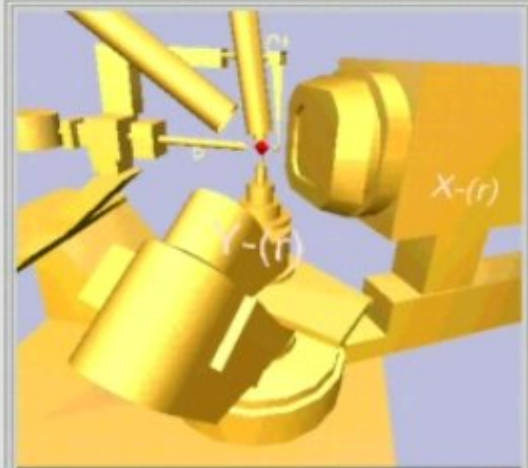
Scan Axis
 Phi Omega

Scan Range:

Image Width:

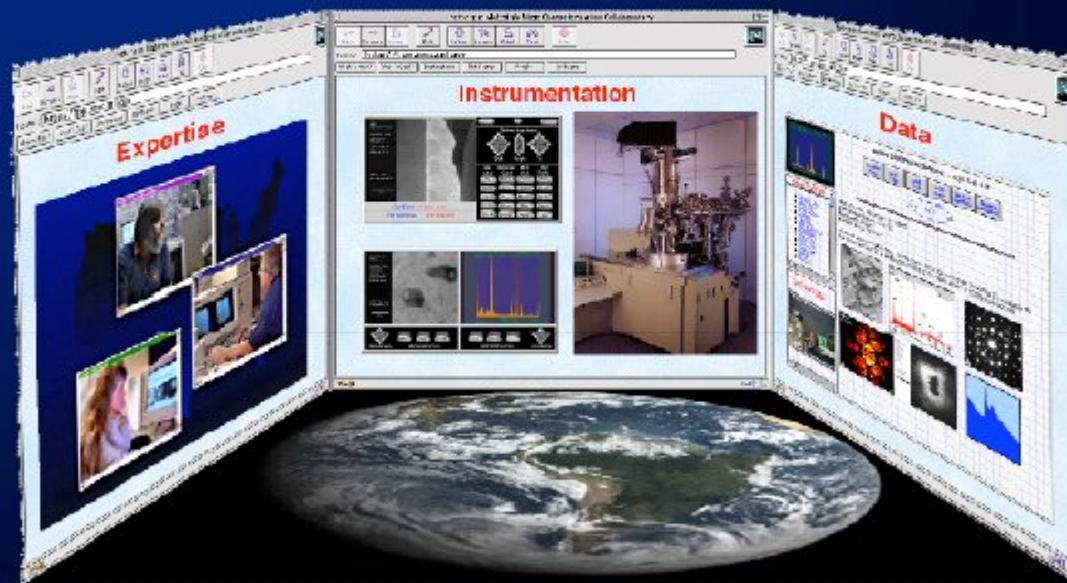
Exposure Time:

Scan Options
 Correlate 2 images New dark image



Browser Driven Remote Instrument Control

The TelePresence Microscopy Collaboratory : Evolving the Paradigm.



Nestor J. Zaluzec
Zaluzec@esem.eme.pnl.gov

TelePresence Collaboration

Provides Access to:

- Tele-Conferencing
- Instrument Room
- Instrument Status
- Experimental Data
Pre/RT/Post Expt.
- On-Line Control

August 4, 1995
12:48:46 PM

The interface is divided into several sections:

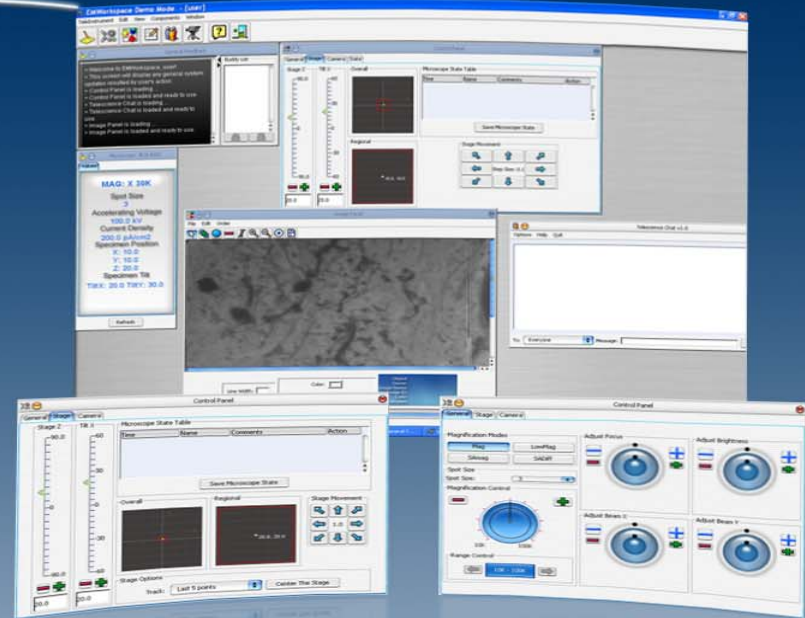
- Top Left:** A video feed showing a person in a laboratory setting with various instruments and equipment.
- Top Right:** A 2x2 grid of video feeds showing four participants in a teleconference.
- Bottom Left:** A data window titled "Data" showing experimental parameters and a table of data points.
- Bottom Right:** A window showing a close-up of a textured surface, possibly a sample or a component of the instrument.

