P.03.01.1

Acta Cryst. (2005). A**61**, C163

***Lafire*: a Software for Automatic Protein Structure Refinement**

Yong Zhou, Min Yao, Isao Tanaka, *Division of Biological Sciences, Graduate School of Science, Hokkaido University,Sapporo, 060-0810, Japan.* E-mail: zy_dut@hotmail.com

Refining an initial protein model to its final structure is usually composed of rounds of refinement performed by programs such as CNS and REFMAC, and manual model modification that includes linking and extending fragments, and fitting the ill matched residues of model by using the computer graphics program such as O. The manual model modification requires expertise of crystallography to recognize structural conformation based on electron density, and it is a time consuming process.

For the purpose of reducing the time and manual intervention of refinement, we developed a software named LAFIRE (Local-correlation-coefficient-based Automatic FItting for REfinement) to automate the whole refinement process. Four function modules are designed: building the missing parts in the current model, fitting the model to the electron density map, monitor program and an interface for combining the first two modules and the refinement programs CNS and REFMAC5.

The LAFIRE is already in the state that builds the whole model from fragments by iterative approach, and performs structural refinement process without manual intervention in a few hours or days. LAFIRE is also available on http://altair.sci.hokudai.ac.jp/g6/Research/Lafire_English.html. The overview of LAFIRE, methods of building and fitting in LAFIRE, and refinement applications will be give in this presentation.

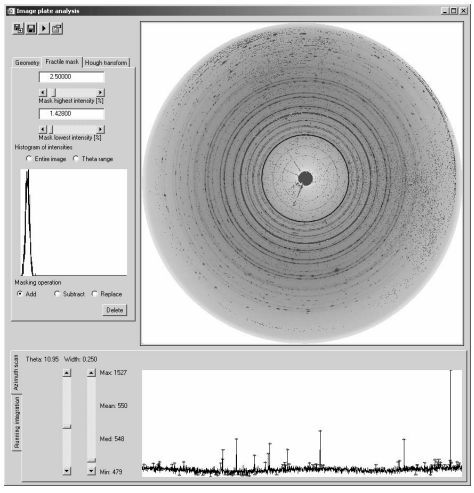
Keywords: automatic refinement, software, Lafire

P.03.01.2

Acta Cryst. (2005). A**61**, C163

Powder3D: Towards Automatic Image Plate Analysis

Bernd Hinrichsen, Robert E. Dinnebier, Martin Jansen, *Max-Planck-Institute for Solid State Research, Stuttgart, Germany.* E-mail: b.hinrichsen@fkf.mpg.de



Large area detectors produce vast amounts of data automatically, however, filtering data by means of masking is a manual task, [1]. Alternative processing methods are required.

Powder3D has facilitated the data reduction and analysis of large numbers of powder diffraction patterns, [2]. A new module utilizing hough transforms and fractile statistics for automated image plate analysis and filtering is presented.

[1] Hammersley A.P., Svensson S.O., Hanfland M., Fitch A.N., Hausermann D., *High Pressure Research*, 1996, **14**, 235. [2] Hinrichsen B., Dinnebier R.E., Jansen M., 2005, *to be published*.

Keywords: powder diffraction software, image plates, time-resolved diffraction

P.03.01.3

Acta Cryst. (2005). A**61**, C163

HipHop. A Novel Refinement Method for Protein Structures

Jan Ondráček, *Department of Recombinant Expression and Structural Biology, Institute of Molecular Genetics, Prague, Czech Republic*. E-mail: ondracek@img.cas.cz

A novel refinement method called HipHop refinement is described. Although HipHop refinement seems to be similar to simulated annealing refinement it is based on a different philosophy - namely that it is in principle impossible to determine a complete structure at a limited resolution. Thus, the limited resolution and the inaccuracy of the underlying X-ray data cause not only errors in the refined structural parameters but principal structural errors in the single model, which is usually used to explain the data.

HipHop refinement is performed in several steps. In the first step, a proper number of pseudo waters corresponding to maxima in the difference Fourier map is added to the model (HIP step, $\mathbf{H}_2\mathbf{O}$ **inp**ut). In the next step, the model is refined and waters not fulfilling density, shape or position criteria are removed from the model (steps HOP, $\mathbf{H}_2\mathbf{O}$ **outp**ut). The process is in fact jumping between local minima – HipHop. During HipHop cycles not only the water arrangement but also side/main chain orientation is changed. The best presentation of HipHop refinement is a multi conformer PDB file.

The method was tested on several different protein structures with excellent results [1,2] The programs are available on http://www.img.cas.cz/hiphop/.

[1] Ondráček J., Weiss M.S., Mesters J.R., *Acta Cryst*., manuscript *in preparation*. [2] Ondráček J., Weiss M.S., Brynda J., Fiala J., Jursík F., Řezáčová P., Jenner L.B., Sedláček J., *Acta Crys.*, *submitted for publication.*

Keywords: protein refinement methods, protein water analysis, protein disorder

P.03.01.4

Acta Cryst. (2005). A**61**, C163

Deconvolution of X-ray Diffraction Profile by Using the Regularization Technique

Vladyslav Piskarov, Joachim Wagner, Rolf Hempelmann, *Saarland University, Physical Chemistry, Germany.* E-mail: v.piskarov@mx.uni-saarland.de

The deconvolution of the instrumental function in X-Ray diffraction profile analysis is a basic step in order to obtain reliable results on the microstructure (crystallite size, lattice microstrain, *etc*.) and is a typical example of ill-posed inverse problems. The implementation of an eigen function method with different regularization techniques is investigated and a simple regularization algorithm is proposed.

A simulation of an instrumental-broadened profile superimposed with random noise and background signals is used to investigate the reliability and efficiency of the proposed technique. For the simulation an experimentally defined instrument function based on an accurate mathematical model for Cu emission profile, the geometry of the diffractometer and the physical properties of the specimen are used. The parameters for this instrumental function are obtained by least squares fitting of experimental data sets resulting from the reference materials LaB_6 and Al_2O_3.

Compared to established algorithms, the proposed route is faster and more reliable in terms of stability, especially in the case of large experimental noise. The evaluation of experimental diffraction data of nanocrystalline gold with respect to grain size and microstrain and the comparison with standard evaluation technique is done.

[1] Kurashov V.N., Kurashov A.V., Piskarev V.L., *Proc. SPIE*, 1997, **3317**, 36. [2] Ida T., Toraya H., *J. Appl. Cryst.*, 2002, **35**, 58. [3] Sanchez-Bajo F., Cumbrera F.L., *J. Appl. Cryst.*, 2000, **33**, 259.

Keywords: powder diffraction, profile analysis, regularization

P.03.01.5

Acta Cryst. (2005). A**61**, C163-C164

Faster Least-Squares Refinement of Larger Molecules using the Program CRYSTALS

Stefan D. Pantos[a], D. J. Watkin[a], R. I. Cooper[b], [a]*Chemical Crystallography, University of Oxford, Oxford, UK.* [b]*Oxford Diffraction Ltd, Abingdon, Oxfordshire. UK.* E-mail: stefan.pantos@chem.ox.ac.uk

Least-squares is both powerful and the most widely used method of structure refinement for small molecules. However normal matrix