The
SER-CAT SPECTRUM

Biannual Newsletter of the Southeast Regional Collaborative Access Team · Vol. 7, No. 2 · Winter 2009

Director's Message

Bi-Cheng Wang

Welcome to the December 2009 issue of The SER-CAT Spectrum. This issue again reports relevant news on SER-CAT's recent advances, planned activities, and things good to know.

An important milestone on SER-CAT's beam time allocation is the optional 12-hour shifts scheme, a further advancement of the virtual home synchrotron concept. It took place during the fall run on 22ID. A new staff member was hired to assist with the establishment of this program. In this issue we report user opinions from four SER-CAT groups concerning their remote data collection experiences. Other SER-CAT advances, reported by SER-CAT Sector Manager John Chrzas, include the development and implementation of procedures into SERgui for checking/alignment of the sample goniometer and precise crystal centering by diffraction patterns.

For the GOOD TO KNOW section, you might be interested in reading a summary by Patrick Stewart on microseeding of crystals. For some up-coming activities, please mark your calendar for the SER-CAT Symposium and Executive Board Meeting to be hosted by Leighton Coates on March 19-20, 2010 at the Spallation Neutron Source (SNS), Oak Ridge National Laboratory. Please also let your colleagues know that on July 24, 2010, prior to the annual ACA2010 meeting in Chicago, there will be an ACA Workshop on Sulfur-SAD Data Collection and Phasing.

SER-CAT extends a warm welcome to Dr. Unmesh N. Chinte as our new second shift support person. We are also pleased to share a recent SER-CAT structure by Wang, Opperman, Wickens and Hall of NIEHS. We believe you will enjoy seeing the Season's Greetings in this beautiful structure! I thank all of you for help in making SER-CAT a highly productive facility. I wish you a Happy Holiday Session and a prosperous 2010!

7th SER-CAT Symposium and Board Meeting March 19-20, 2010

Spallation Neutron Source (SNS), Oak Ridge National Laboratory

The 2010 SER-CAT symposium will be hosted by Dr. Leighton Coates at the Spallation Neutron Source (SNS), Oak Ridge National Laboratory on March 19, 2010. The symposium highlights SER-CAT science and technical development. All SER-CAT users and others interested in structural science are welcome to attend. Detailed Symposium information will be available shortly. The SER-CAT Board Meeting will be held on Saturday, March 20, 2010 . Click on the ORNL SER-CAT symposium site for additional details as they are developed:

http://neutrons.ornl.gov/conf/ser-cat2010/index.shtml

Nominations, Please

Nominations for the two annual SER-CAT Awards are requested. Please send your nominations for the 2010 SER-CAT Young Investigator Award and/or the Outstanding Science Award to **John Rose** before January 22, 2010. For detailed information, click on one of the links below:

2010 SER-CAT Young Investigator Award

2010 SER-CAT Outstanding Science Award

or

Send John Rose an email.

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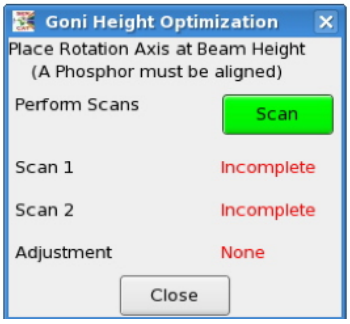
SER-CAT Advance

