

Introduction to Fullprof

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Fullprof Suite

<https://www.ill.eu/sites/fullprof/>



FullProf Suite
Crystallographic tools for diffraction

[Home](#) | [Documentation](#) | [Download](#) | [References](#) | [Contact](#)

**NEWS!**

We are engaged in modernizing the complete **FullProf Suite** and we have started by refurbishing the Web page. We are changing all the GUIs by moving from **Winteracter** to **PySide6**. Presently the new Toolbar is nearly finished and the most important change up to now is the new **FullProf Studio** program. The new FullProf Suite will be developed and will coexist with the **CLASSIC one**.

A simple video (about ten minutes!) showing how to work with the new Toolbar can be visualised here: [View FPS and FP_Studio](#)

Crystallographic tools for Rietveld, profile matching and integrated intensity refinements

The FullProf Suite is formed by a set of crystallographic programs mainly developed for Rietveld analysis (structure profile refinement) of neutron (constant wavelength, time of flight, nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant or variable step in scattering angle 2θ .

[Download](#) | [Features](#)

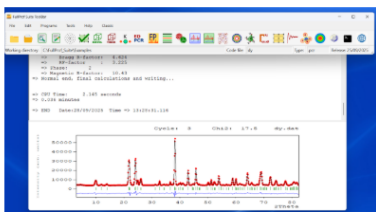
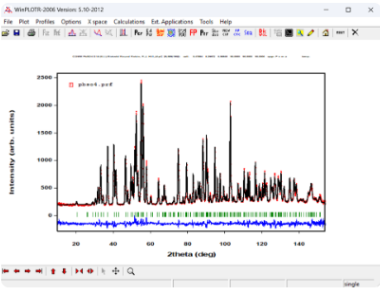
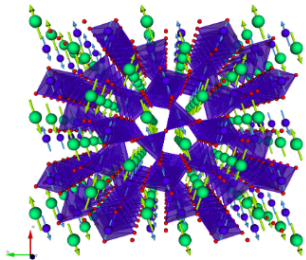


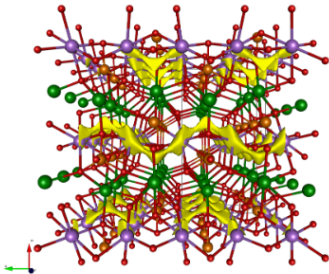
Image gallery



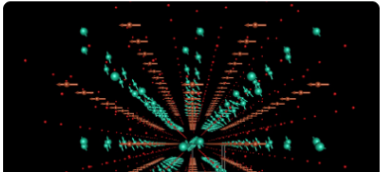
Rietveld analysis

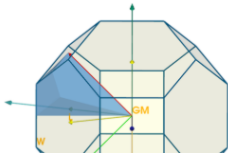


Crystal structure visualization



Bond-valence calculations







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Downloads and updates

- Fullprof has been around since the 1990's
- The main EdPCR GUI has had the same look for a while, but Fullprof has undergone constant development (including a new toolbar).
 - Well optimized for magnetic refinements with latest developments.

The screenshot shows the FullProf Suite website with a navigation bar (Home, Documentation, Download, References, Contact) and a news section. The main content area displays download options for three operating systems: Windows, Linux, and macOS. Each system has a 'Classic FullProf Suite' and a 'New FullProf Suite' (where applicable). The Windows section has two red circles highlighting the 'Classic FullProf Suite' and the 'New FullProf Suite'. The Linux and macOS sections also show download buttons. A 'Previous FPSuite versions' link is at the bottom right.

FullProf Suite
Crystallographic tools for diffraction

Home Documentation Download References Contact

NEWS!

The second version of the **FullProf Suite**, which runs under a Python graphical environment for Windows and Linux, is now available. A macOS version will be released soon. Installation is straightforward: simply unzip the downloaded file and run the **tftp** executable. We have observed some issues with certain Linux distributions, which are due to the wide variety of Linux distros and incompatibilities of system libraries. For now, the distributed versions work well on Linux Mint (Version 22.2, Zora) and Ubuntu (Version Ubuntu 22.04.5 LTS). We will also prepare instructions for using the source code directly from Python. This will allow users on Linux, MacOS, and Windows to work directly with the Python code and potentially contribute to its development. We have added a link to the Web page of the program **iPowder**, which runs under PySide6 only on Windows for the moment (See **References** for details).

