PROGRAM: Ref_UB_Laue

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Program for refining the cell parameters and instrumental, or image parameters, from point coordinates and indices of spots obtained from a series of Laue images. The input file is an appropriate CFL file called, for instance, `My_Lref_file.cfl`. The program can also be run using a script file of extension `.reflaue`.

The relevant content of this script file is the following:

```
CFL_FILE  my_initial_cfl_File.cfl
N_IMAGES  num  rewrite_cfls  reindex_tol rval
image_name_1
image_name_2
........
image_name_num
```

The program prepares individual CFL files corresponding to each image copying the initial CFL file and changing the name of the peak file to that of the image as `image_name_n_peaks.inf` (for image `image_name_n.tif`) it is supposed that the file `image_name_n_peaks.inf` has been previously created by **Esmeralda** or **Laue_Simulator** (or even **Laue_Orient**). All the images are treated one after the other using the same conditions of refinement for all of them. If the keyword **`rewrite_cfls`** is given in the same line as **`N_IMAGES`**, the initial CFL files are replaced by the newest ones instead of creating `filecode_new.cfl` files. If the keyword **`reindex_tol`** is given, followed by its value `rval` in *mm*, the corresponding value is used for re-indexing reflections. Otherwise the value `rval=2.5` *mm* is used.

The CFL input control file should contain the cell parameters and offsets of the instrumental parameters, as well as the refinement conditions. It contains also the name of the spots file and the name of the instrumental file.

The free parameters are named as:

`a`, `b`, `c`, `alpha`, `beta`, `gamma` (at least one length axis should be fixed)

`Phi_x`, `Phi_y`, `Phi_z` (angles corresponding to the U-matrix, normally all should be refined)

The instrumental parameters are taken into account for the refinement. What can be refined is an offset of certain input instrumental parameters. The instrument file should contain at least the following items:

```
DET_TYPE     Cyl          <- Needed information
ROT_ORDER    xzy          <- Needed information
DIST_DET     159.155      <- Shift can be refined
GN_CENTRE  0.000  0.000   <- offsets can be refined (flat detector gamma & nu of the centre)
TILT_ANGLES  0.000   0.000   0.000    <- offsets can be refined
DISP_CENTRE  0.000   0.000   0.000    <- offsets can be refined  (Centre of reference system)
```

Additional refinable parameters are the spot position shifts modelled with Chebychev polynomials.
The program uses least squares to optimize the function:

$$\Delta = \sum_i w_i \{(x_{oi} - x_i)^2 + (z_{oi} - z_i)^2\}$$

The weight w_i is presently taken as a constant for all observations (x_{oi}, z_{oi}) coordinates expressed in *mm*. The instrumental parameters plus the offsets are used as effective instrumental parameters for the calculation of spot positions (x_i, z_i).

A template of the input CFL file is created by the program **Laue_Orient**. An example is given below:

```
Title  UB-Refinement file for Laue data (Template generated by Laue_Orient)
!          a         b         c        alpha     beta     gamma
Cell     17.2596   11.9890   10.0770   90.000  116.140   90.000
!     Space Group
SpGr  C 2/m
!     External Files
PEAKS_FILE     feind_peaks.inf
INSTR          vivaldi.inf
!           Phi_x      Phi_y     Phi_z   of  Busing-Levy U-matrix
ORIENT     182.77878   16.63562  263.84879

OFFSETS
   Dist       0.0
   Tilt_x     0.0
   Tilt_y     0.0
   Tilt_z     0.0
   Gamma_c    0.0
   Nu_c       0.0
   rOD_x      0.0
   rOD_y      0.0
   rOD_z      0.0
END_OFFSETS

CHEBYCHEV     6
  0.0  0.0    0.0  0.0    0.0  0.0       !x
  0.0  0.0    0.0  0.0    0.0  0.0       !z
END_CHEBYCHEV

LSQ_CONDITIONS
  Corrmax 50
  Maxfun  1000
  Tol     1.0e-6
END_LSQ_CONDITIONS

!VARY a b c alpha beta gamma
!VARY Phi_angls
!VARY Phi_x Phi_y
!VARY Cheb all
!VARY Chebychev  1 3 4
!VARY Spindle_Offsets
!VARY Spindle_Offset  1 2 4 5
!VARY Offsets all
!VARY Dist_offset rOD_x_offset  rOD_z_offset
!VARY Tilt_x_offset Tilt_y_offset  Tilt_z_offset
```

Notice that the **VARY** instructions have to be uncommented and modified for the particular problem by the user of the program. Normally the cell parameters (except one of them) and rotation angles should be refined

```
VARY b c  beta
VARY Phi_angls
```

This pair of **VARY** instructions corresponds to the refinement of the orientation matrix.
For cylindrical detectors the following offsets can be refined: `Tilt_x_offset`, `Tilt_y_offset`, `Tilt_z_offset`, `rOD_x_offset`, `rOD_y_offset`, `rOD_z_offset` and the spindle offsets when using simultaneously several images.
For flat detectors `Gamma_c_offset` and `Nu_c_offset` can also be refined.
Unknown distortions of the images are modelled using Chebychev polynomials (presently the same coefficients for all images: one can run the program with a script treating independently all the images). A refinement of everything can be done but strong correlations appear. The user should check the output file `My_Lref_file.ubr`.

(The program is under development and additional output files are under consideration)