Data Window Content:

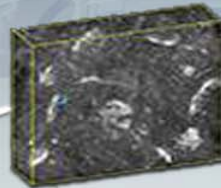
Mod: STM 888Z Replication 20 x 0% 000000 Stage Coordinates
HT: 100.000V Duration 100.0 s 00:00:00 Gain per 10x **
Excitation: 0.750A Screen Position/Desk Field: 00:00:00 SE 100 10.0
Tip: 0.0000 Probe Scan 00 00.0 00.000 0 m V 00 0.0
Focus: 0.000V Probe In C.L. 0000 00.0 00.000

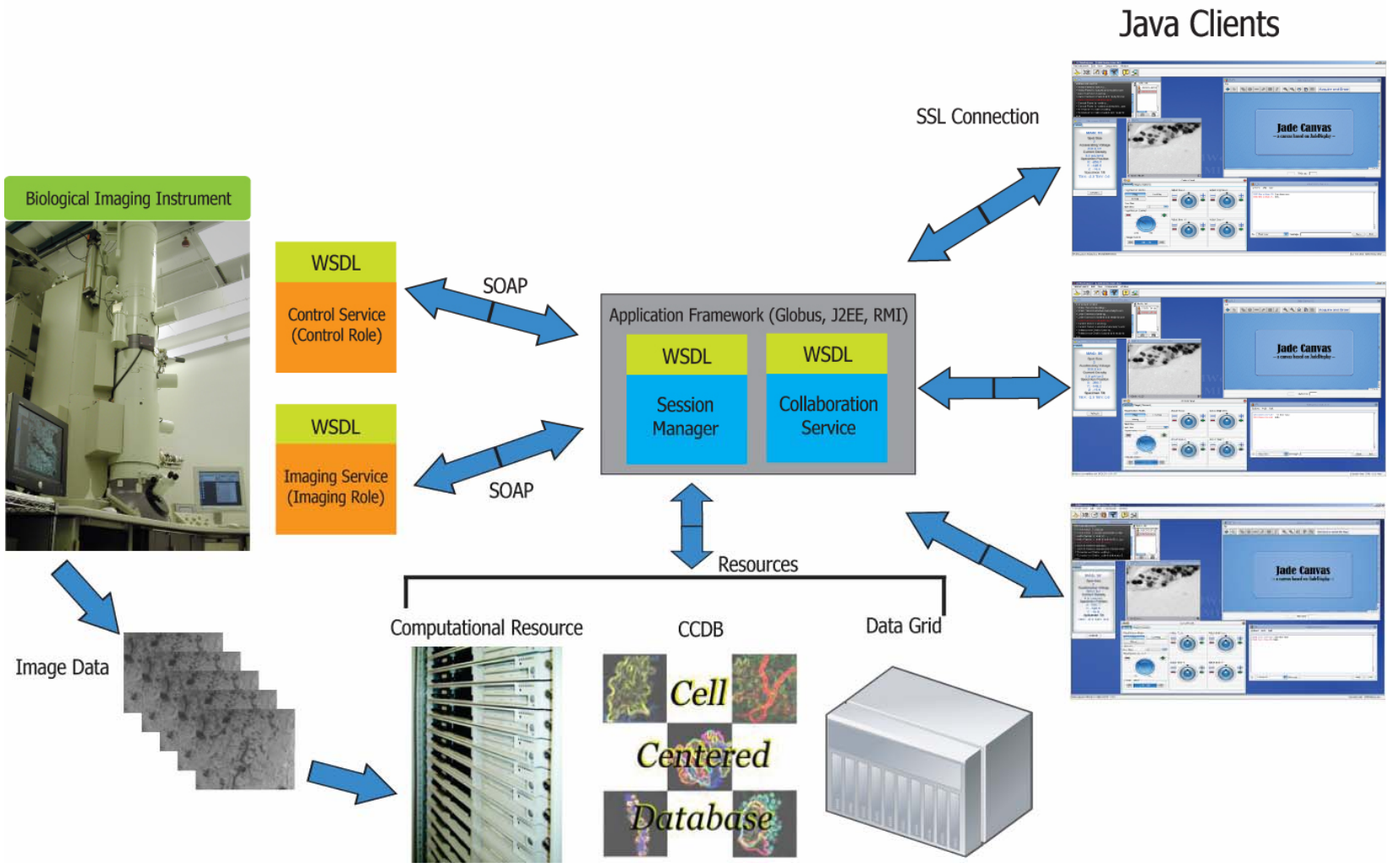
| Stage | Coordinates | Amplitude | Phase |
|--------------|-------------|-----------|--------|
| Condition 1 | 0.0000 | 0.0000 | 0.0000 |
| Condition 2 | 0.0000 | 0.0000 | 0.0000 |
| Condition 3 | 0.0000 | 0.0000 | 0.0000 |
| Condition 4 | 0.0000 | 0.0000 | 0.0000 |
| Condition 5 | 0.0000 | 0.0000 | 0.0000 |
| Condition 6 | 0.0000 | 0.0000 | 0.0000 |
| Condition 7 | 0.0000 | 0.0000 | 0.0000 |
| Condition 8 | 0.0000 | 0.0000 | 0.0000 |
| Condition 9 | 0.0000 | 0.0000 | 0.0000 |
| Condition 10 | 0.0000 | 0.0000 | 0.0000 |
| Condition 11 | 0.0000 | 0.0000 | 0.0000 |
| Condition 12 | 0.0000 | 0.0000 | 0.0000 |
| Condition 13 | 0.0000 | 0.0000 | 0.0000 |
| Condition 14 | 0.0000 | 0.0000 | 0.0000 |
| Condition 15 | 0.0000 | 0.0000 | 0.0000 |
| Condition 16 | 0.0000 | 0.0000 | 0.0000 |
| Condition 17 | 0.0000 | 0.0000 | 0.0000 |
| Condition 18 | 0.0000 | 0.0000 | 0.0000 |
| Condition 19 | 0.0000 | 0.0000 | 0.0000 |
| Condition 20 | 0.0000 | 0.0000 | 0.0000 |