The **Classic FullProf Suite** distribution has been simplified: now the new Intel Fortran compiler (**ifx**) is exclusively used. Users are encouraged to report any issues so that the corresponding executable can be fixed promptly. The program PANDA may not work properly in the Linux distributions for the reasons stated above.

There is also available a tool for automated Rietveld analysis of powder diffraction patterns using FullProf as refinement engine, the **FullProfApp**. This tool requires a previous installation of the **Classic FullProf Suite** and it is designed to easily handle large chunks of diffraction data generated by high-throughput screening (HTS) experiments as well as by in situ and operando studies at large user facilities such as Synchrotron and Neutron sources.

Installation instructions for the FullProf Suite: <https://fpsuite-doc.readthedocs.io/en/latest/pages/installation/installation.html>

Installation instructions for the FullProfApp: <https://fullprofapp.readthedocs.io/en/stable/>

What is new in the classic FullProf Suite: https://www2017.ill.eu/sites/fullprof/Old_FP/php/FullProf_News.htm

Windows

- Classic FullProf Suite**
GUI: Winteracter
Date: 19 June 2026
[Download](#)
- New FullProf Suite**
GUI: PySide6 + Winteracter
Date: 19 June 2026
[Download](#)
- FullProfApp**
GUI: PyQt
Date: 9 April 2025
[Download](#)
- iPowder**

Linux

- Classic FullProf Suite**
GUI: Winteracter
Date: 19 June 2026
System: Linux Mint 22.2
[Download](#)
- New FullProf Suite**
GUI: PySide6 + Winteracter
Date: 19 June 2026
System: Linux Mint 22.2
[Download](#)
- New FullProf Suite**
GUI: PySide6 + Winteracter
Date: 25 April 2026
System: Ubuntu 22.04.5 LTS
[Download](#)

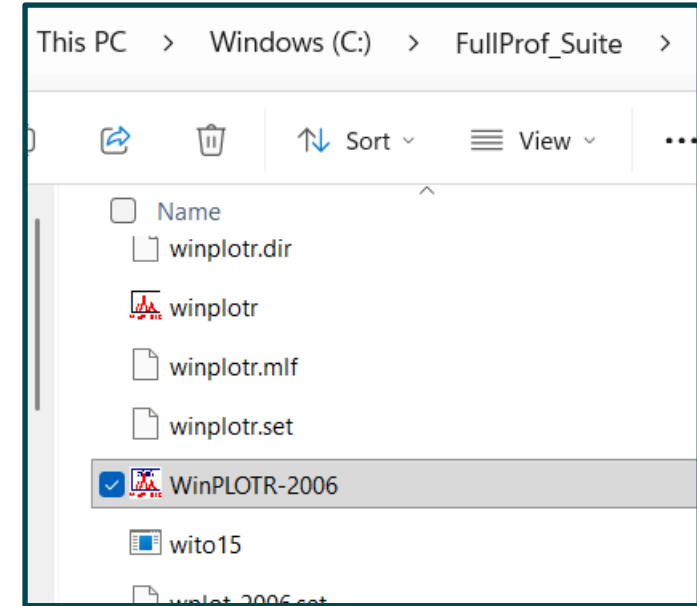
macOS

- Classic FullProf Suite - Linux like**
GUI: Winteracter
Date: 27 February 2025
[Download](#)
- Classic FullProf Suite - dmg**
GUI: Winteracter
Date: 25 February 2025
[Download](#)
- [Previous FPSuite versions](#)

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Downloads and updates

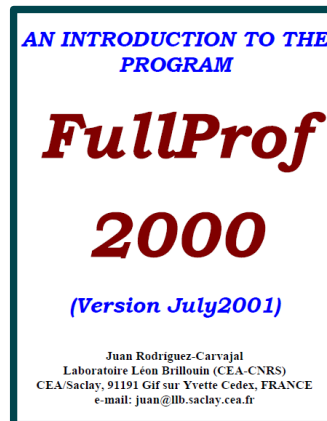
- For windows the “Classic Fullprof Suite” download is typically in the C drive
- The “New Fullprof Suite” works wherever you want to put it
- Look in these folders to see all the programs and other useful folders and files.



