

Experiences with the SER-CAT Remote User Participation Program

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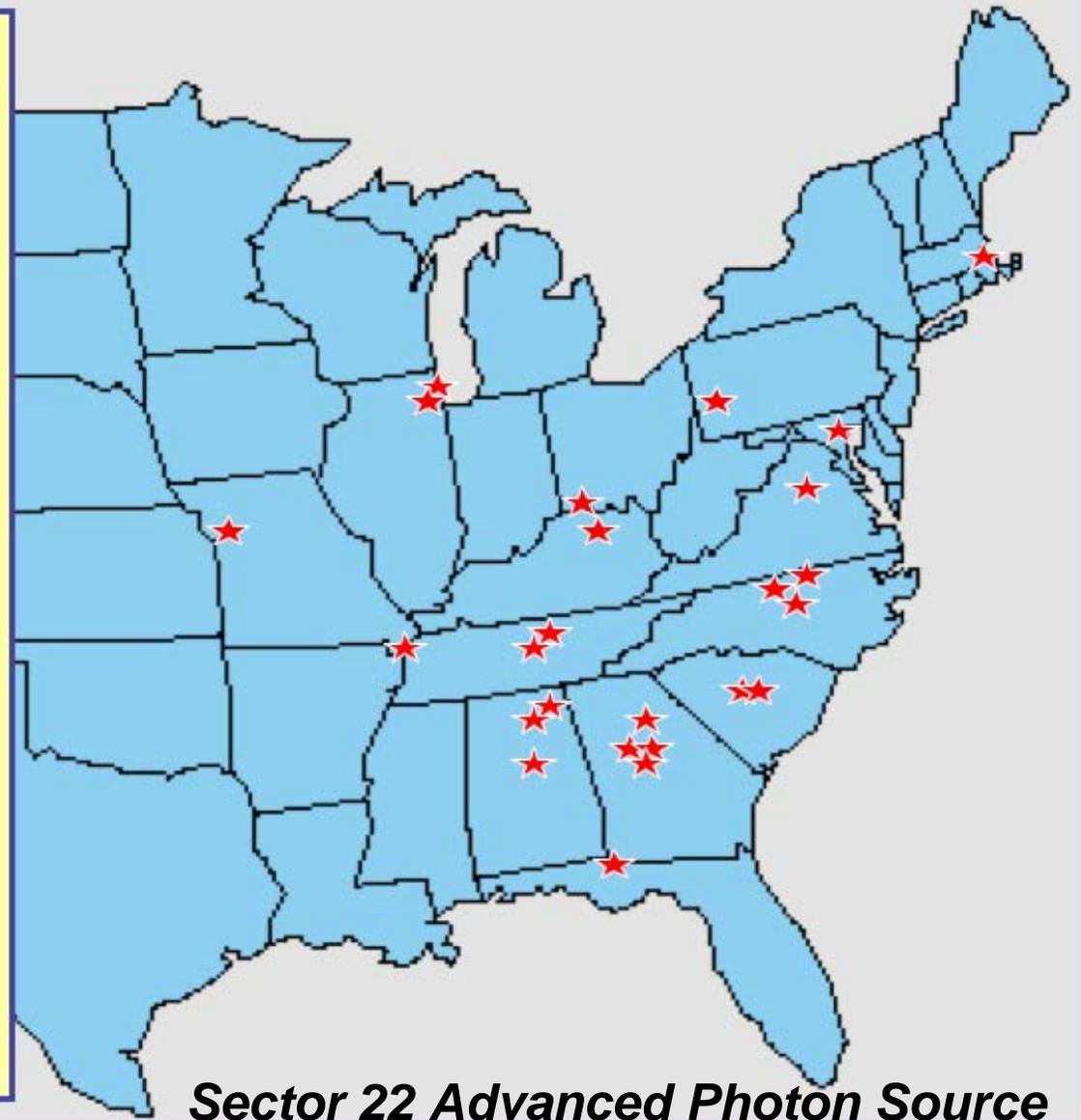
SER-CAT, APS, Argonne National Laboratory
and
Department of Biochemistry and Molecular Biology,
University of Georgia, Athens, GA 30602



SER-CAT *Southeast Regional Collaborative Access Team*

25 Member Institutions in 14 states

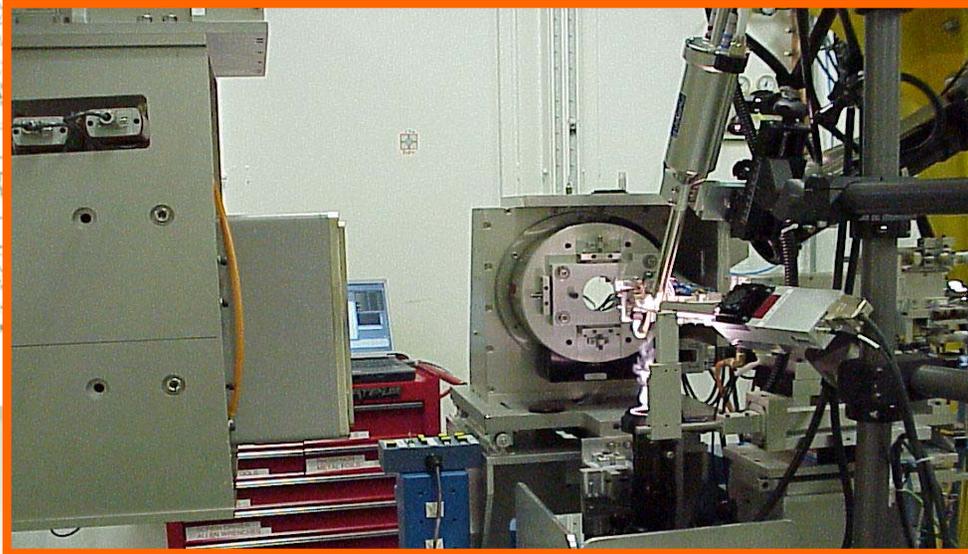
Duke University
Emory University
RFUHS / The Chicago Medical School
Florida State University
Georgia State University
Georgia Tech Research Corporation
Medical University of South Carolina
NASA George C. Marshall Space Flight Ctr.
NIH Intramural Research Program
North Carolina State University
The Procter and Gamble Company
St. Jude Children's Research Hospital
University of Alabama at Birmingham
University of Alabama at Huntsville
University of Georgia
University of Kentucky Research Foundation
University of Illinois at Chicago
University of Missouri at Kansas City
University of North Carolina at Chapel Hill
University of Pittsburgh
University of South Carolina
University of Virginia
Vanderbilt University
Vanderbilt University Medical Center
Wyeth Pharmaceuticals



