

*SouthEast Regional Collaborative Access Team (SER-CAT)  
Facility Presentation*

*for the*

*Cross-cut Review:  
Macromolecular Crystallography at the APS*

*January 24th, 2007*

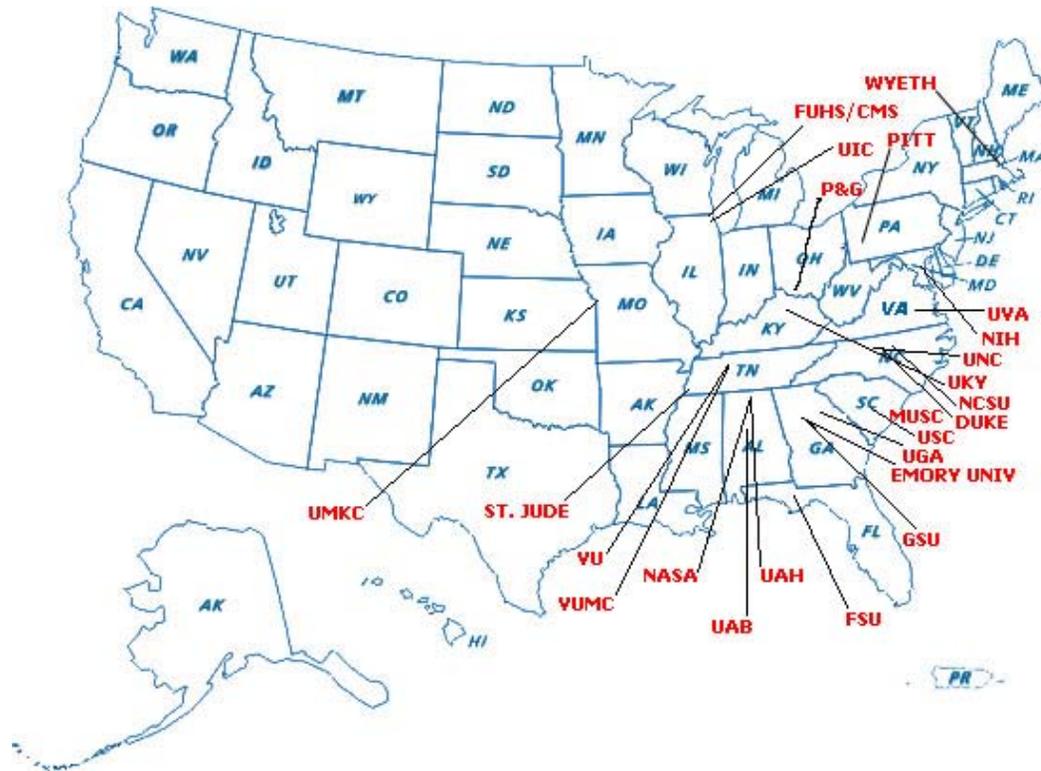
*by*

*John Chrzas  
SER-CAT Sector Manager*

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SER-CAT is comprised of 24 members from 13 states, representing a wide range of scientific interests. The SER-CAT APS facilities consist of an undulator A (22ID) and bending magnet beamline (22BM).

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# SER-CAT Science

## Research Type

- Protein
- Protein-DNA
- DNA
- Virus
  
- Large unit cells
- Large structures
- Micro Crystals
  
- Methods

## Research Focus

- HIV/AIDS
- Cancer
- Cell signaling
- Tropical disease
- Membrane proteins
- Trafficking
- Protein Folding
- Virology
- Drug Design
- Structural genomics
- Methodology
  - Automation
  - Remote studies
  - Soft X-ray Phasing

## Research Funding

- NIH/NCI
- NSF
- DOD
- ONR
- AMFAR
- State
- Industry

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# *Mission Statement*

The SER-CAT Operations Team will provide a world-class synchrotron facility for Macromolecular Crystallography by *optimizing the performance and utilization of the beamlines* and by providing a user friendly environment for SER-CAT members and General Users to conduct their research.

