**s8b.m3.p1** **SIR2000: a parallel package**. M.C. Burla[b], M. Camalli[c], B. Carrozzini[d], G.L. Cascarano[d], V. Di Martino[e], C. Giacovazzo[ad], G. Polidori[b], D. Siliqi[e], R. Spagna[c], [a]*Dipartimento Geomineralogico, Università di Bari, Campus Universitario, Via Orabona 4, 70125 Bari ,Italy,* [b]*Dipartimento di Scienze della Terra - Piazza Universita', 06100 Perugia, Italy,* [c]*Istituto di Strutturistica Chimica "G. Giacomello", CNR, C.P. 10 - Monterotondo Stazione - 00016 Roma, Italy,* [d]*IRMEC c/o Dipartimento Geomineralogico, Università di Bari, Campus Universitario, Via Orabona 4, 70125 Bari, Italy,* [e]*Consorzio per le Applicazioni di Supercalcolo Per Universita' e Ricerca (CASPUR) c/o CICS Universita' di Roma "La Sapienza" Piazzale Aldo Moro 5 00185 Roma, Italy.*
Keywords: direct methods, proteins, crystallographic computing.

SIR2000 [1] is a direct method package aiming at solving *ab initio* complex crystal structures. Protein molecules up to 2000 atoms in the asymmetric unit have been solved, provided date resolution is about 1.1 Å. The computing time for obtaining a correct model for very large structures is usually not negligible, and will probably increase as soon as larger structures will be attempted. We therefore decided to set a parallel version of SIR2000 to take the maximum advantage of local network of workstation eventually available in the user lab. The computation time for solving proteins crystal structures grows with the number of trials. Since the trials are independents a direct implementation of the parallel SIR2000 version may be used. We inserted the standard MPI library call to manage the parallel execution of SIR2000. We tested SIR2000 on a MPICH 1.2.0 installation at our labs, where a cluster of different ALPHA workstation is available. We took care to implement a load balance correction so that heterogeneous clusters of workstations may efficiently run the code.

Owing the full portability of MPI standard, the code may run also on proprietary architectures with optimized MPI. It is important to notice that communication to computation ratio is very low because the problem is an embarrassing parallelism one. Optimal speedup is already achieved also with low cost clusters of workstation, starting from PC clusters connected with fast ethernet switch. We test the parallel code on a PC cluster at CASPUR, and we expect that users may run SIR2000 on doyourself clusters without any problem.

[1] Burla M.C, Camalli M. Carrozzini B., Cascarano G.L., Giacovazzo C., Polidori G., Spagna R.. "SIR2000, a program for the automatic *ab initio* crystal structure solution of proteins ", Acta Cryst , (2000), A56: 000-000.

**s8b.m3.p2** **SYSTER: a program for the evaluation of systematic errors in reflection data.** J.M.M. Smits, R. de Gelder, *Department of Inorganic Chemistry, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands.*
Keywords: systematic errors, data evaluation, error visualization.

Detailed insight into the differences between $F_o$ and $F_c$ can be very helpful during the validation of a structural model and its underlying reflection data. The recently defined R tensor[1], which was developed to signal *e.g.* problems like twinning, shows the anisotropy of the error distribution. However, it does not reveal resolution or measuring order dependencies of the errors due to its averaging over theta and the loss of, in the first place, the link between individual, symmetry equivalent reflections and, in the second place, the link between the order in which the data were collected and the input to the least squares refinement procedure.

Information on the differences between $F_o$ and $F_c$ as a function of measuring order, theta, $F_o$ or position in reciprocal space can show drifts and trends that may point to systematic errors related to instrumental malfunctioning, to data reduction problems (e.g. sloppy correction for crystal decay), to wrong absorption correction or to errors in the structural model.

We developed a program, called SYSTER, that is able to show drifts and trends of $F_o$ *vs* $F_c$ with respect to a large variety of variables. The results can be visualized in the form of two-dimensional plots and/or three-dimensional Ewald spheres (which can be rotated interactively on screen using RasMol[3] as a graphical interface).

A number of examples is given in which the program SYSTER is used to reveal the effect of drift correction and the use of several absorption correction methods on the nature of the error distributions in reciprocal space.

The program requires three SHELXL[2] files: an *.hkl file, an *.fcf file and a *.ref file. The reflections in the *.hkl file should be in the order in which they were measured.

The visualization uses OpenGL and GLUT and has been kept separate from the data interpretation program to ease adaptation to other platforms or other, functionally equivalent, input data files. The two FORTRAN programs are developed for IRIX 6.5 (Silicon Graphics) but platform dependent functions, like dynamic memory functions, are grouped together and can easily be replaced, even by fixed memory allocations.

The program is available, free of charge, at http://www.sci.kun.nl/software/syster.html.

A functionally equivalent Windows95 executable will become available.

[1] Parkin, S. Expansion of scalar validation criteria to three dimensions: the R tensor. Acta Cryst. (2000), **A56**: 157-162.
[2] Sheldrick, G.M. SHELXL-97. program for the refinement of crystal structures; University of Göttingen: Germany, 1997.
[3] Sayle, R. RasMol v2.5. Biomolecular Structure, Glaxo Research and Development, Greenford, Middlesex, U.K.