Fullprof manual and updates

https://www2017.ill.eu/sites/fullprof/Old_FP/php/FullProf_News.htm

- There is an old manual
(C:\FullProf_Suite\Docs\Fullprof_Manual.pdf)
- There is a new file explaining commands
 - FP_COMMANDS.pdf
- There are also manuals for some of the other programs.
- FullProf News contains all latest updates.



FullProf News

This document contains information about new features and corrected bugs of FullProf.2k and related programs. It may be used as an extension to the manual of FullProf.

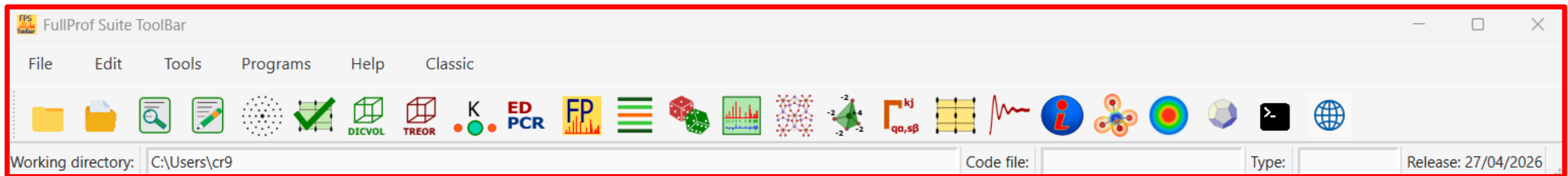
Last version

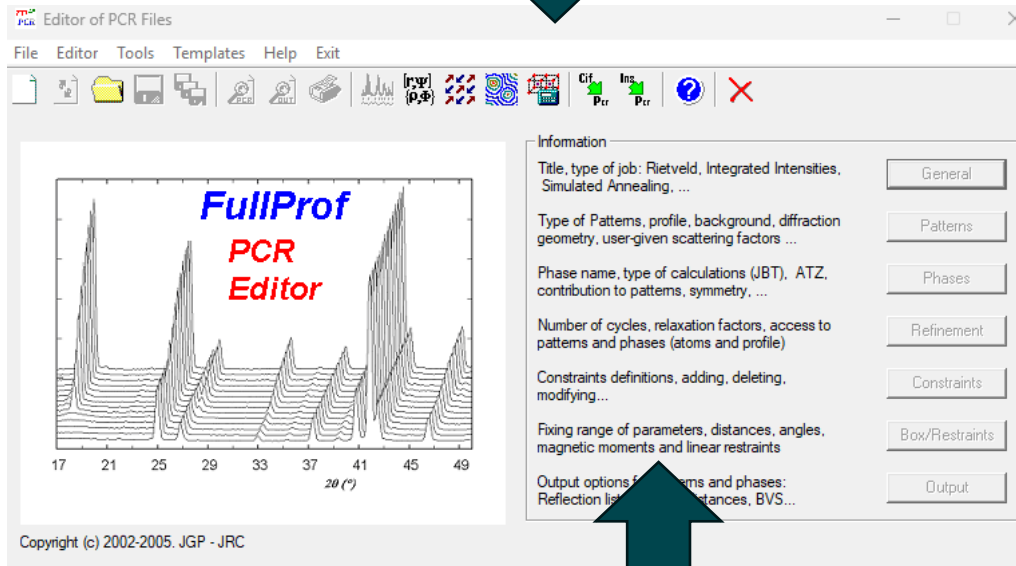
** PROGRAM FullProf.2k (Version 8.40 - Feb2026-ILL JRC) **

2026
[Full 2026 year in plain text](#)
2025
[Full 2025 year in plain text](#)
2024
[Full 2024 year in plain text](#)
2023
[Full 2023 year in plain text](#)
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2013
[Full 2013 year in plain text](#)
2012



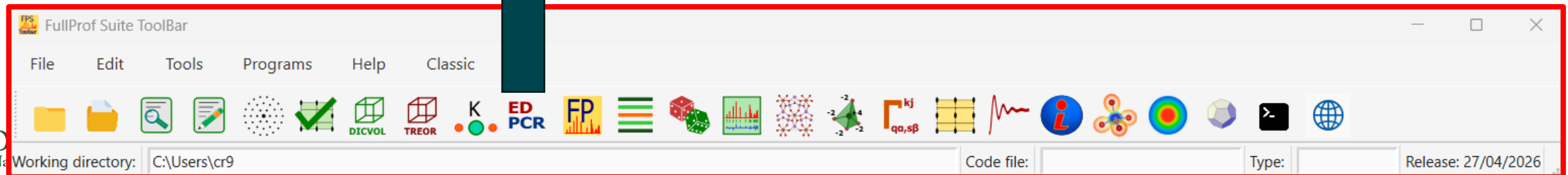
- Fullprof suite toolbar(s)
 - Contains all the different capabilities of Fullprof
 - Selecting the working directory each time you do a refinement is the best way to run refinements and use all the tools without problems.

