

## Program: New\_Argonne\_Boxes

Program to integrate reflections of Laue Patterns.

Written originally by Clive Wilkinson & Garry McIntyre with adds-on by Ross Piltz and J. Rodriguez-Carvajal.

Published use of this program should refer to:

Wilkinson C, Khamis HW, Stansfield RFD, McIntyre GJ, *J. Appl. Cryst.* **21** (1988) 471-478.

A Fortran module has been constructed from the program `Argonne_Boxes` that was written by Clive Wilkinson and Garry McIntyre and it uses Clive's peak integration routines similar to the program `Racer`. The version provided by Ross Spiltz has been used as starting point for changes. It has been transformed to Fortran 90 by using the program `to_f90n` (derived from `to_f90` by Allan Miller) and by hand editing. Many arrays have been made allocatable and the dependencies on VIVALDI/KOALA have been eliminated.

The main program uses this module and runs as the original Fortran 77 program.

This version of the program works using directly TIFF files and hkl-files generated by `Ref_UB_LAUE` that contain corrected (refined) peak positions both in mm and pixels.

The old program has been converted into a subroutine called `Integrate_Vgain` that is called by the new main program called `New_Argonne_Boxes`.

`New_Argonne_Boxes` needs an input file that is automatically generated by `Ref_UB_LAUE` or by `Esmeralda` (it may be created by hand with an editor), containing the number of images to treat the code of the files (xxxx for `xxxx.tif`, `xxxx.hkl`) and the conditions for treatment.

The default extension of this file is `*.abx`.

Running the program without arguments in the command line provides the information needed for running properly the program. The following text is output:

```
Prompt>new_argonne_boxes <cr>
```

Usage of `New_Argonne_Boxes` program for integrating Laue patterns:

Syntax: `Prompt> New_Argonne_Boxes argonne_boxes_input_file.abx`

Example of `argonne_boxes_input_file.abx`:

```
----- Start of argonne_boxes_input_file.abx -----
Nfiles: 3      TIFF
!      gainmax cutoff_m   cont  fill  arfac  cor_mult  cutoff_a  cutoff_neigh
codfil1    0.0      0.0     0.6   0.8   4.0     1.5      0.0      10.0
codfil2    default
codfil3    interactive
! Name of the instrument file
INSTR  instrument_file.inf
----- End of argonne_boxes_input_file.abx -----
```

If TIFF is absent, then `*.reo`, `*.ldm` and `*.geasc` files are expected as input files.

Where `codfil` stands for common code for `codfil.lmd`, `codfil.geasc` and `codfil.reo`

If TIFF is present then the input files are: `codfil.tif` and `codfil.hkl`

If `default` is used, the program uses calculated or suggested values for all parameters.

If `interactive` appears somewhere, the program asks the user for parameter values for all files.

The instrument file name is needed only when TIFF images are input.

TIFF and REO input files cannot be mixed in a single `*.abx` file.