Microscopy Remote Control



EMWORKSPACE

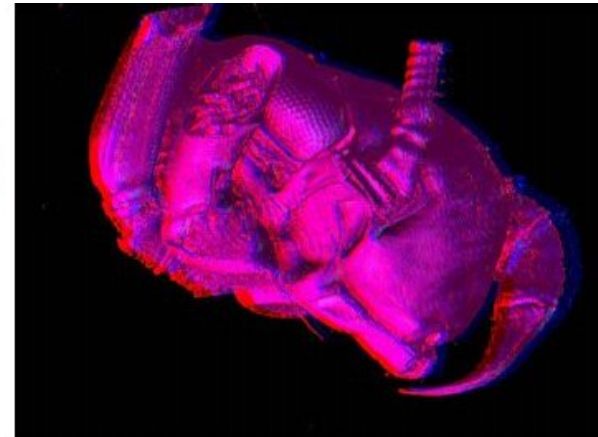
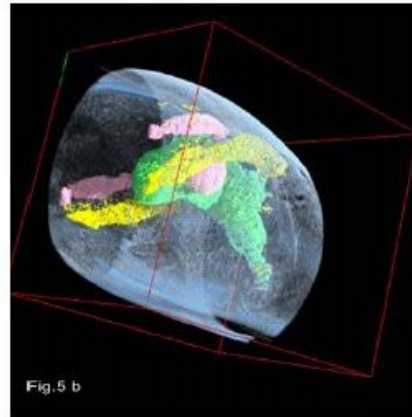
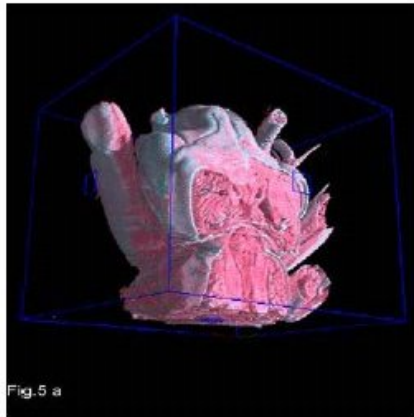




-2k x 2k x 2 bytes x (60 images) = 480MB

-4k x 4k x 2 bytes x (60 images) = 1.9 GB

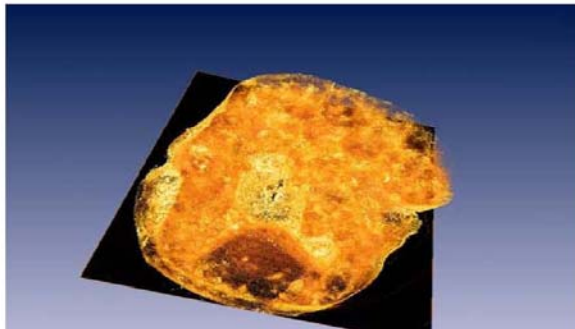
Tomography at Beamline 2BM of the APS:



