The
SER-CAT SPECTRUM

A Biannual Newsletter of the Southeast Regional Collaborative Access Team • Vol. 4, No. 2 • Fall 2006

Director's Message

Bi-Cheng Wang

Welcome to the Fall 2006 issue of *The SER-CAT Spectrum*. It has been a busy and productive period, as we've experienced an array of scientific meetings and conferences at SER-CAT. As you'll read in this issue, these include the annual SER-CAT Executive Board Meeting, the third annual SER-CAT Research Symposium, completion of our second sector review by the Advanced Photon Source, the SER-CAT Booth at the annual ACA meeting in Honolulu, Hawaii and the Study on High-Speed Data Transfer from SER-CAT.

In March we held our third annual SER-CAT symposium at Georgia State University where a team of colleagues from Georgia State University, the Argonne National Laboratory, the University of Georgia and the Southern Light Rail successfully demonstrated the use of a high-speed, direct point-to-point connection between Georgia State University and the Argonne National Laboratory in Chicago. The demonstration brought the ultra fast data transfer capability and the concept of a "virtual synchrotron for the home laboratory" a step closer to reality.

During this period, SER-CAT has also had a steady flow of scientific productivity from both our membership and the General Users. The ID and BM beamlines have undergone changes, as they have become more mature and improvements have continued.

We are making strides and look forward to accomplishing even more in the coming months. Through our membership and dedicated staff, we continue to reinforce the goals of SER-CAT by offering a user-friendly research facility that provides accessibility and precise synchrotron quality.

On the operational and administrative front, we are pleased to have two new staff members onboard. Please join me in welcoming Dr. Zheng-Qing (Albert) Fu and Ms. Sylvia White. We have more information about them later in this edition of *The SER-CAT Spectrum*.

Please continue reading about our events of the past months and aims for the future. We look forward to bringing you more information and updates on our progress, as we strive to provide enhanced services for our members. Feel free to contact us with suggestions or comments and be sure to visit us online at www.ser-cat.org.

3rd Annual SER-CAT Symposium at Georgia State University

The third annual SER-CAT Symposium entitled, *"Interesting Structures, Methods and Advances in SER-CAT Facilities"* was held at Georgia State University in Atlanta, Georgia on March 10, 2006. The goal of this year's symposium was to combine stimulating structural discoveries with practical aspects of the tools and improvements made at the SER-CAT beamlines from a user's perspective.

Symposium participants gather outside GSU for a group photo.

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Interesting Structures

The morning session opened with an award presentation for the new SER-CAT Service Award (please read more about this later on in the newsletter). Talks during the session were devoted to the topic of "Interesting Structures" and it was chaired by Xiaodong Cheng. The session began with a talk by Theodore Jardetzky (Northwestern University), titled, "Extreme machines: the paramyxovirus fusion protein," where he discussed how this research provides insight into how viruses infect target cell membranes.

Stephen White (St. Jude Children's Research Hospital) followed with a presentation entitled, "Looking at active sites from a drug design perspective – focus on bacterial fatty acid and folate synthesis," in which he talked about working to solve the crystal structure of fatty acid synthesis enzymes and the evolution of the two-step enzyme mechanism.

Brian Geisbrecht (University of Missouri-Kansas City) presented, "Structural and Mechanistic Studies of Immunomodulatory Virulence Factors from *Staphylococcus aureus*," which focused on the study of staphylococcus pathogens and their effect on infections in the nervous system.

Karl Volz (University of Illinois Chicago) spoke on, "Structure of Iron Regulatory Protein-1:Ferritin IRE Complex," and the use of protein crystallography and molecular biology to analyze the structural determinants of protein function in a variety of cellular regulatory processes.

Interesting Methods and Approaches

Structural image of a HIV protease protein.

The focus of the afternoon session of the symposium was on the methods and approaches that are of interest to structural biologists in general. Presentations during this time included Pat Weber, Consultant to ExSAR, who discussed, "Using H/D exchange to design recombinant proteins more likely to crystallize," and Alex Wlodawer (National Cancer Institute) on, "The structure of HTLV-1 protease – hard to solve, but worth it," an oncovirus that affects over 30 million people. It is hoped that this structure will spur better drug development in the fight against both AIDS and leukemia.