Sector 22 Advanced Photon Source

OPERATES INSERTION DEVICE AND BENDING MAGNET BEAMLINES AT APS

22ID SER-CAT



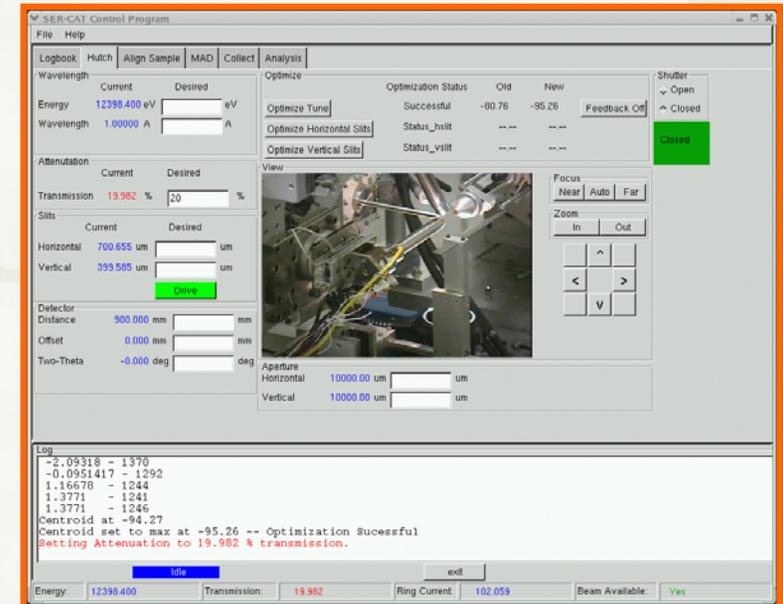
22ID End Station

22ID SER-CAT

Rosenbaum optics and A-frame goniometer
MAR 300mm CCD detector
SERUI² User interface

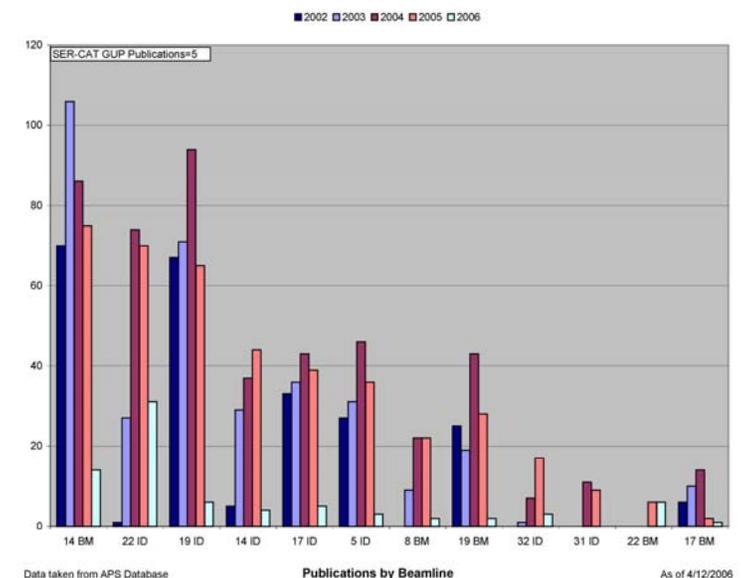
MAD/SAD capable

Operational envelope 6-20 keV
Brilliance 6×10^{11} photons sec^{-1} ($100 \times 100 \mu\text{m}^2$)
Resolution $\Delta E/E$ 5×10^{-5} (Si 220)



SERUI² User Interface

22ID Publications



22ID Now Accepting General Users

22BM SER-CAT

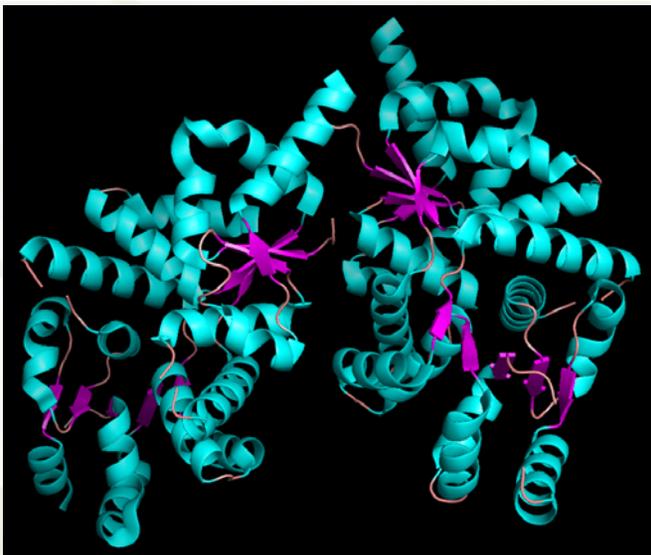


22BM SER-CAT

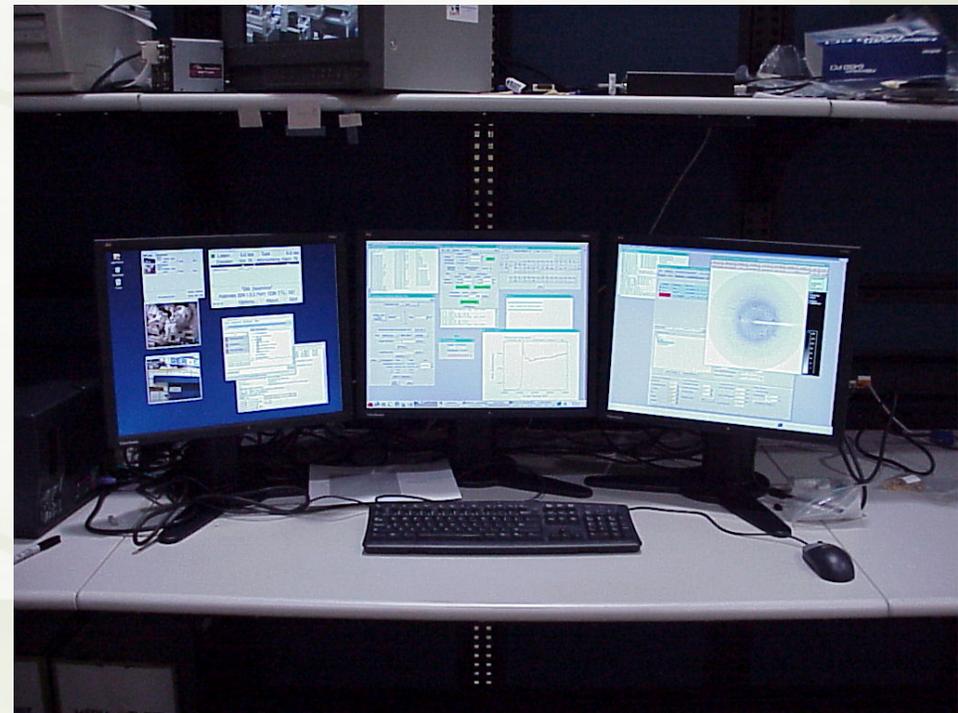
Rosenbaum optics and A-frame goniometer
MAR 200mm CCD detector
ALS style automounter
SERUI² User interface

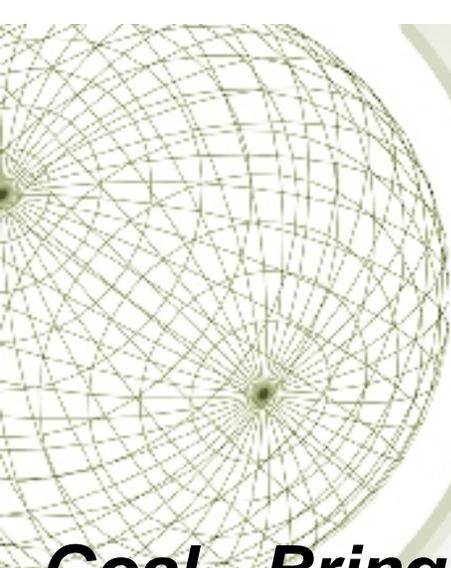
MAD/SAD capable

Operational envelope 6-20 keV
Brilliance $2-3 \times 10^{11}$ photons sec^{-1} ($80 \times 80 \mu\text{m}^2$)
Resolution $\Delta E/E$ 1×10^{-4} (Si 111)
Remote access test bed