**To achieve the objectives of our mission statement a 3-year strategic plan was developed in 2004.**

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# *First Strategic Plan*

## **Major Strategies of the first 3-year strategic plan (ending Oct 2006):**

- *Develop strong outreach program to our membership and potential general user base to build the SER-CAT community*
- Fully Commission 22BM
- Implement sample changing robotics on 22BM
- Develop experimental envelopes that would allow our users to fully utilize the facilities with minimal staff interaction – easy to use
- Develop low energy sulfur data collection capability
- *Working towards providing our membership with remote access capability using 22BM as the test bed – implementation of Access Grid*

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# Outreach Program

- SER-CAT has had a Booth at the annual ACA meetings for the last 5 years.
- SER-CAT's 4<sup>th</sup> annual scientific symposium, "Interesting Structures, Methods and Advances in SER-CAT Facilities", will be hosted by the National Cancer Institute in Frederick, Maryland on Friday, March 16, 2007.
- SER-CAT has implemented a yearly Outstanding Science award, which is open to any user of the SER-CAT facilities. Bin Zhao of Vanderbilt University received the 2<sup>nd</sup> award, recognizing the scientific impact of his work on active site water molecules and substrate hydroxyl groups in oxygen activation.
- SER-CAT has implemented a yearly Young Investigator Award. The 2<sup>nd</sup> award was presented to Jianhua Gan of the National Cancer Institute-Frederick, recognizing his work on structural insight into the mechanism of double-stranded RNA processing.
- **Last years Young Investigator winner, Nicole LaRonde-LeBlanc (NCI) won the 2005 Federation of European Biochemical Societies Journal Prize for best first author paper published in FEBS in 2005 by a graduate student or young post-doctoral scientist.**
- SER-CAT was featured on the TV program World Business Review, which aired on the Bravo network in February 2005.

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Group photo from SER-CAT's 3<sup>rd</sup> Annual Symposium, hosted by Georgia State University

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4th Annual Southeast Regional Collaborative Access Team (SER-CAT) Symposium  
NCI-Frederick, March 16th and 17th, 2007



4<sup>th</sup> Annual SER-CAT Symposium: “Interesting Structures, Methods and Advances in SER-CAT Facilities”, hosted by the National Cancer Institute in Frederick, Maryland on **Friday, March 16, 2007**

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# *Remote Access Program*

For SER-CAT, remote access is defined as providing our membership with a secure capability to perform their experiments at the SER-CAT APS facilities from the comfort of their lab, office, or home. In effect, providing our membership with their own virtual synchrotron at their home institutions.

