

SSRL Remote Synchrotron Access Workshop, February 9, University of Melbourne.

Summary

A remote synchrotron data collection workshop was held on February 9 2007, in the new Learning Laboratory at the University of Melbourne. Following suggestions from Profs Hans Freeman and Mitchell Guss from the University of Sydney, the workshop was organized by Aina Cohen and Mike Soltis from the SSRL, and Peter Turner from the University of Sydney. The SSRL staff presenting the workshop were Aina Cohen, Clyde Smith, Graeme Card and Mike Hollenbeck, together with Edward Snell from the Hauptman-Woodward Medical Research Institute. Attending were 28 participants representing 12 universities and research institutions from Australia, and a participant from Massey University in New Zealand, Geoff Jameson.



The one day workshop provided participants with an opportunity to remotely operate two SSRL macromolecular crystallography beamlines, and the associated SAM crystal mounting robots, and to remotely process and analyse data from these beamlines. The SSRL beamlines have much in common with those under construction at the Australian Synchrotron. A morning overview and demonstration session was followed by split afternoon sessions with one group having hands-on remote beamline control training, and the second being shown how to use the SSRL sample pucks and cryo-tools. Mid-afternoon the groups swapped sessions to complete the workshop. Prior to the workshop Paul Carr from the ANU and Jason Schmidberger, a PhD student with Mathew Wilce at Monash University, had sent their own samples to SSRL, and were able to screen and then collect data from these samples during the workshop. The crystals and data were further analysed after the workshop, with Paul connecting to the SSRL from his hotel room and Jason from the comfort of home. Both Paul and Jason report excellent data and are very pleased with the results.

The workshop concluded with the participants filling in anonymous survey forms and it was clear from the responses that the workshop was an outstanding success. Contributing to the success was the 'state-of-the-art' multi-level Learning Laboratory at the University of Melbourne, which was made available by Professor Frank Larkins and Prof Ken Ghiggino. Professor Peter Tregloan provided on-site organizational assistance and advice, Carlo D'souza provided technical support for the Learning Lab and Inorganic Chemistry Lab manager Sioe See Volaric provided laboratory space and support. The workshop was jointly funded by the SSRL and the ARC Molecular and Materials Structure Network (MMSN). Further details will be available at mmsn.net.au.

Report

The workshop opened with a presentation by Julian Adams describing the current status of the protein crystallography beamlines at the Australian Synchrotron (AS). In particular, beamline 3BM1, which will be commissioned over the next few months, will be used for high-throughput structural biology and will support remote access in a similar manner to that provided at the SSRL. The 3BM1 beamline includes the use of the Stanford Automated Mounting System (SAM) and SSRL Blu-ice control software. Since remote users of the AS will use the same sample storage and shipping cassettes and same control software as SSRL users, they will be able to take advantage of the remote access programs offered by both facilities; particularly while the macromolecular crystallography beam lines at the AS are under development. The second single crystal crystallography beam line to be commissioned at the AS, 3ID, is to be dedicated to obtaining diffraction data from weakly diffracting micro-crystals.



Aina Cohen followed Julian's presentation with an overview of the macromolecular crystallography facilities available at SSRL, including the SAM system and Blu-ice beam line control software. The remote access program was described in detail and participants were shown how to apply for beam time at SSRL and gained insight into what to expect during a remote data collection.



Following Aina, Clyde Smith (SSRL) gave a 'live' demonstration of remote data collection and processing. Crystals were mounted, fluorescence scans recorded and data collection initiated. The lecture room watched as the blu-ice GUI displayed images from several video cameras, and saw the diffraction images as they appeared. The presentation included a description of Web-Ice developments; Web-Ice is a remote data viewing application used for screening and analysis that combines scoring crystal quality with automatic indexing, resolution estimation, strategy determination and, more recently, the ability to run RADDPOSE and BEST to optimize a data collection.



