



The SER-CAT SPECTRUM

A Biannual Newsletter of the Southeast Regional Collaborative Access Team · Vol. 5, No. 2 · Fall 2007

Director's Message

Bi-Cheng Wang



Welcome to the Volume 5, Fall 2007 issue of *The SER-CAT Spectrum*!

In June 2007, SER-CAT marked its tenth anniversary. I am pleased to say that over the years the work of our organization has lead to several significant scientific contributions in the crystallographic community.

This includes solving five structures on site at SER-CAT at the end of 2004 and having SER-CAT place as one of the top ten beamlines in the world for the past three years! We have seen many successes over our ten-year term and have begun to see encouraging results towards routine sulfur phasing. You may find the slides presented at the 9th International Conference on Biology and Synchrotron Radiation (held in Manchester, UK, Aug. 13-17, 2007) titled "Remaining Challenges in Long Wavelength Phasing: The SER-CAT Approach," on our website (www.ser-cat.org). We look forward to even more research advancements in the future.

On a personal note, this has been a very rewarding year for me, as both SER-CAT Director and as a crystallographic researcher. After receiving the first ever SER-CAT Magnolia Award in March, it was announced recently that I would also receive the 2008 Patterson Award from the American Crystallographic Association. I would like to humbly say thanks to all SER-CAT Members, staff and the operational team for helping make SER-CAT one of the most premier beamline facilities in the world. I would also like to say thanks to the crystallographic community for first adopting the use of single isomorphous replacement phasing, and now for its routine use of single-wavelength anomalous scattering phasing that I strongly believed in beginning in the early 1980's.

The current newsletter will also highlight some new applications at the SER-CAT facility, including remote data collection, and routine sulfur-phasing capabilities, reported by John Rose. In addition, SER-CAT's Sector Manager, John Chrzas, will give readers an overview of the new projects and equipment at the facility in a brief technical update.

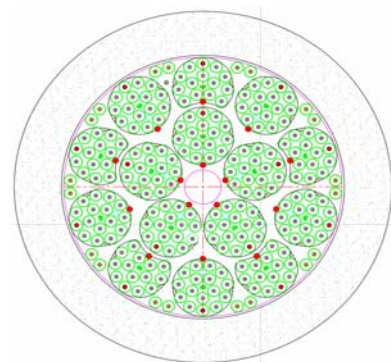
Finally, on the organizational front, more changes are occurring as we say, "Hello" to Sharon Granger, our new User Support Coordinator at the APS, and "Goodbye" to our Assistant Editor, Sylvia White, in the SER-CAT administrative office. You may read more about these changes later on in this edition.

We thank you for your continued support of our program and hope that you will enjoy this issue of *The SER-CAT Spectrum*! Best wishes to you for a wonderful fall season. Please feel free to contact us online at www.ser-cat.org with any comments or questions.

Improved Crystal Automounter at SER-CAT

by John Rose

SER-CAT continues to expand its program in crystal mounting and data collection automation. Shown at right is the new and improved Dewar design for the crystal mounter on 22ID. The new Dewar is capable of holding 230 crystals as well as an assortment of beam alignment tools.



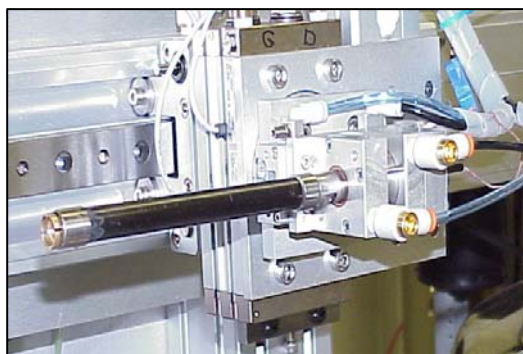
Drawing of the new crystal mounter at SER-CAT

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Crystal Automounter, from Page 1

Designed by John Gonczy, Jim Fait and John Chrzas, the new Dewar/lid assembly has a heat leak of less than 20 Watts. The new design also incorporates an improved LN2 fill system that reduces turbulence within the Dewar during filling, a common cause of crystal icing.