Diffraction Based Centering

John Chrzas

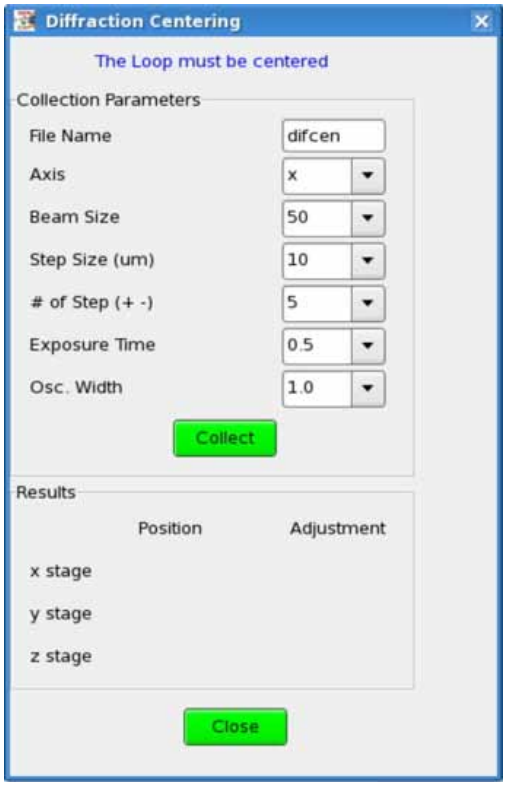
One of the major problems that any crystallographer encounters at all synchrotron facilities is the alignment of that hard to find sample. Whether your loop is clouded with a thin sheet of ice or you have a thin plate or needle that is impossible to "see" in one orientation, everyone has encountered the problem of having diffraction in 3 out of 4 phi positions. The problem can be divided into 2 major categories: goniometer and sample alignment.

If the rotation axis of the sample goniometer is not properly aligned to the height of the incident x-ray beam, then even a properly aligned sample may rotate in and out of the x-ray beam with phi. So the first step should be to check the alignment of your goniometer. The alignment of the sample rotation axis and the x-ray beam can be experimentally determined by the use of the SERgui Goni Height Optimization tool, which is found under the setup menu bar at the top of SERgui



When the Scan button is pushed (note that a phosphor needs to mounted and aligned), the system will translate the sample is z such that the pin intersects the beam and then 2 scans will be performed. The two scans are of the goniometer height at 2 different phi values. Each scan (pin1.dat and pin2.dat located in your archive directory) should represent a square well function as the pin scans thought the x-ray beam. The data from these 2 scans can be used to place the sample rotation axis at the incident x-ray beam height. After the scans are complete and the data processed, the goniometer height will be moved to the correct position. The user then needs to use the phosphor to position the goniometer horizontal position. The operations staff is in the process of replacing this capability with a much simpler process in which a YAG crystal is placed at the sample position and image analysis of the resulting image is used to position the goniometer in both the vertical and horizontal direction – preliminary experiments are promising and the process only takes a few seconds.

Once the user is confident that the sample goniometer is aligned properly, then the next step is to optically align your sample. SERgui now provides 2-point alignment of your sample at any initial phi position. This feature is located in the lower left hand corner of the sample page. Once the button is pushed the user moves the cursor onto the image display and clicks the left mouse button. The sample will then rotate in phi and the user then clicks the left mouse button a second time. The sample will then be moved and rotated to your initial phi position. The problems arise when you really can not see the sample. If you can get any diffraction, then you can use the new Diffraction Centering capability to optimize your sample alignment. The Diffraction Centering GUI can be found under the Automation menu bar on SERgui.



The Diffraction Centering GUI will allow the user to define a linear search of either x, y, or z to optimize diffraction of their sample. The user defines the experiment by use of the pull down menus for each variable. The number of images collected will be 2 times the # of steps plus 1. For the x and y axis, the sample goniometer is rotated so that the correct sample stage is aligned perpendicular to the incident x-ray beam. The sample is then moved thought he defined positions with a diffraction image collected at each step. After the last image is collected (which takes ~90 seconds for 11 images) the data is processed and the sample stage moved to the position with the most found spots. The data processing involves a peak search of each image using the D*Trek function dtfind with the ice ring detection option turned on. The step takes about 30 seconds for 11 images. The whole process takes about 2 minute per axis using 11 images, so that a sample can be aligned in all 3 dimensions in about 6 minutes, and if you use an exposure time of 0.1 seconds you will expose your sample for a total of 3.3 seconds. This capability is now available on both the ID and BM SER-CAT beamlines and has been tested on a variety of different sample morphologies.

