

SIR2002: its heir SIR2004 and IL MILIONE

Giampiero Polidori^a, Maria Cristina Burla^a, Benedetta Carrozzini^b, Giovanni Luca Cascarano^b, Carmelo Giacobazzo^b, Dritan Siliqi^b. *^aDipartimento di Scienze della Terra, Piazza Università, 06100 Perugia, Italy.*
^bIstituto di Cristallografia, CNR, Via G. Amendola 122/O, 70125 Bari, Italy.

Keywords: **Crystallographic Computing, Direct Methods**

SIR2002 is a well established program for the ab initio crystal structure solution of small-, medium - and macro-molecules ([1]Burla et al. 2003). It does not need prior information but requires atomic resolution for the experimental data. The heir of **SIR2002**, the package **SIR2004**, is under beta-testing. It shows several advantages :

- 1) the sequential procedure of **SIR2002** (all the trials provided by the tangent procedure are sequentially refined in direct space) is replaced by a faster procedure using early figures of merit just after the tangent step. This eliminates non promising trials and makes the procedure much faster.
- 2) the phasing process has been powered , and allows to solve protein structures even if data have quasi-atomic resolution (1.4 Å) ([2] Burla et al. 2003).

SIR2004 has been implemented into the package **IL MILIONE** , a set of programs designed for global phasing.

It is able :

- 1) to combine direct methods with SIR-MIR, SIRAS-MIRAS, SAD-MAD techniques (i.e., substructure determination, structure factor phasing, solvent flattening).
- 2) to solve and refine crystal structures from powder data.

[1] M.C. Burla, M. Camalli, B. Carrozzini, G.L. Cascarano, C. Giacobazzo, G. Polidori, R. Spagna. *J. Appl. Cryst.* (2003), **36**, 1103.

[2] M.C. Burla, B. Carrozzini, R. Caliandro, G.L. Cascarano, L. De Caro, C. Giacobazzo, G. Polidori. *Acta Cryst.* (2003), **A59**, 560-568.