PDB Entry 1Y82 first 22BM structure





Remote User Participation

Vision and Goal

October 2004

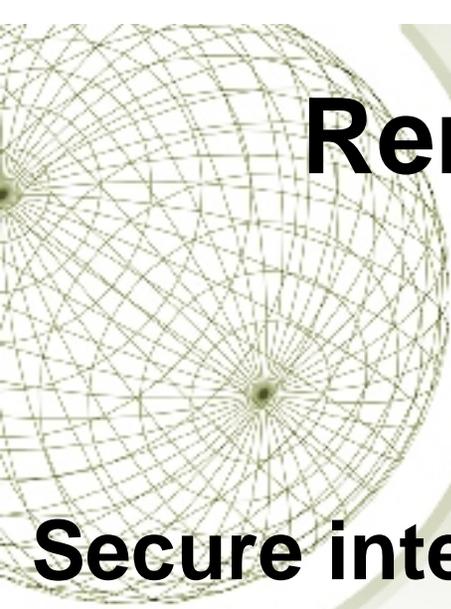
Goal - Bring 22BM online as a fully automated beamline with remote access capabilities

Dramatically increase the productivity of SER-CAT beamlines

Provide users the option of real-time participation in SER-CAT data collection experiments from their home lab

Reduce users travel costs and time away from their lab

Restructure beam time allocation into shorter, but more frequent time slots

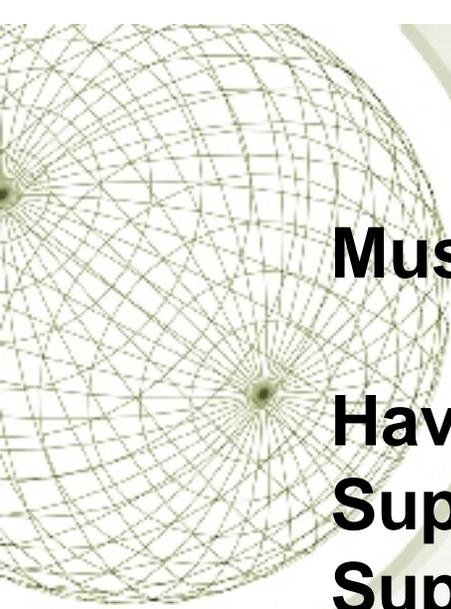
A decorative wireframe sphere is located in the top-left corner of the slide. It consists of a grid of lines forming a spherical shape, with a central point and lines radiating outwards to form a grid of squares and circles.

Remote Access Requirements

Secure internet communications backbone

A unified beamline/experiment control interface

Automated crystal mounting, centering and retrieval



Secure internet backbone

Must be secure - ANL/APS policies

Have low bandwidth requirements

Support video, audio and VNC connections

Support multiple remote connections

Have a means of controlling user access

Have a large existing user base

Have local expertise

Windows or Linux versions available

Easy to install

Low cost (free)

Low maintenance

Selected ANL developed Access Grid



www.accessgrid.org

The Access Grid communications backbone developed by the MCS Division, Argonne National Laboratory allows for secure communication (audio, video and VNC based software applications) between the beamline and the remote user workstation.

The Access Grid is an ensemble of resources including multimedia large-format displays, presentation and interactive environments, and interfaces to Grid middleware and to visualization environments.

These resources are used to support group-to-group interactions across the WEB. For example, the Access Grid (AG) is used for large-scale distributed meetings, collaborative work sessions, seminars, lectures, tutorials, and training. Thus, Access Grid differs from desktop-to-desktop tools that focus on individual communication.

Each remote user must be registered in the Access Grid database and verified via a certificate in order to access the GRID and its venues. The Access Grid has issued over 3,400 certificates to users across 47 countries.

IMPORTANT: only those users scheduled for data collection with a valid certificate will have access to the SER-CAT beamlines.

Unified beamline/experiment control interface

Must provide basic beamline controls

- Beam energy
- Beam position
- Beam focus
- Beam size

Must provide basic goniometer controls

- Shutter control
- Detector distance
- Detector angle
- ϕ rotation

Must provide experiment setup

- Fluorescence scans/analysis
- Data Collection (MAD/SAD)
- Image display/analysis

Must provide interface to sample mounting automation

Should be easy to use

Developed SERGUI²

SERGUI²

File Help

Logbook Hutch Sample MAD Collect Analysis

Alignment
Phi 270.000
+X -X
+Y -Y

Select Camera
 Top bottom

Fine Adjustment
Up
Left Right
Down

Top Camera Zoom
 1 X 2 X

AutoAlign Save Image Lights
Align Snap Off

Robot
Puck Pin
Dismount 1 6
Mount 1 6
Go

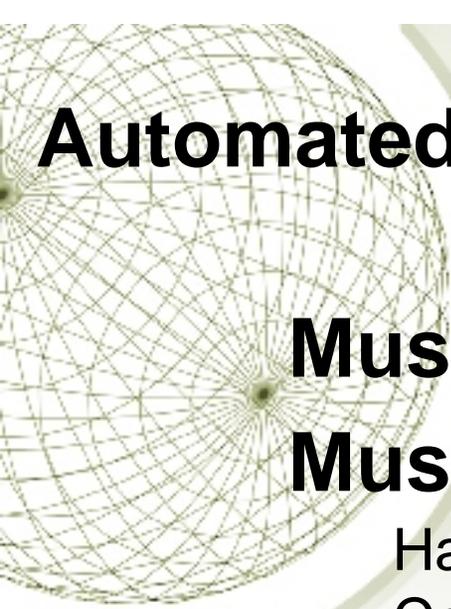
x: 138.841um y: 134.974um z: -1443.122um

```
frame: 52 52.0 time: 5.0 test_1_4.0052 (12431.998540727227, 0, '')  
frame: 53 53.0 time: 5.0 test_1_4.0053 (12431.998540727227, 0, '')  
frame: 54 54.0 time: 5.0 test_1_4.0054 (12431.998540727227, 0, '')  
frame: 55 55.0 time: 5.0 test_1_4.0055 (12431.998540727227, 0, '')  
frame: 56 56.0 time: 5.0 test_1_4.0056 (12431.998540727227, 0, '')  
frame: 57 57.0 time: 5.0 test_1_4.0057 (12431.99235431817, 0, '')  
frame: 58 58.0 time: 5.0 test_1_4.0058 (12431.99235431817, 0, '')  
frame: 59 59.0 time: 5.0 test_1_4.0059 (12431.998540727227, 0, '')  
frame: 60 60.0 time: 5.0 test_1_4.0060 (12431.99235431817, 0, '')
```

