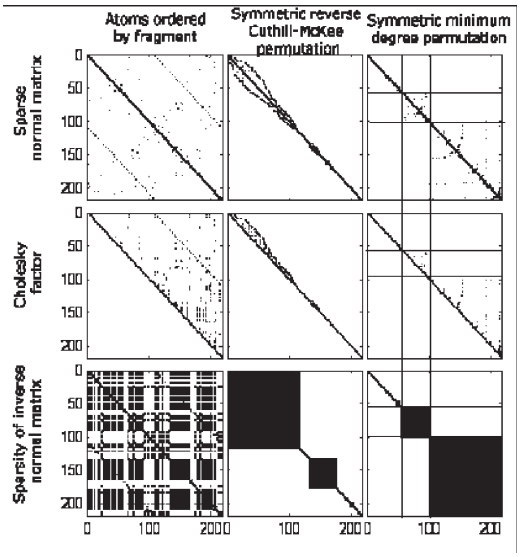
s1.m3.p8 **Evaluation of different treatments of the normal matrix.** S. D. Pantos, R. I. Cooper and D. J. Watkin, *Chemical Crystallography, Chemical Research Laboratory, University of Oxford, Oxford, OX1 3TA, UK. E-mail: d922qg@mac.com*

Keywords: Refinement; Least-Squares; Sparse Matrices

During the method of least-squares a large normal matrix is produced which has to be accumulated and inverted. This is both expensive in computation time and storage. For small structures this is usually insignificant, but time and storage increase rapidly with the number of parameters being refined. Improvements may be made by using sparse matrices, as not storing zero elements reduces the memory footprint and memory access during computation. Efficient storage of a square matrix also depends on the ordering of the rows and columns. The figure shows some preliminary work with sparse matrices at different stages of the inversion process (rows). Some different orderings of the normal matrix (columns) are also shown. Near-zero elements have been omitted to demonstrate the sparsity in the normal matrix. The structure contains some large off-diagonal correlation elements due to the asymmetric unit containing a pseudo-center. Inversion of the matrix produces many more non-zero elements. The first column shows the normal matrix which has not been reordered. The parameters are ordered by adjacent atoms. It can be seen that storing the inverted matrix sparsely would be inefficient. Columns 2 and 3 show MATLAB reordered normal matrices and the results of their inversion [1, 2]. The results of these reorderings produce matrices which are efficiently stored in sparse matrix form and thereby decreasing the storage and the computation required.

The poster shows an evaluation of different orderings of the normal matrix on crystallographic least-squares refinement and the effect of elimination of near-zero elements on the accuracy and convergence of the refinement.



[1] George, Alan and Joseph Liu, *Computer Solution of Large Sparse Positive Definite Systems*, Prentice-Hall, 1981

[2] George, Alan, Liu, Jos, "The Evolution of the Minimum Degree Ordering Algorithm," *SIAM Review*, **1989**, 31:1-19

s1.m3.p9 **SAD / MAD techniques in "il Milione".** Giampiero Polidori[a], Maria Cristina Burla[a], Benedetta Carrozzini[b], Giovanni Luca Cascarano[b], Carmelo Giacovazzo[b,c],. [a]*Dipartimento di Scienze della Terra, Piazza Universita', 06100 Perugia, Italy.* [b]*Istituto di Cristallografia, CNR, c/o Dipartimento Geomineralogico, Universita' di Bari, Campus Universitario, Via Orabona 4, 70125 Bari , Italy cDipartimento Geomineralogico, Universita' di Bari, Campus Universitario, Via Orabona 4, 70125 Bari, Italy. E-mail: giampiero.polidori@unipg.it*

Keywords: SAD; MAD; Anomalous Scatterers

SAD and MAD techniques play an important role in the crystal structure solution of macromolecules.

A new theoretical approach, applying the method of joint probability distribution has bees recently proposed ([1] [2] Burla *et al*. 2002, 2003) to estimate the amplitudes of the structure factors of the anomalously scattering substructure given the experimental diffraction moduli. Its advantage is that the estimates can simultaneously exploit the anomalous and the dispersive differences from several wavelength data.

An automatic procedure has been devised which performs the structural determination of the sub-structure both in SAD and MAD cases. The procedure is able to to select the most informative wavelength combination and determine the best limit for data.

The procedure has been tested on a large set of SAD and MAD data and has been introduced in the Direct Methods Program SIR2004, which will be distributed as part of the package "il Milione". This new package is able to solve crystal structures in the following cases: a) ab initio, for small, medium and for protein structures; b) SIR-MIR, SIRAS-MIRAS, SAD-MAD cases for proteins; c) powder data.

[1] Burla, M.C., Carrozzini, B., Cascarano, G.L., Giacovazzo, C., Polidori, G. & Siliqi, D. (2002). *Acta Cryst*. D**58**, 928-935

[2] Burla, M.C., Carrozzini, B., Cascarano, G.L., Giacovazzo, C., & Polidori, G. (2003). *Acta Cryst*. D**59**, 662-669