



The SER-CAT SPECTRUM

A Biannual Newsletter of the Southeast Regional Collaborative Access Team • Summer 2003

Director's Message

Bi-Cheng Wang



Welcome to *The SER-CAT Spectrum*. It brings me great pleasure to reintroduce our bi-annual newsletter to you and to share some current activities taking place at the SER-CAT facility. Although the newsletter was on my mind a great deal, it just was not possible to produce until now due to various time constraints.

Recently, however, SER-CAT hired Ms. Lisa Edge Horanyi as our new Administrative Secretary to assist us in the administrative office. She comes to us with a Bachelor's Degree from the College of Journalism and Mass Communication at the University of Georgia. Now that she is on board, we plan to publish the newsletter on a more frequent biannual basis to keep the membership up-to-date on SER-CAT's accomplishments and research programs.

Since the last newsletter was published, many things have transpired at the SER-CAT facility. One of the most exciting events took place on October 18, 2002, with a ribbon cutting ceremony for the ID beamline. During this ceremony, SER-CAT proudly turned over the facility to its members and welcomed in the operational component of the project. Now that SER-CAT is able to collect usable data on the ID beamline, our main focus is being turned towards completing the



Ribbon Cutting Ceremony, October 2002

BM beamline, further developing our research capabilities for macromolecular crystallography and serving our members.

In this newsletter we emphasize recent activities and current capabilities, introduce you to our staff and some of the exciting goals and research methods planned for the future, as well as highlight some of the scientific accomplishments of our members. We also include information on the upcoming events planned for the SER-CAT community at the upcoming ACA meeting and in October at APS. I hope you enjoy the newsletter and look forward to hearing your comments and suggestions about future editions of *The SER-CAT Spectrum*. News items for upcoming issues are welcomed. Have a GREAT summer!

SER-CAT Staff Highlight

In order to facilitate interactions between members and SER-CAT personnel, this section of *The SER-CAT Spectrum* will highlight the responsibilities of all the SER-CAT staff, both full and part-time. Since most of your communications will be directly with the on-site operational staff, we will highlight this group first in the list. This will allow you to become familiar with their duties and help you to identify them personally during your next visit. We at SER-CAT are dedicated to making your data collection experience pleasant and look forward to assisting you at the facility.

On-Site Operational Team



John Chrzas

John Chrzas, Sector Manager

John is responsible for the overall day-to-day management of the local operations programs. He is in charge of the development and administration of the sector, the local operational budget, commissioning, maintenance and expansion of the SER-CAT's scientific capabilities for our members.

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Stephen Foundling

Stephen Foundling, Macromolecular Crystallographer

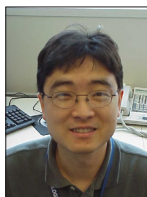
Stephen Foundling, the newest member of the SER-CAT Operations Team serves as wet lab manager and Hazardous Waste Coordinator. He manages the chemical inventory system, provides user support for visiting scientists and handles beamline maintenance and the installation of new equipment.



Marie Graham

Marie Graham, User Support Coordinator

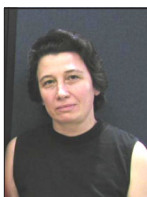
Marie is the first point of contact for on-site beamline related issues. She provides administrative support to the users and local staff and secretarial assistance to the Sector Manager. Marie is also responsible for developing and maintaining the operational section of the SER-CAT web page and maintaining the operational schedules.



Zhongmin Jin

Zhongmin Jin, Macromolecular Crystallographer

Zhongmin Jin's primary responsibilities include: administration of the computer network and the mail-in crystallography program; user support for visiting scientists; maintenance and development of the operations web page; and installation and maintenance of experimental software.



Nadia Leyarvoska

Nadia Leyarvoska, Beamline Scientist

Nadia Leyarvoska handles maintenance of the beamline performance and assists with the installation and commissioning of the beamline. She is responsible for installing new experimental equipment and PMAC programming. She also serves as the Chemical Safety Coordinator and provides user support for visiting scientists.

James Fait, Beamline Control Scientist, and John Gonczy, Beamline Engineer, currently working on construction of the BM beamline, will move to the Operations Team full-time effective in October 2003. Please see the Construction Team's information below for more detailed description of their job responsibilities.

Construction Team



Gerold Rosenbaum

Gerold Rosenbaum, Project Director

Gerold Rosenbaum is the selected builder for the beamline facility and is responsible for the overall design and construction of the SER-CAT site. He oversees the management and construction efforts locally and is in charge of implementing beamline automation.