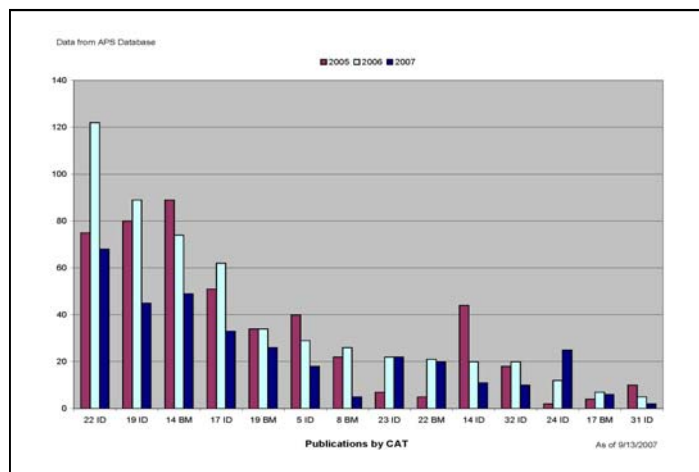


The 22ID automounter also hosts an enhanced crystal gripper (shown above), which has improved thermal properties and is mechanically much more robust than the original ALS designed gripper currently used on 22BM.

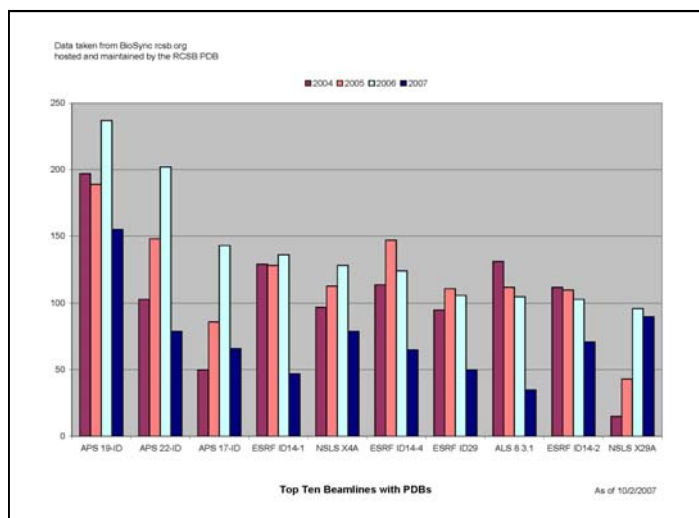
Using the 22ID crystal mounter, and a remote connection, researchers at Wyeth Pharmaceuticals were able to collect over 300 GBytes of data from their home lab in Connecticut during the last run at the SER-CAT facility.

SER-CAT's 2007 Productivity!

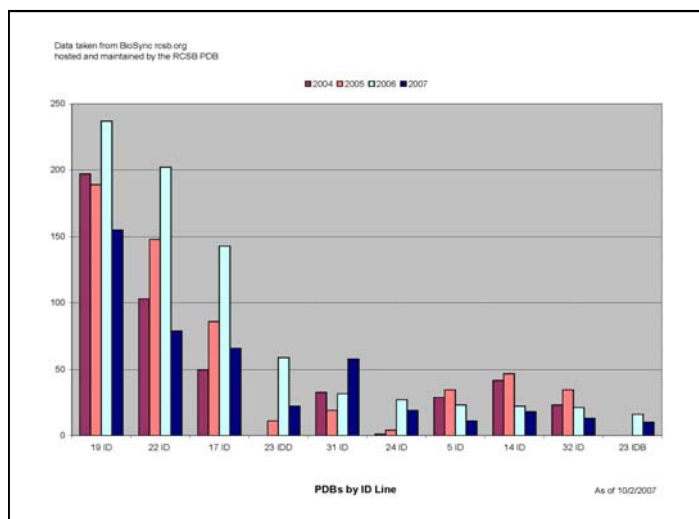
Providing users with a beneficial research environment with positive results is an essential part of SER-CAT's mission, and once again we are pleased to announce our productivity standings for the year. The graphs below reflect our progress at the 22-ID beamline, where we currently have the highest number of publications at the APS for the year! We are also comfortably stationed in the *top five* of the most productive beamlines in the world for the year in PDB submissions, and the 22-ID beamline is once again featured as one of the leading facilities at the APS in PDB depositions!



