Second 2025 Edition of the School on Neutron Diffraction Data Treatment using the FullProf Suite

JUAN RODRIGUEZ-CARVAJAL

DIFFRACTION GROUP

INSTITUT LAUE-LANGEVIN

Grenoble, October 2025

Introduction to the FullProf Suite

History of FullProf: From 1980 to 1986

• I started to work with the Rietveld method in Barcelona in 1982 after receiving a tape from Ray Young in which he sent me the complete source code of the program (DBW) he published in 1981 in J. Appl. Cryst.

• I learnt the subtleties of the Rietveld method, obliged to modify and correct bugs, in order to use the program for my own data taken in laboratory X-ray powder diffractometers (Using CDC, PDP-11, VAX and later IBM-PC computers)

• I had a version of the DBW program that I introduced in the Bertaut's Lab (I was regularly working in Grenoble during summers to complete my PhD)

History of FullProf: Origins ... summer 1987

STRAP package (December 1987)

STRAP

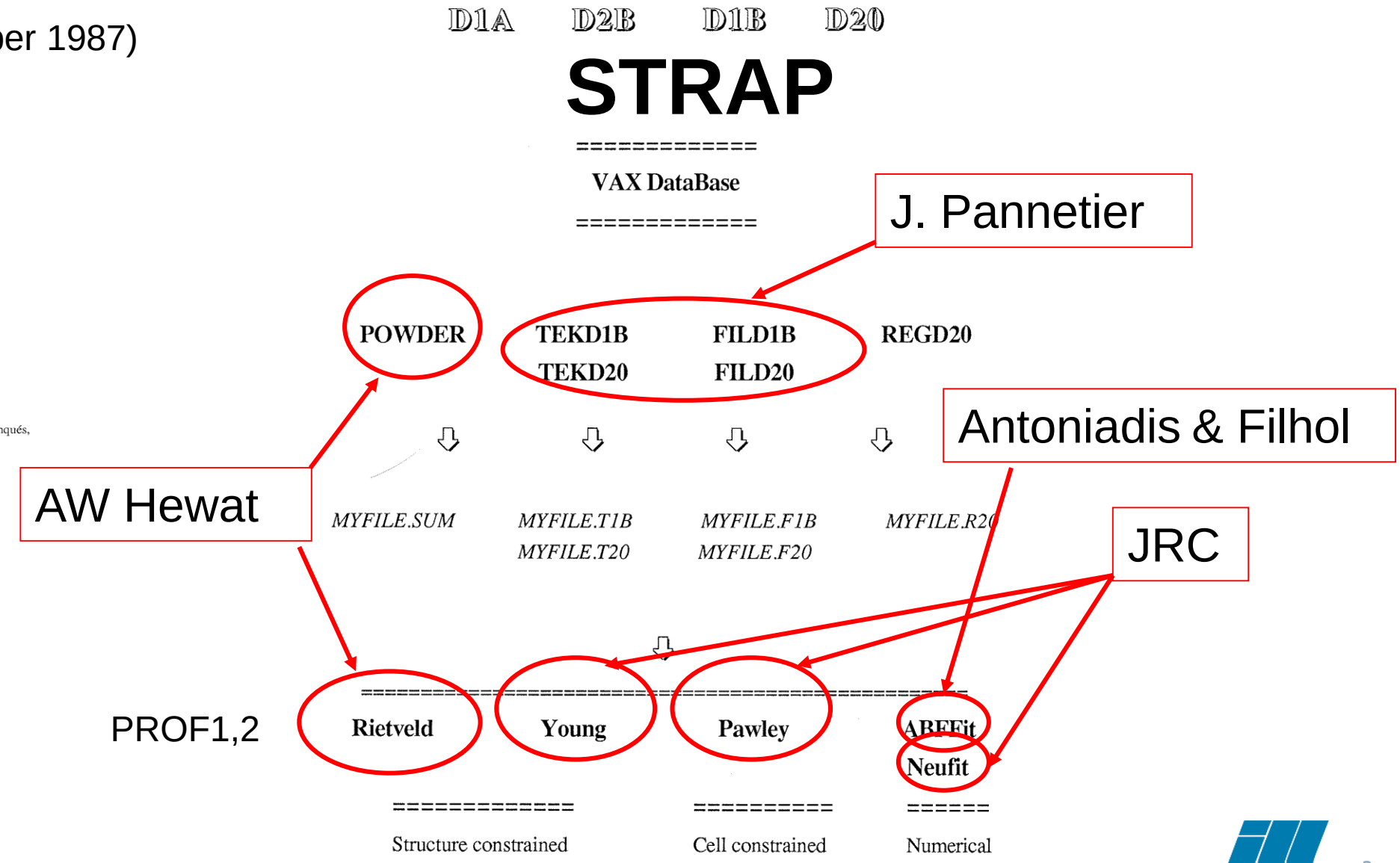
a System for Time-Resolved Data Analysis

(Powder Diffraction Patterns)

a Simple Tutorial

by J. Rodriguez*, M. Anne * * and J. Pannetier * * *

* Instituto de Ciencia de Materiales de Barcelona, CSIC, c/Marti i Franqués, s/n., 08028 Barcelona (Spain)
* * Laboratoire de Cristallographie du CNRS, 166X, 38042 Grenoble
* * * ILL. 156X, 38042 Grenoble



At ILL during the summer of 1987

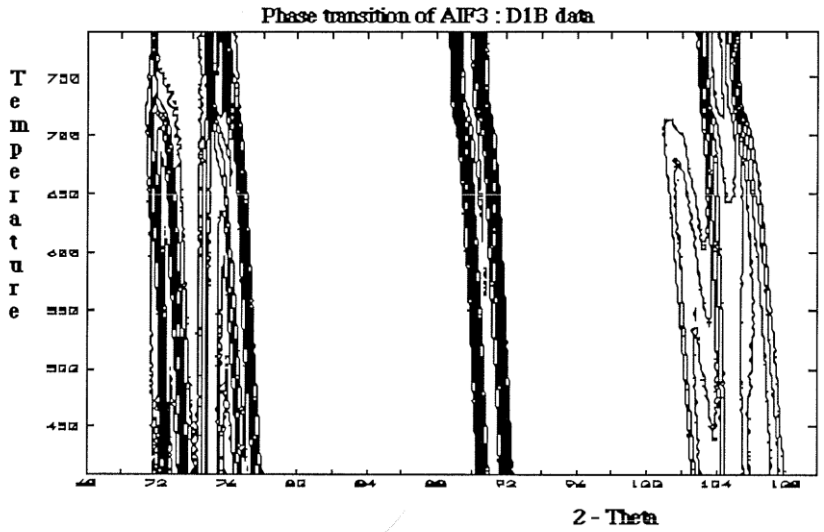


Fig. 2 : Contour map (option 3 of P3DNEW)