James Fait

James Fait, Beamline Control Scientist

James Fait is responsible for the installation and maintenance of SER-CAT's beamline control hardware. He handles the PMAC programming, network administration, fire wall management and operational web page development. He is also SER-CAT's Electrical Safety Coordinator. James will move full time to the Operations Team beginning October 1, 2003.



John Gonczy

John Gonczy, Beamline Engineer

John Gonczy is the primary engineer on the construction project. He is responsible for maintenance of beamline and experimental hardware, beamline vacuum systems and the monochromator liquid nitrogen pump system. He is also SER-CAT's Safety Coordinator. John will also move to the Operations Team full time October 1, 2003.



John Unik

John Unik, Project Administrator

John Unik is the on-site administrator responsible for the fiscal components of the construction effort. He handles the local procurements of beamline equipment and serves as a liaison with the APS. John is also responsible for preparing various technical reports and providing progress updates to the SER-CAT Director.

Administrative Office

Bi-Cheng Wang, SER-CAT Director

Bi-Cheng Wang is responsible for the overall management and direction of the SER-CAT Program. This includes membership activities, financial management and technical direction of the entire CAT facility. He is responsible for carrying out all the duties assigned by the SER-CAT Bylaws and for reporting to the membership.



Lisa Horanyi

Lisa Horanyi, Administrative Secretary

Lisa Horanyi is the newest staff member to join SER-CAT and we would like to welcome her to the Administrative Office. Lisa's responsibilities include providing accounting and secretarial assistance to the SER-CAT program and coordinating our communication activities. She is also responsible for producing *The SER-CAT Spectrum*.



Kathy Morris

Kathy S. Morris, Administrative Coordinator

Kathy Morris serves as the official Secretary to the SER-CAT Board and as Administrative Assistant to the Director. She is responsible for the overall SER-CAT budget, membership negotiations and financial reporting. She maintains the official records on behalf of the SER-CAT program.



John Rose

John P. Rose, Assistant Director of SER-CAT

John Rose assists the SER-CAT Director in the overall management and operations of the facility. He also serves as Chair of SER-CAT's Operations Management Planning Committee and is a member of the APS Users Organization Steering Committee.



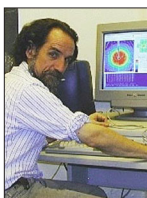
Craig Smith

Craig Smith, Project Coordinator

Craig Smith from the University of Alabama at Birmingham serves as the SER-CAT Project Coordinator for the construction effort. He is responsible for attending and reporting at board meetings and serves as a liaison for the membership.

End-Station Program Support

The SER-CAT operations team has been active in securing adequate programming support for the myriad of projects planned for the upcoming year. We have secured the services of both Andrew Howard and William Lavender to help us provide the best facility to our membership.



Andy Howard

Andrew Howard

Andrew Howard, Associate Professor of Biology at the Illinois Institute of Technology and Chief Scientific Officer of IMCA-CAT, will be working part time with SER-CAT staff this summer in the development of a new SER-CAT control GUI. Professor Howard's participation in the project will be in the software development of a

CCD image display program. The display program will be able to display a wide variety of CCD image formats, as well as provide a number of useful diagnostic tools. The program will incorporate some data processing tools, indexing, strategy development, integration, and scaling using XGEN. The SER-CAT staff is looking forward to working with Andy on this project, as well as possible opportunities in the future.



Bill Lavender

William Lavender

Dr. William Lavender is working part-time with the SER-CAT Operations Team. Dr. Lavender will continue the maintenance and development of his MX beamline control program. Other major projects that Dr. Lavender will be involved in include the software integration of the ALS robotics system as well as integrating the RONTEC fluorescence detector with the XIA multi-channel analyzer, which will provide a large bandwidth energy dispersive fluorescence monitor. There has been a marked increase in the number of zinc-finger and small samples during the last run, which have been very problematic for the current fluorescence detector, and the SER-CAT members should see an immediate impact upon the commissioning of the new fluorescence detector system.

Beamline Capabilities and Future Enhancements

Current Capabilities

The 22-ID construction project is nearing completion, pending the installation of a white beam adjustable primary aperture. This final component will reduce the amount of non-usable radiation in the monochromator, thereby reducing the amount and scattered radiation and reducing thermal effects.