GOOD TO KNOW

Microseed it!

Patrick Shaw Stewart,
Douglas Instruments

A new technique has been sweeping through the crystallization labs of Europe, but it seems to be less well-known in the USA.

For years, crystallizers have known that they can often initiate crystallization in samples by adding seed crystals to the mixture. This often works dramatically for proteins, and scientists have used it routinely for optimization - by seeding into conditions identical or similar to conditions that gave hits before.

What is less well-known is that the same approach can be used in the screening step of crystallization. Simply adding say 100 nl of crushed crystals (suspended in the reservoir solution that gave the hit) can increase dramatically both the number and quality of crystals obtained. This has several advantages: firstly, screening experiments are generally much easier to automate than optimization experiments. Secondly, it can be done without significant planning – simply crush the crystals in a well, transfer to a tube containing the appropriate solution, vortex to break up the crystals even more (the Hampton "Seed Bead" helps here) and add to a normal screen. Thirdly, the seed stocks freeze really well – so you can almost guarantee to reproduce crystals of any protein that you have ever crystallized – even years later.

For Douglas Instruments, the story began in 2006 when Allan D'Arcy (Novartis, Basel) asked us to write a "matrix-seeding script". This simply involved picking up seed stock from the stage of the Oryx robot in exactly the same way as protein, and adding it to all the wells of a screening experiment alongside the protein. Allan published the spectacular results of the technique in 2007 (Acta Cryst. D63, 550-554). For five target proteins that he worked with, it increased the number of hits by a factor of 7. Allan dubbed the method "MMS" (matrix microseed screening), following Ireton and Stoddard (although Allan's approach differed from theirs in several important respects).

Labs that use MMS routinely tell me that it gives an improvement in 75 to 80% of cases. For example, one industrial group uses the method whenever they get hits (good or bad), and they have had good results with cross-seeding – using crystals of a protein to seed similar proteins or complexes. Cross-seeding often works when there is some homology, so try crystals of different mutants and with different ligands (but don't expect lysozme crystals to help with your new target protein – the structures must be related!).

It may not be completely obvious why this method works so well. Remember that the phase diagram of a protein often includes a large area called the "metastable zone" (see Figure 1). If you put crystals into the metastable zone they will grow. However, nothing happens if you set up experiments in this zone but fail to add crystals. Generally speaking, you will get the best crystals from experiments that start in, or at least move through, the metastable zone.

You can imagine a screening experiment as a set of points landing randomly on a phase diagram (shown as arrows above because I'm assuming a vapor-diffusion setup). With normal screening experiments, you will only see hits that land in the nucleation zone (blue arrows), whereas if you set up MMS microseeding experiments, you will also pick up all the potential hits that land in the metastable zone (red arrows).

There are a few pitfalls to avoid. The seed stock may not be stable at room temperature – most labs keep it on ice and freeze it as soon as possible. Also, the seed stock must be very finely crushed to be compatible with some robots (not a problem for robots such as Oryx that use contact dispensing). However, we believe that MMS microseeding should be part of your routine crystallization scheme – even if you set up experiments by hand!

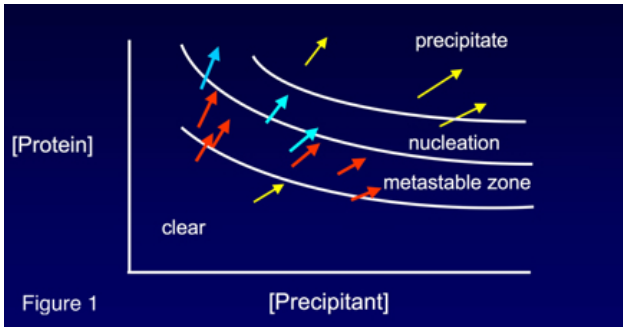
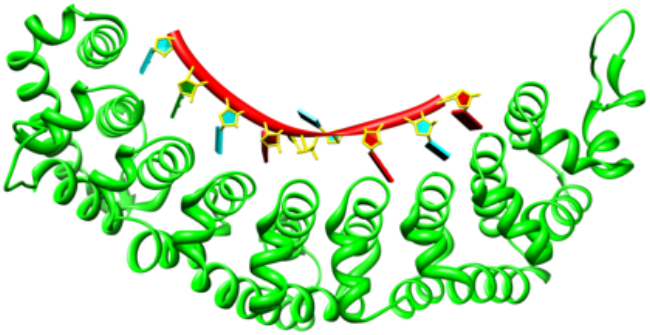


