



The SER-CAT SPECTRUM

A Biannual Newsletter of the Southeast Regional Collaborative Access Team • Winter 2005

Director's Message

Bi-Cheng Wang



Seaon's Greetings from all of us at SER-CAT! As 2004 is coming to an end, we can look back with a smile on what has been accomplished this year and confidently face the changes coming in the New Year. Many achievements have been made over the past year, including some significant advancements since the newsletter in July. Thanks to the hard work of our

members and the dedication of our staff, SER-CAT has grown from a stage of adolescence to maturity. I am very excited about sharing SER-CAT's successes with you, and other activities that may be of interest.

One significant milestone for SER-CAT is the introduction in January 2005 of the General User program on the 22-ID beamline. Members will continue to have the benefit of convenient time slots on 22-ID, as well as additional beamtime on 22-BM scheduled for SER-CAT members only. Productivity on 22-ID has greatly increased this year, in both publications and protein structure submissions to the PDB. In fact, there have been more publications credited to 22-ID than any other ID beamline at the APS!

The capability for high-throughput structure determination has also increased at SER-CAT this year. This has allowed our members to solve more structures than ever at a remarkable speed. On a recent visit from the University of Georgia, researchers determined five structures in the first 23 hours of data collection, with a total of seven structures determined on-site during one visit! This is not only a wonderful achievement for the scientists, but also an excellent testimony to the outstanding efforts of the SER-CAT Operations Team.

In addition to our progress at the beamline, SER-CAT has continued to be involved in various outreach efforts. As in the past, SER-CAT had a very strong presence at the 2004 ACA Meeting in several ways. In addition to our exhibit booth, there were several SER-CAT members and staff that played a significant role in organizing the meeting, whom will be recognized later in this issue. In March 2004, the University of Alabama at Birmingham hosted a productive symposium on Synchrotrons and Structural Biology. For 2005, we will have our second member-hosted symposium at St. Jude's Children's Research Hospital in Memphis, Tennessee, on Friday, March 18.

Also new in 2005 is the introduction of the SER-CAT Young Investigator Award and the SER-CAT Outstanding Science Award. The deadline for nominations for both awards is quickly approaching, so please be sure to read on for additional details regarding how to nominate yourself or a deserving colleague!

I believe that all of the new developments over the past year will serve to enhance the benefits of SER-CAT membership, but we are always open to new ideas for improving our program. Please feel free to contact us with any suggestions on how we might better serve you. Best wishes for a healthy, happy and prosperous 2005!

SER-CAT General User Program Begins

The APS General User Program for 22-ID goes in to effect on January 1, 2005, and the applications are already coming in. It seems that all of our dynamic scientific achievements have not gone unnoticed! We, of course, will continue to first serve the interests of our members; however, the General User Program will now account for 25% of available beamtime on 22-ID. Fortunately, the APS Beamtime Allocation Committee is helping ease this

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General User Program Begins, from Page 1

transition by allowing us a percentage of well rounded users that will benefit our scientific program and possibly our membership as well.

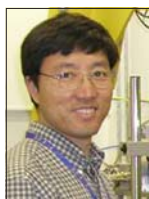
Many of our members have taken advantage of using the 22-BM beamline throughout 2004, and beamtime will be scheduled separately for members only beginning in January. Sector Manager, John Chrzas, reports that members are routinely collecting data on 22-BM without incident. Schedules for both beamlines are available at www.ser-cat.org.

Publications and Structures

We have made great strides in the number of SER-CAT publications and structures in 2004. As our beamline capabilities have increased, our members have become more diligent in their efforts to acknowledge SER-CAT. In addition, our User Support Coordinator, Marie Graham, has actively been conducting detective work to find any publications or structures that may have fallen through the cracks. This is helping us by ensuring that SER-CAT's efforts are properly counted.

We are happy to report that to date, SER-CAT has 83 publications in the APS database, and this number is constantly growing! This is more than any other ID beamline at the APS in 2004 – quite an achievement! We have also reached and surpassed the milestone of 100 structures deposited into the Protein Data Bank.