The commissioning phase of 22-ID is progressing according to schedule. The beamline systems are being vigorously tested to provide a robust and reliable facility. The current beamline capabilities include:

Operational energy range:	6 – 13.6 keV
Full energy range:	5.6 – 25keV
Monochromator optics:	Si (220)
$\Delta E/E$ (12keV):	0.5×10^{-4}
Harmonic contamination:	< 0.1%
Vertical focusing:	Elliptically bent mirror
Horizontal focusing:	Sagittal focusing second monochromator crystal
Working focused beam size:	0.3 x 0.3 mm
Minimal focus:	0.06 x 0.03 mm
Flux full beam @ 12 keV:	7×10^{12}
Exp. beam size:	0.1 mm square (using beamline slits)
Exp. flux @12 keV:	3×10^{12}
Beamline control:	MX with staff-generated GUI's
Beamline alignment:	Automated through GUI's
Sample alignment:	Automated through GUI's
Beam stability:	Controlled through feedback systems
Scientific software:	HKL2000, MARf1m, DPS MOSSFLM, SOLVE, CNS, CCP4
Production detector:	MAR 165 CCD
Experimental techniques:	Single wavelength native data collection, single and multiple wavelengths anomalous scattering data collection

The 22-BM construction project has been delayed some due to the effort required to optimize the performance of 22-ID. The 22-BM beamline commissioning program will begin in August 2003, with the crystallographic commissioning scheduled to begin during late 2003.

Upcoming Improvements

Although the 22-ID has performed very well during its commissioning phase, it has encountered a few growing pains during this period. Therefore, the staff is currently working on various upgrades to the system and the following improvements should be implemented in the next year:

- Improved sample visualization using visible light
- Sample visualization using UV
- Sample alignment using diffraction
- Automated sample alignment using different visualization techniques
- Resolve thermal issues associated with the third undulator harmonic for data collection at shorter wavelengths
- Provide a "fixed" exit capability
- Commissioning of a float silicon diode energy dispersive fluorescence detector

Detector Selections

As per the discussions at the March 1, 2003 SER-CAT Executive Board Meeting, both a MAR 225 and a MAR 300 CCD detector system have been ordered for installation on the beamlines. The MAR 225 is ready for delivery in late July or early August of 2003. Upon successful implementation of the MAR 225 detector, the MAR 300 is scheduled for delivery in March 2004.

Future Enhancements

Although the majority of our efforts are significantly focused on completing the construction of SER-CAT's beamlines and refining the operational procedures, we are also pursuing various areas of research to further enhance the overall facility. Described below are just a few of the research activities being developed to provide members with the most state-of-the-art research facility for synchrotron macromolecular crystallography.

Mail-in-Crystallography

As a service to the members for reducing travel expenses associated with on-site data collection, one of SER-CAT's future goals is to realize the concept of providing long-distance remote access to its beamlines. To date, SER-CAT has started a mail-in crystallography program to work out the logistics of administering such a program. In the 2003-2 run, (January – March 2003), a total of 24 hours beam time in five slots were allocated to the mail-in program, and SER-CAT staff collected data for nine research groups from seven institutions. There is indeed a disadvantage with mail-in crystallography, since the users do not actively participate in hands on data collection at the facility; however, the SER-CAT staff is planning to test the feasibility of remote user participation through fast internet connectivity. Once implemented, users may be sitting ten feet or 1,200 miles from the experimental hutch to conduct research with active participation in the data collection and interactions directly with on-site SER-CAT staff.

Integrated Experiment Control

SER-CAT's staff is currently working on an integrated GUI for beamline control system, which is comparable to other designs such as BLU-ICE.

Sample Placement/Centering Automation

SER-CAT is currently collaborating with researchers at the Advanced Light Source (ALS) to integrate the ALS sample changer into SER-CAT's experiment control systems. As shown during previous presentations, automation could increase the beamline usage efficiency by as much as 300% to 500%. The ALS unit will first be installed and tested on 22BM. Installation is planned for late 2003.

Data Collection Using Softer X-Rays

For most elements, including phosphorus and sulfur, the anomalous scattering signal ($\Delta f''$) using 6 - 7 keV X-rays are significantly larger than that observed using 12 keV X-rays. Thus, softer X-rays offer great potential for macromolecular structure determination when these elements are present in the crystal. However, the use of longer wavelength X-rays (1.75 – 2.3 Å, for example) has not been well tested in the past by the synchrotron community. SER-CAT will test and implement procedures for the optimal use of softer X-rays for macromolecular structure determination. To assist this development, a confocal Cr-radiation X-ray source ($\lambda = 2.29$ Å) at the University of Georgia will serve as a test bed of developing softer X-ray data collection and structure determination strategies.