Idle Exit

Energy: 12431.999 Transmission: 100.000 Ring Current: 9.666 Beam Available: Yes

Tab note book look and feel similar to Blu-ICE



Automated crystal mounting, centering and retrieval

Must be reliable

Must be easily integrated into beamline

Hardware

Control

Must be on-site repairable

We can fix ourselves if needed

Must be compatible with user tools

Pins

Dry shippers

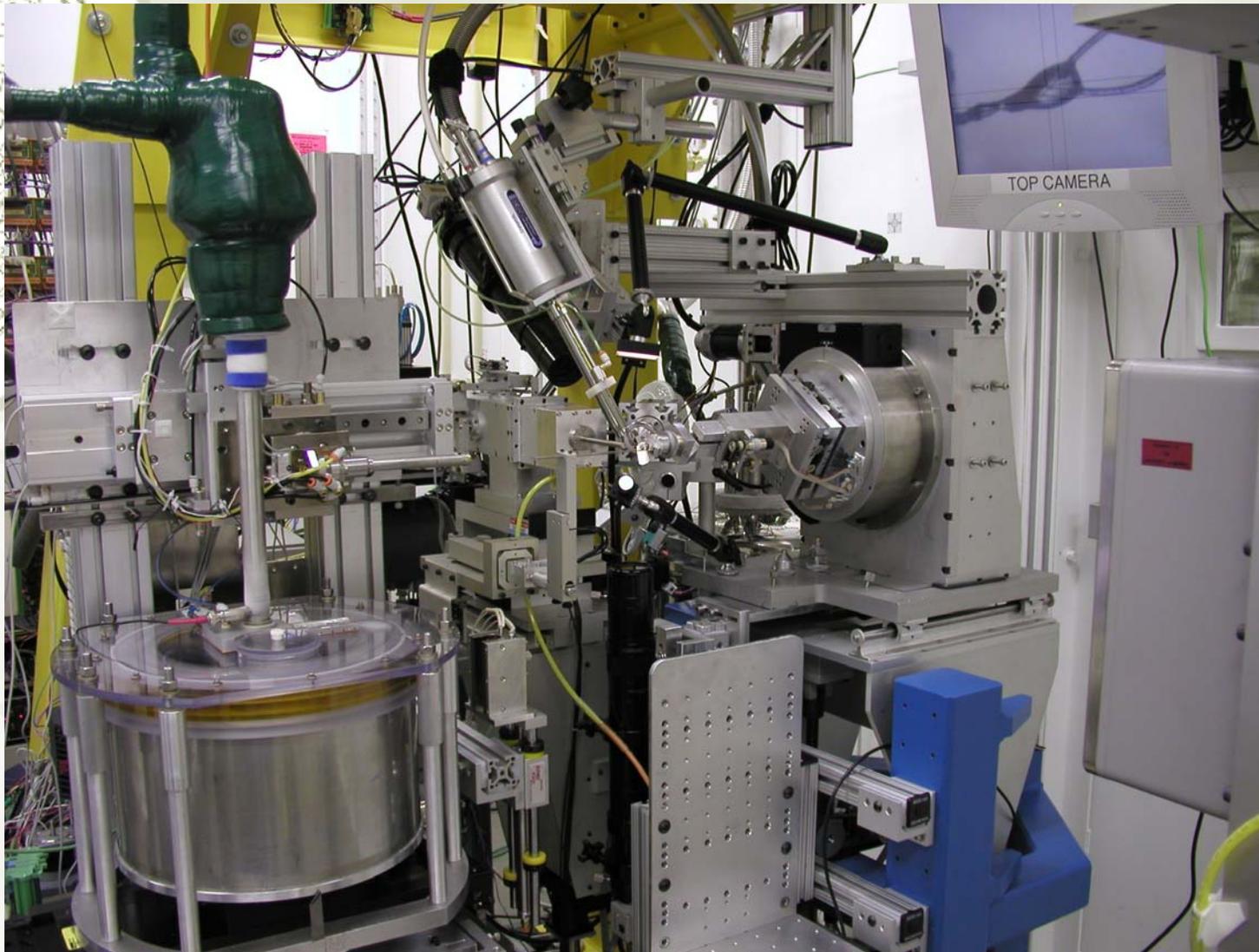
Must have a user community

Must maintain the crystal below 120K

All steps in the process

Choose the ALS automounter

The SER-CAT Automounter



Allows uninterrupted screening or data collection on up to 96 samples

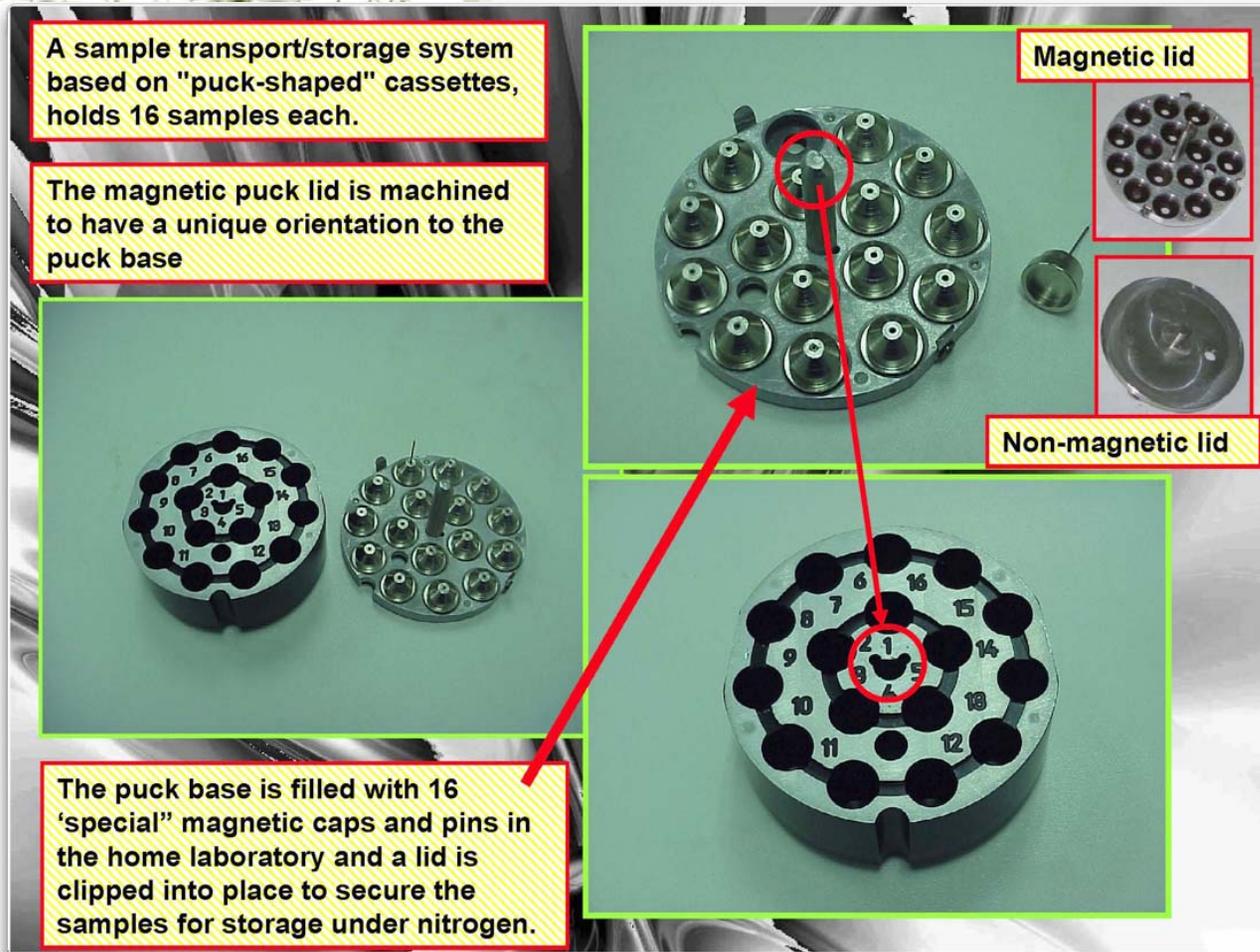
Mounting of the crystal takes less than five seconds

