

*Macromolecular Crystallography Division of Cornell High Energy Synchrotron Source, Cornell University*

MacCHESS is the organization supporting Macromolecular crystallography at CHESS, the Cornell High Energy Synchrotron Source. CHESS provides high-quality x-ray beams and MacCHESS provides the equipment and personnel to enable structural biologists to make good use of these beams; the two organizations are independent, yet intimately entwined. The predominant funding source for MacCHESS has been the P41 grant awarded by the NCRP of the National Institute of Health (NIH) since 1983.

Productivity in all areas of the research resource (technological research and development, collaborative research, training and dissemination, and service) has continued high. The storage ring has been running well and upgrades to the CHESS stations have been proceeding as planned. The recently expanded MacCHESS staff has been continually improving hardware and software capabilities of the facility.

The resource is completing year 5 of its five-year award period. During this period the average time of each user's visit has been only about 40 hours, and the time to obtain a data set is typically less than 6 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 140 MacCHESS-related publications were released over the past 12 months. Details of our progress are provided below.

In the area of **high heatload optics**, the main development has been the installation and use of a white beam, collimating mirror as the first optic on A-line. This device, similar to one already installed on F-line, removes higher energy radiation, thus reducing background as well as heat load on the x-ray optics, and provides a high degree of collimation of the beam entering each monochromator.

To complement the **MAD/SAD** capacities offered by F2, the X-ray energy at F1 has recently been set to 50eV above the Br K-edge to allow fast SAD experiments with Br-soaking.

The MacCHESS beamlines A1 and F2 are each equipped with a **large-format CCD detector**, the Q-210 from Area Detector Systems. However, there are cases in which an area even larger than that of the Q-210 is needed, and a flexible arrangement of two detectors has several advantages over a single large area detector. A **dual CCD** support device has now

been designed and constructed by Mike Cook, and has been tested by MacCHESS staff as well as outside users on F1. Details of this device are described in Marian Szebenyi's article on page 17.

All three beamlines are now equipped with **cryocooling** systems from Oxford Cryosystems. The systems operate between 80 and 400° K with temperature stability of 0.1° K, are relatively insensitive to humidity variations, and have simple startup, shutdown, and temperature-changing procedures. The position of the cold head can be adjusted to accommodate a variety of goniometer heads. In addition, the F1 and F2 stations are now equipped with an automatic refill system for liquid nitrogen which keeps the dewars of the cryostats filled. A1 will be upgraded shortly.

With modern beam intensities, detectors, and computers, the actual time to record a series of x-ray diffraction images is short; mounting, centering, and screening crystals become time consuming. Efforts to alleviate this problem through automation are underway at many synchrotron sources. Construction of a **crystal-mounting robot** for MacCHESS has begun, following the model of a machine at Lawrence Berkeley Lab. In addition, a prototype of a semi-automated crystal-centering system has been developed by Dave Schuller, Richard Gillilan, and others.

**Microcollimation** continues to be a top priority of MacCHESS. Work over the past year has focused on the use of a slit assembly as an alternative to a single collimator. A recent experiment used two sets of slits, each set consisting of a horizontal and a vertical slit, with a separate stepping motor controlling each side of each slit (a total of eight motors). The motors are operated by **SPEC**, the standard motor-control software on the beamline computers, and **SPEC** macros can be defined to operate sets of motors in a coordinated way.

The areas of **implementation of data processing and phasing software** in the synchrotron environment have been addressed by several of the MacCHESS staff. The program package **XDS** has been installed at CHESS to provide a third option for data reduction. This program is particularly suited to dealing with data collected with very small oscillation angles. Art Weaver has tested the program on a variety of data sets, and has developed a graphical user interface for it, **webXDS**, for experimental

use by MacCHESS users. This preliminary version utilizes only one processor, but the code has been designed to distribute the data processing task to multiple processors in a Linux cluster environment in future releases. Quan Hao has pursued development of his program **SAPI** for determining heavy atom positions from SAD or MAD data. A number of users have employed this program to attempt structure solutions while at CHESS.

