

## From the Staff

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).