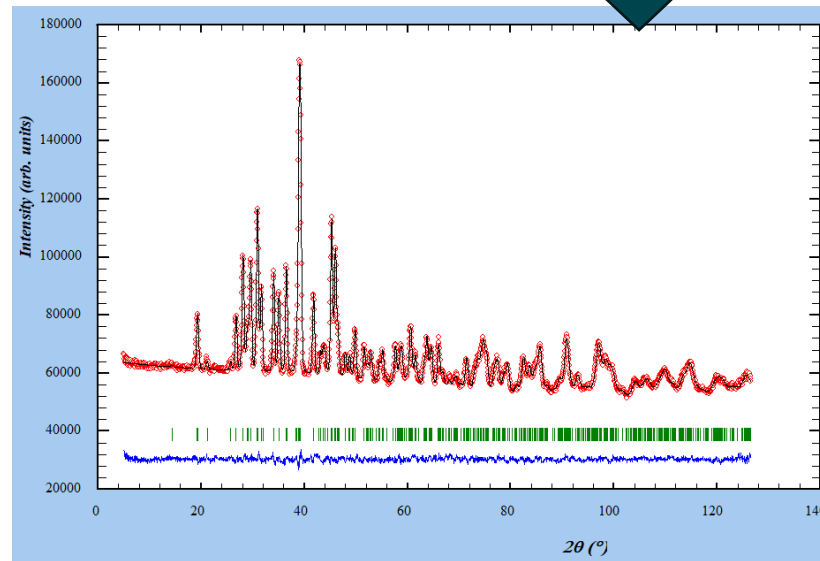




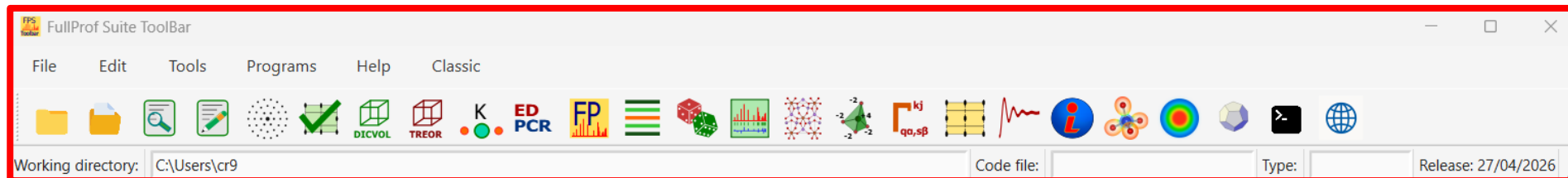
• EdPCr

- Main GUI we'll use for running refinements.
- This reads a text file (.pcr) that we will also edit.





- WinPlotr (only in classic Toolbar)
 - Visualize the refinement against data.
 - Lots of other features.
 - Sequential refinements
 - Instrument resolution
 - Background modelling
 - Various ways to plot and manipulate data
 -
 - Can even run refinements directly from here