Five Structures in 23 Hours and 7 Structures Total On-Site at SER-CAT



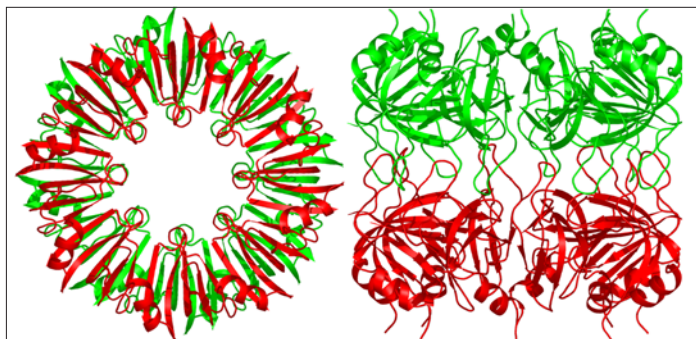
Dr. Zhi-Jie
(James) Liu

On a recent visit, a team from the University of Georgia led by Dr. Zhi-Jie (James) Liu was able to solve five structures in 23 hours at SER-CAT. Eight structures total were solved from the data collection, and seven of these were solved on-site during the visit. User Coordinator Marie Graham announced, "It's got to be a record!" Indeed, it is a record for SER-CAT, and possibly a world record for work performed at a synchrotron facility. *The SER-CAT Spectrum*

asked Dr. Liu to comment on this outstanding achievement, how it was accomplished and what it may bring for the future.

Dr. Liu feels this achievement is a culmination of advancements to the SER-CAT beamline and the recent changes to the infrastructure within the Southeast Collaboratory for Structural Genomics (SECSG), where Dr. Liu is leader of the newly formed "Crystallomics" group. Prior to this visit, the best trip that Liu's team had to SER-CAT was one where three structures were obtained in 24 hours. Dr. Liu commented, "Nothing like this has ever happened before. This is a great opportunity to show how high-throughput structure determination is possible. We are achieving

our goals and can also offer this capability to the scientific community."



Top view and side view of Pfu-1806301: The seventh structure solved in one visit by Liu's team on-site at the SER-CAT facility.

The UGA team used a combination of different techniques and technologies to produce these results. One key technique is the use of "Direct Crystallography," a theory proposed by Dr. Bi-Cheng Wang in which only single wavelength anomalous scattering data is used. Dr. Liu's team is also highly trained in sulfur phasing and has developed suitable procedures for collecting best diffraction data as accurate as possible from given crystals. After data is processed at the beamline, a SCA file is produced, and the team submits a calculation through the web interface to a 128-processor cluster at UGA using a HTP structure determination pipeline called "SC2Structure". The UGA pipeline has hundreds of jobs running simultaneously, and results are checked via the web. The pipeline makes the high-throughput structure determination possible. "We are fortunate to have this time-saving tool," says Liu. "Most crystallographers run a job then check results. Our program combines the jobs and screens all the parameters. It is like having hundreds of crystallographers working together."

While several techniques were utilized on-site, Dr. Liu acknowledged that this event could not have been achieved without proper preparation before the beamtime. "All crystals are mounted and screened at our home source using a state-of-the-art ACTOR robot, which can scan 100 crystals in eight hours," Liu explains. "This gives us a good idea of what we have before we get to the beamline, so we really save time and money – an important step for the most productive use of valuable synchrotron beamtime."

Advancements to our beamlines over the past year have greatly aided Dr. Liu in his research. Liu remarks, "SER-CAT has been constantly improving, and we see the difference on each visit. There are two elements that I believe have greatly contributed to our success. First, the beam is really stable – this is the key to excellent data. Second is the ease of using SERGUI for beamline control. This program is very intuitive, so there is no tedious work involved in operating the beamline. We routinely use SERGUI, and while it is still under development, it continues to get better and better. Overall, SER-CAT has a well thought out

Five Structures in 23 Hours, from Page 2

design that has helped us achieve many goals.” The staff at SER-CAT is pleased with this recent example of what our beamlines can do, and others at APS are taking notice as well. Ms. Susan Bar Strasser, Manager, APS User Administration and Support, has already congratulated the staff on this spectacular achievement.