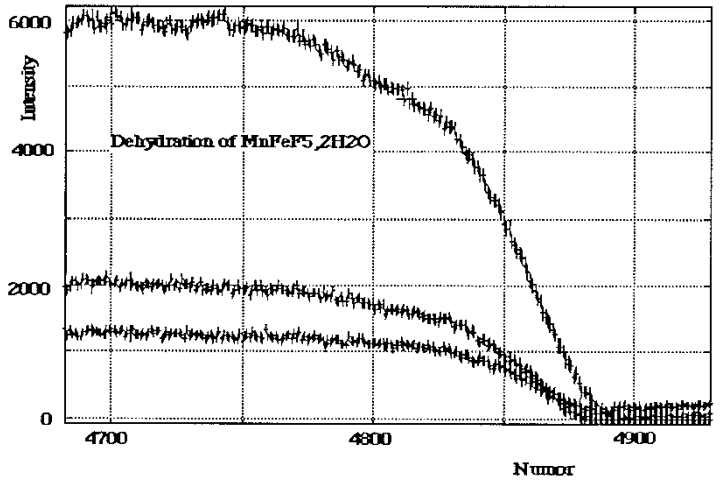
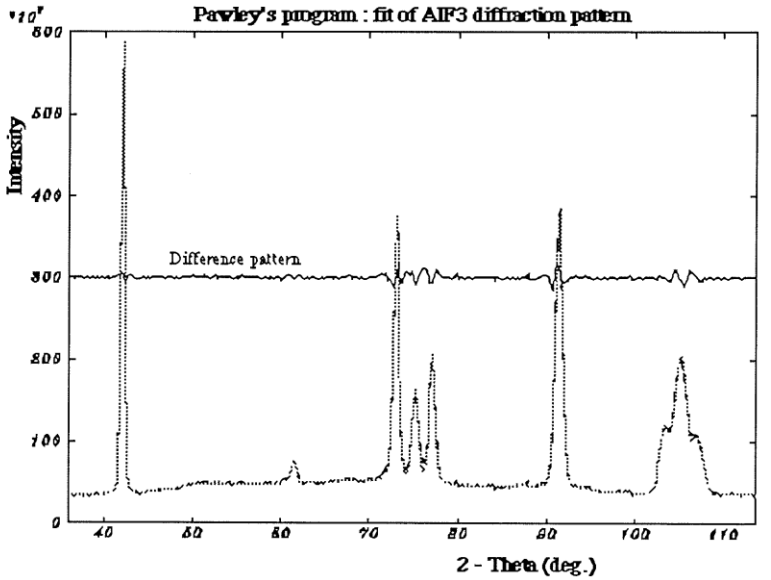


Fig. 10 : Graphic output from Dispaw

- PLOTPOW : produces observed, calculated & difference plots from data stored in FILIN.PRO (see Fig. 8)
  This program is rather interactive and its use will not be further detailed.



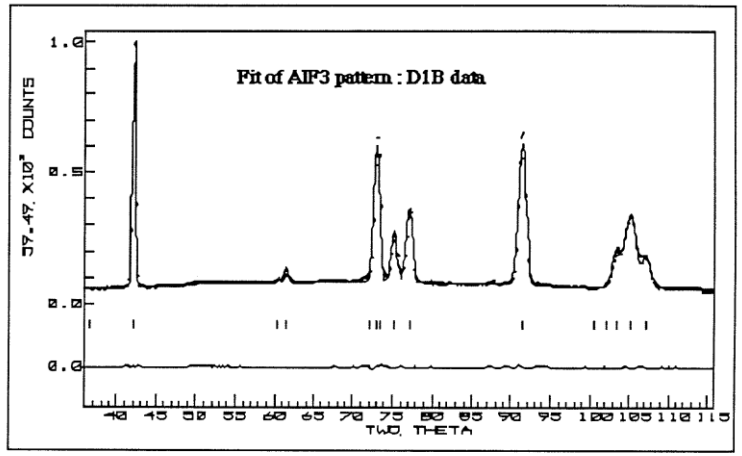


Fig. 14 : Graphic output from RIETYNG

History of FullProf: From 1988 to 1992 @ILL

Implementation in the program **FullProf** the **formalism of propagation vectors** that was able to treat all kind of magnetic structures including incommensurate structures.

This was presented in a Satellite of IUCr congress in Bordeaux on powder diffraction (1990) and, with more complete options, in the
WORKSHOP ON THE USE OF NEUTRONS AND X-RAYS IN THE STUDY OF MAGNETISM (Grenoble, January 21-23, 1993)

Published in **Physica B 192, 55-69 (1993)**

~ 31 years ago!

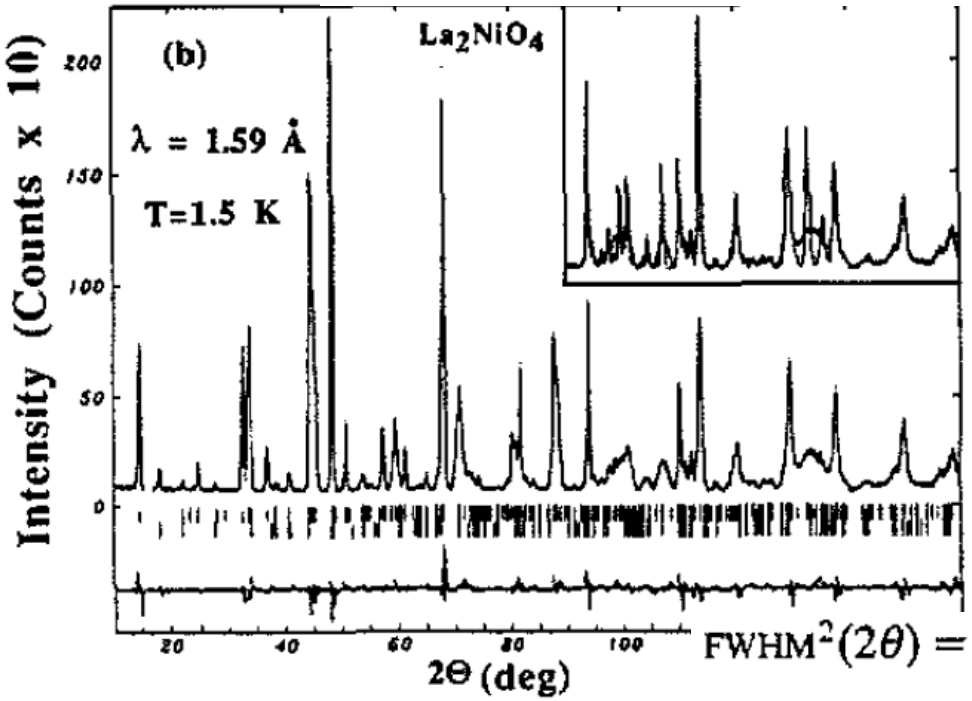
The early development of FullProf

Neutron diffraction study on structural and magnetic properties of La_2NiO_4

J. Phys. Condens. Matter 3 (1991) 3215-3234

J Rodríguez-Carvajal, M T Fernández-Díaz and J L Martínez
Institut Laue–Langevin, 156 X, F-38042 Grenoble Cédex, France

Appendix. Anisotropic broadening of Bragg reflections and Rietveld method



$$P(x) = \frac{1}{\sigma(\alpha)}(2\pi)^{1/2}\exp\left(-\frac{1}{2}\frac{(x-\alpha)^2}{\sigma^2(\alpha)}\right)$$

$$M_{hkl} = 1/d^2_{hkl} = M(\alpha_i; hkl)$$

$$\langle M_{hkl}\rangle = M(\langle\alpha_i\rangle; hkl)$$

$$\sigma^2(M_{hkl}) = \sum_i \sum_j S_{ij}\frac{\partial M}{\partial \alpha_i}\frac{\partial M}{\partial \alpha_j}.$$

$$\sigma^2(2\theta)_s = [\sigma^2(M_{hkl})/M^2_{hkl}]\tan^2\theta$$

$$\mathrm{FWHM}^2(2\theta) = \{U + (8\ln 2)[\sigma^2(M_{hkl})/M^2_{hkl}]\}\tan^2\theta + V\tan\theta + W.$$

THE REFERENCE PAPER OF FULLPROF

Recent advances in magnetic structure determination by neutron powder diffraction

Physica B 192, 55 (1993)