Crystal temperature is maintained well below 120 K

The crystal (loop) can be centered either manually or automatically

Automation of the SER-CAT BM Beamline

Sample handling using the ALS style puck



Sample positions 1-3

- #1 Phosphor
- #2 alignment pin
- #3 empty loop

Phosphor

- Beam size
- Beam shape
- Beam focus

Alignment pin

- Beam alignment

Empty loop

- Defines pin length



The Road Map

October 2004

1. Implementation of Access Grid technology at SER-CAT and UGA

Access Grid

Developed by the ANL Math and Computer Science Division

Satisfies all Internet security logistics imposed by ANL, APS and UGA

2. Automation of the SER-CAT BM beamline.

Installation and integration of the ALS sample automounter into 22BM

Significant retooling of dewar

3. Development of a secure user-friendly beamline control interface compatible with Access Grid

SERGUI² a tab notebook style user interface

Beamline control

Automated sample mounting/centering

Experiment setup

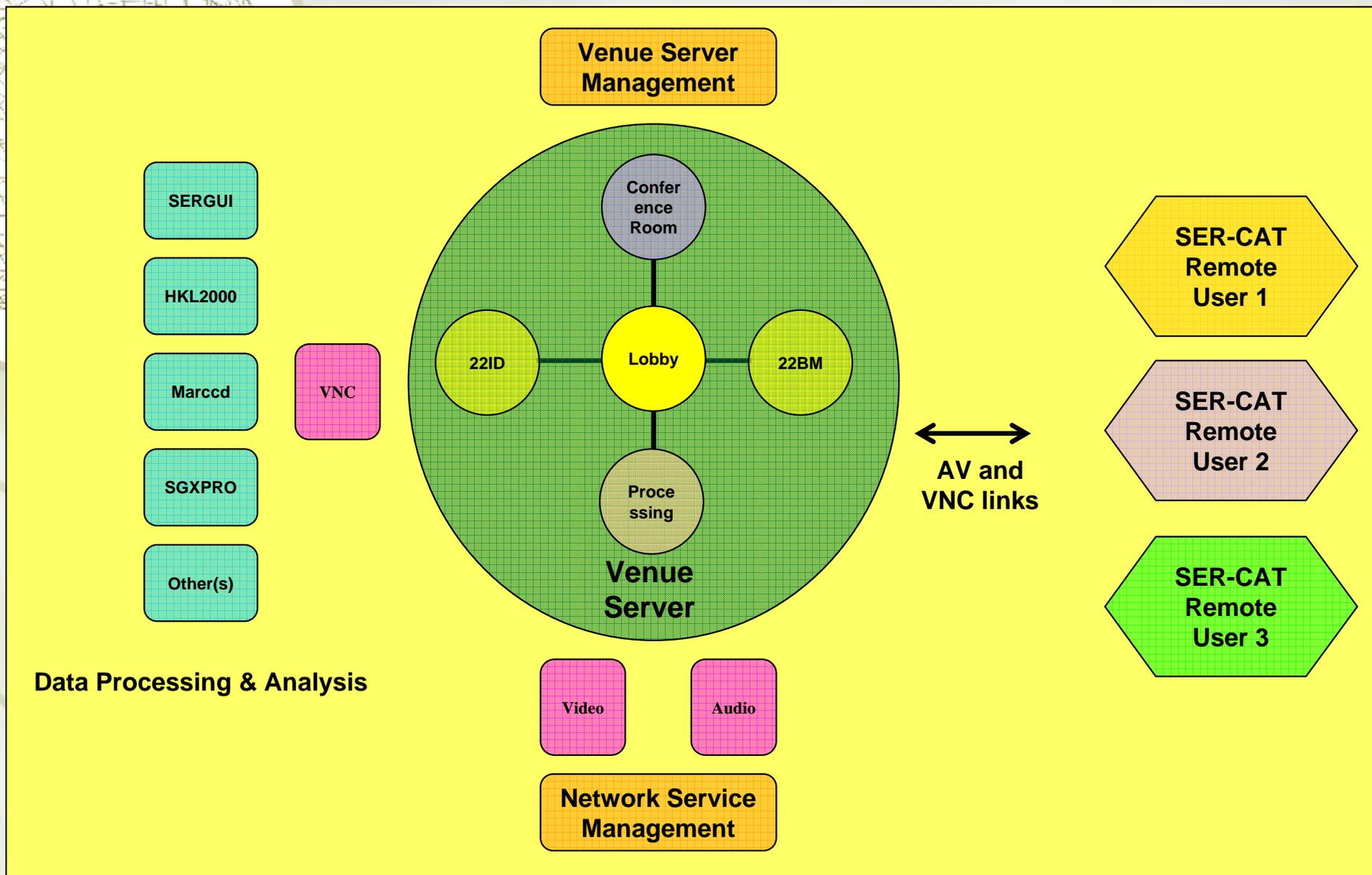
4. Implementation of virtual display and communication systems at SER-CAT and at the UGA test site