Eddie Snell then provided practical tips from the users' point of view covering experiences from 10 remote data collection runs. Eddie mentioned that there are SSRL users at the Hauptman-Woodward Medical Research Institute, who have yet to travel to the synchrotron. During his presentation Eddie showed a photo of the snow covered landscape surrounding his home in Buffalo, NY and expressed his gratitude to be in Melbourne enjoying the Australian summer.



After a lunch break the workshop split into two groups. One group was led by Clyde Smith together with Graeme Card and Edward Snell, who made sure that the remote access software installed and operated on the participants laptop computers. The SSRL remote access system uses the NX remote desktop software to provide access to the beamline control software. With NX installed and a connection made, the participants were able to take control of two of the beamlines at SSRL. The group mounted crystals, moved detectors, changed wavelengths, undertook screening and edge scans, collected X-ray data and processed data. All of this being done remotely from sunny Melbourne.



As mentioned earlier, Paul Carr from the ANU and Jason Schmidberger, a PhD student with Mathew Wilce at Monash University, had sent crystals to the SSRL in advance of the workshop. Accordingly they were able to screen and undertake data collections on their own samples. Screening of these crystals began during this session., and the data collection and analysis continued after the close of the workshop. Paul returned to his hotel room to remotely collect a full data set for a sample of an engineered variant of a promising bioremediation enzyme. Data were remotely collected to a resolution of approximately 1.2\AA ; by far the best data ever collected from this system. Jason was able to screen a series of SeMet crystals during the workshop, and later remotely collected a complete MAD data collection in about 4 hours. The diffraction data was indexed and integrated with Mosflm, and the structure was solved by Solve/Resolve and the model is currently being refined. The structure, which Jason has been trying to determine for more than a year, was obtained within a few days of the remote data collection.



While the first group participated in the 'hands-on' remote access session, the second group attended a practical session run by Aina Cohen and Mike Hollenbeck in a chemistry laboratory in the School of Chemistry. The session started with a description of proper sample pin preparation. The kinds of things to avoid and look out for were covered in detail, including practical examples of mistakes made by other experimenters.



The group donned safety shields, glasses and gloves, the liquid nitrogen came out and everyone had a chance to mount at least one sample in a cassette and practice the techniques involved. Participants learned how to load samples into uni-pucks, a new type of sample storage container compatible with several robotic sample mounting systems in use at synchrotrons. There were discussions between the participants and practical ideas were exchanged.



After a coffee break the groups swapped locations. The day concluded with a wrap up question and answer session - and a reminder to attend the upcoming Crystal XXV meeting being held in April in the Hunter Valley of NSW. Participants were asked to fill-out a questionnaire describing their experiences, with a view to improving future training sessions. Some of the feedback is listed at the end of this report. The participants provided many helpful suggestions and described the workshop as excellent and very worthwhile. Many expressed interest using the SSRL remote access facilities, and looked forward to using the same system at the Australian Synchrotron. The workshop clearly re-affirmed the strong relationship between the SSRL and the macromolecular structure community in Australia.



The success of the workshop was in large part due to the support of several people at the University of Melbourne. Professor Frank Larkins, Deputy Vice-Chancellor, and Prof Ken Ghiggino, head of the School of Chemistry, made the Learning Lab available for the lectures and computing hands-on session at not cost. In the School of Chemistry Professor Peter Tregloan provided on-site organizational assistance and advice. Carlo D'souza and his assistant Michael helped with technical issues at the Learning Lab. Inorganic Chemistry Lab manager Sioe See Volaric was essential to the cryo-tools hands-on session and provided laboratory space and logistical support including a constant supply of liquid nitrogen. She also took many of the photos in this report (other photographers include Peter Turner, Edward Snell and Michael Hollenbeck.). The workshop was jointly funded by the SSRL and the ARC Molecular and Materials Structure Network. The group from SSRL is very grateful to everyone who helped with the organization of this very successful event!



Eddie Snell (HWI), Clyde Smith (SSRL), Aina Cohen (SSRL), Peter Turner (USyd), Mike Hollenbeck (SSRL) and Graeme Card (SSRL).

