

WinPLOTTR news

June 22

- New `skip_header_lines` item in the [OPTIONS] section of the `winplotr.ini` setting file allows to define the number of header lines to skip when reading a powder diffraction data file.

February 21

- **File / select files** dialog box is now limited to a maximum of 100 patterns, even if `Max_Patterns` value, defined in the `winplotr.set` setting file, is larger. Routine to create the select file dialog box has been slightly modified to avoid (definitively ?) **WinPLOTTR** crash (RealWin bug ?).

November 20

- Minor changes in the reading of `.PGF` files containing several patterns with the "`# DATA: X Y COMMENT`" format. This allows to obtain comment for every point of all the patterns when clicking on a particular point.

October 20

- Lines containing `*` character as first character in the data file header are considered as comment lines, as well as for `!` or `#` characters. This allows to read and plot `.dat` or `.xy` data files coming from Rigaku diffractometers. Please use "`1. X,Y data + INSTRM =10`" data file format.

June 20

- **File/Open File/ XY data** menu option can read `.csv` file containing comma separated values (X,Y) without any header (coming from ICSD for example).

May 20

- Cosmetic changes in the treatment of excluded regions for Rietveld type files (FullProf, Jana, Rietan, CIF)

April 20

- **Tools / hkl list generation** is now creating a kind of Debye-Scherrer film with same intensities Bragg peaks. The format of this pattern is a `.PGF` file with "`data_type=3`" and "`DATA: X COMM`" identifiers.

- New **PRF_header** item in the [OPTIONS] section of the **winplotr.ini** setting file : allows reading .PRF file created by **CRYSCALC** and containing a file header with profile parameters and structural informations (PRF_header = 1 in the [PATTERN SIMULATION] section of the **CRYSCALC.ini** setting file).

March 20

- **WinPLOTTR** web site moved from <http://www.cdifx.univ-rennes1.fr/winplotr> to <https://cdifx.univ-rennes1.fr/winplotr>

December 19

- **Tools / Molecular weight calculation** can manage real values for stoichiometry (thanks to JGP for the suggestion). Chemical formula can also be input (ie. La1 Mn1 O3).
- New **Plot / Cancel shifts/offsets** menu option : allows to cancel the effects on data of successive shifts and offsets.

April 19

- **WinPLOTTR** can now read .XRDML files created by new version of DataCollector V6.1 (<intensities unit="counts"> </intensities> tags has been changed to <counts unit="counts"></counts> tags).

November 18

- **File / save data as / save data as multicolumns file** : If several files has been read, corresponding sigmas can be saved in multicolumns file only if **sigma_arrays = Y** in the [OPTIONS] section of the setting file.
- **RIETAN2000/IGOR** format : sigmas are now reading in the file and corresponding extension can be different than .INT.

October 18

- **File / save data as / save UXD-XRDML as single scans** : if temperature is contained in the raw multiscan file, the created buffer file is directly compatible with the external temperature file used by FullProf in sequential mode.

September 18

- **File/Open a setting file** routine has been corrected. User can now select particular setting file name with different settings (**winplotr.set** setting file present in the **WinPLOTTR** folder was always used).

July 18

- New **Rietveld plot options / plot tics out of X range menu option** : acts as a switch, plotting or not vertical tics (Bragg positions) appearing out of X range. This can be usefull in order

to avoid displaying tics of Bragg peaks appearing at angles values higher than the last angular point of the measured pattern but contributing to the counting at this angular point and then present in the reflections list.

- Rietved/profile files (XRFIT, Rietan, CIF ...) can be plotted in different scales (Log, SQRT ...)
- A new routine to calculate difference curve and reflections tics positions has been implemented.

June 18

- .PRF files created by **JANA2006** can be plotted in log scale.

March 18

- When **WinPLOT**R is launched in command line and using a buffer file as argument, the data file format can be deduced from the extension of the first file in the buffer. In case of identical extension for different formats (ex : **.dat**), the associated format can be specified in the MY COMMAND LINE DEFAULT FORMATS section of the **winplotr.set** setting file.

July 17

- In case of zoom, normalization procedure is now performed towards the maximum of countings in the zoomed range and not the whole pattern..

February 17

- The script to be ran by **FullProf** is correctly created in the particular case of sequential mode refinement of multi-patterns (write **multi-pattern** as "data file code" item in the **FPCYC/WinPLOT**R dialog box).

September 16

- **Plot / Offset X,Y / for a particular file** routine has been corrected (offset values were not initialized)

May 16

- **PRF+/PRF-** buttons were corrupted
- search satellites from .PRF : presence of excluded regions is now considered
- save as **.sat** file : check if file extension is given for created file
- **Select files** dialog boxes routine has been changed to avoid **WinPLOT**R crash (RealWin bug?). This new routine is applied for number of loaded patterns smaller than 25.
- **Change graduations tex** menu option has been reactivated.

March 16

- Changes in the routine of reading `.dis` files created by **FullProf**

October 15

- Header of output files created by **WinPLOT**R (`.XY`, `.XYY`, `INSTRM_0.dat`) contain values of used wavelengths.

September 15

- Cursor position provides $2\theta(^{\circ})$ and $d(A)$ values if a single pattern of a PRF **FullProf** file is present on screen and plotted in 2θ space.

August 15

- Data coming from `.UXD` (Bruker) and `.XRDML` (Panalytical) can be plotted in counts per sec. This can be specified through the `data_cps=Y/N` keyword in the [OPTIONS] section of the **WinPLOT**R.set setting file. If not, a dialog box opens.
- Correction of bug in the reading of `.XYY` files created by **WinPLOT**R.

June 15

- The extension of the **WinPLOT**R command file can be specified in the setting file through the `command_file_extension=` keyword in the [OPTIONS] section :
`command_file_extension = .cfe ! winplotr command file extension`
Default value for this command file extension is `.cmd`

March 15

- A **REDO** button has been added in the toolbar, allowing to execute in the same conditions the previous program launched from **WinPLOT**R. This can be useful for example to launch **FullProf** with the same arguments as the previous **FullProf** run.
- Default of filenames number to write can be defined in the [OPTIONS] section of the setting file and the following line :
`max_write_filenames = 15`
- Graphic options (color, marker, style) and X/Y multipliers can now be defined for an individual data file
- New **Text/Display filenames in a window** menu option (not yet fixed)
- Correction in reading new `*_dis.SEQ` files created by **FullProf**

February 15

- Number of linked external programs with the "@" character that can be launched from the toolbar has been extended from 3 to 5.

- Minor changes in the code of "exit" procedure.
- **Rietveld plot options** are activated for **RIETAN2000** .PRF file

June 14

- New parameter in the [OPTIONS] section of the WinPLOTR.set setting file, allowing to select Y scale for the plot :
`Y_scale = LINEAR/LOG/SQRT/YQ2`
 Default value = LINEAR

April 14

- **Noisy data** item has been added in the peak search and background points search procedures dialog boxes

March 14

- **Points selection / Automatic satellites search** menu option has been implemented. This option is available only after plotting a PRF file and allows to perform peak search on the difference curve. Results can then be saved for **K_search** program to search propagation vector components of a magnetic phase.

Feb. 14

- After a files summation, difference or average, the resulting file can be saved with corresponding esd's. Of course, **sigma_arrays** item has to be equal to 1 (or Y) in the **winplotr.set** setting file.

Nov. 13

- New sections in the WinPLOTR.set file :
 - [3D PLOT OPTIONS] (used to customize automatic pseudo-3D plots)


```
3D_color      = RGB(255, 0, 255)
3D_style      = 0
3D_marker     = 1
3D_size       = 2
3D_pen_width  = 1
3D_lines_step = 0
```
 - [SCREEN RESOLUTION] (used for creation of BMP output graphic files)


```
screen_width=1200
screen_height=800
```
 - New tool in **Tools** menu : **Remove blank lines in a file** allows to remove all empty lines in a selected file.
 - **save esd's** item has been added in **Save data / save data as XY file** dialog box
-

Oct. 13

- A bug in reading .PRF files created by **Jana2006** has been corrected
- External programs can be launched directly from the toolbar (max. = 3) : these programs have to be specified in the [RUN PROGRAMS] section of the **winplotr.set** setting file through the '@' character before the identifier of the program.
ex: @ MENDEL = mendel ! My period table ! Windows version
- WinPLOTTR can handle .PRF files created by **CALC_PDF** : The observed and calculated PDF are represented as well as the difference curve. Tick marks correspond to atom pairs distances that can be directly inspected.
- New item in the sequential refinement dialog box : temperatures file can be specified see **fp2k.inf** (25 sept. 2013) for more details

Sept. 13

- Bugs have been corrected :
 - Different columns for different multicolumns files (WinPLOTTR format #1) can not be mixed.
 - **Calculation / Multiply X-Y** and **Plot / Offset X-Y** menu option procedures are now corrected after **CANCEL** handling
 - Wavelength is correctly read in XRDML Panalytical format files

July 13

- Implementation (in CRYSFML) of a new treatment for asymmetry parameters due to axial divergency (Finger et al. JAC 27, 892, 1992)
- Buffer file can contain the title of the plot in the first line if begun by **COMMENT** or **TITLE** command.
- New loaded data are still plotted in the current *Y* mode, even if it a non linear mode (log, SQRT ...)
- New RAW data file format : multiscan XRDML (from PANalytical) can now be read (**WinPLOTTR** format = 58). The **Calculation / Multiscan normalisation** can be applied to these data to create a **INSTRM10** data file for **FullProf**.