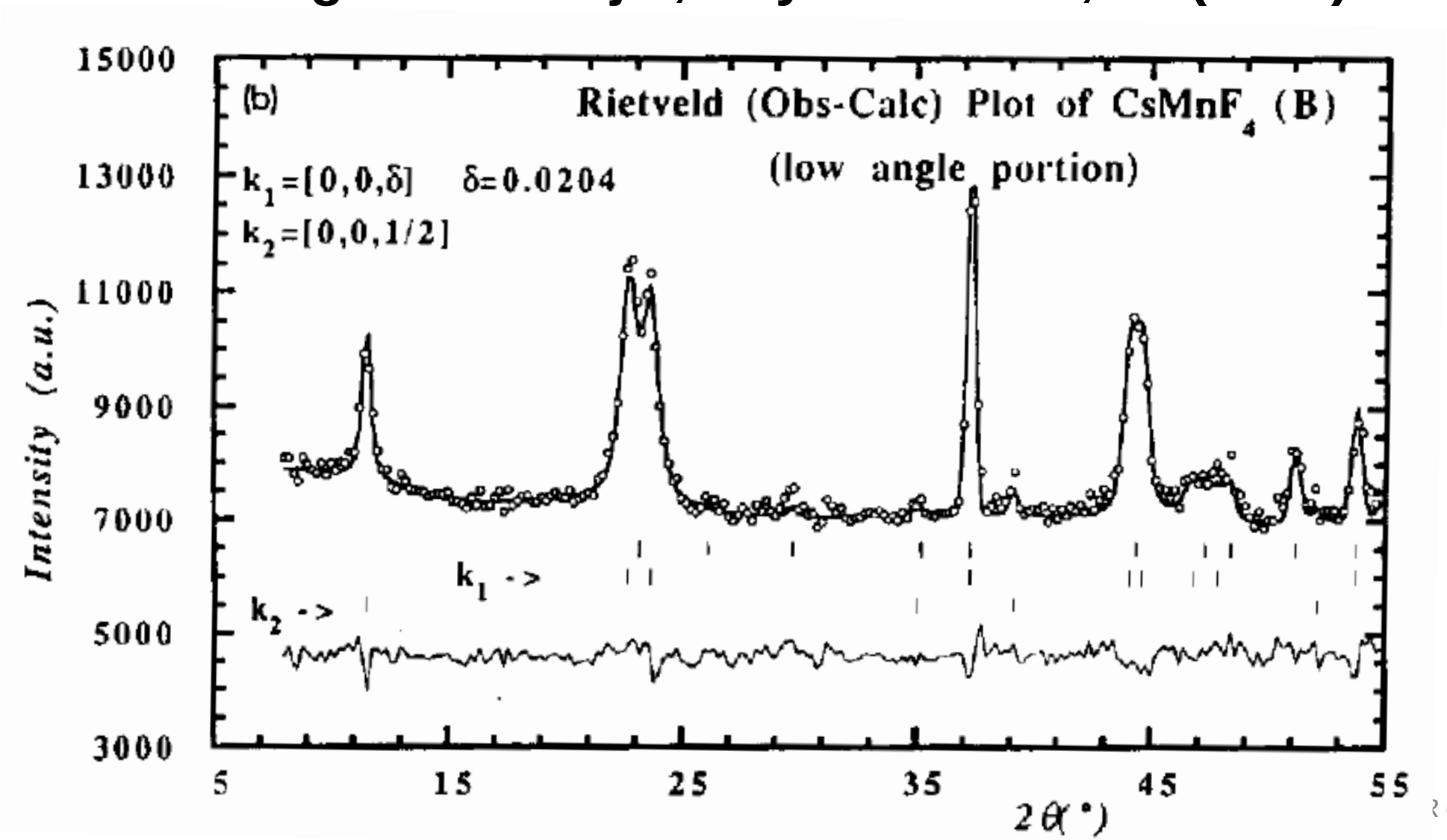
Juan Rodríguez-Carvajal

Laboratoire Léon Brillouin (CEA-CNRS), Centre d'Etudes de Saclay, Gif sur Yvette, France and Institut Laue–Langevin, Grenoble, France

In spite of intrinsic limitations, neutron powder diffraction is, and will still be in the future, the primary and most straightforward technique for magnetic structure determination. In this paper some recent improvements in the analysis of magnetic neutron powder diffraction data are discussed. After an introduction to the subject, the main formulas governing the analysis of the Bragg magnetic scattering are summarized and shortly discussed. Next, we discuss the method of profile fitting without a structural model to get precise integrated intensities and refine the propagation vector(s) of the magnetic structure. The simulated annealing approach for magnetic structure determination is briefly discussed and, finally, some features of the program FullProf concerning the magnetic structure refinement are presented and discussed. The different themes are illustrated with simple examples.

The reference paper of FullProf

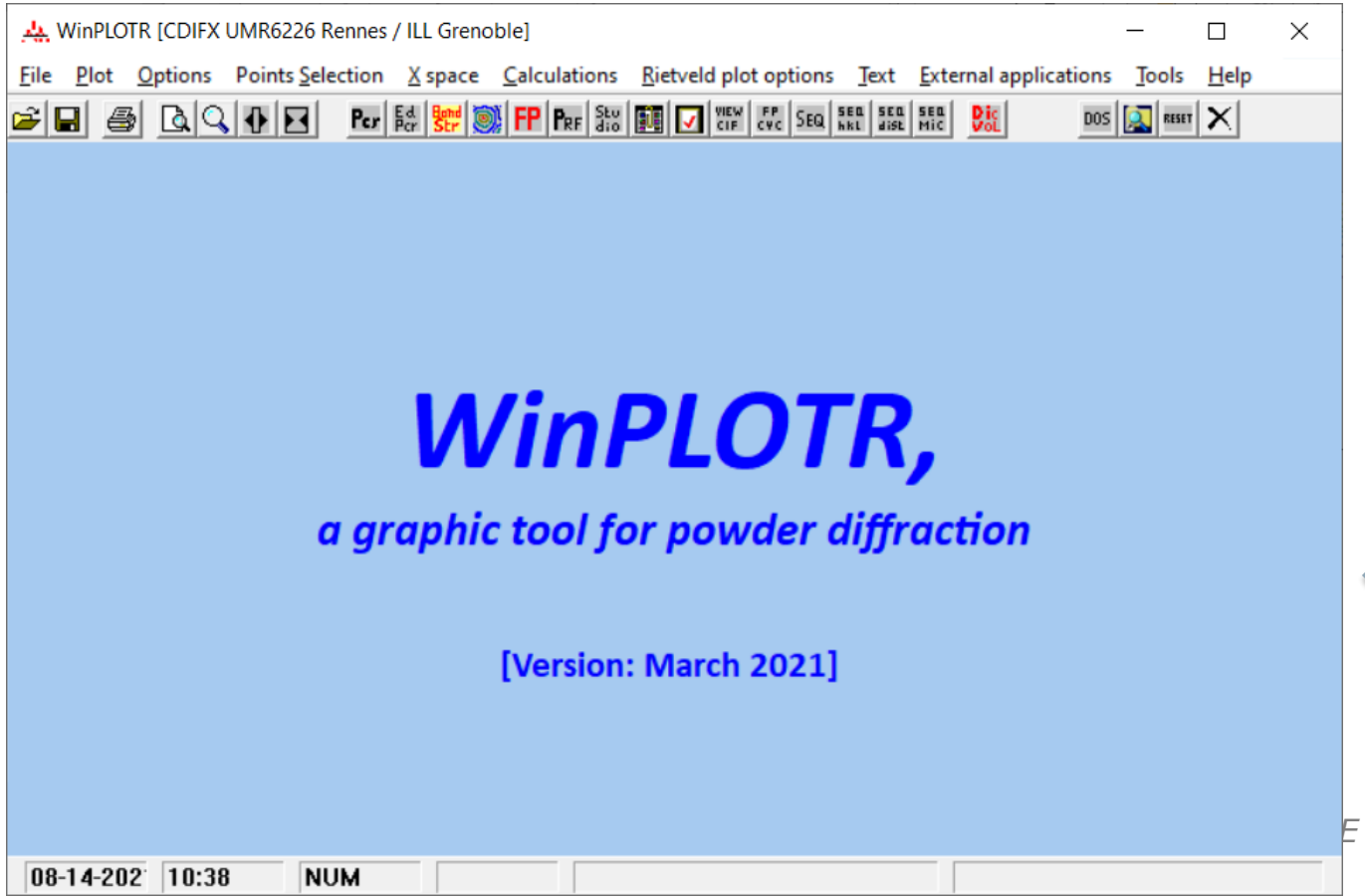
J. Rodriguez-Carvajal, Physica B 192, 55 (1993)



The early development of FullProf

The middle of the nineties

Development of WinPLOTR with Thierry Roisnel at LLB (Fortran 90 + RealWin): a high impact in the distribution of FullProf