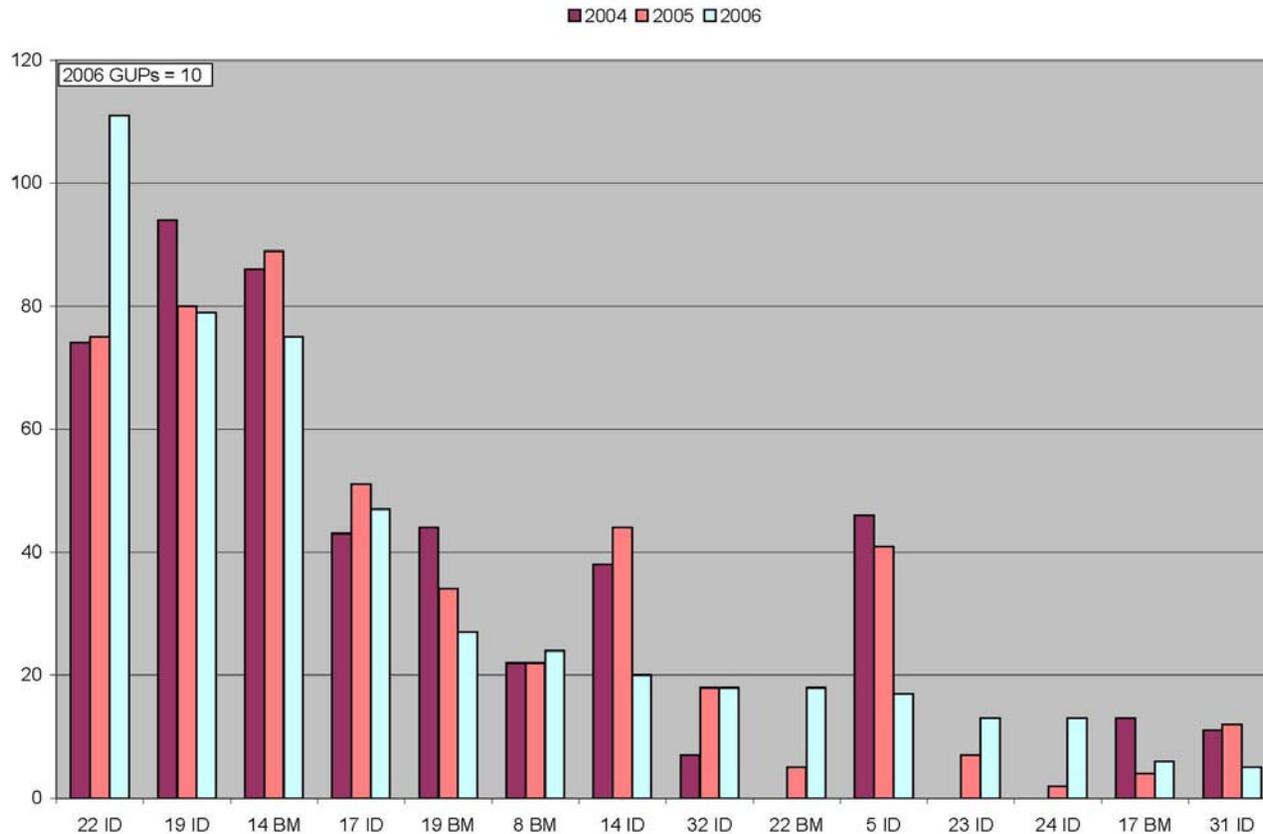
- **Beamline hardware and Software (sergui) designed to support remote operation**
- **AccessGrid Software (<http://www.accessgrid.com>) used for secure tunnel into the APS**
- **25% of membership have successfully tested remote operation on 22BM**
- **22-ID capability will be up and running within 3 months**
- **Will help optimize beam time usage by allowing SER-CAT to change the beamtime allocation structure from 24 hours to 4-6 hours increments**

