Data Analysis, Visualization, and Modeling Software Developments

This has been an exciting year in the area of data visualization and analysis software development with numerous additions to the NCNR's growing suite of software tools as well as many enhanced capabilities in the existing software. Version 1.0 of DAVE (the Data Analysis and Visualization Environment), is a comprehensive set of software tools developed for the interpretation of inelastic neutron scattering data, and was released last year (see Fig. 1). DAVE is a feature-rich application under extensive development as its user base grows and additional requests are accommodated. Some of the new capabilities added this year include enhancements in visualization with fully customizable plots in one and two dimensions, proper handling for single crystal time-of-flight data, new capabilities for exploring and analyzing multiple datasets, and a new module allowing users to fit parameterized models of $S(Q,\omega)$ to 2-dimensional data. These additions are currently undergoing extensive beta testing and are available in the current development version of DAVE (http://www.ncnr.nist.gov/dave/).

The *Igor Pro*-based SANS data reduction and analysis software developed at the NCNR has proven to be very popular with facility users. The Ultra Small-Angle Neutron Scattering (USANS) instrument at BT-5 extends the lowest momentum transfer Q reached by SANS by nearly two orders of magnitude. In response to users' needs, *Igor Pro*-based software has been developed to allow user-friendly reduction of USANS data sets. The software allows experimenters to inspect raw USANS data and to interactively reduce them into a fully corrected USANS data set (see Fig. 2).

A team from the NCNR, the University of Maryland, Baltimore County, and from Los Alamos National Laboratory (LANL) are developing a SANS-Modeler software package. This package is a web-based (http://sans.chem.umbc.edu/) molecular modeling tool to aid users performing Small Angle Neutron Scattering experiments on biological macromolecules. The web site is a compilation of software developed over the years at both the NIST Center for Neutron Research and LANL.

Photography by Lynn A. Shuman

Fig. 1. Victoria Garcia-Sakai and Janna Maranas (Pennsylvania State University) inspect some of their DCS data using the DAVE software package.

Currently users can calculate the contrast factor for nucleic acids and proteins as well as for protein/nucleic acid complexes, simulate a molecular structure using simple shapes such as spheres, cylinders and helices and generate model SANS data, and align two macromolecular structures from which the model SANS data can be calculated. Furthermore users can calculate model SANS data from high-resolution x-ray crystallography or NMR structures that are written in the format recognized by the Research Collaboratory for Structural Bioinformatics (RCSB) Protein Data Bank (PDB). In addition to the on-line modeling capabilities SANS-Modeler also allows 3-D visualization of protein structures. Currently, SANS-Modeler is being tested and planned release to the general SANS community is scheduled for later this year.

Over the past year our reflectometry fitting software has been greatly refined and it is now available for different operating system platforms, including Linux, Windows, Mac OS/X, and SGI's IRIX. Installation is as simple as dragging a single file onto the desktop. With its context sensitive help facility and graphical user interface it is easy for novice users to analyze their data. With access to the underlying scripting language, it is a powerful and flexible tool for experts. This software is gaining wide acceptance in the NCNR reflectivity user community as the standard tool for data reduction and analysis. From the NOBUGS

2002 conference in November and from presentations inside NIST, we are now interacting with other US neutron facilities to further improve the software and explore the possibility for broader use.

EXPGUI, the NCNR-developed graphical interface to the Los Alamos GSAS crystallography package continues to impact the Rietveld community. In the past year, the software was downloaded well over a thousand times and the web pages were viewed more than one hundred thousand times. The user-friendly nature of the EXPGUI package is attractive to students and the program has now been integrated into a number of university courses. It has also been widely taught in workshops, for example at the recent Oak Ridge National Lab's NICEST workshop, the Georgia Tech Advanced Rietveld Short Course and the American Crystallographic Society's annual summer crystallography course. Requests for program enhancements, as well as new features added to the software, are tracked on the NCNR website (www.ncnr.nist.gov/xtal/software/expgui/wishlist.html). In FY2003, requests outstripped the Crystallography team's ability to respond. The major new features added to the code were:

- CIF: The IUCr's standard format, the crystallographic information file (CIF), including the powder diffraction extensions (pdCIF) have been implemented.