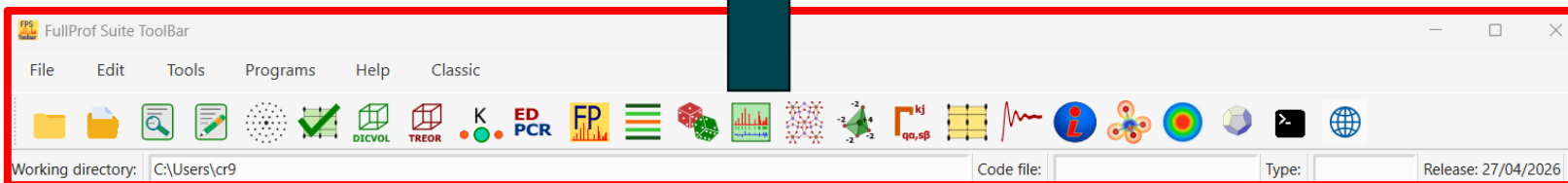
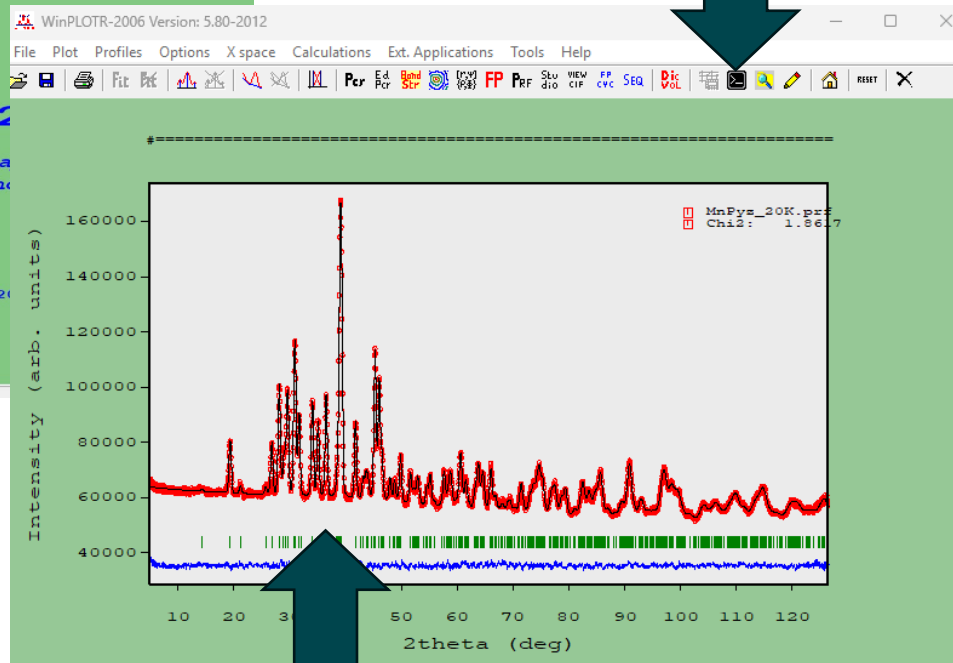


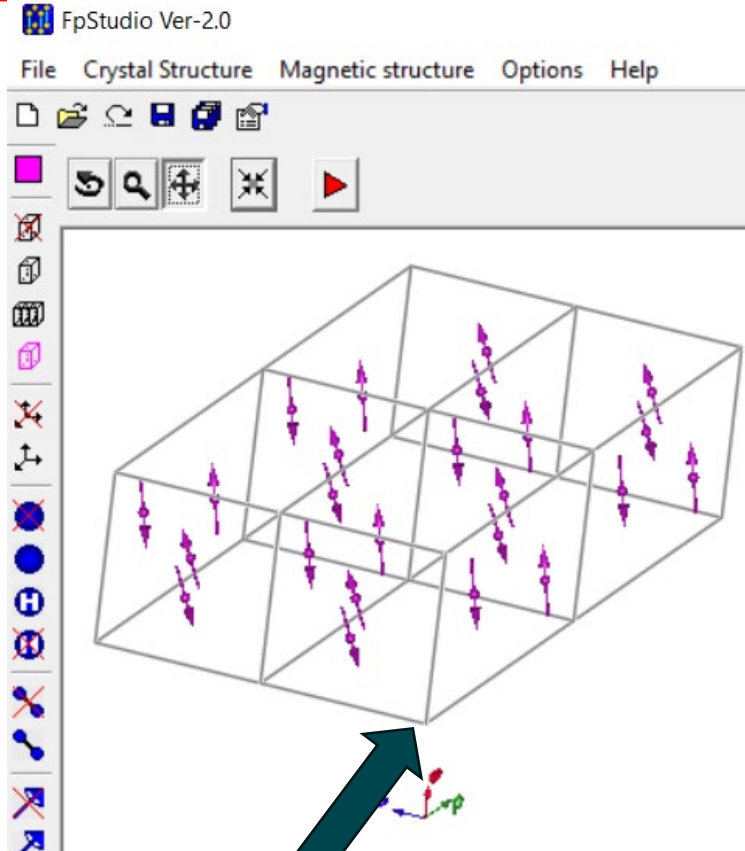


- WinPlotr-2006
- Plot data, refinement
- **k-search**
- Lots of other features.