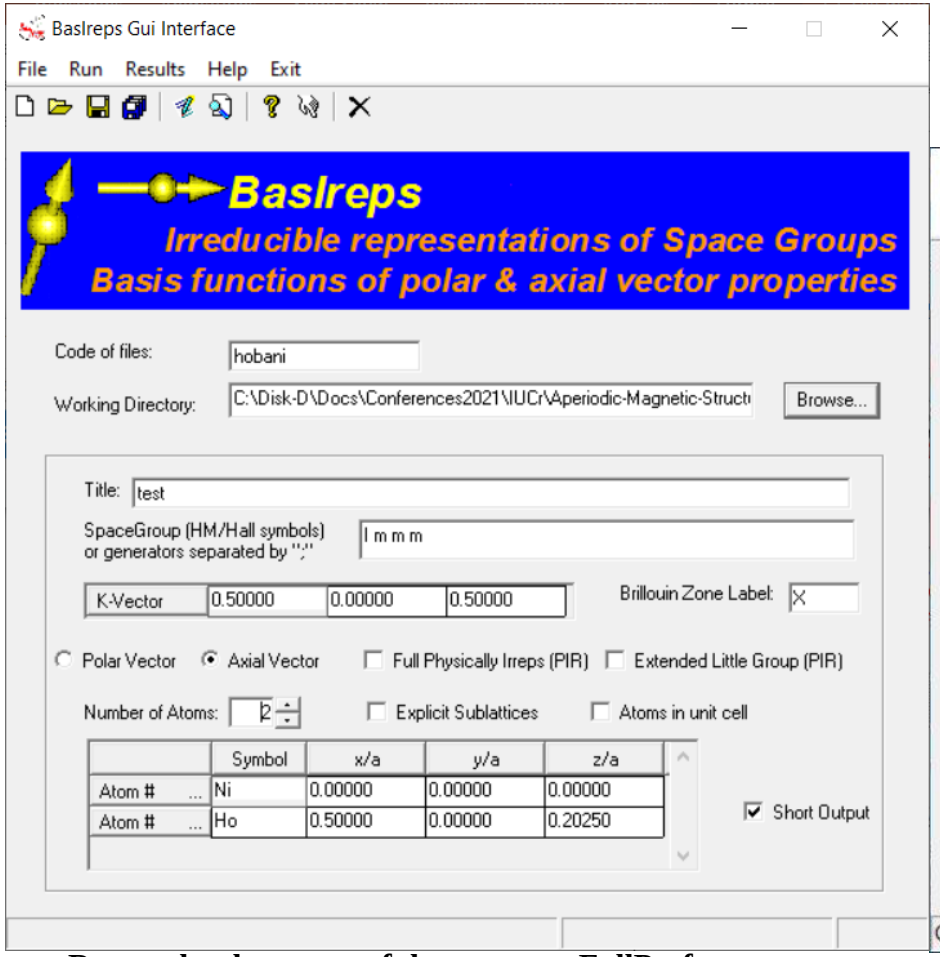


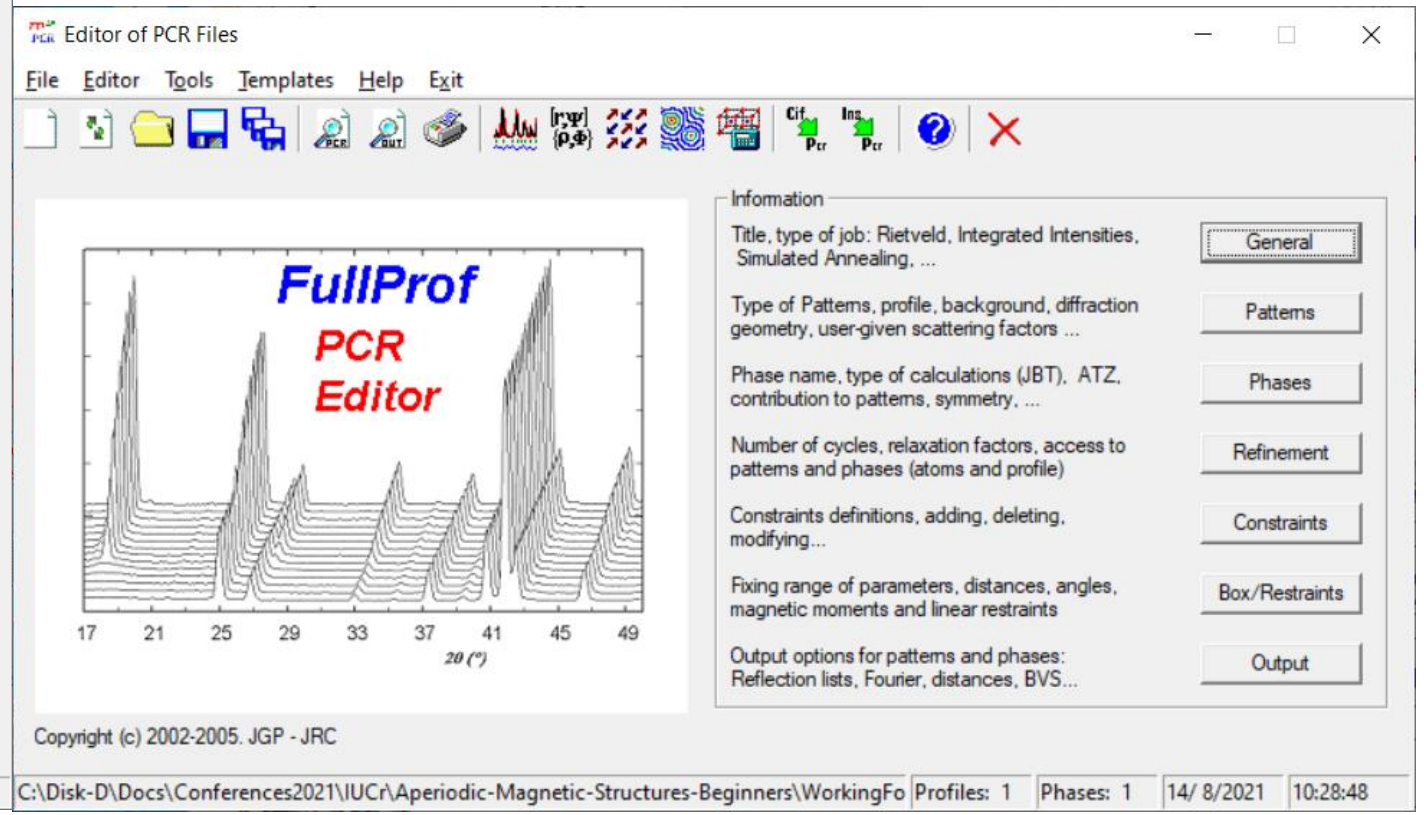
- Visualization of powder patterns
- Peak search, background generation
- Fitting capabilities
- Run FullProf from WinPLOTR
- Interoperability with other programs: BondStr, DICVOL, TREOR, etc.

A recent version of WinPLOTR that works only in Windows and it is a 32 bit application. I will not be working in the future.

The early development of FullProf

The end of the nineties to the new century





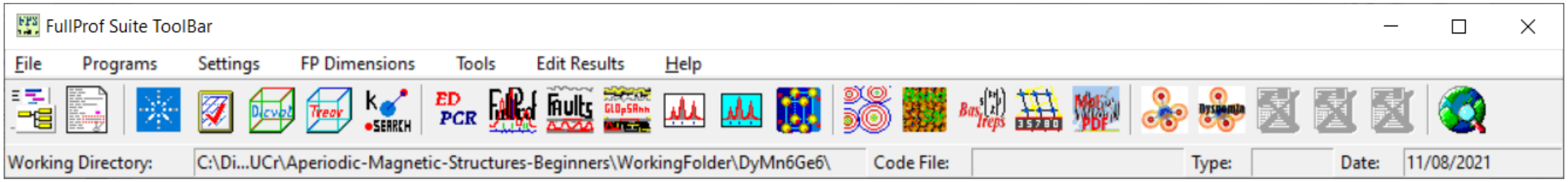
Recent developments of the program FullProf
Juan Rodríguez-Carvajal
Commission for Powder Diffraction, IUCr, Newsletter **26**, 12-19 (2001).