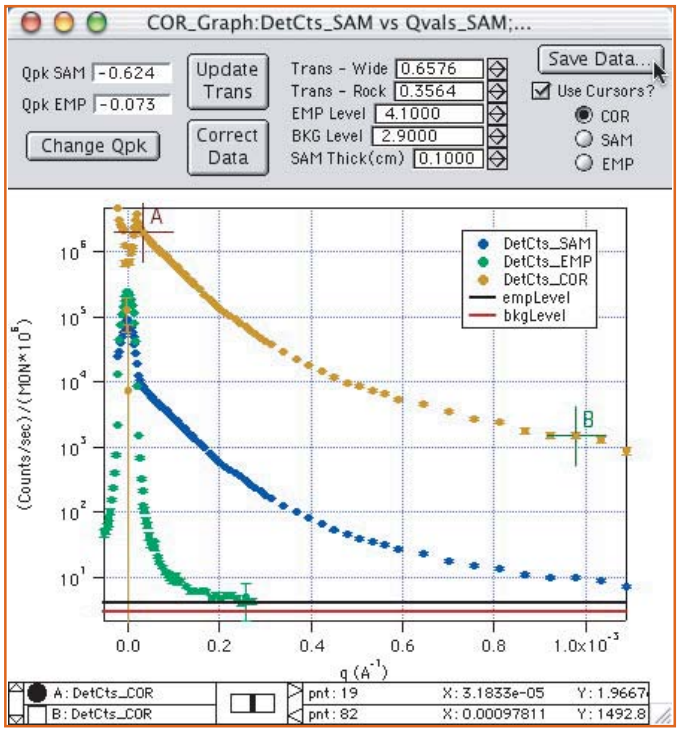

Fig. 2. A screenshot of USANS data reduction software, showing the raw scattering of the sample and empty cell, and the (rescaled) corrected USANS data. The user can override any of the automatically determined parameters, and the effects are directly visualized in the graph.

[Toby, B. H., Von Dreele, R. B. & Larson, A. C. "Reporting of Rietveld Results Using pdCIF: *GSAS2CIF*," J. Appl. Cryst. **36**, 1290 (2003).]

- Instrument parameter file editor: GSAS instrument parameter files describe the diffraction instrument and provide a starting point for the refinement. While users at the NCNR receive an accurate file for BT-1, building or finding an appropriate file for many other instruments has been a major trouble spot for many other users. The new editor shows the contents of the file and the options in an easy-to-understand fashion. It can also be used to create new instrument parameter files "from scratch."
- POWPREF warning: The POWPREF program is used in GSAS to map reflections to the powder diffraction data points. It must be rerun when the data range changes or if phases are added. Neophyte (and occasionally experienced) users may run into problems when they fail to run this program. EXPGUI now tracks these types of actions and reminds users to run the POWPREF program before attempting a refinement.
- Other enhancements include: new data and coordinate export abilities, ability to read in multiple datasets in a single step. Also, all reported bugs were fixed.

Data Acquisition and Instrument Control

Nearly every NCNR instrument relies on motors to position neutron optical elements and to orient the sample. The NCNR is in the process of replacing the motor control hardware with a new architecture to improve the serviceability and reliability of these critical systems (Fig. 3). The new architecture employs VME-based computers and motor indexers with an NCNR-designed chassis for multiple motor driver modules. Extensive use is made of commercial, off-the-shelf components through vendor-neutral interfaces. The chassis system features standardized connectors, jumpers and dip-switches to facilitate configuring the motor control system in the field. The complete system is capable of controlling up to 64 encoder-equipped motors using a full spectrum of motion control features. The new system has been deployed on the BT-8 DARTS instrument and on the NG-7 reflectometer.

Another major standardization effort has been the development of a standard control and readout interface for linear and area neutron detectors. This system is a PC-based histogrammer that interfaces with the detectors through either vendor-

supplied electronics or through standard NIM hardware using a high-speed digital I/O bus that is controlled over Ethernet using a simple, NCNR-designed protocol. Over the past year, this system has been successfully used on the NG-1 reflectometer, NG-1 SANS, and the NG-5 Neutron Spin Echo Spectrometer.

Sample Environment Equipment

There have been a number of improvements made to the equipment pool and support infrastructure for sample environments at the NCNR. The 9 Tesla horizontal field superconducting magnet with single crystal windows has been customized for SANS and USANS studies (Fig. 4). A pulse tube refrigerator capable of temperatures in the range of 4 K to 300 K has been integrated into the BT-1 powder diffractometer as a dedicated unit. A new closed-cycle refrigerator was added for general purpose use providing sample temperatures over a wide range: 7 K to 800 K. A new liquid helium cryostat, designed especially for the DCS instrument, was purchased and provides temperatures in the range of 1.5 K to 300 K. New support equipment includes: needle valve heaters for clearing blocked liquid helium cryostats, helium transfer stations at key locations, a new equipment preparation area at the north end of the Guide Hall, and new or updated user manuals for most of the equipment.

BT-7 Double Focusing Triple Axis Spectrometer Development

A new double focusing triple axis spectrometer for BT-7, is at an advanced stage of development, with installation planned for early next year. Highlights from this year's activities include delivery of the monochromator drum shields, completion of the double focused monochromator using Cu(311) and PG(002), installation of the instrument shutter system and incident beam collimation system, completion of the sample goniometer "bucket," and final testing of the air pad floor system. Final design, fabrication and testing are currently underway for the new analyzer system and for the data acquisition and instrument control system.

Photography by Lynn A. Shuman

Fig. 3. Doris Kendig (NCNR) adjusts motor drivers on the new motor control system.

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Fig. 4. Rachel Anderman (NCNR) fills the new 9T horizontal field superconducting magnet with helium.