s9.m31.p5 **Developments in Data Harvesting within CCP4.** M. D. Winn, P. Patel, E. Krissinel[a], *CCLRC Daresbury Laboratory, Warrington, Cheshire, WA4 4AD. UK.* [a]*European Bioinformatics Institute, Wellcome Trust Genome Campus, Cambridge, CB10 4SD. UK. E-mail: p.patel@ccp4.ac.uk*

Keywords: CCP4; Data harvesting; Protein crystallography

Data harvesting is a process using software for structure solution to output to a file certain items of metadata. This will enable the user who is solving the structure to have an organised collection of files which holds the details of how the model was obtained, which are then sent to the deposition centre and should bypass some of the manual data processing at deposition. CCP4 has programs which have been modified to output these harvesting files. These are Mosflm, Scala, Truncate, Mlphare and Refmac [1].

A few changes have been made to the way in which harvesting is carried out and managed in CCP4i. The options for creation of harvesting files has changed slightly. Also under development is a CCP4i interface to help manage harvesting files produced. This 'Harvesting Manager' will be able to run small tasks to validate the harvesting files in terms of syntax, to make sure the file produced is a correctly written mmCIF file and to convert files from mmCIF into XML. It does not take away from the user their responsibility of managing harvesting files, but its intention is to assist the user in the management of these files and in preparation for deposition. Other functionalities are being planned in the near future. An overview of additional tools in CCP4 5.0 is also given.

http://www.ccp4.ac.uk/ccp4/html/harvesting.html

s9.m31.p6 **Fityk - Peak Fitting Software with Support for Powder Patterns Analysis.** Marcin Wojdyr, Stanislaw Gierlotka and Bogdan Palosz, *High Pressure Research Center of Polish Academy of Sciences 'Unipress' Sokolowska 29/37 Warsaw 01-242, Poland. E-mail: wojdyr@unipress.waw.pl*

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Fityk (fityk.sf.net) is a free open-source software for nonlinear curve fitting and data analysis. It is written in C++ and available for Unix and MS Windows systems. The program was originally developed to analyze powder diffraction patterns, and then extended to allow for analysis of any experimental data that show maxima of an observed parameter. Apart from crystallography *fityk* is reported to be used also in chromatography, molecular photonics and other fields.

The program can be controlled via graphical or command line interface. Simple internal scripting language allows for automation of common data analysis tasks. Program usage begins with building a formula (model), that will be fitted to the experimental data. In *fityk* the model is given as a sum of predefined functions (polynomial, Pearson VII, Voigt, etc.). Parameters of these functions can be constrained. Powder diffraction module realizes Pawley-type data analysis. It takes wavelengths cell parameters, a set of HKL's, zero-shift and sample-displacement, and translates those numbers into a set of analytical peak-shaped funtions with constrained positions. Widths and shapes of the peaks can be fitted independently or constrained using formulae known from the Rietveld-analysis software. In terms of fitting the program currently provides three nonlinear optimization algorithms: Levenberg-Marquard gradient-based method, Nelder-Mead downhill simplex method and Genetic Algorithms. User can easily switch between these methods, e.g. start fitting with simplex method and then continue with Lev-Mar.

Examples of application of *fityk* to diffraction data will be given.