June 13

- **DOS** button is now opening a DOS window in the working folder

October 12

- New keyword for **WinPLOTTR** command file :
SUBTRACT file_1 file_2 format
 - **file_1** : name of first file
 - **file_2** : name of second file (Y_2 data will be subtracted from Y_1 data)
 - **format** : common **WinPLOTTR** format for **file_1** and **file_2**

September 12

- .spc files created by **DIFFAX** can now be read (format = 16). Only the broadened pattern (column #3) is extracted from the data file.

July 12

- Minor cosmetic changes in PostScript files

June 12

- Cosmetic parameters have been added for plotting .PRF files (Rietveld plot options menu) :
 - tics positions : 2 parameters (**t1** and **t2**) can be specified, relating to the position of the tics for the phase #1 towards the base line, and the interval between tics of different phases respectively. The following formula is used :
$$\text{pos_tics_ph_n} = \text{MIN}(\text{Yobs}, \text{Ycal}) - \text{n} * \text{t2} * (\text{MAX}(\text{Yobs}, \text{Ycal}) - \text{MIN}(\text{Yobs}, \text{Ycal})) / \text{t1}$$
with **t2=1** for **n=1**. The default values for **t1** and **t2** are 20. and 1. respectively but they can be defined in the setting file in the [SHIFT AND OFFSET] section with the help of **prf_tics = keyword**
 - Yobs-Ycalc difference curve position :
$$\text{pos_diff} = \text{MIN}(\text{Yobs}, \text{Ycal}) - (\text{MAX}(\text{Yobs}, \text{Ycal}) - \text{MIN}(\text{Yobs}, \text{Ycal})) * \text{K}$$
with **K = (1. + t3*Nb_phase)/5**. **t3** coefficient can now be specified through the **Tics and diff. curve positions** menu option and default value (0.1875) in the setting file in the [SHIFT AND OFFSET] section with the help of **prf_diff_shift = keyword**.
 - colored tics : switch to use or not different colors for tics of different phases. The default value of this **colored_tics** keyword is false but can be defined in the setting file through the **colored_tics=** string in the [PRF PLOT OPTIONS] section.
 - When points are displayed in excluded regions, those of the Yobs-Ycalc curve are not.
- **Zero shifts in 2theta** menu option has been added to input zero shifts value of a powder diffraction pattern (in the case of 2theta display). The whole zero shift is calculated as :
$$\text{ZERO} = \text{z1} + \text{z2} * \cos(\text{Theta}) + \text{z3} * \sin(\text{Theta})$$
and applied as :
$$\text{new_X} = \text{X} - \text{ZERO}$$

May 12

- Single crystal .UXD scans can now be superimposed.

April 12

- Bugs in Rietveld options (Zero difference, excluded regions) has been corrected.

March 12

- In the [AFTER FULLPROF RUN] section of the **winplotr.set** setting file, **edpocr** keyword can replaced **edit_pcr** keyword : **edpocr** will then be automatically launched with the current .pcr file.

February 12

- **DICVOL** and **TREOR** input file created by **WinPLOT**R after a peak search procedure contains informations about incident wavelength (**wave_1**, **wave_2**, **wave_ratio**). **DICVOL** and **TREOR** have been modified consequently to create **.pcr** files containing these informations

January 12

- **winplotr.set** setting file ([**OPTIONS**] part) :
 - **locked_cursor** = Y line (or 1) provides a new type of cursor. This new option, that is activated if only one pattern is displayed, lockes the position of the cursor to the nearest data point.
 - **follow_tfp_folder** = Y line (or 1) allows **WinPLOT**R to recover the current working directory of the **FullProf** toolbar if **tfp.exe** process is activ.

November 11

- After launching **FullProf** in sequential mode, **WinPLOT**R is creating **.SEQ** files (**xx_SEQ.dis** for distance calculations, **xx_SEQ.hkl** for profile matching refinement, **xx_SEQ.mic** for microstructural analysis) for all phases present in the **.PCR** file.
- Plot microstructural features after a sequential run of **FullProf** is now active.

July 11

- Some changes in the **.PAT** files created by **RIETAN**

January 11

- **WinPLOT**R command file : **PLOT** keyword can have 2 optional arguments, delimiting the range to be displayed
- **winplotr.set** setting file ([**OPTIONS**] part) :
 - **skip_exit_message** = Y line (or 1) can be input to skip the dialog box "*Do you really want to quit WinPLOT*R ?"
 - **pcr_history** = Y line (or 1) can be input to create, when running **FullProf** , a **codefile_PCR_history.lst** file from the current **PCR** file

November 10

- **Exclude_CELL_from_title** item has been added in the [**PRF PLOT OPTIONS**] of **winplotr.set** setting file. Equal to 1, this item allows to exclude every character after **CELL** string from the title of a **.PRF** file.

May 10

- Profile fitting of the X-ray K_{α} Fe doublet has been added
- EDIT_PCR and EDIT_NEW items can be present simultaneously in the setting file
- Save winplotr.set was bugged for [PATTERNS PLOT OPTIONS] section

April 10

- Read PRF files created by **Jana2006** (version April 2010) :
 - **Rietveld plot option** menu is activated
 - if PRF files are associated to **Jana** files in the winplotr.set setting file (see [COMMAND LINE DEFAULT FORMATS] section), the **PRF** button can directly load **Jana** PRF files and **PRF+** and **PRF-** buttons are activated.

March 10

- Correction of bugs
 - Calculation of intrinsic profile components for HG_sample negative values
 - Cratton of WHP file
 - Plot of linear fit

February 10

- **EXPO2009** can now be launched if defined in the setting file
- **Tools / hkl list generation** is creating a txt file that can be read further through the **Text / Open reflexions file** option
- Last point of .XY files was not considered. Now, it is!

September 09

- **WinPLOTTR** has been compiled with new versions of CFML (4.00)

June 09

- small bugs have been corrected :
 - read PANALYTICAL format containing end of lines character in the "<intensities unit='counts'>" section

May 09

- small bugs have been corrected :
 - Export as BMP and Postscript files

April 09

- small bugs have been corrected :
 - min and max values in the **zoom dialog box** after changing X space
 - character strings length extended to 132 in the profile fitting routine

Feb. 09

- **Save as DICVOL points** dialog box : add a check box for **DICVOL06 option** and modify the input file for **DICVOL06**
 - **OPTION = 0** : same as **DICVOL04** (optimised search, to be used with normal quality data)
 - **OPTION = 1** : offers an extended (exhaustive) search (for difficult cases)
- Compared to **DICVOL04** (2004), only one additionnal input parameter is added in **DICVOL06**, i.e. **DV06_OPTION** in card 5
- Read **.PLG** files created by the Rietveld program **XND** of J.F. Bérar. The **WinPLOT**R format is 106. If a **filename.HKL** exists in the same folder than the **.PLG** file, hkl indices are displayed. In the other case, background data will be plotted.

Jan. 09

- **SINGLE_SINGLE_PEAK / FIT_SINGLE_DOUBLE** keywords can have two arguments, corresponding to the X range for profile fitting procedure
- **WinPLOT**R from a command **.CMD** file can be launched through the **WinPLOT**R GUI (**Tools / Run WinPLOT**R **command file** menu option).
- **INSTRM14** (ISIS) data files can now be superimposed.
- **Help/FullProf news/FPS web site** has been added to link to **FullProf Suite** news at the **ILL FullProf Suite** web site.
- New keywords for **WinPLOT**R command file :
 - **SHIFT_X shift_X_value** : shift X values by **shift_X_value**
 - **SHIFT_Y shift_Y_value** : shift Y values by **shift_Y_value**
 - **OFFSET_X offset_X_value** : offset X values by **offset_X_value**
 - **OFFSET_Y offset_Y_value** : offset Y values by **offset_Y_value**
 - **MULTIPLY_X coef_X** : multiply X values by **coef_X** value
 - **MULTIPLY_Y coef_Y** : multiply Y values by **coef_Y** value
 - **PLOT** : plot the open file
 - **BITMAP** : create a **BITMAP** file (not compatible with **PLOT** keyword)
 - **EPS** : create a PostScript file (not compatible with **PLOT** keyword)
 - **NORM_UXD** : constant time normalization of **.UXD** multi scans files.
- Read **.PGL** files created by the Rietveld program **XND** by J.F. Bérar. The **WinPLOT**R format is 106.

- The routine to read .IPC files created by **WinPLOT**R has been corrected.
- Microstructural analysis : the max_strain value, expressed in %% (1E-04), was not correct but just multiplied by 1000 rather than 10000.