Dr. Liu believes that the data collection technique used by his team will be able to help many crystallographers. “Lots of crystallographers know, but beginners may not be aware of all factors that can affect data quality. We will publish this technique and also show what to avoid during data collection,” says Liu. “In addition, our pipeline – the workhorse of our operation – can be made available to other institutions.”

Dr. Liu’s team works for Dr. Bi-Cheng Wang at the University of Georgia. “All of our operations are under the direction of Dr. Wang,” Liu proclaims. “None of this would be possible without his guidance. I would like to take this opportunity to thank him for his leadership and direction. Also, I would like to emphasize that this achievement is truly a result of team work between our SECSG team and the SER-CAT operations staff.”

ACA Annual Meeting

For the third year in a row, SER-CAT hosted a booth at the ACA meeting. Many of our members played an important role in the success of the 2004 meeting. Notably, Marilyn Yoder of Uni-



2004 Program Chair Marilyn Yoder & Local Chair Karl Volz



2004 Local Chair Bernie Santarsiero

versity of Missouri-Kansas City organized a fascinating, well-rounded program as Program Chair for the meeting, along with Co-Chair Christer Ackero. Members Karl Volz and Bernie Santarsiero of Uni-

versity of Illinois at Chicago served as Local Chairs, coordinating all local arrangements and ensuring that everything ran smoothly. With the meeting held in Chicago, participants were able to take advantage of the short distance to the Advanced Photon Source. Several



Participants at Jim Fait's ACA workshop.

workshops were held at APS, including a very productive hands-on workshop by SER-CAT Beamline Scientist, Jim Fait, on MAD/SAD Phasing, Data Collection, Processing and Structure Solution. Also, Senior Beamline Scientist, Gerd Rosenbaum, contributed to

the meeting at the conference site, organizing a session on radiation damage.

The next ACA Annual Meeting is scheduled for May 28 – June 2, 2005 at the Walt Disney Swan and Dolphin in Orlando, Florida. This year’s program is being chaired by another SER-CAT member, Ed Collins of University of North Carolina at Chapel Hill. Thank you, Ed, for stepping up to this challenging job, and we are looking forward to another enjoyable, informative meeting at a fun location.



Members Ed Collins of UNC Chapel Hill and John Rose and Wolfram Tempel of UGA take a break at the SER-CAT booth at ACA 2004. Dr. Collins is ACA 2005 Program Chair.

Symposium/Board Meeting at St. Jude Children’s Research Hospital

After our 2004 symposium at the University of Alabama Birmingham, Dr. Stephen White of St. Jude graciously offered to host the next SER-CAT Symposium. The 2005 event will be held on Friday, March 18 at St. Jude Children’s Research Hospital in Memphis, Tennessee, and will be followed by the Board meeting on Saturday, March 19. We look forward to an interesting day of talks, demos and workshops from SER-CAT members and staff. Also, this is a great opportunity to see the wonderful facility at St. Jude Children’s Research Hospital and learn more about the latest research activities taking place there. And, while you are in town, you might like to enjoy some good Memphis blues and barbecue!

As part of the 2005 SER-CAT Symposium, award recipients of the SER-CAT Young Investigator and Outstanding Science awards will be given the opportunity to discuss their research activities. More details on these two awards appear in the following article. A full meeting schedule and registration information will be distributed to our members once available. Thank you to Stephen White and his colleagues for providing this opportunity.



St. Jude Children’s Research Hospital

Last Call for Nominations

The SER-CAT Science Awards are new for 2005. They were both introduced to encourage scientific growth in our program and to recognize individuals that have made the most significant achievements in science each year. The deadline for nominations is January 15, 2005, so do not delay! Award recipients will have their name added to a permanent plaque at the SER-CAT facility and will also be invited to present a lecture on their research at the upcoming symposium at St. Jude Children's Research Hospital. Specific details and nomination instructions for each award are as follows.