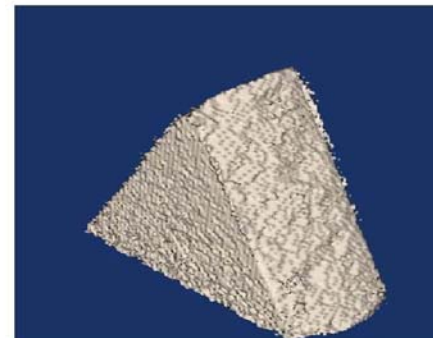
Ceramic coating layers
Anand Kulkarni - NIST



Foam Modeling

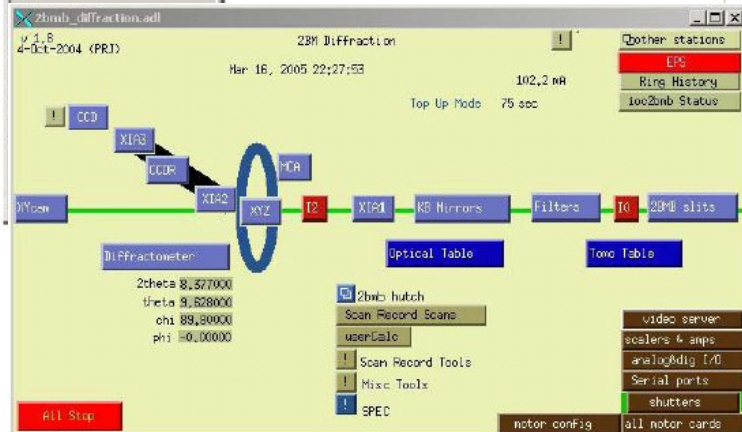


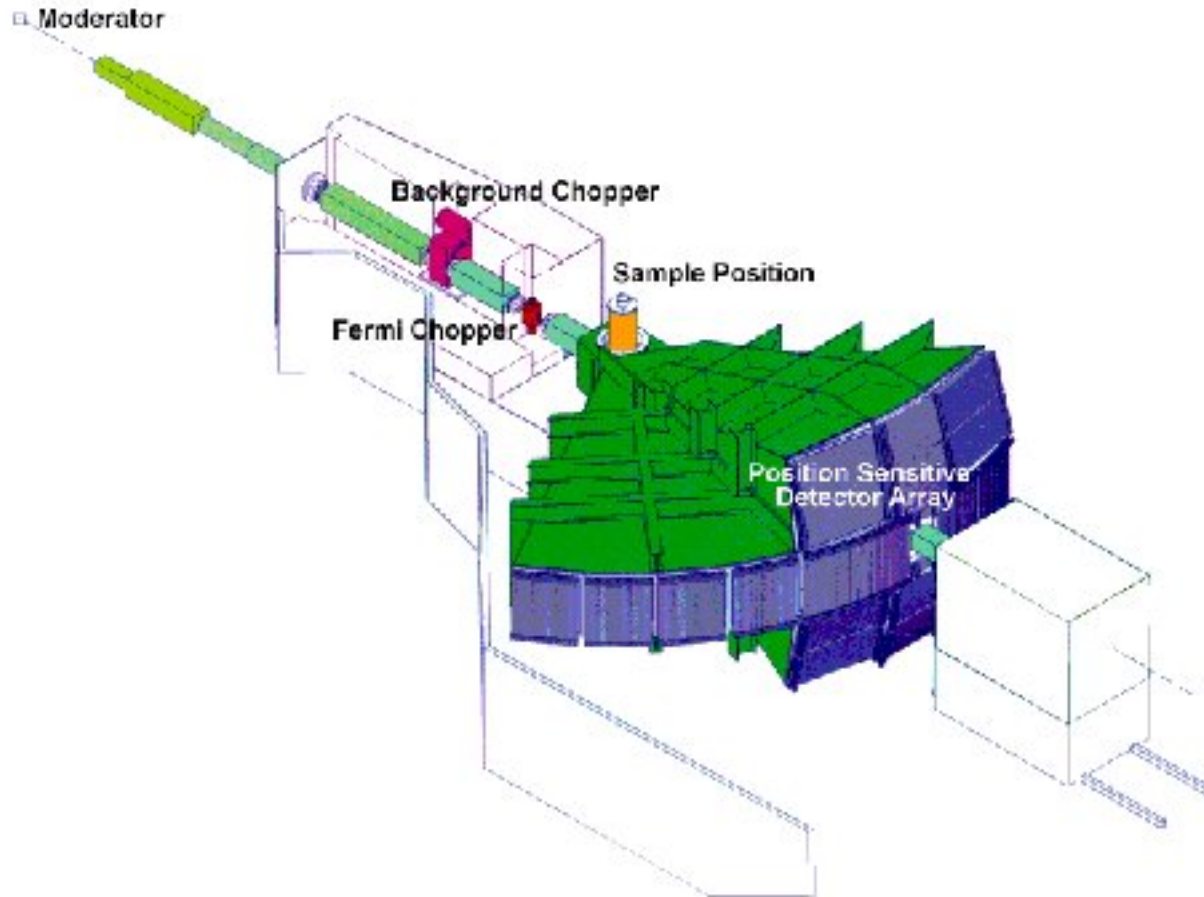
Highly Explosive Materials (PBX-9501) Modeling
Curt Bronkhorst - Los Alamos National Laboratory