Dec. 08

- **X_space/Change_X_space_from_X1_to_X2** menu option has been added, allowing X space transformations from every kind of input data.
- new keywords are available for the **WinPLOT**R command file, for X space transformations :
 - TRANSF_2THETA_TO_Q, TRANSF_2THETA_TO_D, TRANSF_2THETA_TO_STL, TRANSF_2THETA_TO_S
 - TRANSF_Q_TO_2THETA, TRANSF_Q_TO_D, TRANSF_Q_TO_STL, TRANSF_Q_TO_S
 - TRANSF_D_TO_2THETA, TRANSF_D_TO_Q, TRANSF_D_TO_STL, TRANSF_D_TO_S
 - TRANSF_STL_TO_2THETA, TRANSF_STL_TO_Q, TRANSF_STL_TO_D, TRANSF_STL_TO_S
 - TRANSF_S_TO_2THETA, TRANSF_S_TO_Q, TRANSF_S_TO_D, TRANSF_S_TO_STL
- WAVE keyword for **WinPLOT**R command file
- interpolation procedure has been corrected.

Nov. 08

- **WinPLOT**R can read XY multicolumns files with tabulator used as separator

Feb. 08

- Some tools have been added for launching **FullProf** in a sequential mode :
 - FPCYC dialog box
 - * scripts (.bat file) can be created
 - * Plot interatomic distances
 - **Tools/Run scripts** menu option to execute a script file (.bat)
- **Tools / Create buffer** : access to a dialog box to select a particular extension of data files to be stored in a buffer file.
- **File/Save data as/save data as XXX** menu option has been added. Format is compatible with different software as KaleidaGraph, Origin, SignaPlot or Excel.
- **FPCYC hkl** button : arrays and variables are no more reset, allowing display of evolution of different reflexions.

Jan. 08

- **SEQ** button : evolution of different parameters coming from different .SEQ files (created by **FullProf** in cyclic mode) can be simultaneously displayed

Oct. 07

- .PGF files : comments are automatically displayed for X, Y, TEXT data ("DATA: X Y TEXT" in place of "DATA: X Y COMM" where comment is display only after a mouse click on a particular point).

Sept. 07

- .PRF files with $K\alpha_1$ and $K\alpha_2$ wavelength :
 - Only plots versus 2θ are correct
 - The calculated d_{hkl} in the 'Reflections positions list' is now correct
 - **Text/Write reflections text** menu option will only display reflections indices corresponding to the $K\alpha_1$ wavelength

July 07

- Some commands for **WinPLOT**R can be included in a command file called through the command line :
`d:\progs> winplotr winplotr.cmd`
This command file must have .CMD extension and can contain some keywords and related arguments to order to be performed by **WinPLOT**R . Following keywords have been included :
 - **FILE file%name file%format**
The file%name file will be read with the file%format **WinPLOT**R format (see user's guide)
 - **SAVE_AS_XY**
Data of input data file will be saved in a XY 2 columns file
 - **SAVE_AS_INSTRM_0**
Data of input file will be saved as a INSTRM_0 file for FullProf
 - **FIT_SINGLE_PEAK**
Data will be fitted with a single peak profile
 - **FIT_SINGLE_DOUBLET_CU/FIT_SINGLE_DOUBLET_MO/FIT_SINGLE_DOUBLET_CO**
Data will be fitted with a single X-ray doublet profile for Cu, Mo, and Co radiation respectively
- **Calculations / Fit single peak** and **Calculations / Fit single doublet** (for X-ray Cu, Mo and Co $K\alpha$ radiation) has been implemented. This allows automatic profile fitting (without input of parameters through mouse clicking and dialog box).

June 07

- **Calculations / Polymer crystallinity rate** menu option has been added : access to the cursor to select background points corresponding to the amorphous phase of the compound and calculation of the crystallinity rate of a polymer as follows :
 - integration of the amorphous phase intensities (a)
 - integration of the sample intensity (s)
 - $\text{crystallinity_rate} = 1 - a/s$

March 07

- **Tools / PCR space group info** menu option has been added and is active if a .PCR file has been edited : informations about the space group in the current .PCR file are then output in a window.
- Links have been created between structural parameters of the current edited .PCR file and input parameters of the **Tools / hkl list generation** and **tools / unit cell volume calculation** dialog boxes.

Jan. 07

- New facilities in the **Rietveld plot options** menu, activated after loading .PRF files :
 - Save as .PRF template : all the plot features of the Rietveld plot (colors, graduations, text legends, fonts ...) are stored in a template file (extension = *.TPL). The format of this type of file is similar to the .PGF files created by **WinPLOTR**.
 - **Open .PRF template file** : load all the plot features in a .PRF template file (*.TPL) for a Rietveld plot.

Nov. 06

- Data file format coming from a Rigaku Rint diffractometer has been add. The **WinPLOTR** corresponding format number is #15 and the default extension is *.TXT

Oct. 06

- **Help / FullProf Suite Web site** links to the **FullProf Suite** at ILL : <http://www.ill.fr/pages/science/IGroups/diff/Soft/fp>
- **Help / FullProf user's guide / FullProf and microstructural effects** menu option links to `microstructural_effects.pdf` file present in the `\doc` or `\tutorials` folder
- **WinDICVOL04** can create .PCR files for **GSAS** diffraction data files

Sept. 06

- .CIF files created by **GSAS** can be read as profile data files
- **Help / Environment variables** menu option to get informations about environment variables related to **WinPLOTR** and **FullProf**.

July 06

- .CIF files containing experimental and calculated powder diffraction profiles and created by **FullProf** (`xx_prof.CIF`) can now be read through the **File / Open Rietveld-profile file** menu option. The **WinPLOT** corresponding format is 105.

Feb. 06

- **MENDEL** : X rays data for Cobalt radiation has been added
- **Tools / hkl list generation** menu option has been added

Oct. 05

- **FullProf** in cyclic mode :
 - new item in the **Cyclic mode of FullProf** dialog box : the user can select to plot cyclic **FullProf** refined parameters or hkl features (intensity, position) coming from profile matching run of **FullProf**. In this later case, **Save HKL files** has to be activated. A new `filename_FPCYC.HKL` file is then created by **WinPLOT** from the contains of the `filename_1.hkl` files created by **FullProf** for the first phase.
 - New button labelled as **CYC hkl** has been add in the toolbar : its function is to allow to select and read a `FPCYC.hkl` file created by **WinPLOT** when **FullProf** is launch in a cycle mode from the **WinPLOT** interface. The user can then select to plot integrated intensity or Bragg position of a selected hkl towards the external parameter.
hkl- and **hkl+** buttons are then automatically activated to plot previous or next reflexion evolution.
 - Save PCR files of cyclic run of **FullProf** :
 - * before running **FullProf** : initial .PCR file is saved as `filename_save.pcr`
 - * after running **FullProf** : final .PCR file is saved as `filename_final.pcr` and `filename_save.pcr` file is renamed as `initial.pcr`
- News plot features for .PRF files can be read directly in the setting file (after [PRF plot options] part :
`.write_Y_negative_graduations=1/0`
`.write_PRF_filename=1/0`
- **PRF-/PRF+** buttons are now activated after plotting a .PRF file if several .PRF files, are present in the working directory.
- **File/Save UXD file as single scans** menu option has been added : it is active only when multiple scans .UXD files have been plot (load data as RAW data) and allows to split a multiple scans .UXD file to single scan data files (INSTRM10 format)

Sept. 05

- **WDICVOL04** : .PCR files are now created with a zero shift value compatible with **FullProf**. There was a mismatch in the definition of the zero shift between **WDICVOL04** ($2\theta_{real} = 2\theta_{obs} + zero_shift$) and **FullProf** ($2\theta_{real} = 2\theta_{obs} - zero_shift$)

- **Plot single crystal data PRF files** : a check box has been added in the **Select plot type** dialog box to allow/avoid sorting data by increasing X values. This kind of sort was automatically performed in previous versions of **WinPLOT**R to avoid peculiar plots when continuous line is selected for Y_{obs} .
Skipping this sort can allow to access directly to the reflexion index in the raw file by clicking on a particular reflexion.
- **Help / Links to** menu option has been added to access directly to CCP14 (<http://www.ccp14.ac.uk>) and IUCR powder commission (<http://www.iucr.org/iucr-top/comm/cpd>) web sites. Other internet links can be added by the user by defining web sites name and URL address in the [WEB SITES] part of the **winplotr.set** file.
Example :
`CDIFX = "http://www.cdifx.univ-rennes1.fr" ! cdifx (Rennes)`
- **Help / Download WinPLOT**R menu option has been added to access directly to the **winplotr.exe** file at :
`ftp://ftp.cea.fr/pub/llb/divers/winplotr/winplotr.exe`
A browser has to be defined in the **winplotr.set** setting file ([SYSTEM APPLICATIONS] part).
- **Help / Download FullProf Suite** menu option has been added to access directly to the **FullProf Suite** package at :
`ftp://ftp.cea.fr/pub/llb/divers/fullprof.2k/Windows/setup_FullProf_Suite.exe`
A browser has to be defined in the **winplotr.set** setting file ([SYSTEM APPLICATIONS] part).

July 05

- **GSAS** file containing the keyword **TYPE = FXYE** and **TYPE = FXY** can be read.
GSAS file containing several scans can be read.

June 05

- **File / Save as / XY file** option is available if only one pattern on screen. The format of this 2 columns is compatible with the **XCH** software of Socabim (no comments, no header)
- raw data file coming from the new 3T2 multidetector with 50 collimators-detectors bank has been integrated. The type of 3T2 file (20 or 50 detectors) is detected automatically.