Figure 1

See http://www.douglas.co.uk/mms.htm for more information, and http://www.douglas.co.uk/MMS_proc.htm for our suggested method of preparing seed stock.

Recent SER-CAT Structure

PDB# 3K5Q **FBF-2/FBE complex**



Y. Wang, L. Opperman, M. Wickens, T.M.T Hall
NIEHS

Season's Greetings

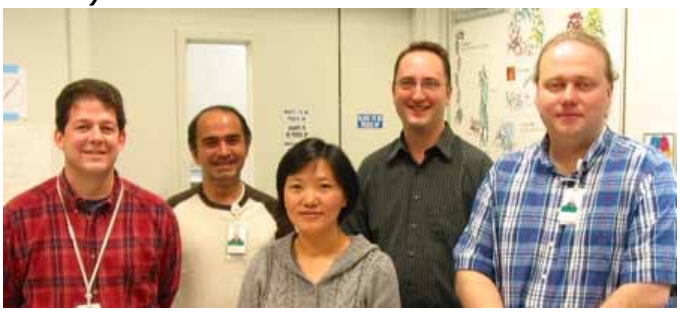
USER OPINION
REMOTE DATA COLLECTION
THE EXPERIENCES OF FOUR GROUPS AT SER-CAT

From **Kevin Parris,** Principal Research Scientist, Pfizer, Cambridge (North), MA

Pfizer Group Photo: L to R, Lidia Mosyak, Yohann Misquitta, Kristine Svenson, Kevin Parris, Andrea Olland, Sean Juo and Joel Bard

Remote data collection at SER-CAT is all about maximizing productivity. By shipping dewars to the staff at SER-CAT, our scientists spend more time in the lab. More importantly, we are able to assign short shifts to many people to do the data collection, avoiding the exhaustion that being up 24 hours brings. The year after we began using remote data collection, we observed a significant increase in the number of structures deposited into our in-house database. There were some learning pains, but those ended when we understood that communication with the support staff is imperative. The software is remarkably stable for us and every run finds significant improvements in it, all of which makes it even easier for us to do remote data collection successfully. There are downfalls, however. At times, we have lost crystals because the robot failed to mount/dismount a sample properly. We have yet to encounter this problem since the software was modified to defrost the gripper on a rigid schedule but we are always aware that it may occur again. We also have gotten use to the data processing session crashing when running HKL2000; fortunately this is only an inconvenience and not a fatal error - like sample loss. One last comment: it is no longer trivial to remove surface ice during remote data collection. When on-site, we would either wick the ice flakes off or wash the sample with liquid nitrogen. When doing remote data collection, you need to weigh the bad prospect of losing your crystal against the good prospect of ice-free data. A trade-off - but one well worth the convenience of collecting data at a synchrotron from your home lab.

From **Tim Rydel ,** Crystallography Lead, Protein Technologies Department (St. Louis) Monsanto GG4345



Monsanto Protein Technologies Group: L to R, Tim Rydel, Fred Moshiri, Meiying Zheng, Eric Sturman, & Artem Evdokimov

The Monsanto crystallography group began collecting data by remote means last March, and since then we've performed eight data collections, ranging from three to 12 hours each. All produced useful data, though our initial experiments contained a fair share of 'learning experience' foibles. In this write-up, my aim is to share with you some things we've learned over this time period.

