Chapter 5.7

SUPERFLIP

Structure Solution by Charge Flipping

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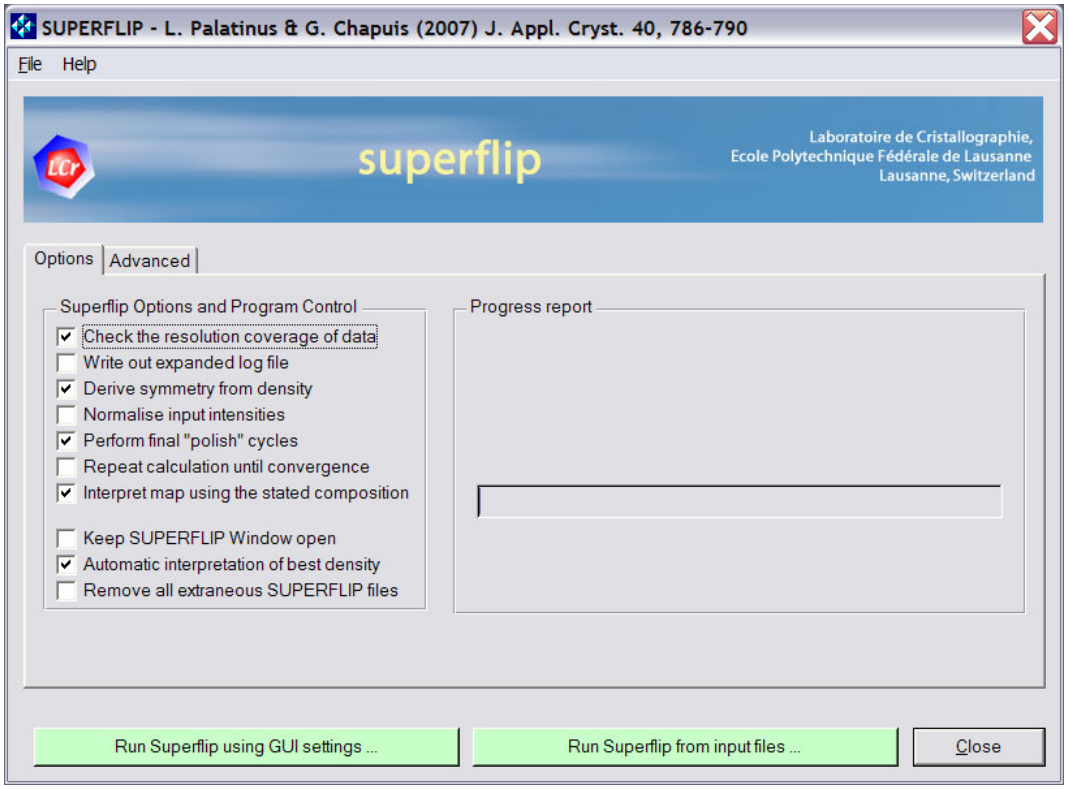
The charge flipping algorithm recently described by Oszlányi & Sütö [1-4] is a surprisingly simple method for *ab initio* crystal structure solution. It involves density modification in real space, and has been implemented in a program **SUPERFLIP** by Palatinus & Chapuis [5]. Although **SUPERFLIP** allows density reconstruction in arbitary dimensions (for instance incommensurate structures may be solved [6]), the WinGX GUI only allows access to a subset of the **SUPERFLIP** commands, for "standard" 3-D crystal structure solution. The **SUPERFLIP** program and its associated documentation may be obtained from the web site at ref 7. The WinGX version uses a slightly modified version of the program **EDMA** [8], which is run after **SUPERFLIP** to interpret the density map.