Some Participant Feedback

“The workshop was stimulating and informative, and there really is no substitute for a hands-on experience - in terms of learning and gaining confidence.”

“I found the workshop provided a valuable insight into using the remote access software for the SSRL which, conveniently, will also be used at the Australian Synchrotron.”

“As a new member of Jenny Martin's group at UQ it was great to see the system that will be available at the Australian synchrotron. I found the workshop informative and useful. I thought the sections were well organized and it was great to meet the people responsible for implementing the system at the SSRL to get help with any problems and ask questions directly to those who designed the system. This was great when being introduced to a new system. I found the sections on helpful tips and the hands on parts the most useful and we are already trying some of the techniques today in the lab. Once again thanks.”

“The workshop went really well. It was very well organized, the lectures and hands on sessions were very useful and very well explained. The time dedicated to each subject was adequate too. Definitely worth attending to the SSRL remote access workshop.”

“Thanks for organising the workshop. It was very informative and in my view a great success. While some of the lecture material was more directed to SSRL users or potential users most of the information will be relevant for the Australian synchrotron. The afternoon session using the cryo kits and blue ice software were helpful. It was good to learn about pin types and issues relating to robots and individual systems. This is one thing that can be quite confusing for non-experienced synchrotron users. Presentations were very good and were pitched well. Speakers presented well. The food was a nice bonus.”

“It was a well organised and extremely useful workshop covering the practical details of remote access operation of the overseas synchrotron facility using BLU-ICE and related software. During the workshop I managed to screen diffraction from crystals of an engineered variant of a useful bioremediation enzyme that we are currently studying. Subsequent to the workshop I managed to collect a full data set to a resolution of $\sim 1.2\text{\AA}$ remotely using the SSRL macromolecular crystallography facility. This is by far the best data ever collected from this system. I am very excited by the prospect of using the techniques learned at the workshop for further data collections at the SSRL and also the Australian Synchrotron. The workshop was very timely given the proposed commencement of operations at the Australian Synchrotron later this year. The same robotic hardware and software will be used for remote access at both facilities.”

“I found the workshop very informative. All the people from SSRL gave clear talks with comprehensible slides and timing of the talks were spot on (which I was very impressed after attending Lorne conference). Lots of hand on and live demonstration was very helpful. I am confident that I could access the blue ice program remotely without much help. It was also fascinating to see how idiot proof blue ice was. Food was very nice. Timetable was well balanced and well informed. Thanks for the opportunity to attend the course. I am more enthusiastic about crystallography. I am sure this program would be immensely useful to people who intend to use Australian Synchrotron, too.”

“It was sufficient to enable anyone with a background in crystallography to learn how to perform remote crystallography at an SSRL-type remote beamline. It has the right combination of theory

and practice. The tutors were very well informed about the material. Furthermore, the multimedia venue was very good and helped make the workshop a success.”

“I thought the SSRL remote-access workshop was thoroughly excellent and, as a hardcore sceptic, I was very impressed that the remote access system did not fail once during the day. My previous experience of robotic systems at beamlines has been to watch crystals fall off, disappear etc. I sincerely hope that the Australian Synchrotron beamline(s) can obtain such high levels of reliability. I think that a wise decision has been taken to use blue-ice etc and I hope links with the SSRL team are maintained. I am grateful to the SSRL crew for taking the trouble to come all this way for the workshop.”

“I find the workshop being extremely useful in terms of knowing alternate ways to obtain data remotely. The experience is extremely useful whether we end up using the radiation source from the Australian synchrotron in Melbourne or that in SSRL. After attending the workshop, I personally found it a bit nervous to use the facility remotely without anyone who already has the experience nearby. Therefore I still prefer, if possible, collect at the site for the first time.”