Recommendations:

• Use at least two standard PC monitors for remote work. It's best to use one monitor for data collection and the other for data processing. Trying to accomplish both on one standard monitor is difficult and stressful (!).

• Follow SER-CAT magnetic cap recommendations. We've used super glue to affix height-adjusted, 20-micron thickness, mounted cryoloops to the Hampton Research (HR) HR4-779 CrystalCap Magnetic ALS caps, and had no problems with robotic mounting or dismounting at SER-CAT. To avoid this assembly work, we used HR CrystalCap HT complete crystal mounts during our initial remote/robotic data collections. Though advertised to work on ALS-style sample mounters, we observed mounting/dismounting problems at SER-CAT about 40% of the time when using them. The moral of this story: use only CrystalCap Magnetic ALS caps at SER-CAT.

• SER-CAT staff can help you transition to remote, robotic data collection. Zhongmin Jin and John Chrzas were particularly helpful to us in making the transition, and Zhongmin lent us the requisite cryo-tools for use until ours arrived. Our existing Taylor-Wharton CX-100 dry shipping dewars work well with the pucks and puck holders

• Make sure you're satisfied with the system performance from the start. Making sure at the beginning of your experimental work that you're satisfied with the performance of the beamline, auto-mounting robot, data collection & processing GUIs, and your data backup, should be something you always strive for; this is especially critical when you're remote from the beamline and have no hands-on way to intervene. Therefore, work with

.....Continued on page 5 .....

your beamline support person(s) from the beginning by phone to ensure things get off to a good start.

While there are big benefits to successfully collecting remote diffraction data, such as eliminating travel costs and the significant time savings, there is a serious down side. You now won't have any easy way to get a tasty hot dog from **Teddy's Red Hots** or a delicious breakfast from **Downers Delight!**

From **Stephen White,** Structural Biology, Room D1024E, St. Jude Children's Research Hospital, 262 Danny Thomas Place, Memphis, TN 38105-3678

Pictured above: Stephen White in front of remote data collection screens at St. Jude facility

As a long time user of synchrotron radiation, either driving from Oxford to Daresbury or taking the train/ferry to Paris and Hamburg in the early days or, more recently, flying from Memphis to Chicago - the concept of remote usage has always been a dream concept. My colleagues and I long realized that 'remote' could just as well be 1000 miles sitting in an office as 10 yards sitting outside the hutch as long as computers and robots are controlling the action. Now that the dream has come true with our ability to access the SER-CAT beam lines from afar, I have not been disappointed. Not only have the obvious benefits of convenience, comfort, sleeping and home cooking come to fruition, but many other unanticipated advantages have emerged.

For one thing, planning has become less of a headache. Rather than deciding well in advance which projects to concentrate on and who is going to travel, then booking airline tickets and frantically praying that the necessary crystals will appear, any sample and project can now be included in a booked session as long as you can make the FEDEX deadline. This improves efficiency because all structural groups can potentially prepare for a session and many more crystals are available if crystals either fail to appear or diffract poorly. Another bonus is that many more people can participate in the session, seasoned vets to provide assistance, advice and the occasional prodding to move things along, and younger investigators who can observe and learn. Also, the non-crystallographers involved in the project have the opportunity to see in real time the fruits of their efforts. In addition, investigators are not wasting time away from their research and families, often sitting around while others are collecting data or spinning their wheels when the beam goes down or there is some other technical hitch. Now during such times, one can simply go back to work during the day or go home and catch a nap during the evening. Finally, remote use has really promoted camaraderie within our department. We have set up a four screen 'remote pseudo station' in a shared area, and people can come and go during data collection to chat, observe, process data, solve preliminary structures on-the-fly and generally help out. Graduate students particularly like this setting; rather than worrying, often alone, outside the hutch wondering if they are screwing up and praying that none of the complicated hardware and software will fail at 2:00 am in the morning, help is always at hand.