SER-CAT Outstanding Science Award

The SER-CAT Science Committee is offering an award for outstanding science carried out at SER-CAT during the previous year. The Outstanding Science Award is open to any researcher or research group carrying out experimental activities at SER-CAT.

The award will be presented at the annual SER-CAT Symposium. The recipient of the award will also be invited to present a 40-minute lecture on his/her research related to the award at the symposium. In addition, the winner's name and institution will be recorded on the master plaque displayed at Sector 22.

Nominations for this award must include the following:

- A one-page description of the work for which the award is proposed (*note SER-CAT must have played an important role in the work described*)
- A single publication related to the work published during the eligible year together with a statement describing the significance and impact of the work (*note SER-CAT must be properly acknowledged in the publication and related PDB files*)
- A current CV
- Names of two individuals that have agreed to write supporting letters
- The signature of the nominator

SER-CAT Young Investigator Award

The SER-CAT Science Committee is offering a Young Investigator Award to recognize an important technical or scientific accomplishment by a young investigator (within two years of his/her Ph.D. degree) at, or of benefit to, SER-CAT. The award is open to both post-doctoral and senior graduate students from any institution carrying out experimental activities at SER-CAT.

The award will be presented at the annual SER-CAT Symposium. The recipient of the award will also be invited to present a 20-minute lecture on his/her research related to the award at this the symposium. In addition, the winner's name and institution will be recorded on the master plaque displayed at Sector 22.

Nominations for this award must include the following:

- A one-page description of the work for which the award is proposed (*note that SER-CAT must have played an important role in the work described*)
- A single publication related to the work together with a statement describing the significance and impact of the work
- A current CV
- For student nominees, a statement of career goals and how they envision the role of the APS in their future
- Names of two individuals who have agreed to write supporting letters
- The signature of the nominator

Please note: It is the responsibility of the nominators to request supporting letters, which should be sent under separate cover.

Complete packages (nominating information and letters) for both the Outstanding Science and Young Investigator awards must be received **no later than January 15, 2005**.

Nominating packages and letters should be sent to:

Prof. John P. Rose
Chairman SER-CAT Science Committee
Room B204B Davison Life Sciences Complex
University of Georgia
Athens, GA 30602

Staff Changes

It is with mixed feelings that we announce the departure of former SER-CAT Beamline Scientist, Nadia Leyarovska. Nadia left her position at SER-CAT in September to accept a position at XFD-BES (Sector 11), also located at the Advanced Photon Source. While we were all sad to see Nadia go, this was a promotion for her, and we are very happy that she has advanced in her career. Nadia joined SER-CAT in July of 2002 and played a very important role in the commissioning and operation of 22-ID, robotics, and user support, among other things. The Operations Team, along with the help of Andy Howard of Illinois Institute of Technology, are all working together to fill her shoes while we search for a talented, hard working replacement. Thank you Nadia, for all you have done for SER-CAT and best wishes in your future endeavors.



We'll miss you Nadia!

Some staff changes took place in the SER-CAT Administrative Office at the University of Georgia as well. Kathy Morris, who has served as Administrative Coordinator since the inception of the SER-CAT program, is now working part-time while back in school pursuing a degree in social work. Lisa Horanyi, who joined

Staff Changes, from Page 4



Trelle Baker

SER-CAT as Administrative Secretary in February 2003, has taken over the other half of Kathy's duties while working part-time on other projects at the University of Georgia. Trelle Baker was hired in September to fill the vacant full-time position of Administrative Secretary. Trelle has several years of university experience and most recently worked in the Human Resources Department. We are very pleased to have her working with us and would like to welcome her to SER-CAT.

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 706-583-8243.

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The SER-CAT Spectrum

Bi-Cheng Wang Director/Editor
Lisa Edge Horanyi Assistant Editor

SER-CAT Administration

Bi-Cheng Wang, Director
John P. Rose, Assistant Director
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Kathy S. Morris, Administrative Coordinator
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John Chrzas, Sector Manager
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SER-CAT Administrative Offices
University of Georgia
B202 Life Sciences Building
Athens, GA 30602-7229

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