- Sequential refinements
- Instrument resolution
- Background modelling
- Various ways to plot and manipulate data
-

- Can even run refinements directly from here

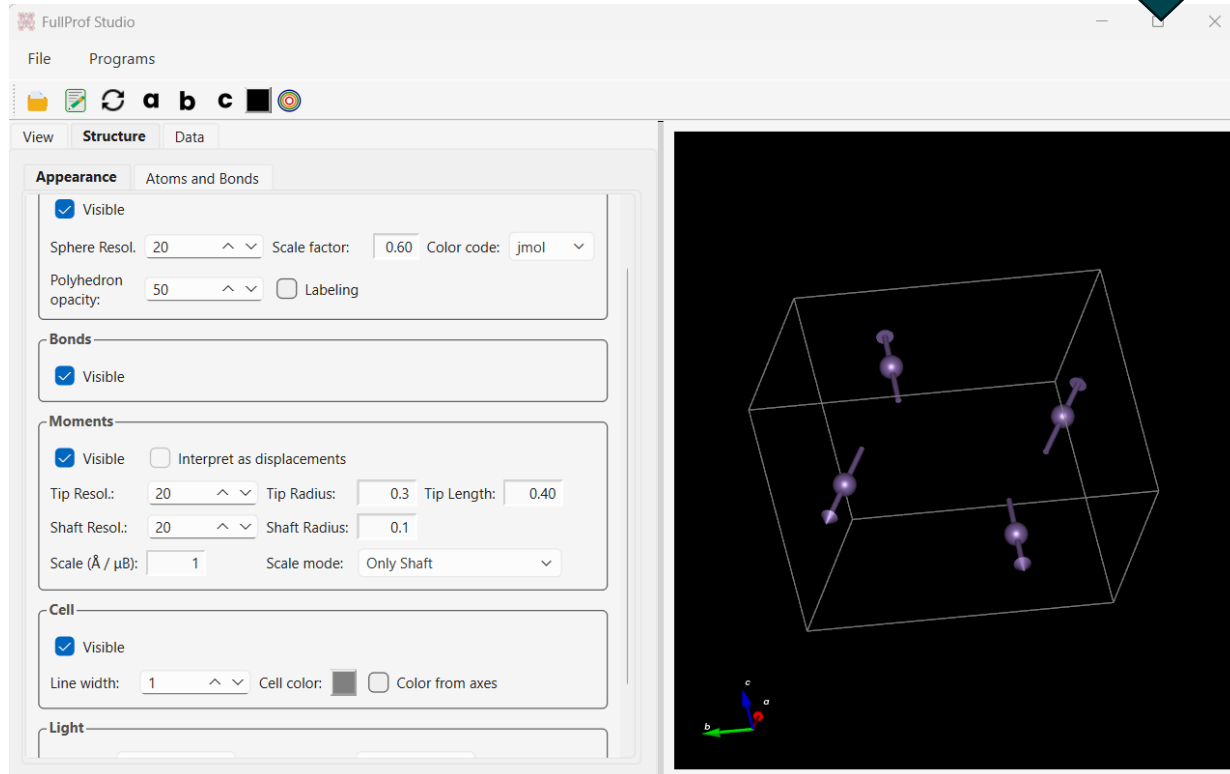




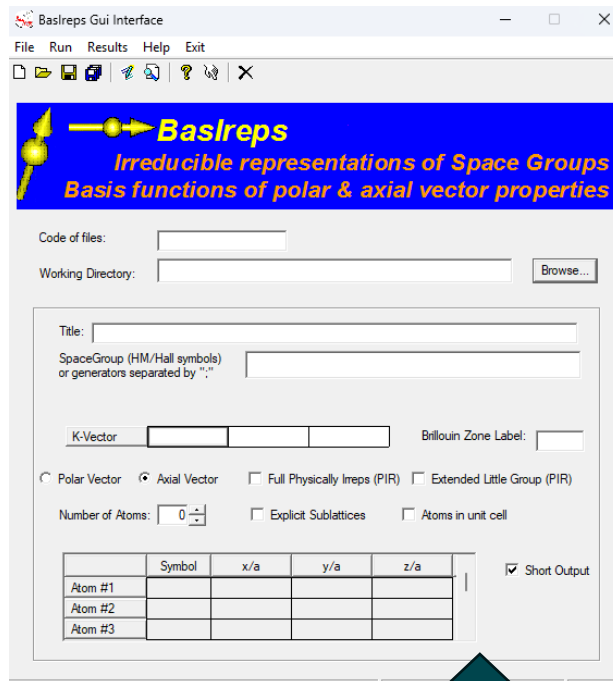
- Fullprof studio

- Visualize crystal and magnetic structure
- Check magnetic moment values from refinements





- New Fullprof studio
 - Loads mcif, cif, .fst
 - Improved graphics



- Basireps
- Representational analysis for magnetic structures.

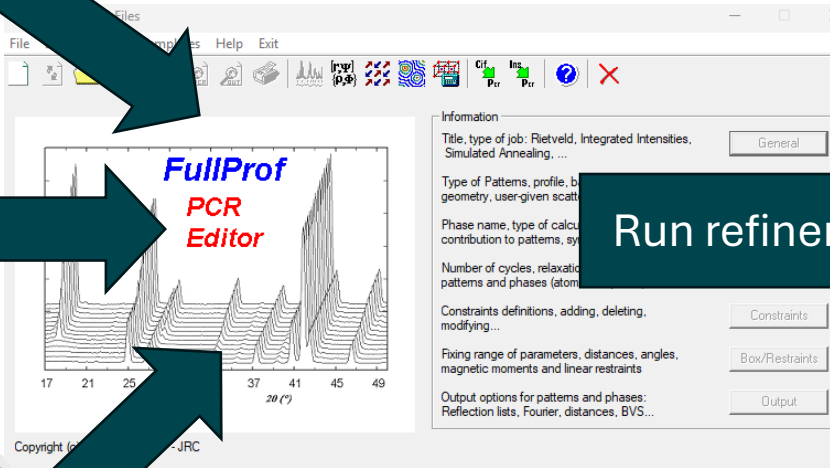


How do we determine the magnetic structure with Fullprof?