2 μ m Ta rods in Si substrate total FOV = 1.3 mm

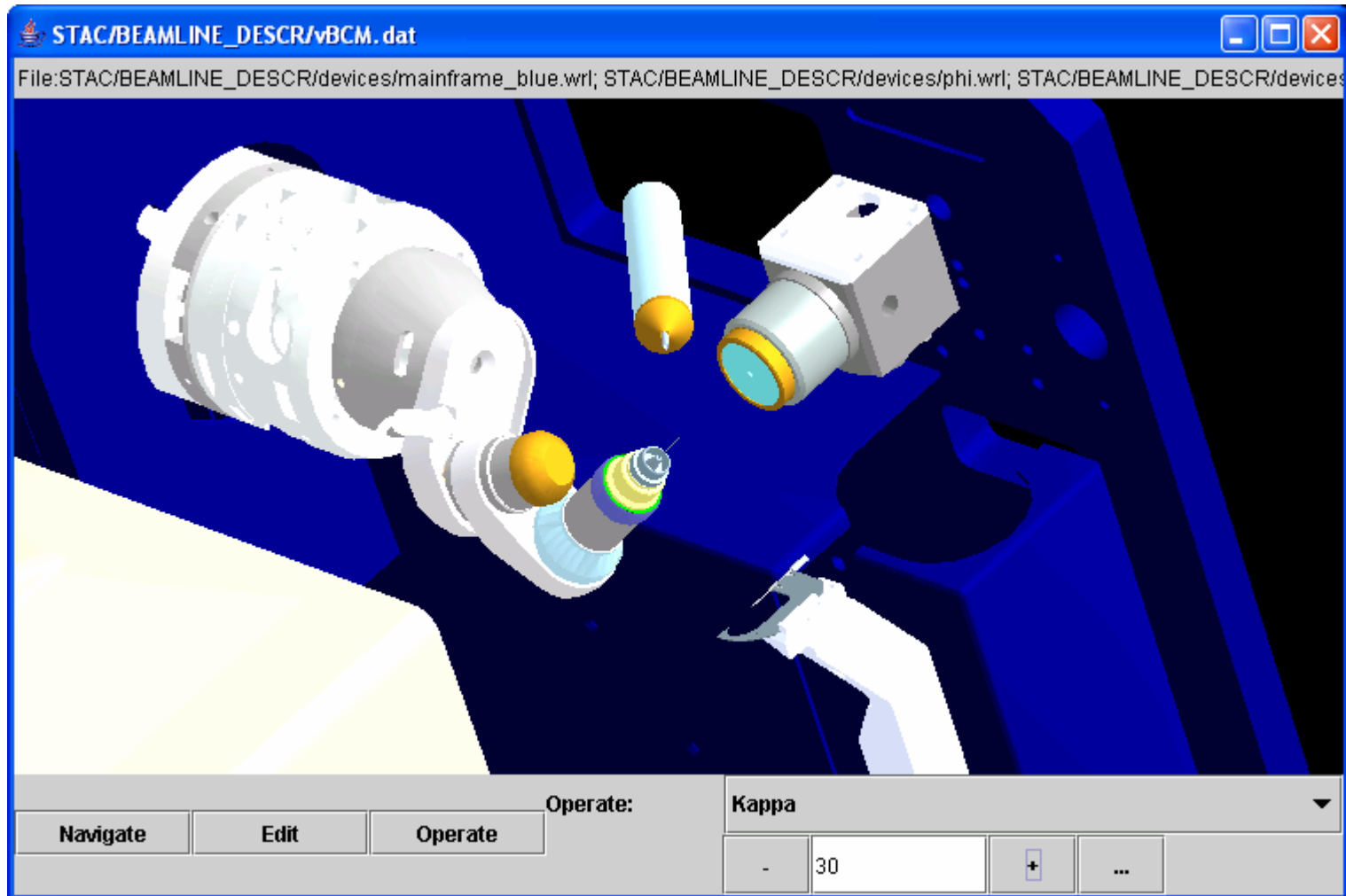
Collaborative Remote Access at 2BM:

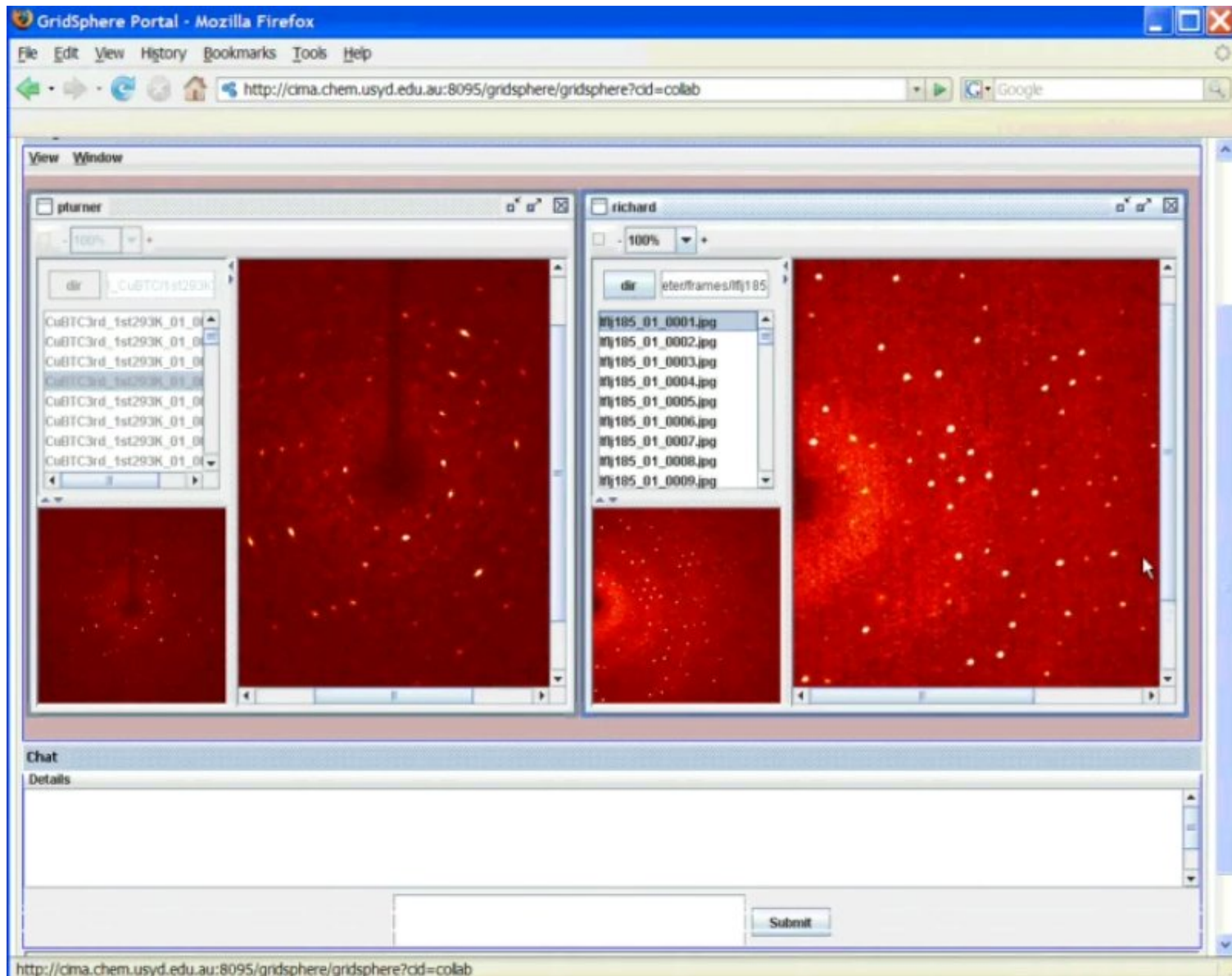




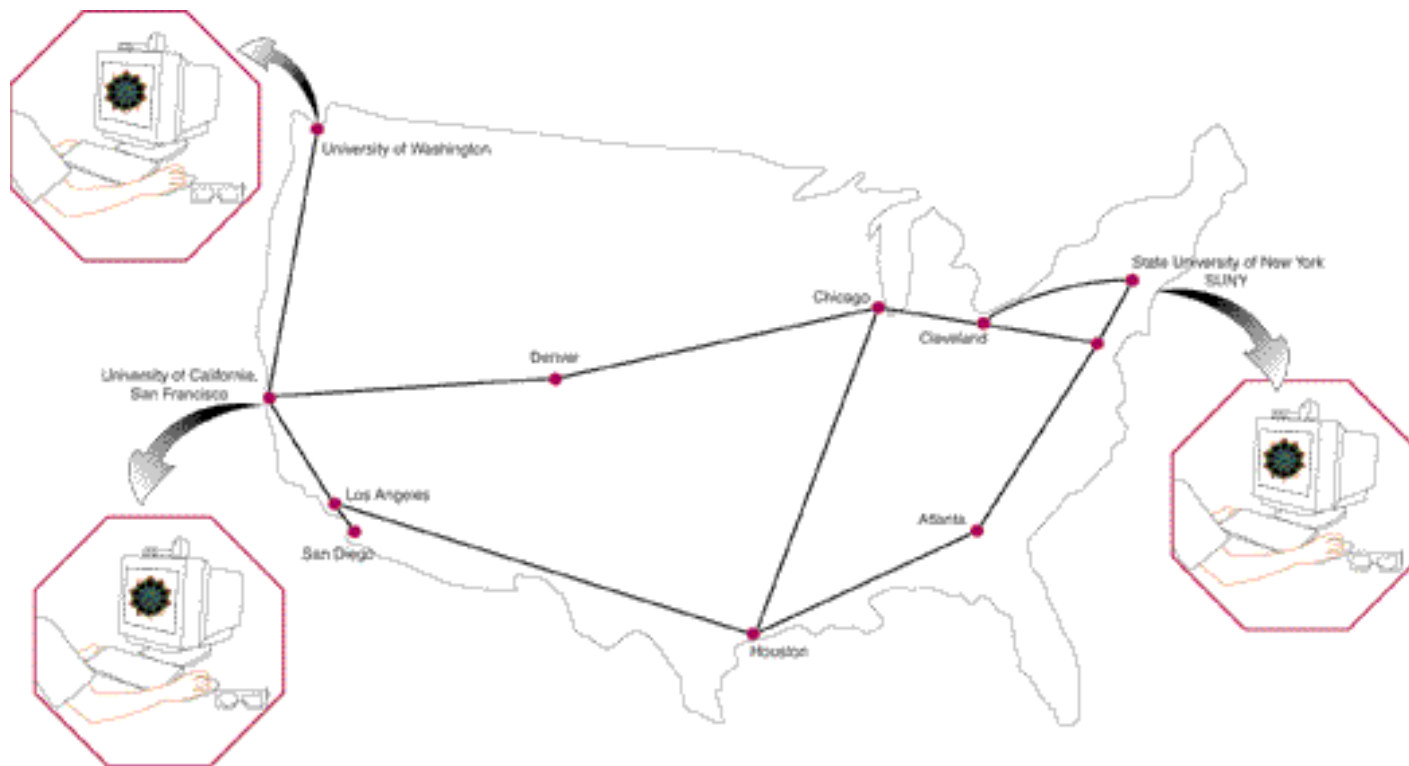
Virtual Neutron Scattering

Virtual Synchrotron Beamline

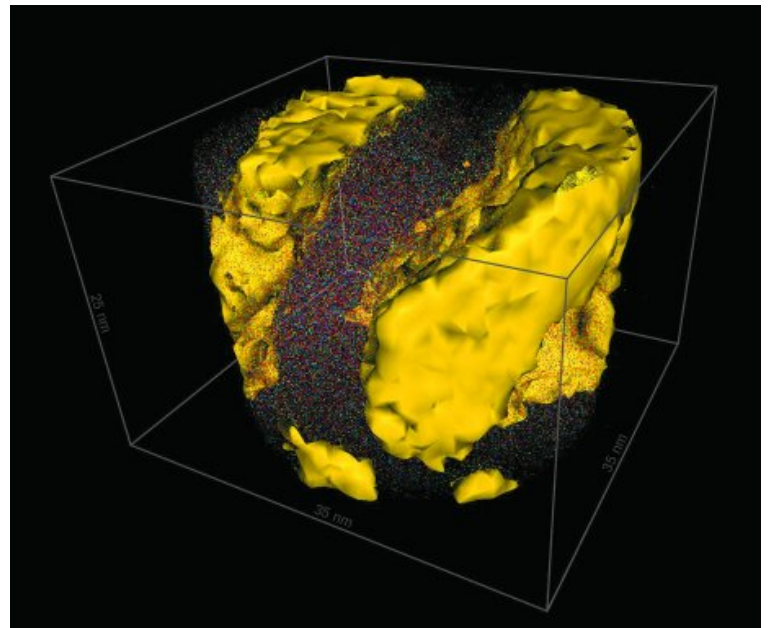
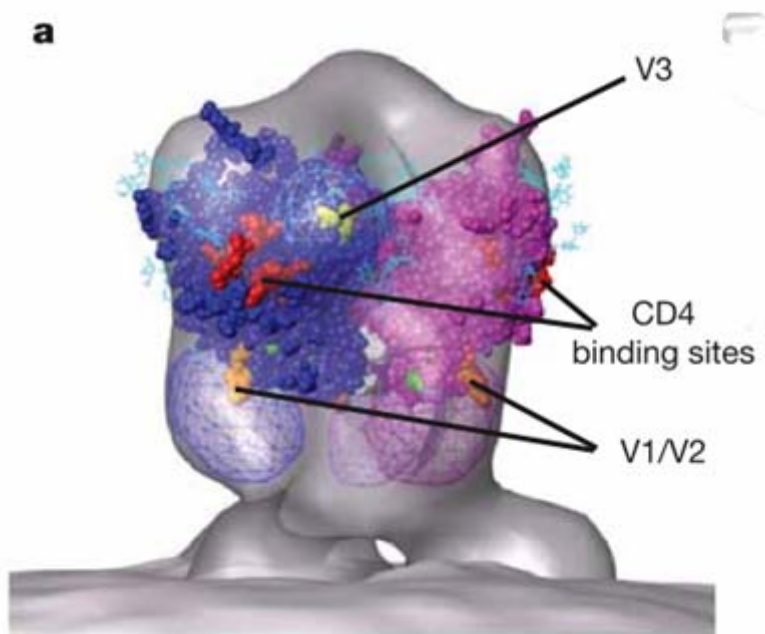
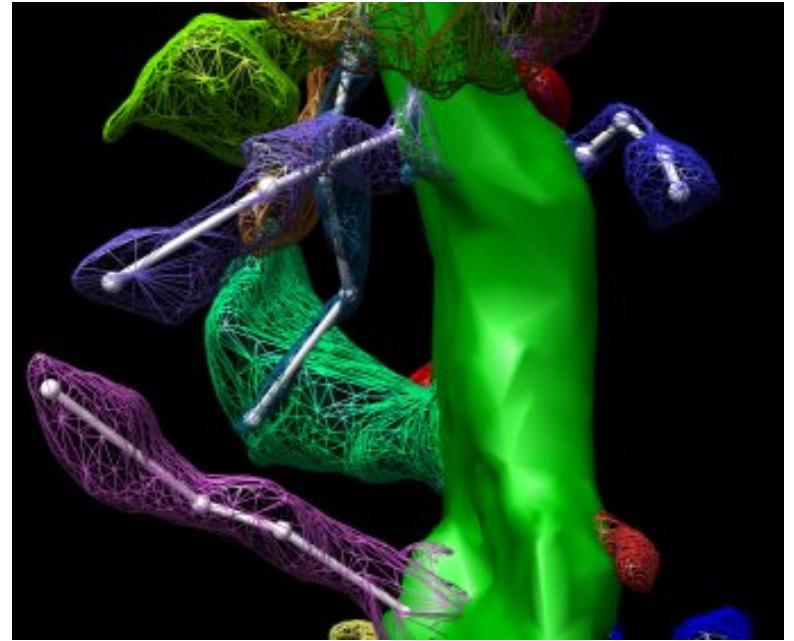