April 05

- **The add peaks/background points** and **remove peaks /background points** menu options are now activated after manual peaks/background points selection.
- The constant time normalization procedure for multiscans .UXD files is now adapted to overlapped scans. If several Y values for a single X value are available, only the first Y value is stored in the INSTR_₁₀ file.
- **WinPLOT**R is compiled with the new Crystallographic Fortran Module Library (JRC and JGP).

Mach 05

- RGB colors code has been corrected and is now in agreement with Red, Green, Blue color code. The user has now to change the R and B columns in the definition of the different colors used by **WinPLOT**R in the `winplotr.set` setting file (`RGB(rrr,ggg,bbb)` parts) in order to get the true colors. The RGB color is now defined as :
`color=RED + 256*GREEN + 256*256*BLUE`

Example :

`RGB(255, 0, 0)` corresponds to pure red

Feb. 05

- Single crystal data coming from the 6T2 neutron diffractometer (LLB, Saclay) is now readable with **WinPLOT**R :
 - multiscan file : Reflections can be plotted ones after others through the **hkl+** or **hkl-** buttons. **Plot / select hkl reflection** menu option has been added to select in the multiscans file a particular reflection to plot.
 - single scan file : **hkl+** or **hkl-** buttons are also activated and allow to change the number of the file to plot file (and then the reflection) in the working folder.
- Fixed bugs : correction of a bug in reading 6T1(LLB) files.
- New buttons to access the programs **GBond_STR** and **GFourier** has been added

Nov. 04

- Minor changes in **WDICVOL04** and **WTREOR90** : Setting files have been created (`wdicvol04.ini` and `wtreor90.ini` respectively), containing the following optional parameters, united in different sections :
 - `[WDICVOL04/WTREOR90 window]` : definition of the size and position of the text window, in screen units (0. - 1.0 range). Default values are :
`x_pos = 0.15`
`y_pos = 0.05`
`width = 0.70`
`height = 0.45`
 - `[FULLPROF]` :
 - * `create_PCR_input_file= item` : creation of PCR input files for **FullProf** (value is y or n)
 - * `IRF_file= item` : definition of IRF file name (IRESO=1 format) : this kind of file can contained some experimental parameters as wavelength, angular range, diffractometer geometry, profile function, resolution parameters ... (see FullProf user's guide)
 - `[CRYSFIRE]` :
 - * `create_CRY_input_file= item` : creation of CRY input files for **CRISFIRE** (value is y or n)
 - `[EXP0]` :

- * `create_EXPO_input_file=` item : creation of input file for **EXPO** (value is y or n). This corresponds to HKL=-2 in the .PCR file of **FullProf** .
- * `space_group`, `structure` and `cell_content` items : definition of space group, structure name and cell content for **EXPO**

These setting files are installed in the **WinPLOT**R folder but can also be copied in the working directory for another setting.

Oct. 04

- **WDICVOL04** (new version of the **DIVOL** program : A. Boulton and D. Louer, J . Appl. Cryst. 2004, 37, 724-731) is distributed through the **WinPLOT**R package and the **FullProf Suite** . Please read the `wdicvol04.ins` user guide and the above article to have the features and improvements of **DICVOL**.

Sept. 04

- Buffer type files can be loaded from the prompt : arguments are the buffer file name and the common **WinPLOT**R format of the data files (1 - 14) :

```
My_prompt> winplotr my_diffraction_exp.buf 2 <cr>
```

- When quitting **WinPLOT**R , name and format of the last selected data file are now saved in the `winplotr.dir` file in the **WinPLOT**R directory. These items are then taken as default in the next **WinPLOT**R run. A `last.PGF` file is also created (in the **WinPLOT**R folder) and can be load rapidly when launch **WinPLOT**R from the prompt by typing the following command :

```
My_prompt> winplotr last <cr>
```

- A new button has been added in the toolbar : click on **Studio** will allow to select a **FST** file and then launch the **FP_studio** program (see `fp2k.inf` file for details concerning this new crystal/magnetic structure visualisation program that is distributed through the **FullProf Suite**).

The **FP_studio** can also be launch automatically after a **FullProf** run (the relative items in the 'PCR has to be adapted consequently) by adding as thirs item the `draw_fst` string in the `winplotr.set` setting file, in the [AFTER FULLPROF RUN] part.

- A new smoothing procedure has been added, using Fourier filtering

July 04

- **Calculation / Constant time normalization** : this new procedure can be execute from .UXD data files containing several scans (different angular ranges with different counting time and step) to create INSTRM10 file with data and sigmas normalized to a constant counting time.
- Profile fitting procedure : if **IRF** is known (and **IRESO**/=4), **U,V,W** resolution parameters are automatically included in the starting parameters dialog box. Consequently, shift values of **FWHM** are fixed to zero.

- *.PIK/*.NEW files for profile fitting : last item of line 1 corresponds to **IRF** and has to be modified by the user. If equal to 1, an .IRF file will be created, containing a list of HG and HL versus 2theta (IRESO=4)

June 04

- Excluded regions and text position can be saved in .PGF files
- display of several 2theta scans contained in .UXD files (**File / raw data file** menu option). Default format associated to .UXD file is 9 (single scan file) but can be modified explicitly in the [MY COMMAND LINE DEFAULT FORMATS] part of the **winplotr.set** file through the third item (first corresponds to .DAT extension and second to .PRF files respectively). The format number associated to this multiple scans .UXD file is 56.
- fixed bugs :
 - .PCR files created by **DICVOL** were not correctly created (wrong values of resolution parameters, profile function, scale factor ...) for neutron data
 - Protection for XY files containing continuous data with identical X values
 - LOG(Y) option : a protection for zero counting data has been included

May 04

- Fixed bugs :
 - Profile fitting after reload data and microstructural analysis
 - Plot .SEQ files :
 - * refined parameters are related to the phase
 - * correct Y legend
 - Run **FullProf** in cyclic mode : last number can be lower than first number (inverse cyclic mode)
 - Protections for the case with all data equal to zero

April 04

- Fixed bugs :
 - **Profile fitting** after automatic peak search procedure
 - plot .XRF file after profile fitting with .PIK input file or after automatic peak search procedure
 - read .PGF files with XMIN XMAX and YMIN AND YMAX items
 - Ymin graduation in manual mode zoom
 - run user's defined programs

March 04

- Line width in .UXD files has been extended to 512 characters to allow a correct reading of lines containing 16 data.
- Cosmetic bugs has been corrected (ex : *pen_width* action)
- **Calculation / I.R.F.** menu option : the FWHM of the pseudo-voigt function is calculated from the HG and HL values and the T.C.H. relationship
- access to the **FullProf** manual in HTML format

Feb. 04

- **Wtregor90** and **WinDIC** are now running with input files stored in directory whose name contains blank character (" ")
- .SEQ file : error barrs are automatically display and their values are taken into account in the min and max values calculation in the plot.
- **Open setting file** menu option has been added. The user can then select the setting file useful for his work. The default name of the setting file is **winplotr.set** but can be more explicit (ex : **wpl_neutron.set**, **wpl_xrays_D8.set** ...).
- a link to **FullProf** news and **WinPLOT** news (HTML format) has been added (these HTML files are distributed in the last **FullProf Suite** package and copied in the **fullprof_suite\docs** folder).
- **FP cyc** button has been added : it allows to launch the DOS version of **FullProf** in a cyclic mode (this version is explicetely defined in the **winplotr.set** file, through the **FP_CONSOLE** item in the **[RUN PROGRAMS]** part. The different arguments to launch cyclic **FullProf** are input by the user in a dialog box.
- .SEQ files (output file created by a cyclic run of **FullProf** and **RPA=-2**) can be displayed (**SEQ** button or automatically after a cyclic run of **FullProf**).
- INSTRM14 data file has been added in the pattern list (corresponding extensions= *.DAT;*.GSS;*.GSA). It corresponds to multi-bank time of flight data (ISIS normalised data)
- .NEW input files can be selected to launch **FullProf**. In that case, it is previously copied to .PCR file (**FullProf** is always running with .PCR input files).

Jan. 04

- .IRF file with **IRESO=4** can contain **WAVE** item before the list of HG and HL values
- new item in the **Peak search parameters** dialog box : *Display Bragg peaks positions*
- cosmetic changes in the **winplotr.set** setting file. Each item is now defined between '[' and ']' characters. This new format is of course compatible with the old one.
- new version of **Wtregor90.exe** : the *_treor_cell.sum file for **Crysfire** was not correctly created in case of hexagonal solutions
- **Tools / space group infos** : space group extinctions rules are output

- For more clearness, the list of the different kind of powder diffraction data has been splitted in several groups :
 - pattern files (13 formats) corresponding to **FullProf** compatible formats
 - raw data files (5 formats) including multiconounters diffractometers data
 - profile type files (5 formats) : WinPLOTTR/XRFIT, FullProf, Jana2000, Rietan2000 and Debye
 - microstructural files

The corresponding **WinPLOTTR** formats ranges (useful for example when **WinPLOTTR** is launching through a command line) are the following ones :

- pattern files : 1 - 13
 - raw files : 51 - 55
 - profile files : 100 - 104
 - microstructural files : 201 - 204
- 3T2 neutron multiconounters diffractometer (LLB-Saclay) raw data file has been included*
 - Fonts are now saved in .wpl files
 - a `winplotr.set` setting file can be present in the working directory. If not, **WinPLOTTR** will use the setting file in the directory associated to the `WINPLOTTR` environment variable (`d:\fullprof_suite` for example). The user can then have in each working directory a settings file adapted to the powder diffraction problem he is dealing with.