INPUT
CRYSTAL
PARAMETERS
(e.g. load in a
cif)

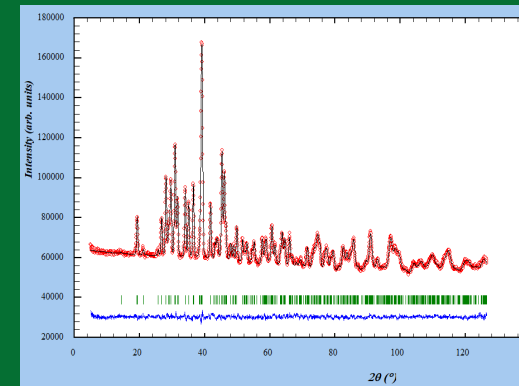
INPUT
MAGNETIC
MODEL (e.g.
use SARAh or
basireps)

INPUT
INSTRUMENT
PARAMETERS
(e.g. load in
an irf)

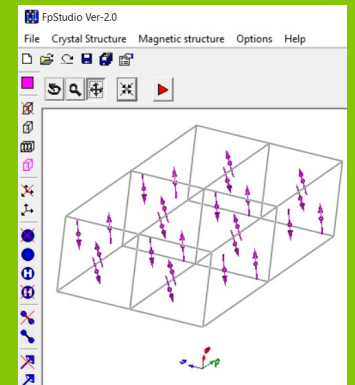


Run refinement

COMPARE THE
REFINED
FULLPROF
CALCULATION
AGAINST THE
NEUTRON DATA



PUBLISH
DETERMINED
MAGNETIC
STRUCTURE



Beyond the EdPCR GUI

- All the inputs to the refinement are contained in a text file, the .pcr file.
- This can be opened and edited.
 - Some features are not in the GUI
 - Often it is faster to edit the text file, after you get used to the format.