Low cost PC based hardware solution

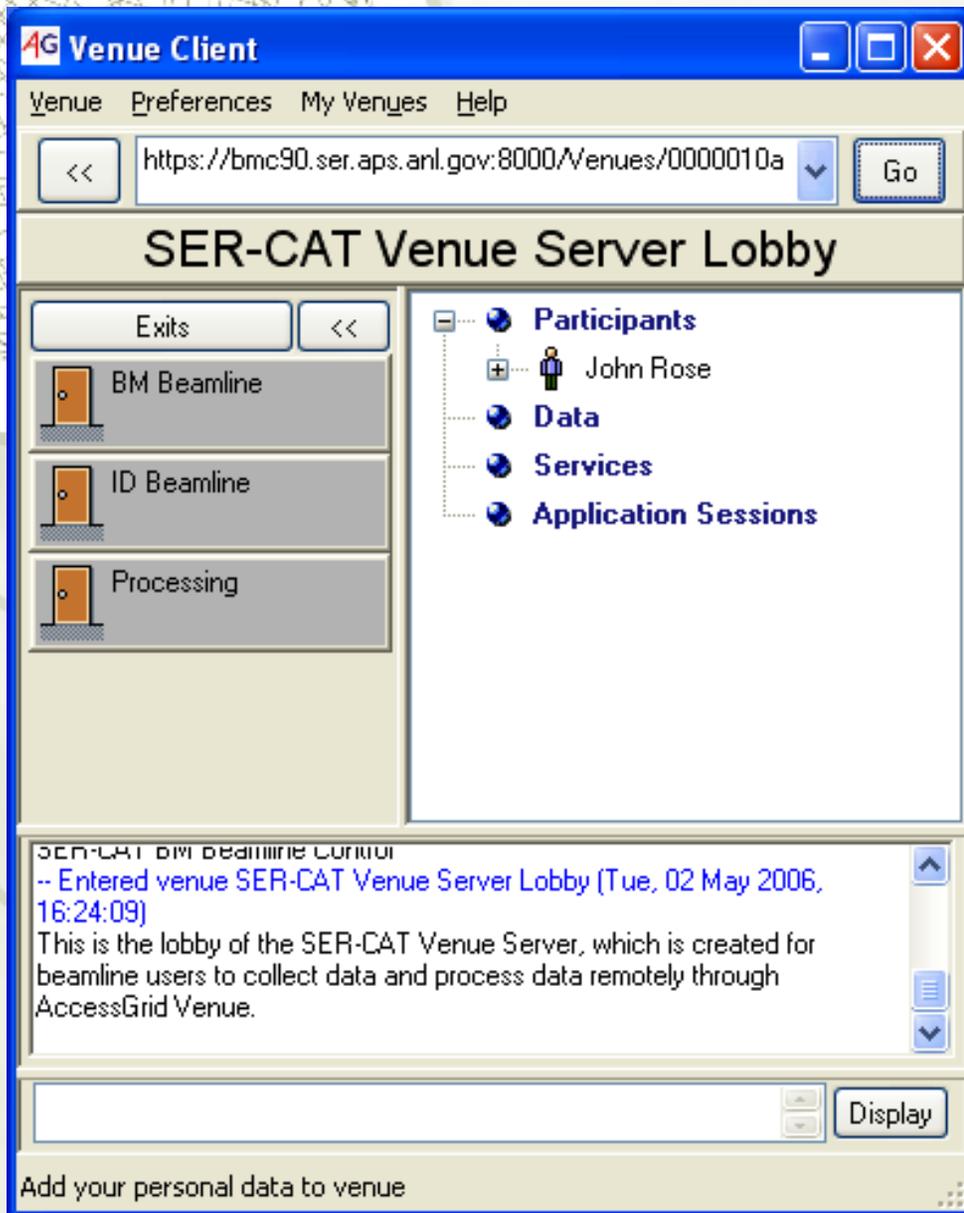
Remote Access Workstation

Access Grid Web Conferencing

The SER-CAT Access Grid Venue



Accessing the SER-CAT AG Venue



Certificate based

Who can access

When user can access

What user can access

BM Beamline

Access to 22BM beamline

ID Beamline

Access to 22ID beamline

Processing

Access to processing servers

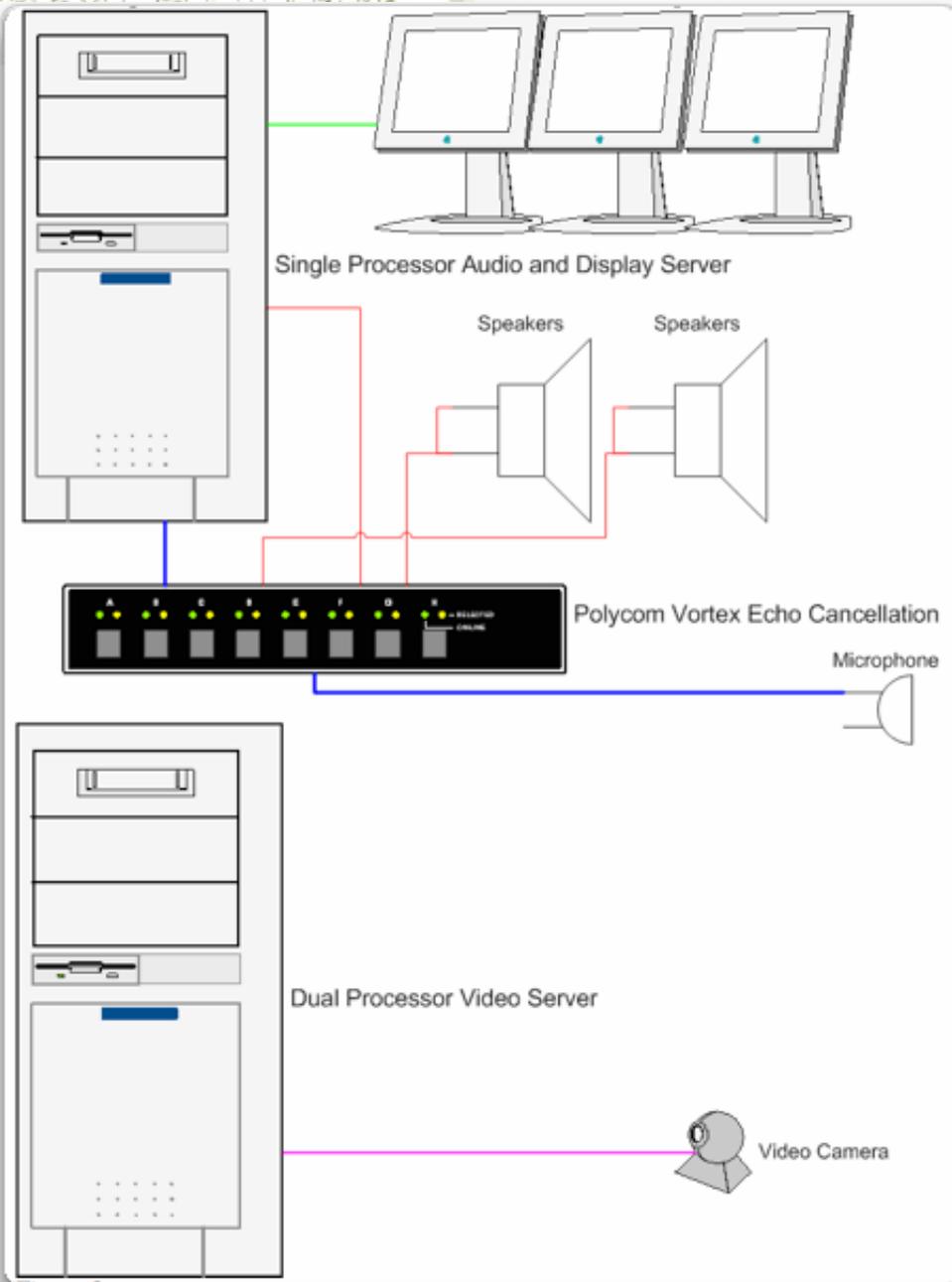
Software

Computer

Disk array

Cluster

Setting Up the Remote Workstation



SER-CAT Remote User Workstation

Display/audio server (mandatory)

Windows/Linux PC

Handles SERCAT - user communications
audio and video feeds

Video server (optional)

Linux PC

Handles User - SERCAT video

lets the people at the beamline see you



Access Grid Remote Workstation Hardware

Display/Audio Server (recommended configuration)

1ea Single (or dual) processor 2.0 GHz or faster computer

1 GB RAM, and an AGP slot

reasonable quality sound card (must be capable of full duplex sound)

keyboard and mouse.

1ea A good quality video card capable of supporting 3 monitors.

NVIDIA chipset cards, one AGP and one PCI.

Jaton 228PCI-Twin (CDW # 567326)

Jaton 3DForce MX4000-64Twin (CDW # 839739).

3ea 19-20 inch monitors capable of at least 1600x1200 pixel resolution.

Viewsonic VP201B (or Planar PL2010) flat panel monitors

Viewsonic G220f CRT monitors

Operating system

Either Windows or Linux (recommended) will work.

Software, other than the device drivers, is available at accessgrid.org

Access Grid Remote Workstation Hardware

Optional Audio Components if you want good quality audio over the internet

1ea Echo cancellation device

Polycom SoundStation2 with the VoIP connector

Polycom Vortex EF2241 (probably overkill for a workstation)

Microphone*

Speakers*

Headset unit*

Speakers*

*Not required if you use the Polycom SoundStation2.

