Oral Contributions

[MS44] Crystallographic Software Fayre introduction
Co-Chairs: Andrea Thorn (UK), Santiago Garcia-Granda (ES)

[MS44-01] New features in Sir2011 Giovanni Luca Cascarano, Benedetta Carrozzini, Carmelo Giacovazzo, Annamaria Mazzone

Istituto di Cristallografia, CNR, Via G.Amendola 122/O, Bari, 70126, Italy.
E-mail: gianluca.cascarano@ic.cnr.it

New algorithms. VLD (Vive La Difference) [1] was originally designed for ab-initio crystal structure solution: it has been successfully applied to small, medium and protein structures, provided that the data resolution is atomic. Sir2011 [2] has been recently modified in order to use VLD (in synergy with EDM and FreeLunch[3,4]), in non ab¬initio cases and when data resolution is not atomic. The procedure has been tested for the Molecular Replacement (data resolution up to 3 Å) [5]. Good preliminary experimental results encouraged us to design a pipeline for leading molecular-replacement solutions to the refined target structure in a fully automated way. The pipeline includes external programs such as Refmac [6] and ARP/wARP [7]. The results of the application of this new procedure will be shown. New graphic tools The graphical interface has been further on improved and allows the straightforward use of the program even in difficult cases. The graphic routines (based on OpenGL) are shared with those written for JAV (Just Another Viewer, unpublished), a program to visualize structural models and electron density maps. JAV, is a stand-alone program; it is distributed as add-on with Sir2011 or included in the package Il Milione [8]. The graphic routines allow the visualization and modification of the current model at any step of the program; they can be used also to produce higher quality images (with respect to the traditional more naïve graphics of SIR2011). In the latest version of the program new GUI's have been designed to face with data format typical of proteins (MTZ, PDB, Fasta sequence) and to set up the necessary environment to face Molecular Replacement problems.

[1] Burla, M. C., Carrozzini, B., Cascarano, G. L., Giacovazzo, C. & Polidori, G. (2011). J. Appl. Cryst. 44, 1143–1151.
[2] Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Mallamo M., Mazzone, A., Polidori, & Spagna R. (2012). J. Appl. Cryst., 45, 357-361.
[3] Caliandro, R., Carrozzini, B., Cascarano, G.L., De Caro, L., Giacovazzo, C. & Siliqi, D. (2005a). Acta. Cryst. D61, 556-565.
[4] Caliandro, R., Carrozzini, B., Cascarano, G.L., De Caro, L., Giacovazzo, C. & Siliqi, D. (2005b). Acta. Cryst. D61, 1080-1087.
[5] Carrozzini, B., Cascarano G.L., Comunale G., Giacovazzo C. Mazzone A. Acta Cryst. (2013). D69, 1038–1044
[6] Murshudov, G. N., Skubak, P., Lebedev, A. A., Pannu, N. S., Steiner, R. A., Nicholls, R. A., Winn, M. D., Long, F. & Vagin, A. (2011). Acta Cryst. D67, 355–367.
[7] Perrakis, A., Morris, R. & Lamzin, V. S. (1999). Nature Struct. Biol. 6, 458–463
[8] Burla M.C., Caliandro R., Camalli M., Carrozzini B., Cascarano G.L., De Caro L., Giacovazzo C., Polidori G., Siliqi D., Spagna (2007) J. Appl. Cryst. 40,609-613.