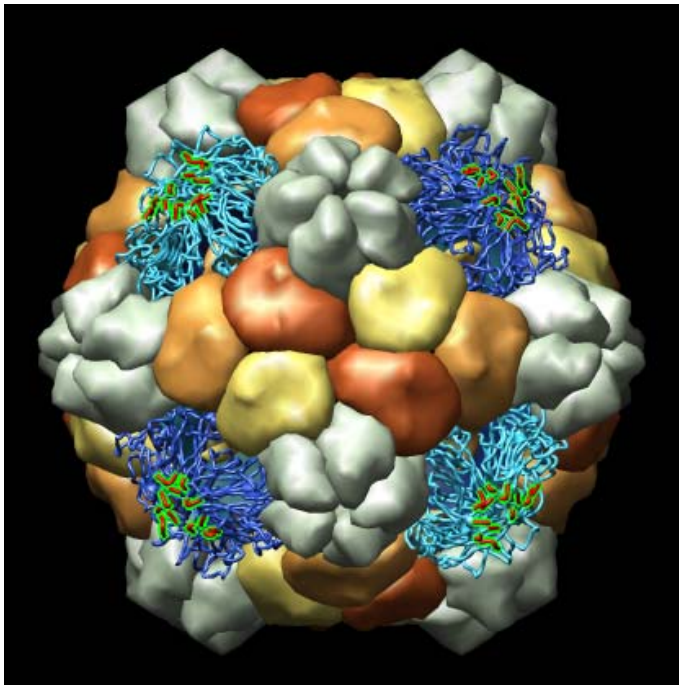




Browser Based Multi-user Collaborative Image Viewing Tool



Chimera Molecular Modelling Collaboratory





NOBUGS 2008 to be held in Australia

(New Opportunities for Better User Group Software)

Meeting emphasis is to find successful scientific software collaborations and find the elements that make them work. Also looking for some cross-pollination of ideas for control systems and data analysis.

WANTED: Astronomy community rep. to join local organising committee.

Contact:

Nick Hauser: nha@ansto.gov.au

Peter Turner: p.turner@chem.usyd.edu.au