“The workshop was excellent. The presentations and hands-on sessions provided a good balance between the requirements from the novice to the seasoned users. Both types of sessions were required because of the specialised nature of the cassettes to be loaded (practical), and the array of requirements that come in crystallography experiments (software). Remote, or not, discussing strategies for collecting data are useful as new apparatus are always affecting the prioritisation of work, and ability to achieve progress. Aside from the formally described components, I was able to speak to the beamline staff and ascertain their levels of confidence in the particular aspects of the beamline access and use. I was able to get a good appreciation of the way in which my experiments would run and what trouble shooting was available. Clearly some aspects of what were shown in the software are under development, as one might expect in any project. In the software we saw aspects that were still a long way from perfect.”

“I found the workshop very well organised and useful. The hands-on sessions, especially sample preparation, as well as tips from the remote user were of particular value. In the future it will likely save many potentially very valuable samples from being ruined because we now know what to watch out for. The demonstration of software that will be used at Australian synchrotron means that we are more or less ready to go using it. Thank you very much for everyone involved.”

“The SSRL workshop was extremely useful, both in getting background into the system and hands-on experience with the hardware and software. The opportunity to interact with the SSRL beamlines remotely during the session made it clear how straight-forward and effective such an access route is - vastly better than the 15 hour flight across the Pacific!”

“I am a Ph.D who attended the SSRL workshop. I thought the hands on experience with the cassettes was very useful - they are a lot easier to load than first thought. I did think the Blu_Ice/Web-Ice workshop was very good, but I thought maybe a split screen set up may have made it a little easier to follow, also if the different windows on the GUI had scroll bars on the side as you do not know a lot of the parameters/settings are there”

“The SSRL remote access workshop held this year at Melbourne University in February, was truly a worthwhile experience. The software is amazing and the robot is very robust in its utility and reliability. To pick and choose and screen crystals in real time whilst being in a different country was such a luxury. The lectures were as informative as you could hope and the inclusion of the “Practical tips” session by Professor Snell was useful to indicate how easy to use and reliable the system is. The afternoon hands on session was great to first have a go at handling the equipment

needed for crystal transport. Having already arranged for the transport of crystals to SSRL for use online in the workshop, I had some experience with the apparatus. What was useful in the hands on session was using the newer versions of the tools for loading crystals and seeing how they have gotten around problems I had with older versions available to us at the time I loaded our crystals. At the end of the day it was our turn to have a drive of the software controlling the system. In a nutshell, it is very easy to use. Whether screening crystals, or deciding on a data collection strategy, the software is nicely integrated to provide a smooth transition between the different functions. I was particularly fortunate to not only be able to screen a series of SeMet crystals I had sent earlier, but to also make a complete MAD data collection. It took about 4 hours to collect peak ($E = 12660.75$ eV), Inflection ($E = 12658.88$ eV) and High Remote ($E = 13500$ eV) data sets. Diffraction data was indexed and integrated with Mosflm/CCP4 and the mtz's were fed into a very useful MAD script (Solve_structure.com). From this the structure was solved by Solve/Resolve and a reasonable model provided. All of this was done online and the structure output within a few days of data collection. The crystals used were not the best diffractors, and this result is a big deal to me as I have been chasing this structure for over a year now. Given the ease and low cost of using the remote access SSRL system, were I not at the end of my PhD project and writing up, I would be applying for as much time there as they would give. It is certainly good to hear that we will soon have a similar system here at the Australian Synchrotron in Melbourne."

"The workshop was comprehensive, covering not only remote access to the SSRL, but also sample loading into the SSRL cassette. The staff presenting the workshop, including Julian Adams from the Australian Synchrotron, were excellent in all respects -- enthusiastic, helpful and very knowledgeable. The real-time hands-on aspects were hugely useful, as this allowed one to experience (not just receive from presentators) what happens in real-time, what problems can occur, and how to recover from errors made in using the software. I, for one, am particularly grateful for the efforts of the local organisers, Peter Turner, in particular, that ensured that access to the workshop was possible for all investors in the Australian Synchrotron. I have been to many workshops, both voluntarily and involuntarily -- this Remote Access Workshop, would be THE very best in terms of usefulness with genuine hands-on experience, and quality of presentation and organisation."