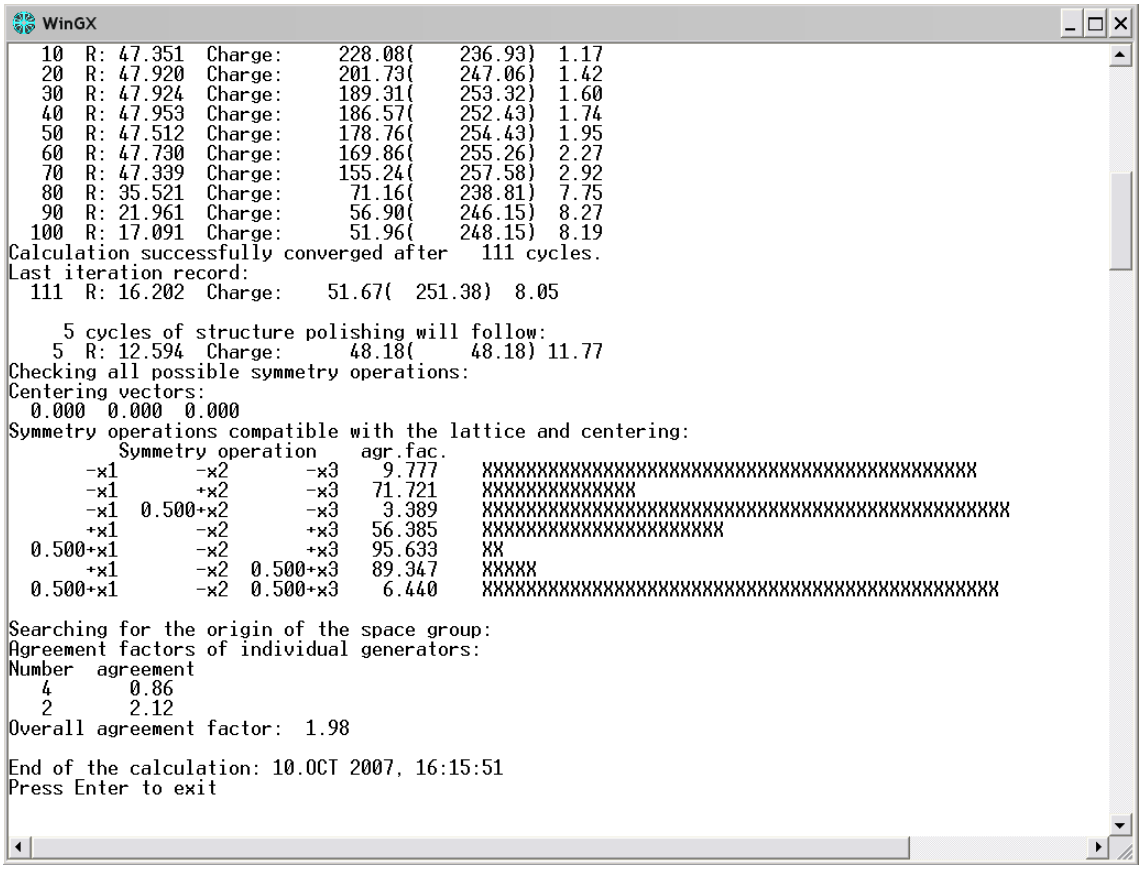
The only required files are *NAME.INS* (which should contain as minimum information the commands CELL, LATT, SYMM, SFAC, UNIT, HKLF), and a **SHELX** style reflection file *NAME.HKL*. No symmetry or cell content information is used by the **SUPERFLIP** program, but the interpretation of the resultant electron density map is greatly aided if the space group symmetry and unit cell contents are known. The program **EDMA** analyses the electron density and produces a **SHELX** style file *NAME.RES* as the output, which is conveniently visualised in the **SXGRAPH** program.

In ***WinGX***, **SUPERFLIP** is run from a GUI, accessed through the "Solve-SUPERFLIP" menu item. This GUI writes the input files for **SUPERFLIP** (*SUPERFLIP.INPUT*) and also for **EDMA** (*EDMA.INPUT*), and executes both programs automatically in sequence using the "Run Superflip using GUI Settings" button, as show below.



The "Advanced" panel allows the user to modify the most commonly changed parameters for **SUPERFLIP**, and also control aspects of the program flow.

