

## MacCHESS Director's Report

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MacCHESS is the organization supporting Macromolecular crystallography at CHESS, the Cornell High Energy Synchrotron Source. The predominant funding source has been the P41 grant awarded by the NCRN of the National Institutes of Health (NIH). With recently renewed funding, MacCHESS is in its 21<sup>st</sup> year of service to the crystallography community. During this past year the average time of each user's visit has been only about 36 hours, and the time to obtain a data set is typically less than 4 hours. This means that a great many users have collected a great many data sets: the MacCHESS facility supported visits from over 300 members of the scientific community and approximately 130 MacCHESS-related publications were released over the past 12 months from data collected on only 3 experimental stations. In October 2003, we were absolutely delighted to hear that our faithful user and collaborator **Rod MacKinnon** (Rockefeller University) shared the 2003 Nobel Prize in Chemistry for determining the beautiful structure and function of ion channels.

Changing directions in high-energy physics research at Cornell now allows CHESS and MacCHESS to enjoy a machine dedicated to x-ray production for a significant portion of the year. Optimized beam conditions enable much longer run times between fills, greater stability, and smaller source sizes. These conditions are a welcome improvement for users collecting Multi-wavelength Anomalous Dispersion (MAD) datasets on our **F2** station; the Quantum 210 detector with fast data readout, combined with a rapid air-bearing rotation system makes this one of our most sought-after stations. **A1** station, which is also equipped with a Quantum 210 detector, has recently been realigned to allow greater sample-to-detector distances and is now tuned 40 eV above the selenium K-edge to allow Single-wavelength Anomalous Dispersion (SAD) experiments with seleno-methionine protein crystals. Both high-resolution and large unit cell crystallography require large detector surface area. MacCHESS offers a unique dual CCD arrangement in which two Quantum 4 detectors can be positioned in a flat or V-shaped

configuration. **F1** station, where the dual detector system is located, also provides a biological isolation environment suitable for some virus work. Additionally, F1 station energy has been tuned just above the bromine edge and so allows for rapid halide soak SAD phasing experiments.

All three MacCHESS stations are now plumbed for liquid nitrogen with cryosystems set to automatically refill without user intervention. Many users are taking advantage of mail-in dry shipper dewars to avoid air-travel problems. Use of our online **express mode** proposal system, a fast and easy method of requesting beamtime, has doubled every year since its inception. Average time between an online proposal submission and actual visit averages less than three weeks.

In addition to serving a worldwide base of users, MacCHESS is engaged in exciting new research and development **initiatives** that will push the limits of sample size, resolution, and unit cell size to new dimensions. These initiatives include:

- Microcrystallography
- Large unit cells
- Ultrahigh resolution diffraction
- High throughput crystallography (robotics)
- Crystallographic software and new phasing procedures
- Crystallographic beamline hardware

MacCHESS organized a **workshop** on novel data collection techniques for macromolecular crystallography in June 2003, in conjunction with the CHESS Users' Meeting. Topics covered included data collection strategies for kinetic crystallography, microfabricated mounts for microcrystals, and microbeam experiments with glass capillaries.

Details of our progress and future directions are described in Marian Szebenyi and Richard Gillilan's articles in this newsletter. The article on page 58 by Ekaterina Heldwein of the Harrison Lab (Harvard) tells an interesting story about how she solved a challenging crystallographic problem with help from MacCHESS technological developments.