WinPLOTR: a Windows tool for powder diffraction patterns analysis
T. Roisnel and J. Rodríguez-Carvajal.

Materials Science Forum **378-381**, 118-123 (2001).

NEUTRONS FOR SOCIETY

The early development of FullProf
The new century: CrysFML and FullProf 2k



- Development of **FullProf Studio** (L.C. Chapon)
- Development of **GBondStr/BondStr** (J. González-Platas)
- Development of the new **WinPLOTR-2006** (O. Baltuano)
- During the first decade of the new century the **FullProf Suite** was continuing developed and largely distributed through the Internet

Crystallographic Fortran Modules Library (CrysFML): A simple toolbox for crystallographic computing programs
Juan Rodríguez-Carvajal and Javier González-Platas
Computing Commission of the International Union of Crystallography.
Compcomm Newsletter **1**, 50-58 (2003).

The Once and Everliving FORTRAN : Why Fortran still goes onward and upward while many of its "replacement" languages have already died
Juan Rodríguez-Carvajal
Computing Commission of the International Union of Crystallography.
Compcomm Newsletter **3**, 32-40 (2004).

PRESENTATION OF THE FULLPROF SUITE

FullProf (may be run in console mode using scripts for thousands of patterns)

- **A program for :**
  - **Simulation of powder diffraction patterns**
  - **Pattern decomposition⇨ integrated intensities**
  - **Structure refinement**
  - **Powder and single crystal data with multiple phases and/or domains**
- **Crystal and magnetic structures: special form factors, rigid bodies, symmetry adapted modes, incommensurate magnetic structures, restraints, microstructure effects, superspace for magnetic structures, etc.**
- **Multiple data sets: simultaneous treatment of several powder diffraction patterns (CW X-rays & neutrons, Energy dispersive X-rays, TOF neutron diffraction)**
- **Combined treatment of single crystal and powder data**
- **Crystal and magnetic Structure determination capabilities:**
  simulated annealing on integrated intensity and profile data
- **Polarized neutrons: Flipping ratio analysis**
- **Single crystal electron diffraction (kinematic only)**

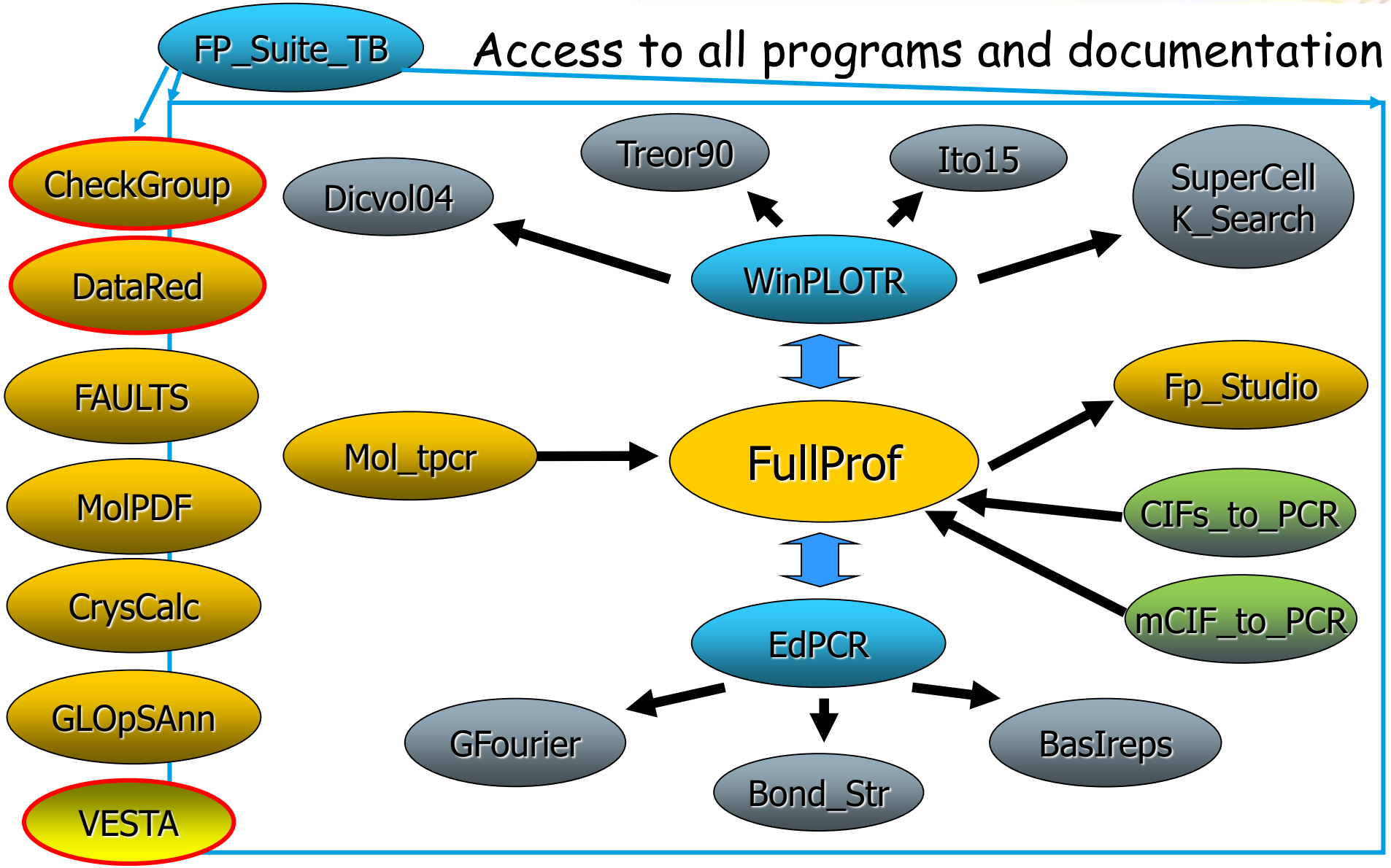
The PCR file

It is a text file containing all instructions for running **FullProf**. A good text editor is needed for using the most advanced options

The PCR file may be produced automatically for combining different patterns and phases using the utilities: **CIFs_to_PCR** or **mCIF_to_PCR**

It may be produced from the scratch by using **EdPCR**

PRESENTATION OF THE FULLPROF SUITE

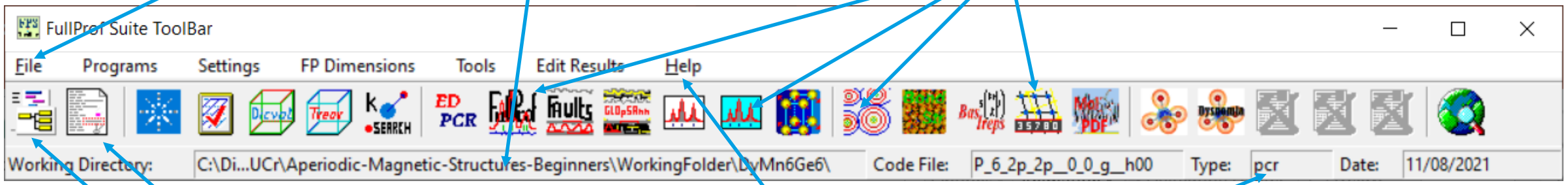


Other utilities:
MHall
TOF_fit_LM
. . .