Brian Savory (Southern Light Rail) presented on, "UltraHigh-speed (GigE) connection for data transmission from SER-CAT." He discussed establishing a connection between locations and enabling a more collaborative research environment between institutions.

Both Jim Fait (SER-CAT) and John Rose presented on "Advances in SER-CAT Facilities," and offered information on sample structures and remote operations in data collection. This and the ultra-high speed connection demonstration brought the concept of virtual synchrotron for the home laboratory a step closer to reality.

John Chrzas, Jim Fait and John Rose fine-tune their remote access demonstration during the symposium.

SER-CAT Award Winners

Michael Cassidy receives SER-CAT's first Service Award from Bi-Cheng Wang.

As part of this year's symposium, SER-CAT presented its second annual Outstanding Science Awards, to recognize exceptional work carried out at the SER-CAT facility and newly established SER-CAT Service Award. During the opening remarks, Mr. Michael Cassidy, President and CEO of the Georgia Research Alliance (GRA) received the first SER-CAT Service Award for his vision and GRA's financial support towards SER-CAT during the initial stages of its development.

Jianhua Gan receives the 2006 Young Investigator Award.

During the afternoon session Dr. Jianhua Gan of the National Cancer Institute won the 2006 SER-CAT Young Investigator Award for his work in the structural biology of double-stranded RNA processing by ribonuclease III.

Bin Zhao receives the 2006 Outstanding Science Award.

Dr. Bin Zhao from Vanderbilt University Medical Center won the SER-CAT Outstanding Science Award for his work in the role of active site water molecules and substrate hydroxyl groups in oxygen activation, which was published in *The Journal of Biological Chemistry*. Both scientific awardees gave presentations on their recognized works at the symposium.

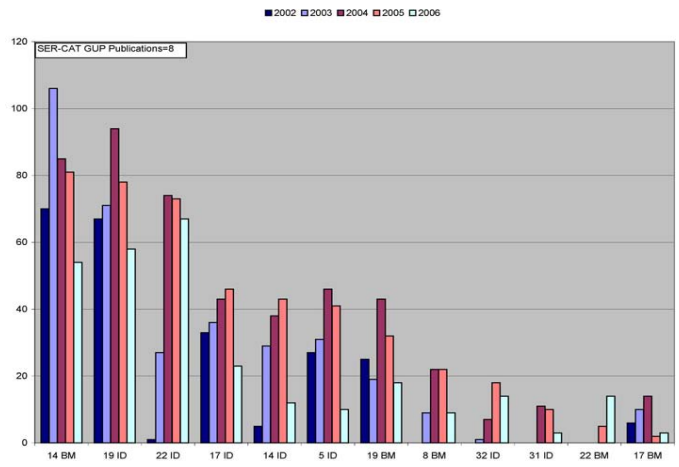
We would like to acknowledge and sincerely thank Irene Weber for hosting the SER-CAT Symposium at Georgia State University. We would also like to thank our 2006 award winners for their outstanding support and acknowledgement of the SER-CAT facility.

If you would like to see additional details on this year's event, including photos, please visit our website at www.ser-cat.org.

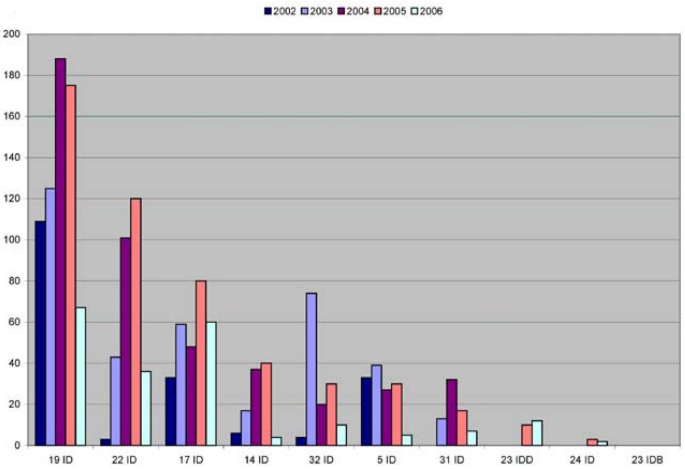
SER-CAT's on the Rise!