Of course, remote use does have its disadvantages and we do have some suggestions for improvements. Although we appreciate the efforts of the SER-CAT staff, support has often been spotty and we are naturally reluctant to phone in when manual intervention is required. Understandably perhaps, staff accessibility drops off severely after 8:00 pm and during the weekend, but this problem needs to be addressed if SER-CAT is truly to be a 24 hour, 7 days-a-week facility as advertised. Also, in our experience, crystals seem to come out of the pucks more icy than at other beamlines and we frequently need to bother staff with the tiresome request to wash the crystals with liquid nitrogen. Whether it be poor freezing techniques by users, sloppy puck handling by staff, or the robot itself, the root cause of this problem needs to be identified and resolved. Changing energy has also proven to be a problem – significant changes always require staff intervention and this is frustrating for folks at both ends of the phone. As a general comment, and this may be apocryphal as are many things at synchrotron facilities in my experience, beam-line reliability at SER-CAT has declined in recent years, especially with respect to the computer interface. If this is a general perception, remote usage will especially suffer because reliability is an absolute must in this mode of operation. If these problems persist and regular staff intervention remains a necessity, we will begin sending one person to SER-CAT during runs, particularly when important and/or difficult data are scheduled for collection.

Overall, St. Jude crystallographers are delighted that remote data collection has now become a reality at SER-CAT, and the benefits in terms of time, efficiency, money saving and results have been considerable. Despite our complaints (users will always complain), we appreciate the efforts of the staff in establishing and maintaining this capability. However, we urge the SER-CAT staff to address the problems and to continue making improvements so that SER-CAT becomes the leader in this technology. As a member of the SER-CAT Board, I can reassure readers that this is a hot topic of conversation and that measures are in hand to address these important issues. As synchrotron time becomes more available worldwide, it is crucial that SER-CAT stays ahead of the pack in terms of quality, ease-of-use and cutting edge technology.

.....Continued on page 6 .....

From **Irene Weber, Yuan-Fang Wang and Johnson Agniswamy,** Department of Chemistry, Georgia State University, Atlanta, Georgia 30302-4098

Georgia State Group: L to R, Yuan-Fang Wang, Irene Weber and Johnson Agniswamy

These comments come from Irene T. Weber, Yuan-Fang Wang and Johnson Agniswamy concerning their experiences with a little over a year of using remote access for data collection. Overall, we get about the same number and quality of crystal structures as with on-site access. The major advantage is the savings in travel time and costs over sending a team of 3 or 4 people, and potentially faster access to beamtime without delay for arranging travel. Moreover, everyone can participate. For example, students can collect data in between their classes. One disadvantage is difficulty in obtaining on-site help after hours, even for simple problems like a stuck pin that requires entering the hutch. Data collection tends to be slower due to a slow transfer rate or technical problems. We have two recommendations we believe would be helpful:

(1) Installing a webcam to see the intensity meter reading and
(2) Use a virtual tour to help new users appreciate the set-up.

Editor's Note: The SER-CAT Administration is pleased to receive and is grateful to the Users' opinions on remote operations, as this is a top priority item at SER-CAT. During the last SER-CAT Executive Board meeting (March 2009), additional funds were approved to provide extended staff coverage to aggressively address some of the issues related to the data collection experiences expressed concerning the evening hours and weekends. Please see the next column on the addition of a new staff member, Dr. Unmesh Chinte, who is now providing second shift user support.

SER-CAT is committed to establishing and maintaining a strong remote operations program in its objective to fully achieve "Light when YOU need it". Please send further comments and suggestions to the operations staff and SER-CAT Director B.-C. Wang, as YOUR opinions are greatly helpful, and allow SER-CAT to locate and address new targets for needed improvements and upgrades.