PRESENTATION OF THE FULLPROF SUITE

File: Select working directory

Run Programs

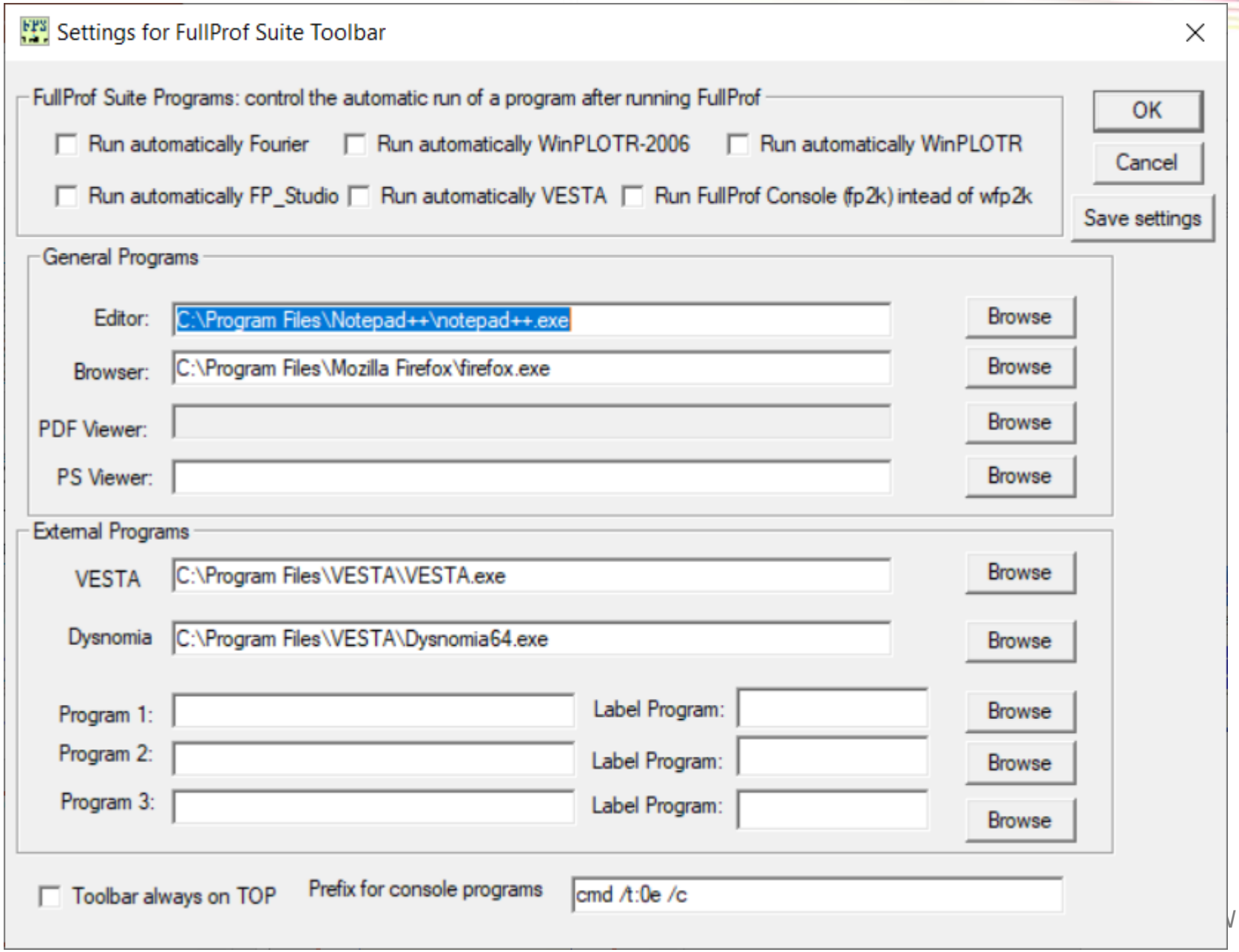


Edit current file

Load PCR or recognised files

Access to documentation

PRESENTATION OF THE FULLPROF SUITE



Select a text Editor

Select a Browser

Locate VESTA exe

Locate External programs

PRESENTATION OF THE FULLPROF SUITE

WinPLOTR

0: Visualizing multiple powder patterns (superimposed or 3D)
1: Automatic peak search for indexing
2: Saving peaks as DICVOL04, Treor90, etc
3: Running indexing programs
4: Automatic generation of PCR file for cell refinement and integrated intensity extraction (Le Bail fit)
5: Making individual peak fits
6: Exporting background files
7: Invoking other programs

EdPCR

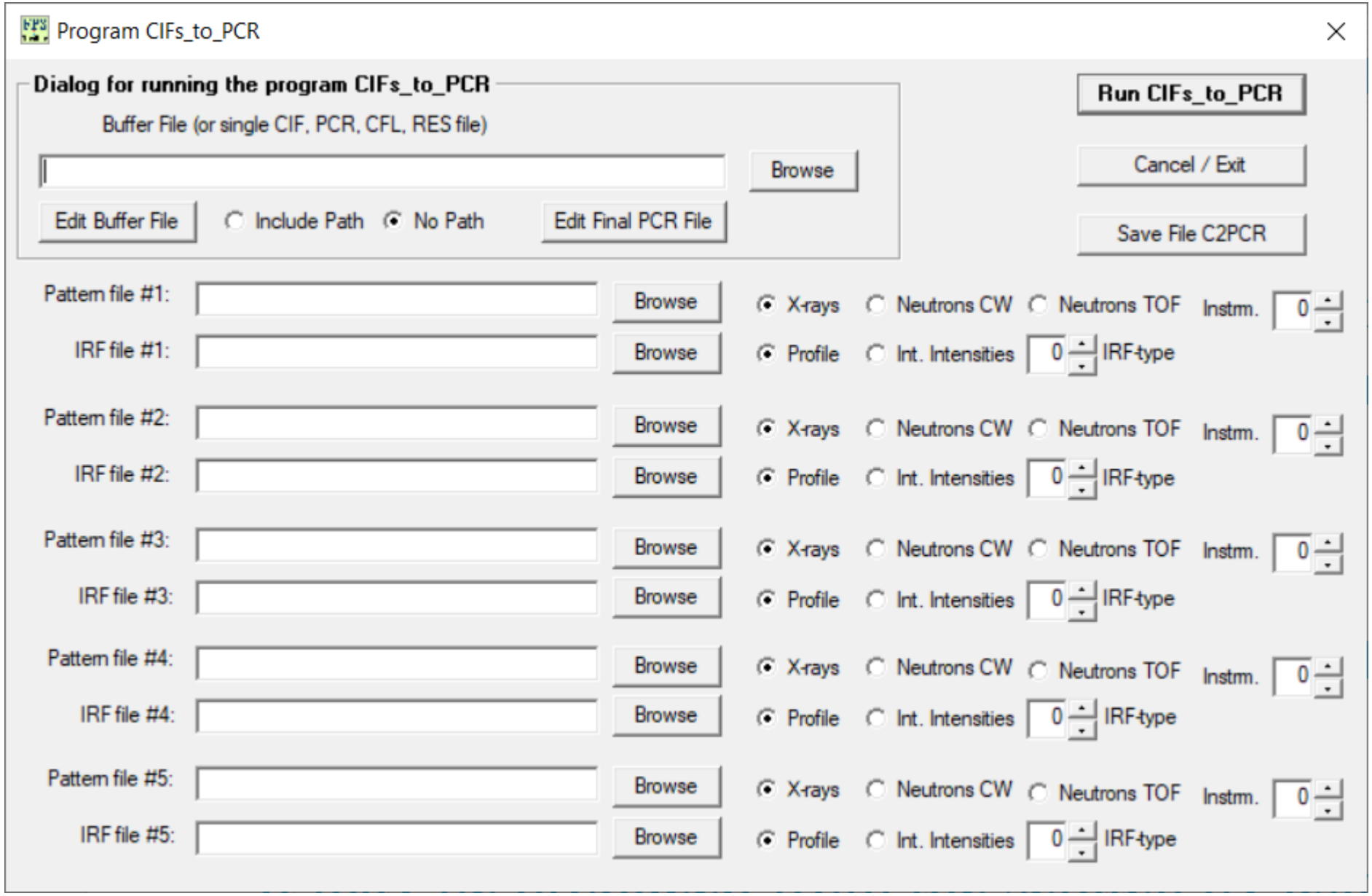
GUI for editing PCR files
Only limited number of options
Shubnikov and superspace groups are not currently available within EdPCR

PRESENTATION OF THE FULLPROF SUITE: CIFs_to_PCR

Select input files with information of the different phases: e.g. a list of CIF files

Select data files containing diffraction patterns and the corresponding features

Select the IRF file of each pattern (radio buttons)



PRESENTATION OF THE FULLPROF SUITE

FAULTS Program to refine powder diffraction patterns (X-rays and neutrons) of crystal systems with any type of coherent planar defect. Based on DIFFaX and CrysFML

MolPDF Program to refine Pair Distribution Function specialized for Molecular systems

GLOpSAnn Global optimization by simulated annealing of crystal structures using a variety of cost functions: R-factors, BVS, distances, torsion angles, etc.