There has been a heavy effort put into development of **fast computing**, including both installation of multiple

state-of-the-art workstations and construction of a **supercomputing cluster** - "SIRIUS" (see Frank Labonte's article on page 16). SIRIUS has already been used for rapid phasing of macromolecular structures. We have used the parallel direct-methods program **SnB** on SIRIUS to solve a variety of heavy-atom substructures as well as an all-atom protein structure at sub-Ångstrom resolution; run times are reduced from the hours typically needed on a single-CPU machine to minutes. Another macromolecular phasing program, **FSEARCH** by Quan Hao, has recently been implemented on SIRIUS. A parallel-aware version, **MPI\_FSEARCH**, has been used successfully to perform an exhaustive 6-dimensional search to phase very low resolution x-ray data using a molecular envelope from EM or solution scattering data.

This past year has seen an enormous increase in on-line **data storage** at MacCHESS. The first 1 TB of RAID storage, which became available in early 2001, has been increased to over 10 TB. Each beamline has a new 1 TB Avistor RAID system attached to the SCSI bus of the Alpha used for data collection, and images are written directly to these devices. In the area of **data transfer**, the gigabit Ethernet begun in early 2001 has been expanded to include most of the MacCHESS computers.

We have implemented a "**FedEx**" **data collection** system, in which users send only their crystals and instructions; MacCHESS staff carry out the collection, and data reduction if requested, and return the results. Shipping a dewar of prefrozen crystals is much cheaper than arranging transportation and lodging for people.

MacCHESS organized a **workshop** on high-throughput crystallography and complementary techniques in June 2002, in conjunction with the CHESS Users' Meeting. Topics covered included automated structure determination, phasing techniques, mass spectrometry and solution scattering as related to crystallography, and supercomputing at MacCHESS.

## Enter...the CHESS On-Line Express Mode

**Ernie Fontes and Lana Walsh**

To encourage even more investigators to visit CHESS and make it easier for them to access the facility, we have recently upgraded our beamtime proposal and user orientation procedures. Our Express Mode (EM) beamtime proposal system has been successful for many years. It started as a short form used to request one or two days of x-ray beamtime at one of the "already set up" protein crystallography stations. The idea was that users needing only short periods of data collection time would be greatly facilitated by having the experimental equipment "set to go" upon their arrival. In addition, since an EM proposal had a more limited experimental scope, the proposal review process could be kept quite short. Our goal now is to get a user group from proposal to visit in less than 4 weeks.

Just this past year we've improved the EM system in three ways: 1) the EM form is now an on-line web page, 2) the form was shortened, and should now take less than 15 minutes to fill in, and 3) the choice of experimental technique now includes high-pressure studies (at the B1 or B2 stations) as well as small-angle x-ray scattering (at D1, C1 and/or G1). We are also open to suggestions of other techniques where users can make use of standard station preparations.

These revisions have had a very positive effect in easing entry of first time CHESS users and greatly reducing the submission-to-schedule lag time. Statistics from the first 5 months of 2002 demonstrate an amazing average turn-around time for crystallography users of 2.5 weeks (actual time between the on-line EM submission date and the first day of data collection).

Once users are scheduled for a visit, a new on-line User Safety Orientation Tour provides all the information needed to quickly familiarize people with CHESS. This can all be done before the users leave home, thus saving precious time upon arrival at CHESS. This tour describes the facility and our experimental capabilities as well as presenting necessary safety policies and procedures. Once the users finish the on-line tour they take a short on-line quiz to verify their knowledge. Completing the tour and quiz are needed prior to the signing-in at the start of a user's first visit.

Users are encouraged to learn more about our new time-saving procedures and forms starting at our home page at [www.chess.cornell.edu](http://www.chess.cornell.edu).