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# Productivity



Data taken from APS Database

Publications by Beamline

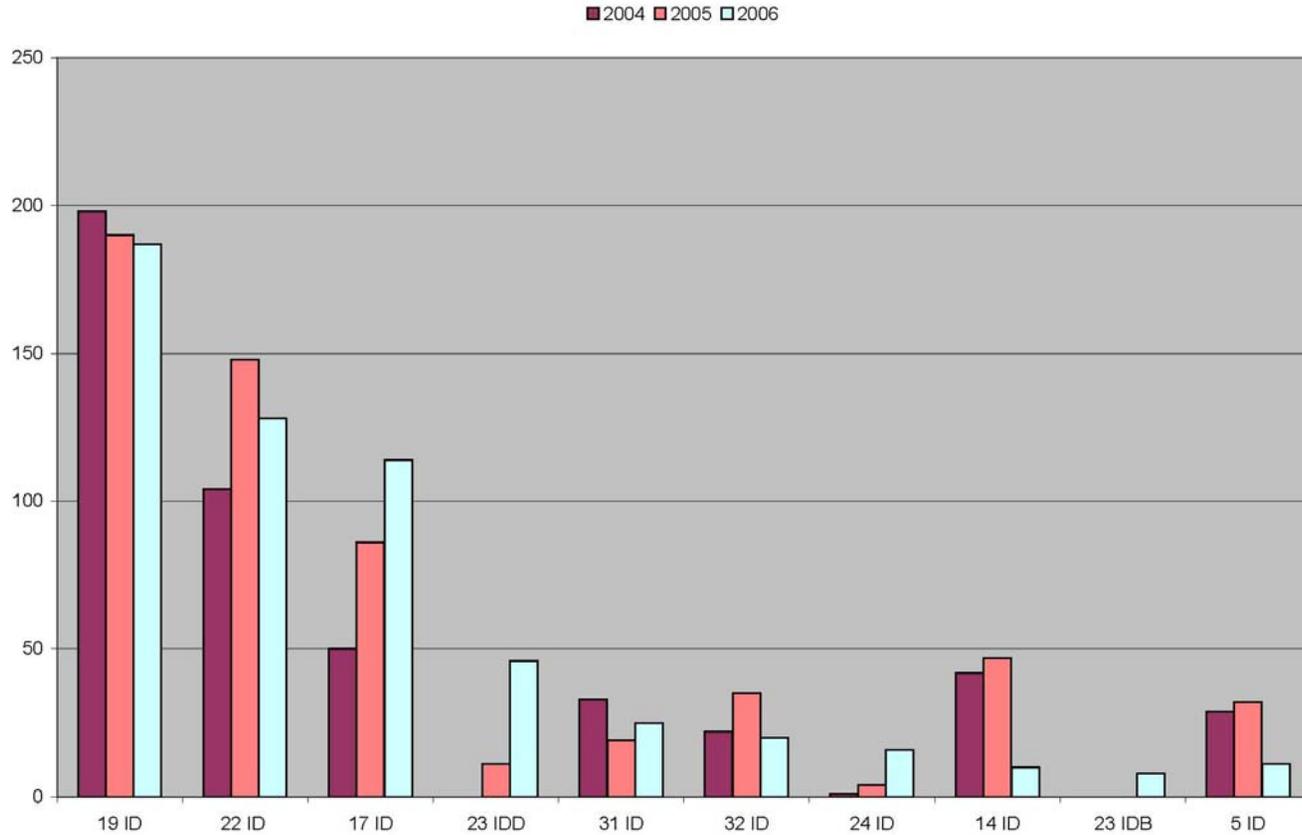
As of 1/18/2007

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# Productivity

Data taken from BioSync.rcs.org hosted  
and maintained by the RCSB PDB



PDBs by ID Line

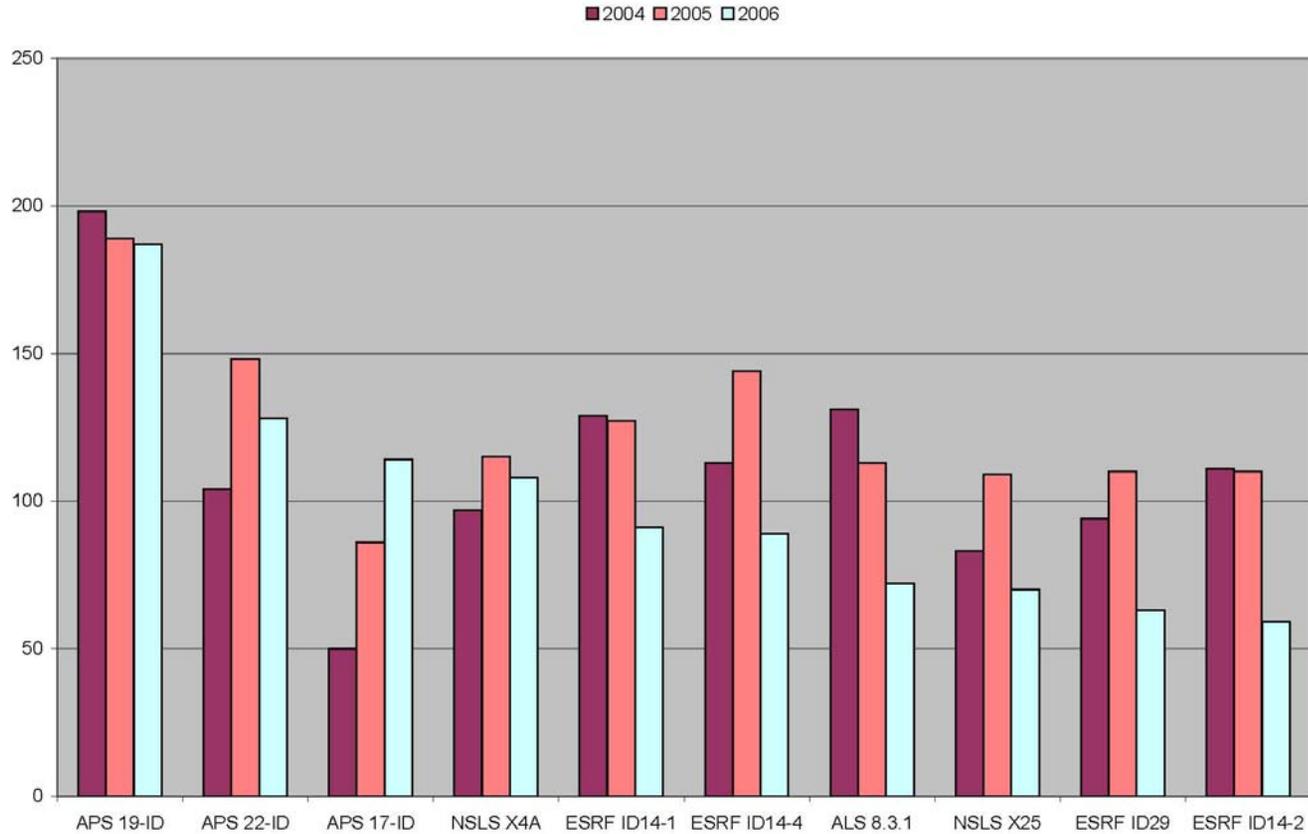
As of 1/18/2007

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# Productivity

Data taken from BioSync.rcsb.org hosted  
and maintained by the RCSB PDB



Top Ten Beamlines with PDBs

As of 1/18/2007

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*Vision for the Future:  
Next 3-year strategic Plan  
(October 2006 – September 2009)*

- *Optimize Optimize Optimize !*
- Implement robotics on 22ID (250 sample capacity)
- *Develop signal based data collection capability*
- Fully Develop/Integrate automated data integration and reduction pipelines
- Fully Develop/Integrate automated structure solution pipelines
- Fully implement remote capability on both beamlines
- *Fully implement the concept of the virtual synchrotron*
- *Radically change beamtime allocation by providing “virtual” shifts as short as 4 hours*

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# *Virtual Synchrotron*

The concept of providing Light When YOU need it! has been evolving over the last 2-3 years. The initial concept included:

- Mail-in data collection services (8 shifts last run)
  - Has been in service for over 3 years now
  - ID and BM line both participate
  - Used over 8 shifts last run
  - 30 data sets collected last run (6 MAD)
- Attended remote access using Access Grid
  - 22BM fully implemented
  - 25% of membership has used remote data collection
  - ID beamline comes online this run

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# *Virtual Synchrotron*

The new concept of providing Light When YOU need it! by providing a virtual synchrotron will not only change the idea of how we use the beamlines, but how we allocate beam time.

*The objective is to optimize the use of the beamlines for quality science!*

- Attended Remote Access
  - Users can effectively use the beamline at any hour of the day from any location
  - Beam time quantum can be reduced from 24 hours to as little as 4 hours
  - Will need to modify how we schedule users
- Un-Attended remote access
  - Not all samples will benefit, but many will – large screening requirements
  - Beamline automation moved to a higher level
  - The objective is to fill in any gaps in beamtime – keep the x-rays flowing!

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# *Signal Based Data Collection*

SER-CAT/UGA have started a program to develop a signal based data collection program, in which either the anomalous signal or data quality of a sample will be measured during data collection. The sample can then be changed when it is no longer viable.

- **Sulfur SAD data collection**
- **Radiation sensitive cryogenic and room temperature samples**
  - **Native**
  - **Anomalous**
  - **High resolution**

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