Nov. 03

- Instrumental parameters can be read from the .IRF file in the starting parameters dialog box of the profile refinement procedure. This new option is valid for TOF data as well as CWL data.
- The profile fitting procedure for TOF data is now running properly. It uses the `NPROF=9` function defined in **FullProf** (convolution of pseudo- Voigt with a pair of back-to-back exponentials).
- Different kinds of IRF files can be used, depending on the item `IRESO` (as in **FullProf**). It can be defined in the `winplotr.set` setting file in the `MY IRF FILE` part : first item corresponds to the `IRESO` value and the second one to the `IRF` file name.

! MY IRF FILE (IRESO IRF_file_name): 4 d:\fullprof_suite\IRF_files\my_irf.IRF

For `IRESO/=4`, the .IRF file contains 6 instrumental resolution parameters (*Uins*, *Vins*, *Wins*, *Xins*, *Yins*, *Zins*) which meanings are dependent of `IRESO` value :

`IRESO=-1` pseudo-Voigt profile

$$H^{*2} = UINS \tan(q) + VINS) * \tan(q) + WINS$$

$$ETA = XINS + YINS * q + ZINS * q * q$$

`IRESO=1` Voigt profile (corresponds to `NPROF=7` in **FullProf**)

$$HG^{**2} = UINS \tan^2(q) + VINS \tan(q) + WINS$$

$$HL = XINS \tan(q) + YINS / \cos(q) + ZINS$$

IRESO=2 Voigt profile

$$HG^{**2} = (UINS \tan(q) + VINS) \tan(q) + WINS$$

$$HL = (XINS * 2q + YINS) * 2q + ZINS$$

IRESO=3 Voigt profile

$$HG^{**2} = (UINS * 2q + VINS) * 2q + WINS$$

$$HL = XINS * 2q + YINS * 2q + ZINS$$

This IRF files are the same as used by **FullProf** and then can contain some informations on the diffractometer setup (see **FullProf** documentation for more details) : WAVE/, GEOM, CTHM

...

For IRESO=4, the .IRF file contains a list of *HG* and *HL* values versus 2theta.

Oct. 03

- new button **Reset** in the toolbar
- a CIF viewer can be defined by the user in the winplotr.set setting file in the ! SYSTEM APPLICATIONS part. This CIF viewer is associated to .CIF files (created by **FullProf** with RPA=-1) and allows to display crystal structure directly through a single click on the **view** CIF button. The authors strongly recommend the **Mercury** program for visualization of molecular crystal structure (<http://www.ccdc.cam.ac.uk/prods/mercury/index.html>)
- **Calculation / data normalization** menu option has been added

Sept. 03

- fonts can be defined by the user in the winplotr.set setting file in the ! TEXT FONTS section :

TEXT FONTS	:	Typeface	point	italic	underline	strikeout	bold
main title	:	Times New Roman	18	F	F	F	F
X legend	:	Times New Roman	18	T	F	F	F
Y legend	:	Times New Roman	18	T	F	F	F
X graduations	:	Courier	14	F	F	F	F
Y graduations	:	Courier	10	F	F	F	F
file name	:	Courier New	10	F	F	F	F
(hkl) indices	:	Times New Roman	10	F	F	F	F
dialog boxes	:	Times New Roman	10	F	F	F	F

- Vertical and horizontal lines can be draw (**Plot / draw vertical-horizontal line** menu option

- HGL viewer can be defined by the user in the **winplotr.set** setting file
- **LOG(Y)** option : a protection for negative data has been included
- A molecular weight calculation has been included : **Tools/molecular weight calculation** menu option
- Some changes in the peak search algorithm : shoulders positions are determined with better accuracy. The number of iterations for data smoothing procedure can be input by the user

July. 03

- Peaks positions can be saved for **McMaille** program (indexing powder patterns by Monte Carlo method, A. LeBail : <http://www.cristal.org/McMaille/McMaille-v3.html>)
- The **CFML** tools are used in **WinPLOT**R :
 - new profile fitting procedure, available for CWL data and TOF data
 - **Tools menu** is added, leading to new crystallographic tools as **Space group info** and **Unit cell volume calculation**
 -

June 03

- several TOF GSAS files can be displayed simultaneously

May 03

- new general graphic file can be created and loaded by **WinPLOT**R . It contents some general features on the graphic plot (legend text, graduations, colors ...) and data in XY format.
- bug in reading .UDF files from Panalytical has been corrected.

April 03

- New input files for **FullProf** (.new can be automatically edited after a **FullProf** run : change the EDIT_PCR string to EDIT_NEW string in the **WinPLOT**R setting file (! AFTER FULLPROF RUN: section). This can be useful if IPC parameter is equal to 2 in the .PCR file.
- Minor change in the INSTRM_0 data file created by **WinPLOT**R : the step item is now written with a F14.6 format, i.e. with 6 decimal numbers. The previous format (F14.4) was not enough accurate for data coming from countinuous scans (step corresponds to an electronic step rather than mechanical step).
- Different Y scales are available : linear, log and SQRT (**Options / Y scale** menu option)

March 03

- Format #17 (Philips X'Pert) and #18 (Philips X'celerator) have been merged into a single PANalytical format. Different kinds of data file formats can be read and are discriminated from their respective extensions : *.UDF, *.CSV, *.JCP and *.XRDML.
Don't forget to change the data file description in the `winplotr.set` setting file (DATA FILES EXTENSIONS: section). It has to be as follows :

```
16      *.CPI                                !16 : CPI (Xrays)
17      *.UDF ;*.JCP ;*.CSV ;*.XRDML        !17 : PANalytical formats
18      *.DAT                                !18 : ESRF multi analysers
```

- the bug in reading .UXD file with _2THETACOUNTS and _2THETACPS is corrected
- The `winplotr.pdf` file containing user's guide can be read through the **WinPLOT**R GUI (**Help / User's guide / winplotr.pdf**) if a PDF reader is defined in the `winplotr.set` setting file
- .XRDML data files from Philips diffractometer has been included. It has been associated to data file format number 18 (Xcelerator)

Feb. 03

- **Select pen_width option** is now compatible with dashed and dotted lines
- cosmetic changes in automatic 3D plots

Jan. 03

- small bugs have been fixed :
 - profile fitting with .UXD file and CPS data
 - launching **WinPLOT**R through a command line for data file (Rietveld or Microstructural files were OK)
- Windows explorer can be launched from the **WinPLOT**R GUI through the **External applications / Explorer** menu option or by a button in the toolbar
- output files created by the profile fitting procedure in **WinPLOT**R are now labelled as `filename_pf.*`.

Dec. 02

- **WinPLOT**R is now distributed via the **FullProf Suite** package (http://www-llb.cea.fr/fullweb/ftp/pub/divers/fullprof_suite/setup_fullprof_suite.exe). This suite contains **FullProf**, **WinPLOT**R, **GFourier**, **EdPCR** ...
- Data file from ESRF multi analysers diffractometers (i.e. : ID31) has been included

- IRF file (IRESO=4 format) can be defined in the `winplotr.set` through the `! MY IRF FILE (IRESO=4)` item
- small change in the **profile fitting parameters** dialog box : `CREATE .IRF FILE / CREATE .IPC FILE / NO OUTPUT FILE` radio button has been added.
- some system applications can be defined in the `winplotr.set` file, in the `! SYSTEM APPLICATIONS` part :

```
Browser           ="C:\Program Files\Netscape\Communicator\Program\netscape.exe"
PostScriptViewer="C:\Program Files\gstools\gsview\gsview32.exe"
PDFreader         ="C:\Program Files\Adobe\Acrobat 4.0\Reader\AcroRd32.exe"
BMPviewer         ="c:\winnt\system32\mspaint.exe"
```

- **Help / WinPLOTR web site** menu option : access to the **WinPLOTR** web site (<http://www-llb.cea.fr/fullweb/winplotr/winplotr.htm>) through the previously defined browser
- **Help / User's guide / FullProf manual** menu option : load the `fullprof_manual.pdf` file (`'fullprof_directory\docs` folder) into the previously defined PDF reader
- **External applications / PostScript viewer** menu option : access to the Windows directories dialog box to select a PostScript file and view it with the previously defined PostScript viewer
- **WinPLOTR** web site can be accessed directly in the **Help** menu option, if a browser has been previously defined in the `winplotr.set` file.
- PostScript files can be viewed through a previously defined PostScript viewer (**External applications / PostScript viewer** menu option).
- some small changes in the procedure to launch **WinPLOTR** from a command line : the two arguments in the command line are not order depending :
`winplotr 101 fullprof_file.PRF`
and
`winplotr fullprof_file.PRF 101`
are correct.