An example of a pcr file

[illegible]

Contains flags for refinement set-up
e.g. Nph is the number of phases

Lambda1	Lambda2	Ratio	Bkpos	Wdt	Cthm	muR	AsyLim	Rpolarz	2nd-muR	-> Patt# 1
2.406700	2.406700	0.000000	60.0000	8.00000	0.00000	0.00000	180.000	0.00000	0.00000	

Instrument and sample specific details

INCY	Eps	R_at	R_an	R_pr	R_g1	Thmin	Step	Thmax	PSD	Sent0
10	0.02	1.00	1.00	1.00	1.00	8.5000	0.069037	128.6940	0.000	0.000

Number of refinement cycles, range, etc

```
26 !Number of refined parameters
```

Number of parameters being refined

Zero	Code	SyCos	Code	SySin	Code	Lambda	Code	MORE	Pattern#
0.26469	0.0	0.00000	0.0	0.00000	0.0	0.000000	0.00	0	
Background coefficients/codes for Pattern# 1 (Polynomial of 6th degree)									
43.885	-13.726	11.683	7.474	-4.415	0.000				
51.00	61.00	71.00	81.00	91.00	0.00				

Zero offset and background

```

Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 3.88 Magnetic R-Factor: 10.37

```

Nuclear and Magnetic Structure of: /srv/www/bcs_branch/www/bcs/www/tmp/Cr2WO6

!Nat	Dis	Ang	Pr1	Pr2	Pr3	Jbt	Irf	Isy	Str	Furth	ATZ	Nvk	Npr	More
4	0	0	0.0	0.0	1.0	10	0	2	0	0	767.677	0	7	0

```
Pn'm number:58.395      <--Magnetic Space group symbol (BNS symbol & number)
```

Transform to standard:

Transform from Parent:

! Nsym	Cen	N_Clat	N_Ant
8	0	0	0

Symmetry operators

```

1 x,y,z,+1
2 -x,-y,-z,-1
3 x,y,-z,+1
4 -x,-y,z,-1
5 -x+1/2,y+1/2,-z+1/2,-1
6 x+1/2,-y+1/2,-z+1/2,+1
7 x+1/2,-y+1/2,z+1/2,+1
8 -x+1/2,y+1/2,z+1/2,-1

```

This section is the phase information for your sample.
Has atomic information, symmetry, occupancy,
thermal parameters

Atom	Type	Mag	Vek	X	Y	Z	Biso	Occ	N_type	Spc/Fftype	/Line below:Codes
	Rx	Ry	Rz	Ix	Iy	Iz		MagPh	/Line below:Codes		
	beta11	beta22	beta33	beta12	beta13	beta23	/Line below:Codes				
W1	W	1	0	0.00000	0.00000	0.00000	1.07060	0.25000	0	0	#
				0.00	0.00	0.00	171.00	0.00			
Cr1	MCR2	1	0	0.00000	0.00000	0.33602	0.32382	0.50000	1	0	#
				0.00	0.00	221.00	181.00	0.00			
	2,24046	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	<-MagPar		
	111.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
O1	O	1	0	0.31675	0.29343	0.00000	0.49453	0.50000	0	0	#
				231.00	241.00	0.00	191.00	0.00			
O2	O	1	0	0.30635	0.29684	0.33979	0.47728	1.00000	0	0	#
				261.00	251.00	211.00	201.00	0.00			

Scale	Shapel	Bov	Str1	Str2	Str3	Strain-Model
1.7086	0.0000	0.0000	0.0000	0.0000	0.0000	0
21.0000	0.000	0.000	0.000	0.000	0.000	
U	V	W	X	Y	GausSiz	LorSiz Size-Model
0.406899	-0.648329	0.315017	0.043578	0.000000	0.000000	0.000000 0
171.000	131.000	141.000	101.000	0.000	0.000	0.000

Here is the scale and peak shape parameters

a	b	c	alpha	beta	gamma	#Cell Info
4.578908	4.582315	8.847304	90.000000	90.000000	90.000000	#
11.00000	31.00000	41.00000	0.00000	0.00000	0.00000	
Pref1	Pref2	Asy1	Asy2	Asy3	Asy4	S_L D_L
1.00000	0.00000	-0.13649	0.00000	0.20758	0.00000	0.04400 0.04400

Lattice constants and any preferred orientation

!	2Th1/TOF1	2Th2/TOF2	Pattern to plot
	8.500	128.694	1

Range to plot the fits (only for visualization)

Now let's start using Fullprof
with some examples!