New SER-CAT Staff Member

Welcome to Dr. Unmesh N. Chinte as a new user support staff member at SER-CAT. Unmesh joined the operational team on August 1, 2009 and is primarily dedicated to providing second shift user support to our Members. He previously worked as a Postdoctoral Research Associate in the Department of Structural Biology at the University of Pittsburgh, where he regularly visited the APS for data collection activities at SER-CAT and other beamline facilities. He received his Ph.D. in Chemical Engineering from the University of Toledo in 2006, and has considerable experience in X-ray crystallography, structure determination, and the optimization of cryogenic cooling of protein crystals. Unmesh is also proficient in various computer software applications, including those with Unix/Linux platforms. Stop by and say hello to Unmesh on your next SER-CAT visit

Workshop on Sulfur-SAD Data Collection and Phasing

The ACA will host a one-day workshop on sulfur-SAD phasing Saturday (July 24, 2010 at the University of Illinois at Chicago Saturday) in conjunction with its annual meeting in Chicago.

The workshop (with lectures in the morning and hands-on exercises in the afternoon) is intended for both students and professionals interested in SAD data collection and phasing. The focus of the workshop will be on sulfur-SAD phasing mainly because it is the most demanding SAD phasing technique in terms of sample preparation, crystal mounting, data collection and data processing.

Morning session lecturers will cover such topics as (1) SAD theory, (2) sample preparation, (3) source/beamline considerations, (4) data collection strategies, (5) data processing theory, (6) anomalous substructure determination and (7) generating initial protein phases and electron density maps.

The afternoon session will focus on hands-on exercises in data reduction and sulfur-SAD phasing. Here attendees will process a set of zinc-free insulin data (51 residues, 3 disulfides, space group $I2_13$, a = 78Å) using common data reduction packages. Then, using the scaled structure factors, attendees will attempt to (1) determine the anomalous scattering substructure (insulin disulfide centroids), (2) determine the correct hand of the disulfide centroids, (3) calculate a set of initial protein phases and (4) interpret the quality of the electron density map produced.

Attendees will also work on the more demanding sulfur-SAD

structure determination of ORF 1382 from *Archaeoglobus fulgidus* (95 amino acids, 5 sulfurs, space group $P4_2$) whose crystals only diffract to 2.65Å resolution.

All workshop attendees will receive a DVD containing lecture materials and a how-to guide for the crystallization of zinc free insulin and crystal cryoprotection protocol together with instructions for crystal mounting and data collection so that they can practice sulfur-SAD data collection and phasing at their home institution, after the workshop.

Workshop instructors: **John Chrzas**, SER-CAT Advanced Photon Source, Argonne National Laboratory; **Zheng-Qing Fu**, SER-CAT Advanced Photon Source, Argonne National Laboratory; **Zhi-Jie Liu**, Institute of Biophysics, Academia Sinica, Beijing, China; **John P. Rose**, University of Georgia; **Bernard Santarsiero**, University of Illinois at Chicago; **Bi-Cheng Wang**, University of Georgia and **Manfred Weiss**, European Molecular Biology Laboratory, Hamburg, Germany, and others.

PDC 2009 at UGA by John Rose

The 67th Annual Pittsburgh Diffraction Conference was held at the Georgia Center for Continuing Education located on the University of Georgia Campus. The three-day conference provided an outstanding forum for experts in the fields of RNA Crystallography, Biological SAXS, Diffraction Studies of Materials, Crystallization of Protein-Protein Complexes and Neutron Small Molecule Crystallography.

The session on RNA Crystallography organized by Joseph Wedekind, University of Rochester School of Medicine & Dentistry covered all aspects of the field from novel RNA specific phasing techniques to ribosome function. Speakers in this session included: Martin Egli, Vanderbilt University School of Medicine (RNA phasing); Ailong Ke, Cornell University (bacteriophage phi 29 prohead self-assembly); Charles Dann III, Indiana University (riboswitchs); Christine M. Dunham, Emory University School of Medicine (ribosome & translation regulation); Graeme Conn, Emory University School of Medicine (antibiotic resistance ribosomal RNA methyltransferases); Joseph Wedekind, University of Rochester School of Medicine & Dentistry (RNA Raman crystallography).