In the second way, if the second argument (data format) is missing, the format is deduced from the file name extension. In the case of `.DAT` files or `.PRF` files, the default corresponding formats can be defined in the `winplotr.set` file through the `! MY COMMAND LINE DEFAULT FORMAT` items. This new option can be helpful to visualize patterns in **WinPLOTR** directly from the Windows Explorer by just clicking on a data file (the corresponding extension has of course to be associated to **WinPLOTR**).

- Microstructural analysis

- new items in the `winplotr.set` :

* ! MY RESOLUTION PARAMETERS: part can contain until 6 parameters values (reals) to define the Instrumental Resolution Function.

Number of
parameters I.R.F.

3	Pseudo-Voigt $H^{**2} = U.\tan^{**2}(\theta) + V.\tan(\theta) + W$
4	Pseudo-Voigt $H^{**2} = U.\tan^{**2}(\theta) + V.\tan(\theta) + W + Z/\cos(\theta)$
5	Voigt $HG^{**2} = U.\tan^{**2}(\theta) + V.\tan(\theta) + W$ $HL = X.\tan(\theta) + Y/\cos(\theta)$
6	Voigt $HG^{**2} = U.\tan^{**2}(\theta) + V.\tan(\theta) + W$ $HL = X.\tan(\theta) + Y/\cos(\theta) + Z$

The last *HG* and *HL* angular dependences are corresponding to the the format `IRESO=1` of `.IRF` file in **FullProf**

* ! DETERMINATION OF INTRINSIC PROFILE COMPONENTS: leads to perform, at the end of a profile fitting procedure, a deconvolution from the instrumental part described just above. Output `.IPC` file (containing intrinsic profile and microstructural parameters) is created.

* **Calculation / Read IRF file (IRESO=4)** menu option :

IRF can be read in a file, containing a list of $2\theta(^{\circ})$, $HG(^{\circ})$, $HL(^{\circ})$ values, as for the `IRESO=4` IRF file format in **FullProf** .

This IRF file is then used after the fitting procedure to perform a microstructural analysis (*HG_instr* and *HL_instr* for the refined positions are calculated through a cubic-spline interpolation of *HG_instr*'s and *HL_instr*'s contained in the IRF file)

- profile fitted angular ranges are now graphically distinguish : they appear with a particular color after **Calculation / reload data file** menu option. These angular ranges are treated as excluded regions. The default color for these ranges is grey (in not defined in the `winplotr.set` file through the `!EXCLUDED REGION COLOR:` item), but it can be changed in the **Plot / excluded regions color** menu option.

Excluded regions in `.PRF` files are now plotted by this way. If you don't want to see any points in these regions, you just have to select for the **Excluded region color** the same color than the **Background plot color**.

- for more clearness, colors in the `winplotr.set` can be now defined using a RGB code :

`color=RED*256*256 + GREEN*256 + BLUE`

Example :

`! BACKGROUND SCREEN:`

`background screen color: RGB(228,255,255)`

and `! BACKGROUND SCREEN:`

`background screen color: 15007743`

are equivalent

- **Calculation / IRF** : access to dialog box to enter instrumental resolution parameters, calculate the I.R.F. and then plot it on the screen.
- peak positions can be saved as .PRN file (**CHECKCELL** format)
- **Add/remove peak** : the list is updated in the text window after clicking with the right mouse button to exit from the procedure
- profile fitting can be followed graphically during the fitting procedure (flag in the starting parameters fitting procedure dialog box)
- PRF files with single crystal data containing flipping ratio refinements can be plotted

Sept. 02

- **WTREOR90** version in the last package was bugged : it has been corrected
- the possibility to read a reflexion list from an external ASCII file has been included (**Text / Open reflexion file** menu option). Then, this file content is written as text over the pattern. The format of this file is the following (lines beginning by '!' or '#' are comments) :

```
!Example of reflexions file
! silicium a=5.4307 Fd-3m
! wave=1.54056 A
! X-ray pattern
!2Theta (hkl)
28.4430      (  1  1  1)  Si
47.3038      (  2  2  0)  Si
50.0000                      <<< impurity ?
56.1236      (  3  1  1)  Si
58.8576      (  2  2  2)  Si
69.1316      (  4  0  0)  Si
76.3780      (  3  3  1)  Si
88.0324      (  4  2  2)  Si
94.9550      (  3  3  3)  Si
94.9550      (  5  1  1)  Si
106.7116     (  4  4  0)  Si
114.0957     (  5  3  1)  Si
116.6474     (  4  4  2)  Si
```

June 02

- data can now be saved in a INSTRM=0 format (available only if one pattern on screen) : interpolation is performed through a cubic spline procedure. The format is compatible also with Rietveld format (*.dat) in **CHECKCELL**
- new facilities in **WinTREOR90** and **WinDICVOL** (thanks to Alain Lafond for suggestions and discussions) :
 - output files (.SUM and .CRY) for the **CHECKCELL** program (J. Laugier and B. Bochu : <http://inpg.fr/LMGP>)
 - corrections of bugs in **WinTREOR90** in the .PCR creation procedure (wavelength, space group)

- New dialog box in the **Save as TREOR points** option in **WinPLOT**R : MONO, CEM, MERIT parameters can be modified by the user
- Profile fitting procedure : sub-profiles (**peaks_n.xy**) are now correctly calculated
- **EdPCR**, the new GUI for editing and modifying the .PCR input files for **FullProf** , is now distributed in the **WinPLOT**R package and can be launched through the **WinPLOT**R interface. Thanks to Javier Gonzalez-Platas and Juan Rodriguez-Carvajal for their hudge work to create this interface.

May 02

- **WinPLOT**R can now be launch through a command line following by two arguments :
 - first argument corresponds to the format number (integer) :
 - * format = 1,2 ... 18 : diffraction pattern with format corresponding to the list number in the **format dialog box**

Example : format=0 for X,Y format
 format=1 for INSTRM=0
 ...

 - * format = 101, ..., 104 : Rieveld format for **FullProf** , **Jana2000**, **Rietan2000** and **Debin** respectively
 - * format = 201, ..., 203 : microstructural file (same order than in the **Open micro-structural file** section)
- second argument correspond to the data file name

Example : > winplotr 101 fullprof_file.PRF
 > winplotr 7 pbso4.dat

This new opportunity can be interesting to be launch by the own user application that can create data file those format is compatible with **WinPLOT**R .

- a **PRF** button has been added in the toolbat to open and display a .PRF **FullProf** file
- the bug to display multipattern .PRF file with NPAT>9 has been corrected
- the **Text / display reflections list** option has been added : it is valid only for .PRF, .XRF file or after an automatic peak search. It allows to display and store the position list (in 2θ (°), $d(\text{\AA})$, $Q(\text{\AA}^{-1})$, $\sin\theta/\lambda(\text{\AA}^{-1})$)
- the **Text / write reflexions text** menu option is valid after the profile fitting procedure
- the **Text font / (hkl) indices font** option is now valid after writing reflexions indices and/or positions
- X_{min} , X_{max} , Y_{min} and Y_{max} values in the zoom dialog box are related only to previous values entered by the user in this dialog box : they are not corresponding the extrema values selected by the mouse. This change has been implemented to help to user to keep some X_{min} ... values.

April 02

- some bugs have been corrected :
 - in the reading *.WPL files procedure
 - display reflection positions
- multi-phases .PRF files created by **Jana2000** are now recognised

March 02

- last version of **Wfp2ks** and **fp2ks** are included (previous one was bugged for .PCR files containing distances and angles constraints)
- wavelengths supplied by the user in the **winplotr.set** file are correctly interpreted
- the bug in the **Save settings** procedure is corrected
- for more clearness, **Exit** right button text is replaced by **Valid & exit**

Feb. 02

- Microstructural .MIC file (created by **FullProf**) can now be read
- **XRFIT.pik** file is created after the validation of the **Profile fitting parameters** dialog box. This file is entirely compatible with the **XRFIT** DOS program. This old program is still useful for a cyclic profile fitting procedure, for example.
- **Exit** tool has been included in the toolbar
- bug in the **save as multicolumns file** menu option has been corrected
- positions of reflexions can be displayed on Rietveld patterns plot : use the **Text / Write reflexions text** menu option

Jan. 02

- some small bugs have been corrected
- Executable file is now compacted. Thanks to M. Oberhumer and L. Molnar for their **UPX** free compactor (<http://upx.sourceforge.net/>)

Oct. 01

- **M'** calculation is included in **DICVOL**, according to the definition in **NTREOR** (ref : *Altomare et al., J. Appl. Cryst. 33, 1180 (2000)*)
- data from the **Fit2D** program (extension=.CHI ; ESRF) has been included the X,Y data formats

Sept. 01

- Problem with **TREOR** and angular 2theta positions lower than 1.0 deg. : remove such kind of data when you are dealing high energy synchrotron data
- data file from X'Pert (Philips) diffractometer has been included
- the **PRF file** format is removed from the data file list and is now only in the Rietveld file format list (!! change the data file list in your setting file!!).