PRESENTATION OF THE FULLPROF SUITE

The programs of the **FullProf Suite** are not black-box-like with a single way of doing the things.

The GUIs are mere help utilities for handling the input control files.

The learning curve for the use of the programs may be steeper than for other programs, however understanding the content of the input files and making manual changes is much faster, once the user is becoming expert, than using the GUIs.

Future of the FullProf Suite

CrysFML → CrysFML20xx

Extension of CrysFML

Algorithm for the identification of crystallographic and magnetic space groups in any arbitrary setting.

CrysFML2008

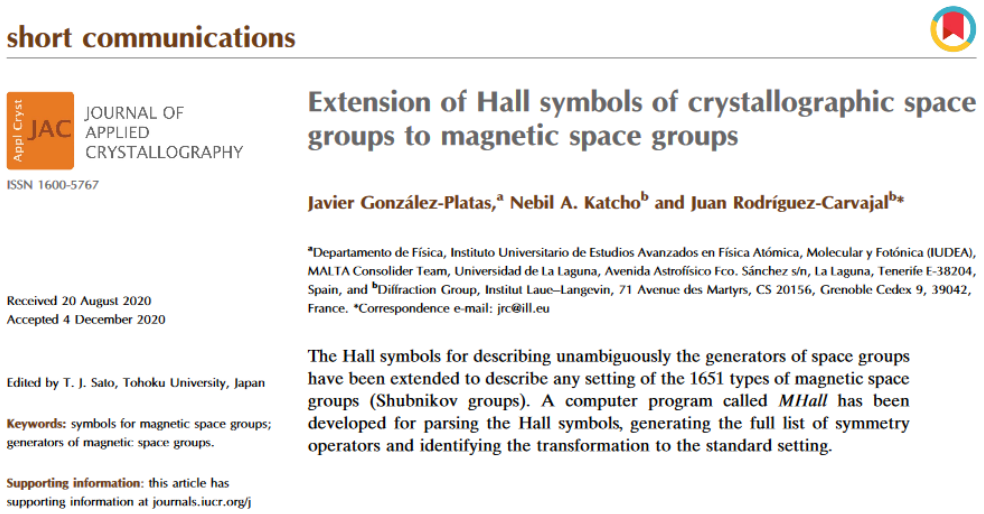
CrysFML written using the latest Fortran standard.

The modules contain now submodules and object-oriented programming is used for the parts containing a profuse use of types.

Almost finished. Core of the new **FullProf 2025**

Example of development using CrysFML08:

Program **MHall**



short communications

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Keywords: symbols for magnetic space groups; generators of magnetic space groups.

Supporting information: this article has supporting information at journals.iucr.org/j

Extension of Hall symbols of crystallographic space groups to magnetic space groups

Javier González-Platas,[a] Nebil A. Katcho[b] and Juan Rodríguez-Carvajal[b]*

[a]Departamento de Física, Instituto Universitario de Estudios Avanzados en Física Atómica, Molecular y Fotónica (IUDEA), MALTA Consolider Team, Universidad de La Laguna, Avenida Astrofísico Fco. Sánchez s/n, La Laguna, Tenerife E-38204, Spain, and [b]Diffraction Group, Institut Laue–Langevin, 71 Avenue des Martyrs, CS 20156, Grenoble Cedex 9, 39042, France. *Correspondence e-mail: jrc@ill.eu

The Hall symbols for describing unambiguously the generators of space groups have been extended to describe any setting of the 1651 types of magnetic space groups (Shubnikov groups). A computer program called *MHall* has been developed for parsing the Hall symbols, generating the full list of symmetry operators and identifying the transformation to the standard setting.

NEUTRONS FOR SOCIETY

FULLPROF UPGRADING

New web site for the FullProf Suite

Windows

FullProf Suite	FullProf Suite	New FullProf Suite	FullProfApp
Fortran compiler: ifort	Fortran compiler: ifx	Fortran compiler: ifort	Fortran compiler: ifort
GUI: Winteracter	GUI: Winteracter	GUI: PySide6 + Winteracter	GUI: PyQt
Date: 24 October 2025	Date: 24 October 2025	Date: 24 October 2025	Date: 9 April 2025
Download	Download	Download	Download

Linux

FullProf Suite	FullProf Suite	New FullProf Suite	FullProfApp
Fortran compiler: ifort	Fortran compiler: ifx	Fortran compiler: ifort	Fortran compiler: ifort
GUI: Winteracter	GUI: Winteracter	GUI: PySide6 + Winteracter	GUI: PyQt
Date: 24 October 2025	Date: 24 October 2025	Date: 24 October 2025	Date: 9 April 2025
Download	Download	Download	Download

macOS

FullProf Suite - Linux like	FullProf Suite - dmg
Fortran compiler: ifort	Fortran compiler: ifort
GUI: Winteracter	GUI: Winteracter
Date: 27 February 2025	Date: 25 February 2025
Download	Download

Previous FPSuite versions

FullProf Suite
Crystallographic tools for Rietveld, profile matching and integrated intensity refinements

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**.

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

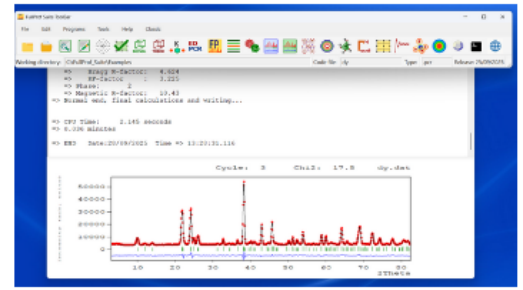
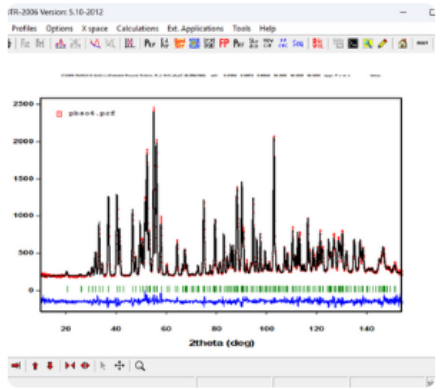
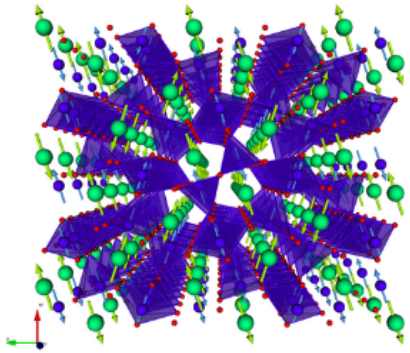


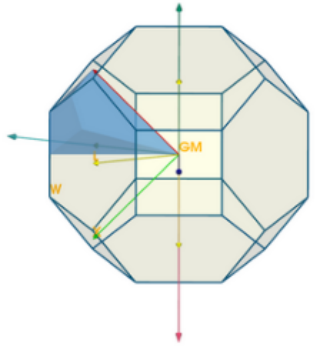
Image gallery



Rietveld analysis



Structure visualization

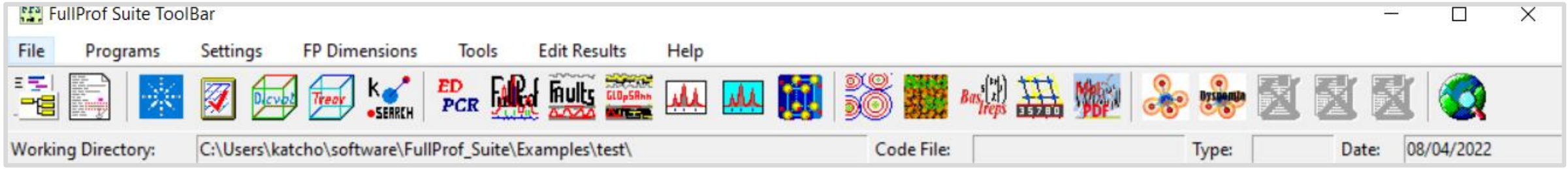


Symmetry analysis

FullProf upgrading

New GUI for coexistence of **classic FullProf Suite** and the new **FullProf Suite 202X**