Publications by Beamline



Top Ten Beamlines Worldwide



Top Ten Beamlines at APS

With the help in submissions of structures and publications by our members and general users, SER-CAT has maintained its standing as one of the better facilities for structural biology research. We sincerely appreciate your diligence in acknowledging SER-CAT in your publications and PDB depositions and ask that you please continue to do so in the future. Information on the proper phrasing for acknowledgements may be found at www.ser-cat.org.

Technical Update

By John Chrzas

I would like to take this opportunity to share with you a few of the projects that the operations team has been working on. In particular, the sample automounting robots and the remote access programs have made a lot of progress during the past year.

Technical Update, from Page 2

Sample Robots

Both beamlines now have sample changing robots installed and operational. We have started to see a steady increase in the number of members using the automounters, and the staff is ready to assist members that may have questions. The 22BM system has a capacity of 96 samples, while the ID system has a capacity of 230 samples. Some important facts about robot usage are:

- (1) Use the correct magnetic caps (The Hampton Research P/N HR4-779)
- (2) Pucks and accessories may be purchased from Boyd Industries, by calling (707) 882-1630 or emailing the company at PBoyd@earthlink.net.
- (3) Pin lengths may vary between 15-24 mm, but should be consistent!

Puck Mounting tools and auto-mounter requirements: the auto-mounter requires a puck tool set, pucks and lids.

Quantity	Item	Price / Each \$	Total \$
1	16" bent cryo tong	\$ 130	\$ 130
1	16" straight cryo tong	\$ 130	\$ 130
1	Puck pusher	\$ 150	\$ 150
1	Puck wand	\$ 150	\$ 150
7	Cryo puck SER-CAT modified *	\$ 60	\$ 420
7	Magnetic cryo puck lid	\$ 110	\$ 770
1	Cryo puck shipping cane	\$1000	\$ 1000
1	Puck separator tool	\$ 350	\$ 3,100

Puck sets are ordered from:
 Peter Boyd, Boyd technologies, Box 95, Manchester, CA 95459.
 Phone (707)-882-1630. Cell (707)-484-7571. Fax (707)-882-1745
 E-mail: pboyd@earthlink.net * request the SER-CAT modified PUCK

Visit us at www.ser.aps.anl.gov/new/robot_automount1.html for more information on the robotic automation at SER-CAT.

The staff has a limited number of pucks and accessories to loan out, but there is no guarantee that the loaners will be available at the time you need them, as they are a hot commodity. We do keep a number of pucks at the beamline, so that members may transfer their samples into the pucks and try out the robots. If you are interested in trying out the robots, please contact the staff so that we may make suitable arrangements to try and best meet your needs.

I would like to thank those of you who helped to debug the hardware and software for the current phase of the robots. Your help was invaluable in providing us with the feedback needed to bring these systems up to their current state. So, as we move forward towards optimized performance and automated screening of samples (something expected in the very near future), we will again ask for more help from the members to ensure that the work is completed quickly and safely.

Remote Access

This past year has been a very busy time for the operations team, as we move forward with the remote access program on both 22ID and 22BM. The success of the sample automounters has been a critical piece of the remote puzzle.