July 01

- data file from X'celerator (Philips) diffractometer has been included
- a bug in the Wito/WinPLOTR interface has been corrected

June 01

- (hkl) reflexions can be displayed on Rietveld patterns plot : **Write reflexions indices (ON/OFF)** in the **Text** menu option
- 3D plots can be realized rapidly (default parameters) : **Plot 3D+/3D-** in the **Plot** menu option

May 01

- The bug in the **Reload data file** menu option is now fixed
- Position of the files names can be specified by the user (**Text / Legends positions**)

April 01

- The following bug has been fixed : . text has microscopic size in the **File / Print** procedure
- Linear fit of microstructural data can be performed

March 01

- Rietveld profiles file created by **Jana2000** (.PRF) has been included
- Bitmap files can be created

Feb. 01

- Plots for a microstructural analysis can be performed :
 - Williamson Hall : integral breath b^* versus $1/d$
 - Average size-strain : $(b^*/d^*)^{**2}$ versus b^*/d^{*2}
- A Windows version of the **ITO15** program (J. Visser) is distributed within the **WinPLOTR.zip** package

- The **DOS command** option has been replaced by the **Open a DOS window** option
- Data file .CPI created by **POUDRIX** (J. Laugier and B. Bochu) has been implemented
- Default version of **FullProf** is **wfp2k.exe**

Jan. 01

- some changed in the profile fitting procedure of doublets have been performed : X-Rays Kalpha1 and Kalpha2 wavelengths can be defined by the user in the **winplotr.set** file by defining two new items :

```
! MY X-Rays WAVALENTHS (A):
Kalpha1_wavelength Kalpha2_wavelength
```

- Text fonts for legends can be changed by the user in the **Text / text fonts** menu options
- Copy text to the clipboard can be realized in text windows
- the Windows calculator can be spawn through **WinPLOTTR**

Dec. 00

- Rietveld files created by **Rietan2000** (.PAT) and **Debvin** (.GRA) Rietveld programs have been included
- IPL2=2 .PRF Rietveld file created by **FullProf** has been included (**IGOR** format)
- Data file (.INT) for **Rietan2000** has been included
- Positions and rotation of the legends texts can be defined by the user (**Text / Legends positions** menu option) and stored in the **winplotr.set** settings file
- Offset X and Y values can be defined for each pattern independently

Nov. 00

- Xray attenuation coefficient and total interaction cross sections have been included in the **MENDEL** program
- .CPI data file format has been included
- **WinDICVOL** and **WinTREOR90** : .CRY files as input files for **CELREF**, **CHEKCELL** are creating

Oct. 00

- Profile fitting procedure : the *HG* and *HL* parameters (*FWHM* of the Gaussian and Lorentzian part respectively, of the Voigt function are calculated from the pseudo Voigt approximation parameters (*Fwhm*, *eta*) using the Thompson-Cox-Hastings formulation : A **FILENAME.IRF** file is created, containaing *HG* and *HL* versus 2θ .
- Powder diffraction pattern can be transformed to another wavelength pattern

Sept. 00

- Correction of a bug in reading time of flight data coming from Argonne

July 00

- After plotting a .PRF file, a .SUB file (created by **FullProf**) is automatically shifted according to the shifts parameters of the .PRF file.
- The calculation of the *FWHM* from the Caglioti formula has been implemented (**Calculation/FWHM(Caglioti)** menu option)
- The number of user's defined editable files has been extended from 2 to 4

June 00

- the bug in **WinDIC** in the triclinic case (display unit cell parameters on the screen and in the .UCP file) has been corrected
- a bug has been corrected in the manual fit dialog box (selected peaks)

May 00

- a bag version of the **INSTALL** program has been installed in the LLB ftp area : it has been corrected

April 00

- some changes in the **Save as TREOR input file** subroutine have been performed in order to interface the last **TREOR** Windows version :
 - first two lines are beginning with the '!' character
 - reflection intensity and background are stored
- new TREOR windows version :
 - after successful run, automatic generation of PCR input file
 - for **FullProf** (profile matching mode)
- **WinDICVOL** window size and position can be defined in the `windic.ini` settings file (stored in the directory associated to **WinPLOT** through the `winplotr` environment variable)

March 00

- new procedure to plot red selected reflexions and selected background points (it would be more rapid with very large of points in the data files - synchrotron data for example-)
- **Help / WinPLOT help file** menu option has been changed
- **Select files** dialog box has been modified (bug with large number of data files)

- **! EDIT FILES:** item in the `winplotr.set` file : definition of files (type + extension) that can be edited in the **External applications / Edit a file** menu option
- Peak search and background points search are running correctly with d spacing data
- **PFE** editor has been removed from the **WinPLOTTR** package
- some bugs in the PostScript and HPGL files have been corrected
- frame features can be modified by the user : line thickness, major and minor ticks thickness and length
- bugs have been corrected in the creating/reading *.WPL files procedures
- **SELECT** option in the **External applications** menu : select an .EXE file to run from **WinPLOTTR**

Feb. 00

- Fitting procedure from a .PIK file can be performed with INSTRM=10 (with sigmas as third column) data files

Jan. 00

- a background subtraction procedure has been implemented in the **Calculation** menu
- small bugs have been corrected in the following menu options
 - **save as TREOR points** : inversion of the VOLmax and BETAmx item values
 - **PRF+** / **PRF-** tools : problem with the '_' character in the directory name
- the **PFE** editor is now distributed with the `winplotr.zip` package and is considered as the default editor
- the `winplotr.set` file can be edited from **WinPLOTTR** through the **External applications / Edit a file / Winplot.set file** menu option

Oct. 99

- the .PRF file can be automatically plotted and .PCR file can be automatically loaded after a **FullProf** run, by defining two new items in the `winplotr.set` file :

```
! AFTER FULLPROF RUN:
item_1 item_2
!
item_1 = plot_prf      => the PRF file is plotted (default value)
        no_plot_prof  => the PRF file is not plotted

item_2 = edit_prf      => the PCR file is edited
        no_edit_prof   => the PCR file is not edited (default value)
```

Sept. 99

- bugs have been corrected in the **Calculation/Integration** and **Calculation/Profile fitting** menu option of the previous **WinPLOTTR** .

July 99

- a new zoom and graduations routine has been implemented.
- a `winplotr.hlp` HELP file has been created. It can be loaded through the **Help / WinPLOTTR help file** menu option.
- The utility launched by **WinPLOTTR** to read the `winplotr.hlp` file is `winhlp32.exe` by default. However, it can be defined in the `winplotr.set` file in the `!/ HELP FILES:` part, as the following :

```
. ! HELP FILES:
.   N   winhelp
```

- some bugs in the peak search routine has been corrected

June 99

- bug in reading the INSTRM=4 data files (Brookhaven format) has been corrected

May 99

- .PRF files (single crystal data) can be displayed as a $F2_{calc} = f(F2_{obs})$ plot
- sorry for the last bad version of the `INSTALL.exe` program : it has been corrected now
- `winplotr.set / !run programs` : program name that will be launched by **WinPLOTTR** can be .LNK files as well as .EXE files
- The number of user's defined programs is extended to 10
- **File / file Infos** menu option : displays in a text window some informations about data file
- `! MY DEFAULT FORMAT:` keyword in the `winplotr.set` file allows to define the default format in the select format dialog box. If no default format has been defined, first format (X, Y format) will be taken as the default one.

April 99

- buffer file can contain some optionnal informations, as for example temperature, experimental conditions ...
- **plot / reverse order** option
- user's DOS program definition in the `winplotr.set` file : the number of arguments accompanying the relative DOS program can be specified in parenthesis at the end of the definition line.
ex : `Fullprof_dos = FULLPROF !FullProf dos version !DOS version (2)`
In this case, **WinPLOTTR** will open two dialog boxes to select the two arguments files for the FullProf program. The following command line is then executed :
`FULLPROF selected_file1.PCR selected_file2.DAT`
If the program comment starts with `fullprof` 'in capital or lower case letters), **WinPLOTTR** will automatically display the last .PRF file created by **FullProf** .