The session on Biological SAXS, organized by Jeff Urbauer, UGA, provided insight into this new and exciting field. Speakers in this session included: Dmitri Svergun, EMBL-Hamburg (BioSAXS today), Greg Hura, Lawrence Berkeley National Laboratory (SAXS assisted proteomics), Alexander Grishaev, NIDDK (SAXS assisted NMR), Thomas Grant, Hauptman-Woodward Medical Research Institute (conformational dynamics), Sam Butcher, University of Wisconsin (RNA structure), Jeff Habel, Lawrence Berkeley National Laboratory (SAXS assisted structural genomics).

The session on Diffraction Studies of Materials organized by Angus Wilkinson, Georgia Institute of Technology, focused on diffraction techniques related to material science. Speakers in this session included: Chris Tulk, ORNL; Scott Childs, Renovo Research (Mercury CSD optimized crystal engineering); Katharine Page, Los Alamos National Laboratory (neutron and X-ray studies of ferroelectric perovskite oxides and related oxynitrides); Matthew Suchomel, Advanced Photon Source, Argonne National Laboratory (high-resolution synchrotron powder diffraction); Angus Wilkinson, Georgia Institute of Technology (negative thermal expansion frameworks).

The session on the Crystallization of Protein-Protein Complexes organized by Joseph Ng, University of Alabama in Huntsville highlighted recent innovations in the field. Speakers in this session included: Peter Sun, NIDDK (current status of the field); Larry DeLucas, University of Alabama at Birmingham (membrane protein complexes); Marc Pusey, iXpressGenes Inc., Huntsville, AL (fluorescence-based approaches to the protein crystallization); Leighton Coates, ORNL (update on the new protein crystallography station at SNS); Janette Hobbs, Molecular Dimensions, UK (crystal optimization); Miranda Byrne-Steele, University of Alabama in Huntsville (hyperthermophilic and pychrophilic proteins).

The session on Small Molecule Neutron Crystallography organized by Christine Hoffmann, ORNL, covered recent developments in the field with talks by a number beamline scientists from facilities in the US and elsewhere. Speakers in this session included: Garry McIntyre, Institute Laue-Langevin (ILL), Grenoble, France (the VIVALDI Laue diffractometer at ILL); Thomas Proffen, Lujan Neutron Scattering Center, Los Alamos National Laboratory (analyzing diffuse neutron scattering); Alison Edwards, Bragg Institute, Australian Nuclear Science and Technology Organization (the KOALA Laue diffractometer at ANSTO); Anna Gardberg, Center for Structural Molecular Biology, ORNL (the joint X-ray-neutron refinement of rubredoxin) Christina Hoffmann, Neutron Scattering Sciences Division, ORNL (the TOPAZ and other neutron diffractometers being development at ORNL).

A new feature of the PDC this year was the Pittsburgh Diffraction Society Future Leaders Symposium organized by Bi-Cheng Wang, University of Georgia, which highlights outstanding research being carried out by a graduate or undergraduate researcher. Speakers (taken from submitted abstracts) in this session included: S. Jason Polizzi, University of Georgia (structural studies of UDP-xylose synthase); Guoxing Fu, Georgia State University (structural studies of executioner caspases); Yuan Hu, Indiana University of Pennsylvania (diffraction studies of $Na_2(Zn_{1-x},Co_x)SiO_4$ (x = 0.50)); Susan D. Orwig, Georgia Institute of Technology (structural studies of acid-β-glucosidase chaperone complexes); J. Tucker Swindell II, University of Georgia, (optimizing data reduction); Norie Sugitani, University of Alabama in Huntsville (structural studies of Mbur_1912 from *E. Methanococcoides burtonii*).

The Chung Soo Yoo award for best student poster went to Jason D. Salter, University of Rochester for his work on the HIV-1 viral infectivity factor (vif). The full program and abstracts is available from the PDS web site www.pittdifsoc.org.

The SER-CAT Spectrum

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