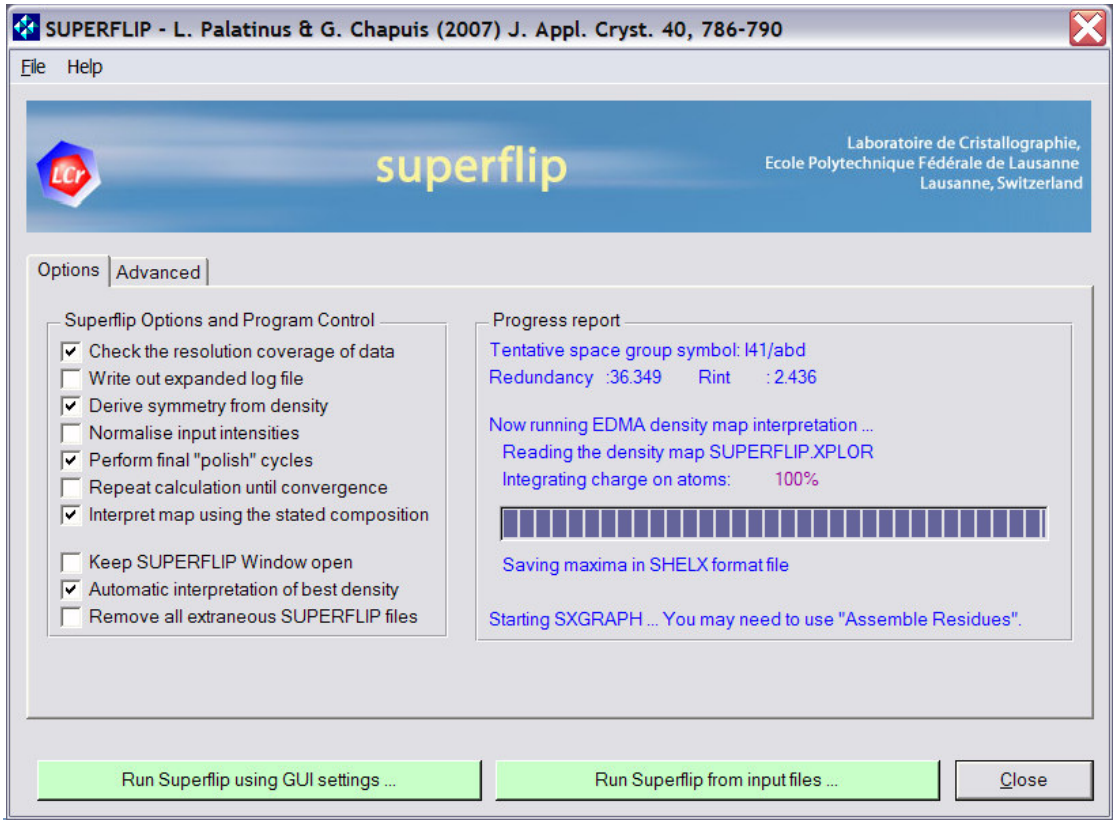
The **SUPERFLIP** executable supplied with the WinGX package is one obtained from the Superflip web-site, and is a DOS style console application. The text output is displayed in a "DOS" box, and by default this window will disappear as soon as **SUPERFLIP** has finished execution. If the user selects the "Keep SUPERFLIP Window open", then the text output may be examined by scrolling the window. The program will expect the user to hit the "Enter" key to dismiss this window. The main GUI window becomes invisible while the SUPERFLIP DOS Window is open.



SUPERFLIP will run through cycles of real-space/reciprocal-space discrete Fourier transforms (10000 by default) until convergence of the charge density is achieved. In the event that the program runs to the 10000 cycles, it is unlikely that the structure will be solved. If the "Repeat calculation until convergence" option is selected, then **SUPERFLIP** will repeat itself until a solution is found. *NOTE - in the event that the structure cannot be solved, the program will enter an infinite loop!* The default mode uses random phases determined by a randomseed, set by the system time. As a result (unlike for other structure solution programs apart from **SHELXD**), the calculation *will in general be different* each time the program is

run. So if a first run of **SUPERFLIP** fails, it is entirely possible that a second (or subsequent) run will result in the structure being solved.