- Windows version of **TREOR** (WTREOR90.exe and the user's guide) are now included in the winplotr.zip file and automatically installed with the INSTALL.exe program.
- user's diffractometer resolution parameters can be defined in the winplotr.set file, via the ! RESOLUTION PARAMETERS (U,V,W): keyword in the winplotr.set
- **save as multicolumns file** option : select X and Y columns to save for each file

March 99

- **Add / remove peaks** options are now available after an automatic background points search
- Windows version of **FullProf** (WFP98.exe and related files) is now included in the WinPLOTTR.zip file. Automatic installations of **WinPLOTTR** and **FullProf** are realized by launching the INSTALL.exe program contained in the WinPLOTTR.zip file.
- **WinPLOTTR** is compatible with dispersive energy data

Feb. 99

- **WinPLOTTR** is a GUI for the **TREOR** program (Windows version) :
 - save selected points as TREOR points to create an input file for **TREOR**
 - edit **TREOR** input file
 - run **TREOR**
- new tools in the toolbar after plot of .PRF or .XRF files : **hkl-** / **hkl+** buttons lead to display in a text window the features of the previous / next Bragg reflexion
- new tools in the toolbar after running the multipatterns version of **FullProf** : **PRF-** / **PRF+** buttons lead to plot previous / next .PRF file.
- **WinPLOTTR** is now compatible with the **FullProf** multi-patterns version (Wmfp99.exe) : just change the appropriate item in the WinPLOTTR.set file

Jan. 99

- **Peak search** dialog box : choice between **search single peaks** and **search Cu Ka1/Ka2 doublets**
- **Plot / 3d lines** menu option
- some changes in the menu presentation :
 - **Options / Background colors** menu option leads to the 'background colors menu'
 - **Text / Text colors** menu option leads to the 'text colors menu'
 - **External Applications / Edit a file** leads to the 'edit a file menu'
 - **External Applications / Run user's programs** leads to the 'run user's programs menu'
- **External Applications / Edit a file** new menu option
- ISNTRM= 1 data file format (data from variable time X-ray data collection) has been included (raw or normalised data)

- **WinPLOT**R can be used as a GUI for **SuperCELL** program (search of commensurate supercell or incommensurate propagation vector) :
 - **Points selection / save as SuperCELL points** option
 - **External applications / edit .SAT file** option
 - **External applications / Run SuperCELL** option
 - **Supercell** program name is stored in the `winplotr.set` file in the ! RUN PROGRAMS: section
- **Help menu** : 'Help Files' option as a switch to display or not help files in windows
- the INSTRM=9 data files are now correctly read
- ! HELP FILES: keyword in the `WinPLOT`R.set file : display or not user's guide files in a window
- a new initialization routine has been implemented : I hope the slowness in the **Reset** and **Run Fullprof** options are now disappeared

Dec. 98

- Colored PostScript files
 - **FullProf** default version is `Wfp98` (Windows version)
 - **Dicvol** default version is `Windic` (Windows version)
 - the '`s=1/d (A-1)`' X space is available
 - multiply *X* values option
 - INSTRM=4 data file format has been included (data from Brookhaven synchrotron)
- position and size of the WinPLOT
- R main window can be defined in the
- `winplotr.set`
- file, via the ! MAIN WINDOW POSITION AND SIZE: keyword. The parameters in the following line are related to the upper-left corner coordinates (
- x*
- and
- y*
-) and the width and height of the window, respectively. These values have to be between 0. and 1.

Nov. 98

- fitting profile procedure will create an **XRF** output file, containing $X(i)$, $Yobs(i)$, $Ycalc(i)$, $Yobs-Ycalc(i)$ and $background(i)$ values and position, intensity, full width at half maximum and eta value for each fitted reflexion.
This **XRF** can then be loaded by **WinPLOT**R and is considered as 5 files. Click with the mouse on reflexions tics will displayed in a window the corresponding position, intensity, fwhm and eta
- some changes in the profile fitting procedure :
 - introduction of U,V,W resolution parameters
 - introduction of an angular dependence of the eta parameter (lorentzian part in the pseudo-Voigt function) :

$$pV(2\Theta) = \text{Eta} * L(2\Theta) + (1 - \text{Eta}) * G(2\Theta)$$

$$\text{Eta} = \text{Eta0} + X * 2\Theta$$

- **Selected points / Add peaks** and **Selected points / Remove peaks** option : lead to the capability to add (or remove) reflexions to (or from) a list of Bragg peaks determined by the automatic peak search procedure : an automatic profile fitting procedure can then be executed, taking into account this new reflexions list
- the user can select and save screen background color, introduction text color and plot background color

Oct. 98

- **File/save as multicolumns file** option : create a multicolumns file with all the data on the screen, with the following format :

```
X_1  Y_1 X_2  Y_2      ....      X_n Y_n
```

- some modifications have been done in the **Win_DICVOL91** program (Windows version of **DICVOL91**) in order to create .PCR files for **FullProf** to test rapidly unit cell solutions proposed by progWin_DICVOL91
- Automatically find peaks can then be stored in a .DIC file for a further automatic search of the unit cell
- an automatic background search procedure has been implemented (**Points selection / automatic peak search** option). The results of this automatic procedure are related to background threshold value, that can be stored in the **winplotr.set** via the **! BACKGROUND THRESHOLD:** keyword. Default value is 0.05.
- an automatic peaks search procedure has been implemented (**Points selection / automatic background** option). The results of this automatic procedure are related to background threshold values, that can be stored in the **winplotr.set** via the **! PEAK SEARCH DETECTION THRESHOLDS:** keyword. These values can be changed by the user, and are defined as follows :
T1 : sensitivity to find 'real peaks'
T2 : sensitivity to find 'shoulder peaks'
Default values are the following : T1 = 0.02 and T2 = 2.
- An automatic profile fitting can be performed after the automatic peak search procedure
- an automatic procedure for installing **WinPLOT**R has been realized : all the **WinPLOT**R and install files are zipped into a **winplot.zip** file. To install **WinPLOT**R on your PC, unzip this file and execute **install.exe**
- **File / save sup file** option :
 - save data created by the calculation options : Summation, Difference, Average, Derivative and Smoothing procedures
 - format = 2 columns X, Y
- a log file can be created to have a trace of that has been done during **WinPLOT**R using. This file creating is related to the **! LOG FILE:** keyword in the **winplotr.set**, and a **winplotr.LOG** file is created in the directory defined by the **WINPLOT**R environment variable.
- order in the format list has been changed : please reload the last **WinPLOT**R.set (in **pub/divers/winplotr** area) or delete the **! DATA FILES EXTENSIONS:** part in yours.
- **INSTRM=8** (data from DMC (PSI) diffractometer) has been implemented
- options **Plot/Excluded regions** and **PRF options/excluded regions** have been implemented

Sept. 98

- problem in **save WinPLOT settings** option has been corrected in the previous version
- user's programs can be executed from the **External applications** menu : the program name, version and comment are defined by the user in the `winplotr.set` file, in the lines following the `! RUN PROGRAMS:` keyword.
example : `PLOT = 'c:\progs\plotr.exe' ! PLOT DOS version`

As for `FullProf`, `Edit` or `Dicvol`, first item on the line is related to the vertical **External applications** menu item, second (after the '=' character) to the program that will be run, and third (after the '!' character) to the text that will appear in the status bar of **WinPLOT**
Remark : a maximum of 5 user's programs can then be defined

- data file extensions can be defined by the user in the `winplotr.set`, via the `! DATA FILES EXTENSIONS:` keyword

example :

1	*.xy	! X,Y data
2	*.dat	! INSTRM = 0
4	*.dat ;*.d1b	! INSTRM = 3

- multicolumns data files are now accepted in **X,Y data** format
- **File/print Setup** option has been removed (unused)
- `INSTRM=10` data file format has been included (with `XYDATA` as keyword in the first line)
- Fit procedure bugs have been corrected
- X,Y file (with '!' or '#' as first character of the lines) are now correctly read
- Link to **DICVOL** program (D. Louer & A. Boultif) :
 - select some points
 - save as **DICVOL** points : fill a **DICVOL** dialog box to create a **DICVOL** file (.DIC)
 - run the Windows version of **DICVOL** (External links)
- **Calculation option** :
 - derivative data
 - smoothing

July 98

- **fit procedure** dialog box :
 - global Fwhm and Eta are displayed as refined parameters values
 - add or remove peaks
 - a `file.XRF` is created (column format) with refined parameters and standard deviations values
- new tools in the toolbar : shrink or expand the plot frame width

June 98

- a bug in the **difference calculation** option, after selection of files to plot (**Files/Select files**), is corrected
- selected points values are displayed in text windows

May 98

- G41 and G61 (LLB) files format has been included
- new tools in the toolbar :
 - arrows : move through the patterns
 - **FP** : run FullProf program
 - **Pcr** : edit .Pcr file
 - **Fit** : access to the profile fitting procedure
- clicks on frame lines have been replaced by clicks on icons in the toolbar (if the zoom or focus option has been previously activated)
- buffer files with empty lines are read without error
- correction of bugs in :
 - **profile fitting** after **select files** among several files
 - **difference calculation** option
- If a WINPLOTR environnement has been defined, the last current directory is stored in the `winplotr.dir` file. This file will be read after each **WinPLOTR** executing to open files in the directory previously visited by **WinPLOTR**.
- left mouse click on frame lines :
 - right frame line : move the pattern to the right
 - left frame line : move the pattern to the left
 - down frame line : move the pattern to the down
 - up frame line : move the pattern to the up

April 98

- After running **FullProf** (Wfp98 Windows version), **WinPLOTR** will plot the last data file used by **FullProf**, if a **FULLPROF** environment variable has been defined.
- link to an editor to edit a `PCR.file` : the editor name can be specified in the `winplotr.set` file. If not, the **notepad** editor will be used. Unfortunately, you have to exit from the editor to run **FullProf** (**WinPLOTR** have to stop a `'call(system) command'`).
- The existence of a sigma data array can be specified by the `! SIGMA ARRAYS:` item in the `winplotr.set` file. Sigmas are then associated to all the data files to plot errors bars.
- Plot error bars

- Save pattern plots as `file.WPL`
- Open templated `file.WPL`
- Choice of the pen width
- Write or not the negative Y graduations
- Change the frame width of the pattern plot
- Profile fitting procedure

March 98

- Birthday of the beta version of **WinPLOT**R