Speaker cable, connectors, etc to hook everything up

Access Grid Remote Workstation Hardware

Optional Video Server (to send your video feed to SER-CAT)*

1ea Dual processor 2.0 GHz or greater PC

1 GB RAM and at least 1 64-bit PCI slot
keyboard and mouse.

1ea Quality camera

Linux - Logitech QuickCam Pro 4000

Windows - Any USB Web Camera or

video capture card (Spectra8 recommended)

camera Canon VC-C4 (or equivalent) that has an RCA output

Cables, KVM switch, monitor (cheap or used) to connect everything up

*Note that video is only needed if you want the people at SER-CAT to see you.

The UGA Remote User Workstation

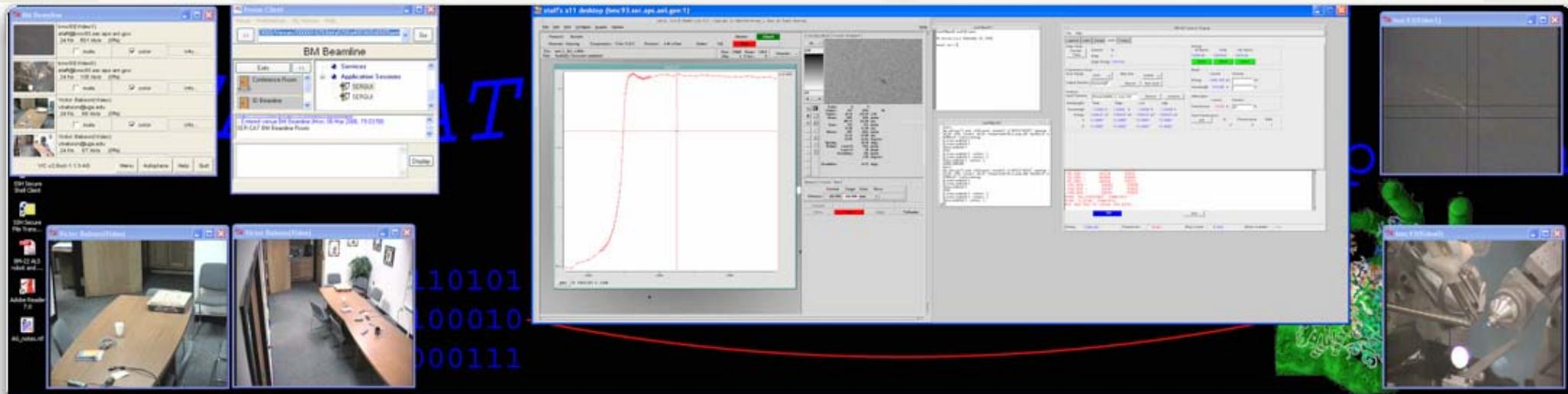


22BM Workstation



UGA Workstation

What the Remote User Sees

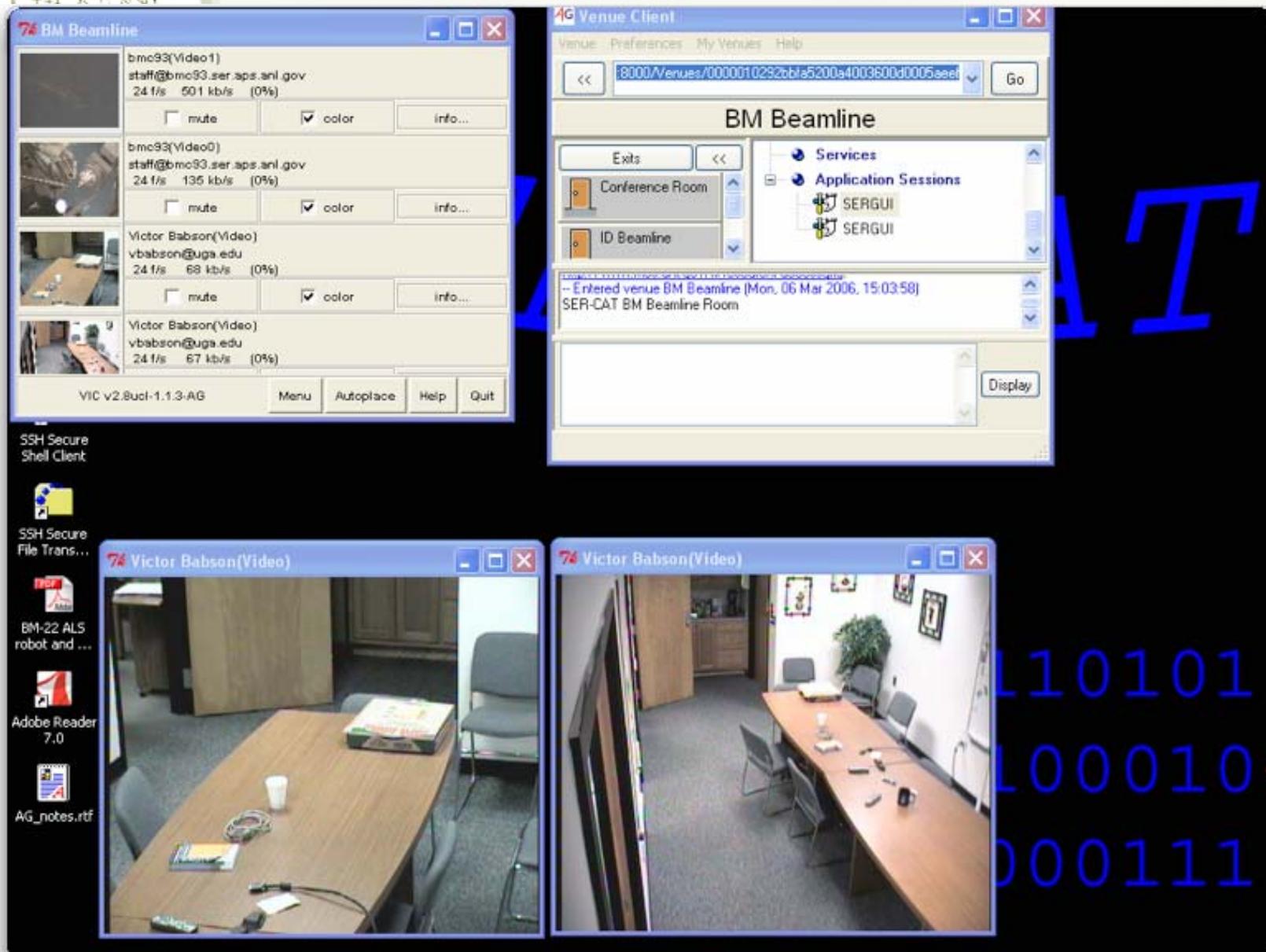


Environment

Analysis

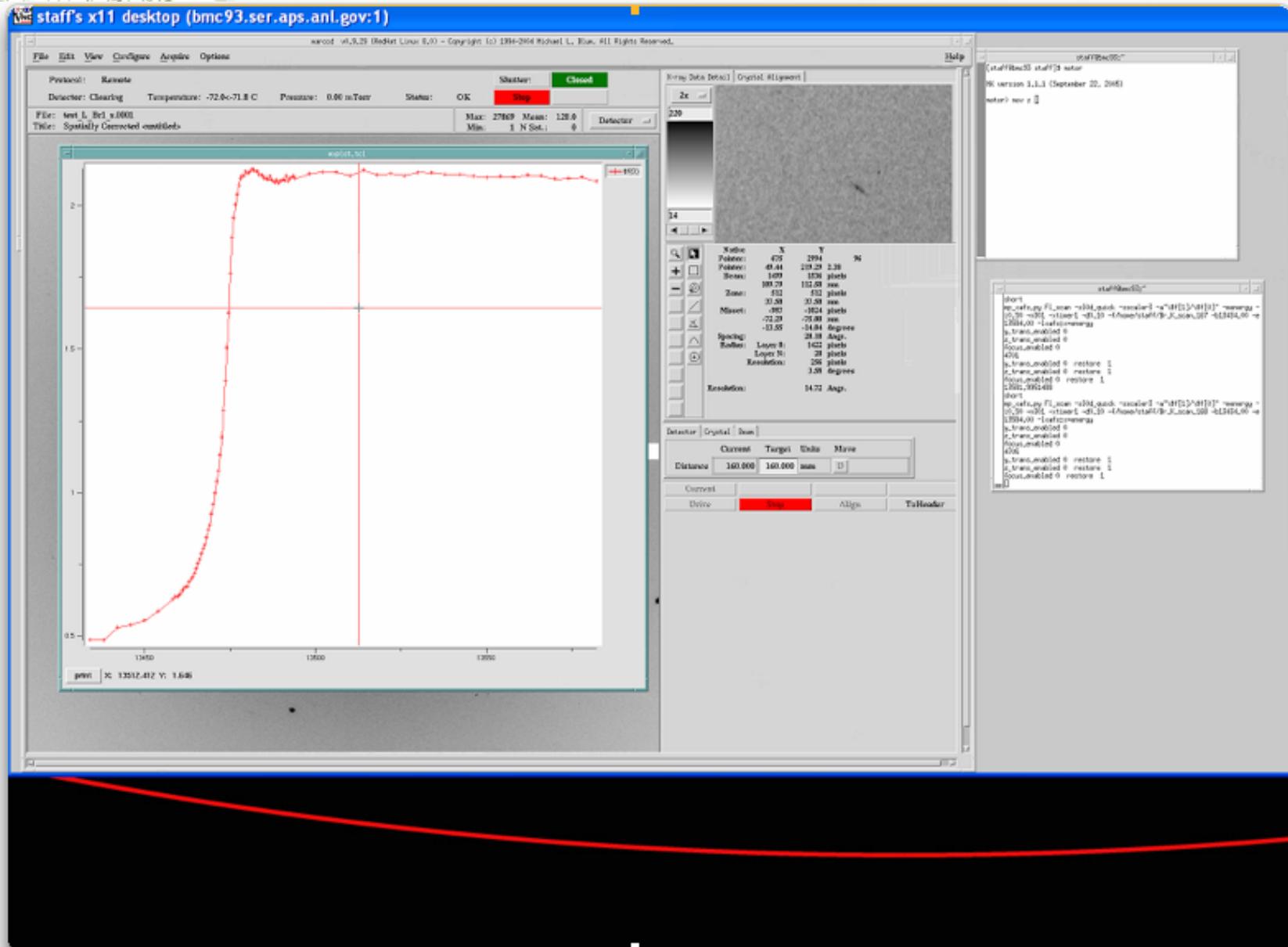
Experiment

The Environment Screen



The **environment screen** is used for Access Grid control functions (audio, video and text messaging).

The Analysis Screen



The **processing screen** is used to run MARCCD, HKL2000 and other data reduction software remotely at the beamline.

The Experiment Screen

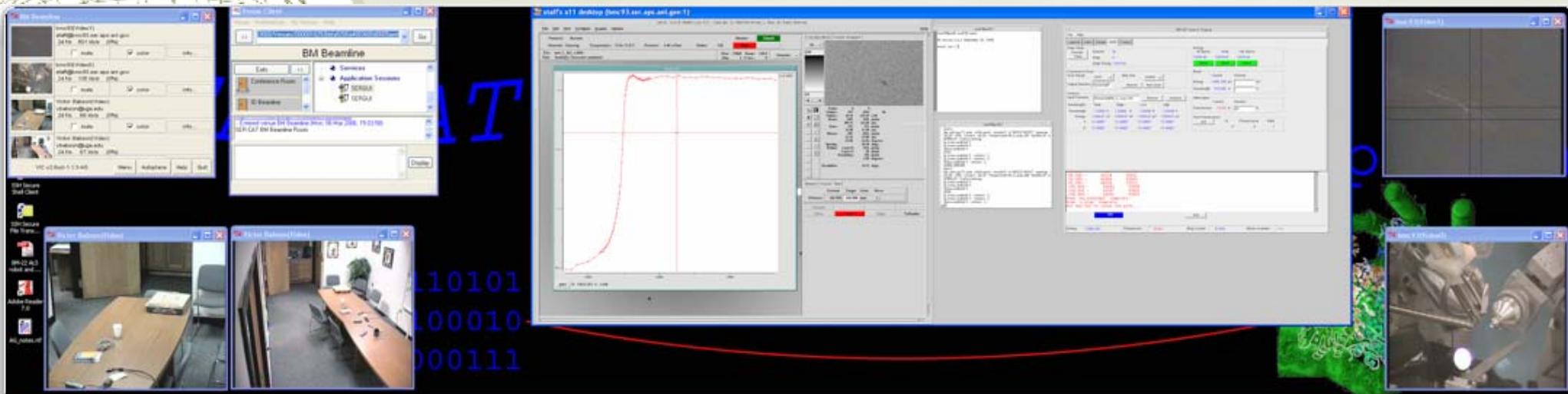
The screenshot displays the SERGUI interface, which is used for setting up and carrying out data collection. The interface is divided into several sections:

- Control Panels:** Includes sections for "Edge Data" (Element, Edge, Edge Energy), "Fluorescence Scan" (Scan Range, Step Size, Output Directory), "Analyze Input Parameters" (Wavelength, Peak, Edge, Low, High), and "Attenuation" (Current, Desired, Transmission, Test Fluorescence Ratio).