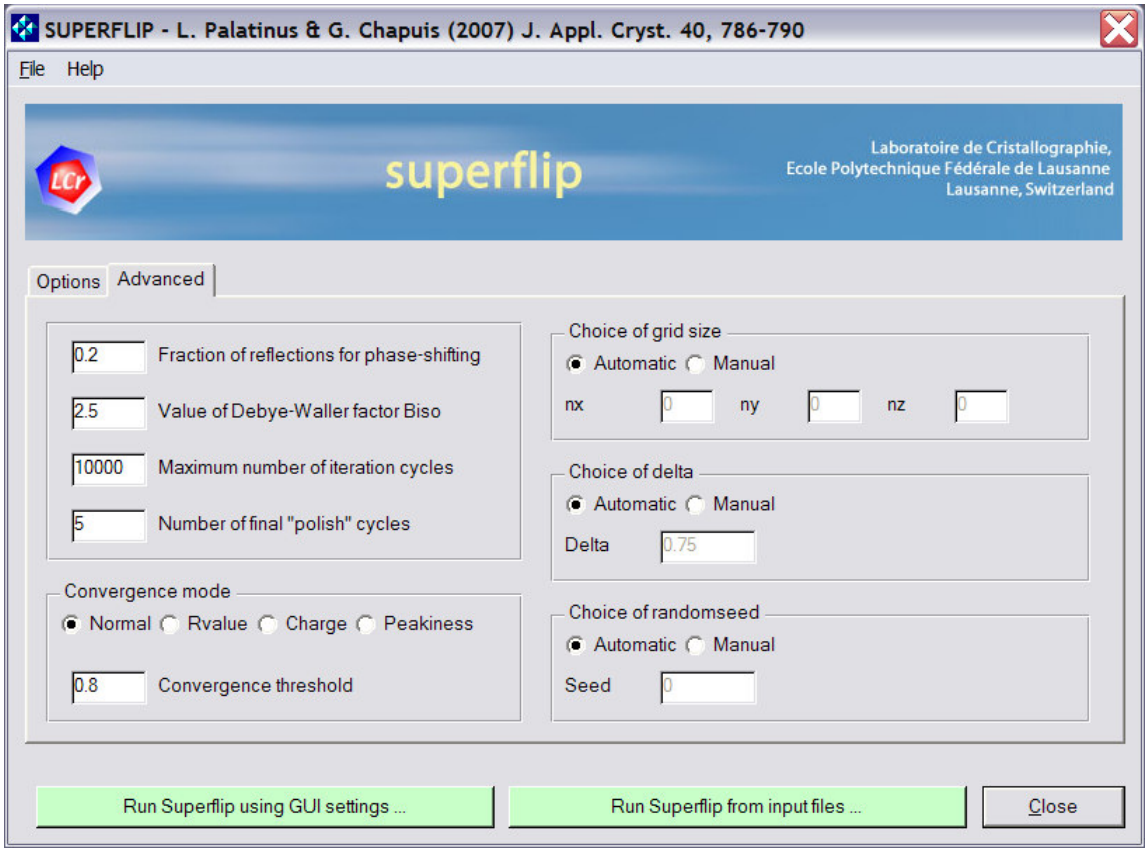
Once **SUPERFLIP** has converged, a density map is written - in the ***WinGX*** environment, this file is always called *SUPERFLIP.XPLOR*. If the option "Automatic interpretation of best density" is selected (the default), the map is then examined by a modified version of **EDMA** [8]. This latter program works exclusively in the background, but sends messages to the GUI, which indicate the progress. A real time resumé of the progress of both Superflip and EDMA is shown in the Progress report box (see below). A file *NAME.RES* is written containing the coordinates of the (hopefully) solved structure. This may be examined and modified by **SXGRAPH** in the normal manner. *One important point is that EDMA will, more often than not, produce a coordinate file which does NOT have the atoms in a connected residue*. To get a connected set of coordinates, just use the Model-Assemble Residues option in **SXGRAPH**.



The listing output from **SUPERFLIP/EDMA** are in the files *SUPERFLIP.LST* and *EDMA.LST*. These files and all other non-essential files will be deleted when the GUI is closed, if the "Remove all extraneous SUPERFLIP files" option is selected (the default).

For more expert users, there is a second advanced pane, which allows the user to modify some of the **SUPERFLIP** parameters (see the **SUPERFLIP** manual for details

of their meanings). It is also possible to manual edit the instruction files *SUPERFLIP.INPUT* and *EDMA.INPUT* using the "File - Edit SUPERFLIP input" and "File - Edit EDMA input" menu items and then run the program directly (by-passing the automatic rewrite of the input file), by using the "Run Superflip from input files" button.



References

1. Oszlányi, G. and Sütö, A. (2004) *Acta Cryst*. **A60**, 134-141.
2. Oszlányi, G. and Sütö, A. (2005) *Acta Cryst*. **A62**, 147-152.
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7. http://superspace.epfl.ch/superflip/
8. van Smaalen S., Palatinus L., Schneider M. (2003), *Acta Cryst*. A**59**, 459-469