One of the goals at SER-CAT is to provide users with a first-rate beamline experience. The two most obvious measures of achievement in the field of crystallography are by depositing the structure coordinates into the PDB and by journal publications. Last year we announced the 2004 scientific productivity results of the 22-ID beamline and even then our numbers were steady and growing.

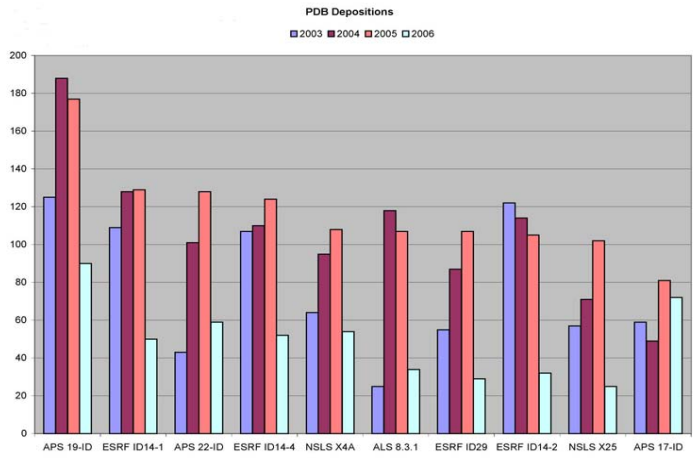
We are thrilled to announce for 2006 that SER-CAT is on the rise in the listings of top beamlines in the world. The graphs below reflect how the user-program at 22-ID has increased in numbers of publications and PDB submissions. As you can see, 2005 was a stellar year and 2006 is shaping up to be yet another! With a little over half the year gone by so far, we are currently ranked as the third top beamline in PDB depositions, third in overall top beamlines and first in publications!



Publications by Beamline



PDB Depositions by ID Line



Top Ten Beamlines

Several elements have helped enhance productivity, including effective use of beamtime by members, as well as, structures and publications submitted by general users conducting research at SER-CAT. SER-CAT currently has a total of 334 PDB entries and 276 journal publications to its credit.

We greatly appreciate the acknowledgments given to us by our users. Please be sure to continue crediting SER-CAT when depositing structures into the PDB and in your publications. Information on the proper phrasing of acknowledgements may be found on our website at www.ser-cat.org.

Researcher Highlight

Brian Geisbrecht,
University of Missouri at Kansas City

As an ongoing feature of the SER-CAT Spectrum, we continue to recognize researchers who are making strides in the crystallographic community with their work. Dr. Brian Geisbrecht of the University of Missouri at Kansas City (UMKC) is becoming one of the new generation of scientists making ground-breaking finds in the field.

We asked Dr Geisbrecht to take a moment to discuss how SER-CAT has helped in his data collection. His energy, when talking about the benefits at the beamline, was both infectious and rewarding to hear.

Dr. Geisbrecht's work at UMKC focuses on immune responses and the structural biology of infectious diseases, all of which has been approached primarily through crystallography, as he says, "We've done three structures that have told us a lot about how bacterial pathogens shut off the host immune system."

"We work on the structural biology of infectious diseases. We're interested in secreted proteins from bacterial pathogens that help make us sick and the way that they do that is through changing or shutting off what we call host defense processes".

Geisbrecht, from Page 3

As he works on publishing his results, Dr. Geisbrecht says that SER-CAT has been instrumental in his research teams findings and an important reason why he enjoys his work at UMKC. As he states, "We've really only been doing active research here [at UMKC] for a year. I don't mean to sound like an advertiser guy, but what's really made that possible is the fact that we have access to the facilities up in Chicago and it allows us to get the most results that we can in the quickest fashion that we can."