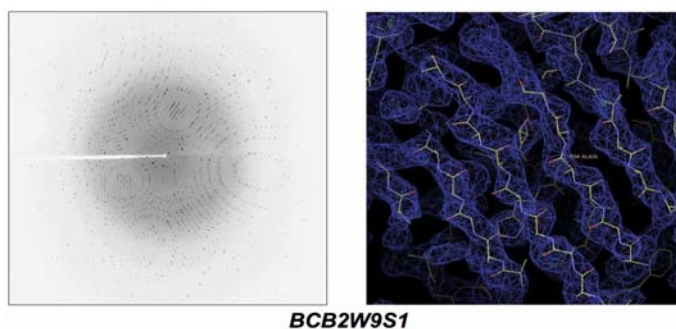
During this last year, we moved away from the Access Grid software in favor of the NX package for providing a secure conduit through the Argonne and APS firewalls. The NX package is easier to install and manage than the Access Grid software, and may be downloaded for free from www.nomachine.com. More importantly, the NX package does a better job at packaging the SERGUI information, which results in a much faster response time for our remote users. If you have not had a chance to look into setting up your remote access to the SER-CAT facilities, now would be a good time to find a few extra minutes to give it a try – we routinely run bench mark tests for members every Tuesday during the APS' scheduled maintenance periods. If you would like some help, please contact either John Chrzas (Chrzas@anl.gov) or Zhongmin Jin (zmjin@anl.gov) for assistance.

We are depending on our membership once again to help debug and optimize the remote access capabilities, as we move towards being able to offer beam time with less than a 24 hour increment. The objective of the remote access program is to bring your SER-CAT beamlines into your every day life, by providing "Light When YOU Need It!"

Progress on Soft X-ray Phasing on 22ID

by John Rose

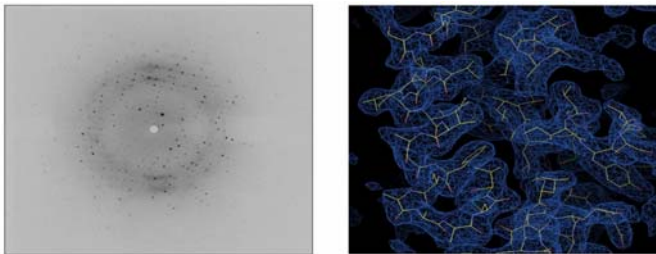
Over the past two years researchers at the University of Georgia together with SER-CAT staff have been working on optimizing the SER-CAT beamlines for sulfur SAS data collection and phasing. In early May, Dr. Liqing Chen (UAH) and his brother Dr. Lirong Chen (UGA) were able to solve a 258-residue protein (BCB2W9S1) using 2Å data collected on ID22 ($\lambda = 1.9\text{\AA}$) based on the anomalous scattering signal from nine sulfur atoms present in the protein. Using SGXPro, the data enabled automatic fitting of 247 of the 258 residues in the protein.



In a more recent example, Mr. Jin-Yi Zhu (UGA), aided by Drs. Lirong Chen (UGA) and Albert Fu (SER-CAT), was able to solve a 95-residue protein (AF1382) based on a 2.3Å data set collected on 22ID ($\lambda = 1.9\text{\AA}$) using the anomalous scattering signal from 5 sulfur atoms. In this case, SGXPro correctly placed 75 of 95 residues in the asymmetric unit. As evident below, the AF1382 crystals did not diffract as strongly as the BCB2W9S1 crystals and two data sets were merged to produce the structure.

(see next page for image)

Soft X-ray Phasing, from Page 3



AF1382

2008 SER-CAT Symposium



Aerial view of the Medical University of South Carolina campus in Charleston, SC.