Scientific Highlights

SER-CAT's 22-ID beamline is still undergoing X-ray commissioning and has been accessible to members since October 2002. Five publications have resulted from the data collected, including one that appears on the cover of the May 2003, Volume 10 issue of *Nature Structural Biology* by S. Bencharit, C.L. Morton, Y. Xue, P.M. Potter, and M.R. Redinbo:

- Sompop Bencharit, Christopher L. Morton, Yu Xue, Philip M. Potter and Matthew R. Redinbo, "Structural basis of heroin and cocaine metabolism by a promiscuous human drug-processing enzyme," *Nature Structural Biology*, **10**, 349-356.
- Allen M. Orville, Joey M. Studts, George T. Lountos, Kevin H. Mitchell, Brian G. Fox, "Crystallization and preliminary analysis of native and N-terminal truncated isoforms of toluene-4-monooxygenase catalytic effector protein," *Acta Crystallographica, D* **59**, 572-575, (2003)
- Gali Prag, Saurav Misra, Eudora A. Jones, Rodolfo Ghirlando, Brian A. Davies, Bruce F. Horazdovsky and James H. Hurley, "Mechanism of Ubiquitin Recognition by the CUE Domain of Vps9p," *Cell*, **113**, 609-620, (2003)



- Silke Suer, Saurav Misra, Layla F. Saidi and James H. Hurley, "Structure of GAT domain of human GGA1: A syntaxin amino-terminal domain fold in an endosomal trafficking adaptor," *Proceedings of the National Academy of Science*, **100**, No. 8, 4451-4456, (2003).
- Alexy Teplyakov, Galina Obmolova, Pavel P. Khil, Andrew J. Howard, R. Daniel Camerini-Otero and Gary L. Gilliland, "Crystal structure of the *Escherichia coli* YcdX protein reveals a trinuclear zinc active site," *Proteins: Structure, Function and Genetics*, **51**, 315-318 (2003).

In addition, numerous publications are currently in preparation or are in press and nine structures citing 22-ID APS have been deposited in the Protein Data Bank. One patent has been filed.

How to Acknowledge SER-CAT

Thank you to those members who completed and returned the review questionnaires requested in April. Much valuable information was collected for the development of the proposal for SER-CAT's first APS Sector Review. Although SER-CAT is still in the commissioning phase, it is becoming even more imperative that members include acknowledgments of SER-CAT's facility and the Advanced Photon Source in any publication or presentation that includes data collected at SER-CAT. One of the criteria for measuring SER-CAT's performance at the APS is based upon the number of publications deposited in the APS Publications Database. Therefore, it is extremely important that you include the following two acknowledgement statements in your publications for work conducted at SER-CAT:

SER-CAT acknowledgement:

Data were collected at Southeast Regional Collaborative Access Team (SER-CAT) 22-ID (or 22-BM) beamline at the Advanced Photon Source, Argonne National Laboratory. Supporting institutions may be found at www.ser.anl.gov/new/members.html.

APS **required** acknowledgment in **all** published reports of work conducted at the APS:

"Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-Eng-38."

ACA 2003 Annual Meeting

For the second year, SER-CAT will have a booth at the American Crystallographic Association (ACA) Annual Meeting. This year's meeting will be held at the Northern Kentucky Convention Center just outside of Cincinnati, Ohio, July 26-31. If you are planning to attend, please be sure to come by and visit with some of the staff at booth # 119. We have found that a formal presence at the ACA meeting is a good conduit for information exchange with our members, provides a mechanism for attracting new members, and will in the future be a valuable tool in attracting general users to the facility.

SER-CAT Board Meeting and Second Annual SER-CAT Symposium

The next SER-CAT Board Meeting has been scheduled for Saturday, October 18, 2003 at the Argonne Guest House, in Argonne, Illinois. In conjunction with the board meeting, SER-CAT and the APS will co-host the Second Annual SER-CAT Symposium at the APS on October 17, 2003. Planned topics include: "Getting the most information from the limited sample life (exposure dose) and other strategies to maximize efficiency of data collection." The symposium is open to all all researchers in the crystallographic community, as well as local APS and CAT personnel. Additional information regarding the symposium will be provided at a later date. Hotel reservations for the board meeting are available through the Argonne Guest House at 800-632-8990. Please be sure to reference "SER-CAT Board Meeting" when calling in to receive the discounted room rate.

The SER-CAT Spectrum is the biannual newsletter of the SER-CAT group. Additional information about SER-CAT and the Advanced Photon Source at Argonne National Laboratory can be found at our website www.ser-cat.org or by contacting the SER-CAT Administrative Office at 706-542-3384.

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The SER-CAT Spectrum

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