Having been at UMKC for only two years, Dr. Geisbrecht completed his post-doctoral work at Johns Hopkins University and then accepted his position with the University of Missouri at Kansas City in August 2004. A hope of getting results from his work in crystallography, via UMKC's access to SER-CAT's beamlines, became a deciding factor for him to move from Baltimore, Maryland to Kansas City, Missouri, as he says, "We simply can't do those kinds of experiments here at our home lab and even from where I came from, we didn't have access to those sorts of facilities at all. I think the biggest reason we've been able to get this much done so quickly is because we've had access to the beamline. For me, that was one of the biggest reasons why I took this job. For me, it was a huge deal."

Dr. Geisbrecht's research is funded by a grant from the University of Missouri Research Board and a grant from the National Institutes of Health, National Institute of Allergy and Infectious Diseases.

For more information, visit: http://www.niaid.nih.gov/dir/ or contact Dr. Geisbrecht by email at: geisbrechtb@umkc.edu

SER-CAT Sector Review Meeting

As part of its three-year scientific review by the APS, SER-CAT presented its accomplishments to the APS Sector Review Panel at the Advanced Photon Source of the Argonne National Laboratory on July 11, 2006. During the review, SER-CAT was asked to provide a profile of the organization and its results over the past several years. Presentations were given by researchers, including a General User, who have made significant exploratory accomplishments in crystallography while collecting data at the SER-CAT beamlines. Dr. Bi-Cheng Wang, SER-CAT Director, also spoke on the past accomplishments and future objectives of the SER-CAT program.

Included in the list of speakers were: Dr. Fred Dyda (National Institutes of Health) who spoke on his work regarding the three dimensional structure of an eukaryotic DNA-transposase; Dr. Joshua Warren (Duke University), who discussed the work of he and Dr. Lorena Beese (the 2005 SER-CAT Outstanding Science Award recipient, also from Duke University) on phasing a large protein/DNA complex at moderate resolution; the 2005 SER-CAT Young Investigator Award winner, Dr. Nicole LaRonde-LeBlanc (National Cancer Institute at Frederick), who presented on the structural studies of the RIO kinases, Atypical Serine Kinases Required for Ribosome Biogenesis and Cell Cycle Progression; Dr. Brian Geisbrecht (University of Missouri at Kansas City) who presented on the structure mechanism of staphylococcal inhibitors; Dr. Zhi-Jie (James) Liu (University of Georgia) who discussed High Throughput Structure Determination at SER-CAT, where he and his research team accomplished an amazing feat of solving five structures in 23 hours; and Dr. Joseph Brunzelle (Northwestern University) who presented his work on the structure and mechanism of the lantibiotic cyclase in nisin biosynthesis.

The day proved to be both successful and enlightening, as a tour of the sector was provided to the reviewers to further highlight the past accomplishments and future work planned at the facility.

The Review Panel was especially interested in the experimental phasing capabilities (such as sulfur phasing) with longer wavelengths and encouraged SER-CAT to further develop this technology, as well as SER-CAT's ongoing Remote Access capabilities.

Thank you to all of our presenters and the SER-CAT staff for their contributions to our Sector Review. SER-CAT would also like to thank the APS and the SRP Committee Members for their review of our continuation plan.

Speakers, from left to right: Zhi-Jie (James) Liu, Bi-Cheng Wang, Nicole LeRonde-LeBlanc, Brian Geisbrecht, Joshua Warren, Joseph Brunzelle and Fred Dyda.

Technical Update

The past year has seen a number of major milestones for the SER-CAT facility. The ID beamline has seen the full implementation of the APS general user program, and the bending magnet beamline has finished its commissioning phase. During this busy time, the operations staff has also been working on a number of projects that will improve the technical and scientific capabilities of the facilities such as the SERGUI control program, the sample changing robot on 22BM, and the remote access program.