The 2008 Annual SER-CAT Symposium will be hosted by Dr. Christopher Davies and the Medical University of South Carolina in Charleston, SC, on March 7-8, 2008. This is our fifth annual event, so please mark your calendars and save the dates. The annual symposium will be held on Friday, March 7th and on Saturday, March 8th, the SER-CAT Annual Board Meeting will convene. SER-CAT members are welcome to attend the open meeting on Saturday.

As with our past symposia, participants will be presented with a day of informative talks, demonstrations and workshops. Included in the presentations are the SER-CAT Service Award, the SER-CAT Young Investigator Award and the SER-CAT Outstanding Science Award. If you would like to make an award nomination, please visit us online at www.ser-cat.org for additional information or contact Dr. John Rose by email at rose@BCL4.bmb.uga.edu. The deadline for nominations is January 14, 2008.

More information on the meeting location and local arrangements will be available on the SER-CAT website in the coming weeks. Again, we would like to extend a warm "thank you" to Dr. Chris Davies for hosting the 2008 meeting. We look forward to seeing all of you there!

Highlights from the 2007 ACA Meeting!



View of Salt Lake City, Utah

Salt Lake City, Utah served as a lovely backdrop for the 2007 American Crystallography Association's (ACA) meeting, as once again SER-CAT hosted a booth at the annual event. This year's meeting was held at the Salt Palace Convention Center, July 21 through 26, 2007.

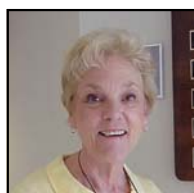
The conference provided attendees with the opportunity to network and share outreach information with individuals and institutions working in the field of crystallography.

Workshops, exhibitions and social ceremonies were spread out over the week, and highlights included contributions by several key SER-CAT personnel and members, including scientific sessions organized by Senior Beamline Scientist, Gerd Rosenbaum and a poster judgment committee organized by Assistant Director, John Rose and arbitrated by SER-CAT members B.C. Wang from the University of Georgia, Edward Collins from the University of North Carolina and Bill Furey from the University of Pittsburgh, along with other scientists in the field. John Horton of Emory University also organized a session talk on "New macromolecular crystal structures," and B.C. Wang of UGA and Manfred Weiss of DESY, Germany conducted a session on "Long Wavelength Phasing." This session was very successful, with the participation of about 120 people and the presentation of good talks, including one by John Rose on SER-CAT's work in this area.

A new generation of researchers also contributed to the conference as University of Georgia graduate student Brett Dillard organized the "Fun Lectures for Young Scientists," entitled, "Vitamin C and Other Essentials for Being a Successful Scientist," and current University of Virginia post-doc and former UGA graduate student, Peter Horanyi, organized the "Margaret C. Etter Early Career Award" session.

This was the sixth year that SER-CAT has hosted a booth at the event, providing participants and users an opportunity to interact with staff on the administrative and operational fronts. We hope you had a chance to visit us and pick up your own "Light When YOU Need It!" flashlight for emergency situations. We hope to see you again next year at the 2008 ACA meeting in Knoxville, TN!

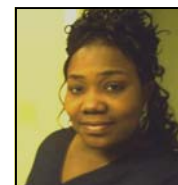
Staff Changes Welcomes & Goodbyes



Sharon Granger

We would like to take this opportunity to say, "Hello" and "Goodbye" to two members of the SER-CAT staff. First, let us welcome Sharon Granger, the new User Support Coordinator on-site at the APS in Argonne, Illinois. Sharon joined SER-CAT in May 2007, after the retirement of Marie Graham. Sharon has several years of administrative and teaching experience in the Chicago area and has already become a key contact for SER-CAT users at the facility. Please join us in welcoming Sharon to the SER-CAT team!

As for our goodbye, we would like to extend our well wishes to *The SER-CAT Spectrum's* Assistant Editor, Sylvia White, as she accepts a new position with the University of Georgia's Carl Vinson Institute of Government. Sylvia's last working day with the SER-CAT Administrative Office is October 24, 2007, so please join us in wishing her much success in her new position. ■



Sylvia White

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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