conference abstracts

Recent advances in the Collaborative Computational Project No. 4 for Protein Crystallography. C. Ballard, *CCLRC Daresbury Laboratory, Warrington, WA4 4AD, UK.*
Keywords: protein, X-ray, software.

The Collaborative Computational Project No. 4 (CCP4) was established in 1979 by the UK Science and Engineering Research Council (now supported by the UK Biotechnology and Biological Sciences Research Council) to support collaboration between groups writing software for macromolecular crystallography. CCP4 provides a large suite of programs covering most of the computations required for macromolecular structure determination by X-ray crystallography. In addition the project supports a number of educational activities to aid crystallographers in applying these, and other, programs to real problems.

Version 4.0.1 of the CCP4 suite was released in Jan 2000 and includes several major changes. In particular automatic data harvesting for structure deposition has been included, CCP4i, the CCP4 graphical user interface, is now an integral part of the suite, and new programs MOLREP, OASIS and SC. Other highlights are major new versions of AMORE, RASMOL, SFCHECK and ARP_WARP (formally ARPP), and a new library for the reading and writing the mmCIF format.

The poster will present an overview of CCP4 activities, as well as details of recent additions to the suite. CCP4 staff will be available to answer questions and provide impromptu demonstrations of the suite.

automar, marFLM, marHKL and marXDS: Data Reduction Software for mar detectors. C. Klein and K.S. Bartels, *X-ray Research GmbH, Segeberger Chaussee 34, D-22850 Norderstedt, Germany.*
Keywords: data reduction, CCD, image plate.

In the last couple of years, considerable progress has been made to automate data reduction of area detector data. Traditionally, the most severe obstacle for getting the data processed has been the indexing step. Available programs differ mostly in the likelihood of obtaining the relevant crystal parameters required for integration.We concentrated our efforts mainly on this task and developed an entirely new data processing package called *automar*.
The program suite includes:

- Spot finding and autoindexing:
  Based on refinement of zone-axes the autoindexing features new algorithms for fully automatic determination of cell parameters and lattice types as well as crystal orientation and mosaicity. The method is extremely reliable and has very high success rates for indexing anything from ruby (5 Ang. cell axes) to virus patterns.
- Spot prediction and integration with various degrees of sophistication including site-dependent experimental and Bayesian profile fitting
- Summation of partials, post-refinement and scaling of intensities
- Calculation of data collection strategies for optimizing data collection time and/or completeness.
- Graphical user interface based on X-Windows/Motif with intuitive look & feel.
- Visual feedback from all stages of data processing and graphical output of results.

The ease of use of *automar* and the success rates of the indexing step encouraged us to adapt the interface to other popular data processing suites, namely MOSFLM, the HKL® suite and XDS. The resulting software provides a single key for processing data with the corresponding data reduction programs. Due to its homogeneity it is especially suited for data processing at synchrotron beam lines. Lack of experience will no longer prevent users from reducing their data with different programs and comparing the results.