SERGUI is the control program that is the hands and eyes of the facility. SERGUI is a WX-Python based tab notebook formatted graphical user interface that controls all aspects of beamline optimization and alignment, as well as actual data

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SER-CAT robot located at BM-22 endstation.

collection (using the MAR remote server protocol). During the last year SERGUI has replaced the MARCCD program as the main user interface to the MAR detectors, which was necessary to achieve the level of control required to move ahead with the remote access program. An image display program is under development, which when completed will totally eliminate the need for the user to interact with the MARCCD program. During the last 6-months, SERGUI has been modified to control the sample changing robot installed on 22BM, and has begun to develop and integrate the tools required to fully support a remote capability such as automated strategy (using the XGEN data processing program) and run list generation, automated data integration and scaling (using XGEN), insitu monitoring of anomalous signal strength (using SGXPro), and automated structure determination and refinement (SGXPro).

During the last 6-months, the sample changing robot on 22BM has reached a mature state of operation. A large number of members have used the robot to screen and collect their data. To facilitate our member's use of the robot, the operations team has purchased a number of spare sets of the equipment required to use the system including: pucks, tools, and sample caps pre-mounted with litho-loops of various sizes. Any member that does not have the required equipment may contact the operation staff and we will supply a short term loan of the equipment to allow you to try the system.

With the maturation of both the SERGUI and the sample-changing robot, the remote access program on 22BM has started its commissioning phase. During the last year we have had a number of successful live remote demonstrations including the ***1st Annual UK-Southeast USA Symposium*** on *"Structural Genomics and proteomics of Membrane and Metalloproteins"* held at University of Georgia on October 16, 2005 and at the 3rd Annual SER-CAT Symposium: *"Interesting Structures, Methods and Advances in SER-CAT Facilities"* held at Georgia State University on March 10, 2006. A few members have also successfully used the remote access program to collect data (NIH and UGA). The operations team is looking for members willing to participate in the commissioning of the remote access program. All interested members may contact John Chrzas for details.

(The above information was supplied by John Chrzas, SER-CAT's Sector Manager)

Study on High-Speed Data Transfer from SER-CAT

In an effort to advance the high-speed Internet connection between outside institutions and the Argonne National Laboratory (ANL), SER-CAT and UGA held a workshop that included key network and security personnel from ANL, APS, SER-CAT, UGA, Georgia Tech and Southern-Light Rail on August 17, 2006 at UGA.

The workshop was a follow-up to a proposal submitted to APS on June 1, 2006 by B. C. Wang with collaborators from SER-CAT, UGA and Southern-Light Rail (SLR), entitled, "A Proposed Feasibility Study of Ultra High-Speed Data Transfer Between APS and SER-CAT Member Institutions". The objective is to provide users with ultra high-speed data transfer capabilities between SER-CAT (Sector 22) and their home institutions, with a transfer rate somewhere between 0.5 and 1 gigabit/second, so that one day's worth of data (300 GB) can be transferred in about one hour.

The primary goal of the workshop was to exchange ideas and to select 2-3 possible ways for testing secured high-speed data transfers. This is a continuing part of SER-CAT's plan for a Remote User Participation Program currently being developed at the SER-CAT facility.

The workshop was organized by David Matthews-Morgan (Associate Director of Network Operations & Infrastructure at UGA) with assistance from B. C. Wang and SER-CAT Administrative staff. Invited out of town participants included Scott Pinkerton (ANL), Ken Sidorowicz (APS), Corey Hall (APS), Warren Matthews (GA Tech), Cas D'Angelo (GA Tech), Brian Savory (SLR) and John Chrzas (SER-CAT).

Group photo of the participants at the High-speed UGA-SLR-ANL Network and Security Workshop at the University of Georgia, August 17, 2006.

Meeting participants enthusiastically contributed various ideas. It was decided to test three possibilities, compare the results and document the findings. Once the feasibility study is complete, the findings will be made available to ANL, APS and SER-CAT member institutions as a resource for Internet policy making purposes. A write up of the findings will also be presented through a joint publication.

We would like to thank all of the meeting participants for their time, effort and interest in the proposed study.

2007 SER-CAT Symposium and Board Meeting

The fourth annual SER-CAT symposium will be hosted at the National Cancer Institute in Frederick, Maryland on Friday March 16, 2007 by Dr. Alex Wlodawer. Please mark the date on your calendar. As always, participants will be offered an enlightening day of events that include talks, demos, workshops, etc. The SER-CAT Annual Board Meeting will be held the following day, Saturday, March 17 at the same location. SER-CAT members are welcome to attend, as it is always an open meeting.