- Data Tables:** A table showing scan results with columns for Wavelength, Energy, and Peak. The table is as follows:

Wavelength	Peak	Edge	Low	High
1.23456 A	1.23456 A	1.23456 A	1.23456 A	1.23456 A
Energy	12345.67 eV	12345.67 eV	12345.67 eV	12345.67 eV
r	12.34567	12.34567	12.34567	12.34567
r'	12.34567	12.34567	12.34567	12.34567
- Video Feeds:** Two video windows labeled "bmc 93(Video1)" and "bmc 93(Video0)" showing a microscope setup with a sample and a bright spot of light.
- Status Bar:** Located at the bottom, it displays "Energy: 12345.670", "Transmission: 19.282", "Pkg Current: 91.025", and "Data Available: 100".

The **experiment screen** is used to setup and carry out data collection via the SERGUI interface.

Where We Are Now



Summary

- ✓ Secure access to SER-CAT beamline control
- ✓ Ability to set experiment parameters
 - wavelength
 - detector distance
 - detector 2θ
 - tune, optimize and focus
- ✓ Ability to mount and center crystals
- ✓ Ability carry out and analyze fluorescence scans
- ✓ Ability to setup and carry out MAD and SAD data collection
- ✓ Ability to process data using SER-CAT computers
- ✓ Ability to analyze data on the SER-CAT cluster
- ✓ Documented guide to setting up the remote user workstation

Future Plans

Beta testing by SER-CAT users has begun

Continued development

Image display within SERGUI

removes need for MARCCD

Crystal Ranking

Auto XGEN

Indexing

diffraction limit

$\langle I/\sigma \rangle$

Mosaicity

strategy

Automated crystal screening

Automated data collection

Auto XGEN

Acknowledgements

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