2007 SER-CAT Symposium, from Page 5

As in the past, the 2007 Symposium will include presentations of the SER-CAT Service Award, Young Investigator Award and Outstanding Science Award. If you would like to nominate someone for these awards, please visit the SER-CAT website at www.ser-cat.org for additional information or contact Dr. John Rose by e-mail at rose@BCL4.bmb.uga.edu or phone at 706-542-1750. The deadline for nominations is January 15, 2007. More information on the meeting and local arrangements will be forthcoming on the SER-CAT website. Thanks to Dr. Alex Wlodawer for his kind offer to host the 2007 event!

A Booth at the American Crystallographic Association Annual Meeting

For the fifth consecutive year, SER-CAT hosted a booth at the American Crystallographic Association's (ACA) Annual Meeting. This year's meeting was held in Honolulu, Hawaii at the Sheraton Waikiki Hotel, July 22 - 27, 2006.

As in the past, the ACA meeting served as a wonderful outreach venue for the SER-CAT program. This year's events included an array of scientific sessions, workshops, exhibitions, and social events over the course of five days.

During the exhibition show, SER-CAT highlighted its ongoing activities and enhancements to the facility over the past year. The meeting also provided an excellent opportunity for users to interact directly with the SER-CAT administrative and scientific staff. So, if you were in Hawaii, we hope you had the opportunity to stop by our SER-CAT booth and say, "Aloha!"

Well Done!

Congratulations go out to the 2005 SER-CAT Young Investigator Award recipient, Nicole LaRonde-LeBlanc, a postdoctoral fellow in the laboratory of Dr. Alexander Wlodawer, National Cancer Institute. The editors of the ***Federation of European Biochemical Societies (FEBS) Journal*** selected her paper on RIO serine kinases, which served as the basis for her 2005 SER-CAT Award, as the best paper published in the journal in 2005 by a young scientist.

In addition to receiving a cash prize, Dr. LaRonde-LeBlanc was invited to present her work at the FEBS Congress in Istanbul in June 2006. She will also be moving to the University of Maryland to assume a faculty position in August 2006. We wish her much success in all endeavors and again congratulate her on this prestigious recognition.

Staff Changes

There have been a few changes behind the scenes at SER-CAT and we would like to take this opportunity to acknowledge and introduce you to our new staff members.

Zheng-Qing (Albert) Fu

As of April 1, 2006, Dr. Zheng-Qing (Albert) Fu, formerly of the SECSG program at the University of Georgia in Athens, GA, joined the SER-CAT Operations team located in Argonne, Illinois on a full-time basis. Dr. Fu assumed the position previously held by Dr. Stephen Foundling and serves as a Protein Crystallographer assisting in user support beginning with the Summer 2006 Run.

Dr. Fu received his Ph.D. in physics from the Chinese Academy of Sciences studying topology, symmetry and phasing of aperiodic crystals under the supervision of Professor Haifu Fan. Dr. Fu joined Dr. B.C. Wang's group as an associate research scientist at UGA in 2001 and has developed new methods and software for evaluating anomalous signal to noise ratio and the automation of structure-solving processes of protein crystals. During his tenure at UGA, Dr. Fu worked to solve structures on some of the most difficult cases for the SECSG program sponsored by the National Institutes or Health, NIGMS.

Sylvia White

We would also like to introduce you to a new administrative team member, Ms. Sylvia White. As some of you may already know, Ms. White joined SER-CAT in March 2006 as an Administrative Assistant. She has previously held an array of administrative positions for the federal government, with her last position being at the Department of Health & Human Services, Office for Civil Rights in Philadelphia, PA.

Ms. White holds the position once held by Ms. Lisa Horanyi. She, along with the operational staff, maintains the SER-CAT website and serves as the assistant editor of *The SER-CAT Spectrum*. Please join us in welcoming both Albert and Sylvia to the SER-CAT team. ■

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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