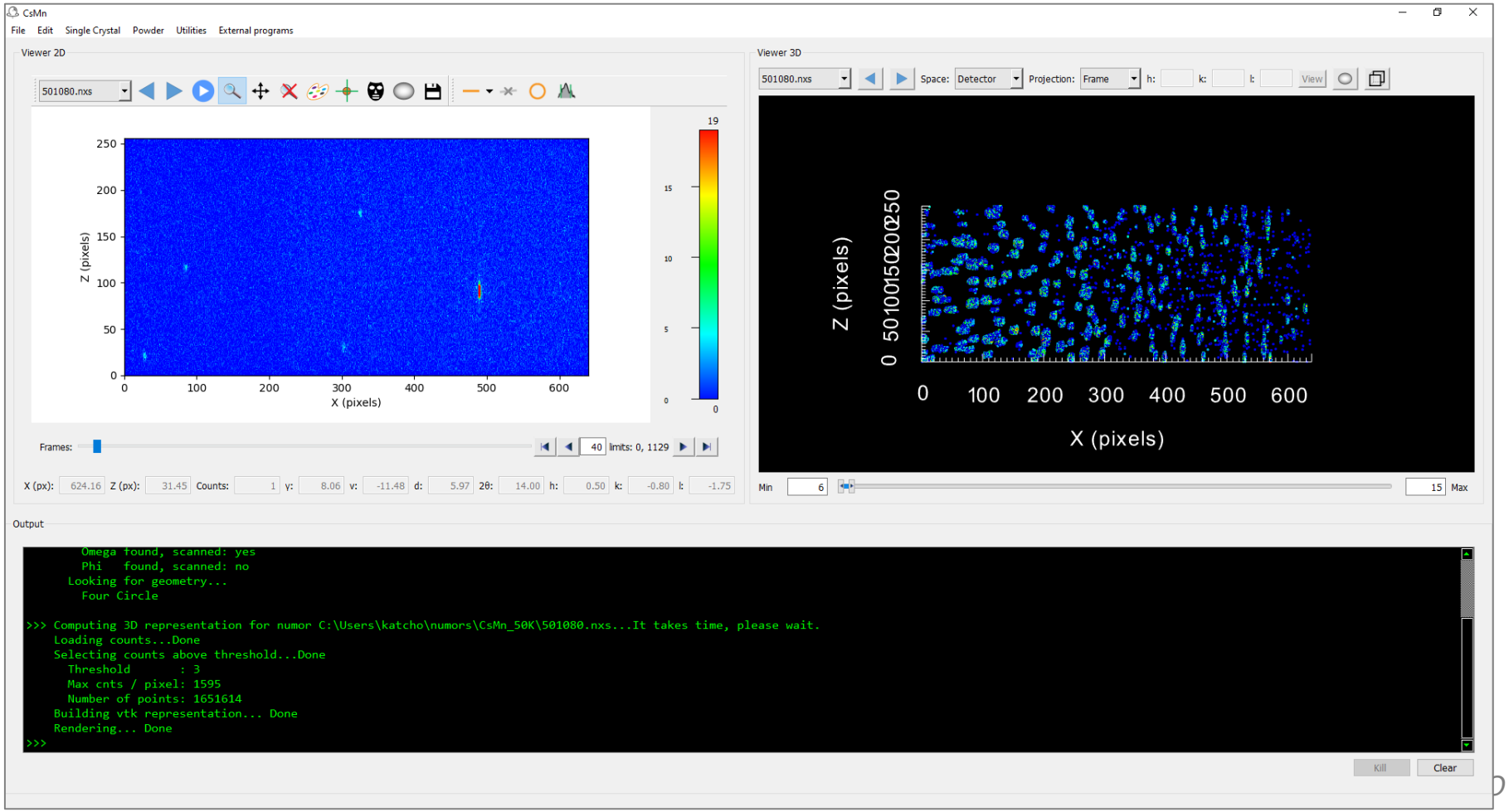
Classic



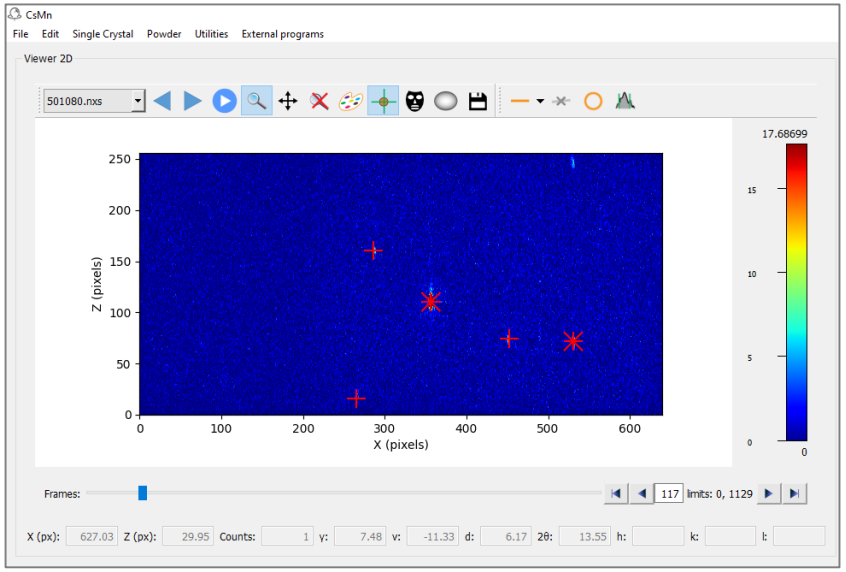
FullProf Suite 202X

The future GUI for FullProf Suite will be similar to that of the Int3D GUI

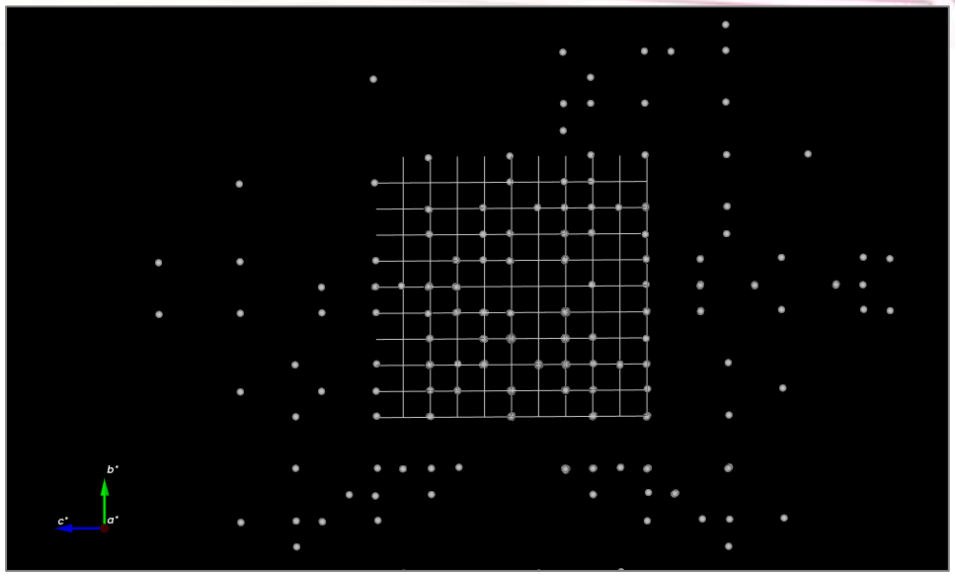
The GUI consists of a **menu bar**, a **2D viewer** (left), a **3D viewer** (right) and a **terminal** (bottom)



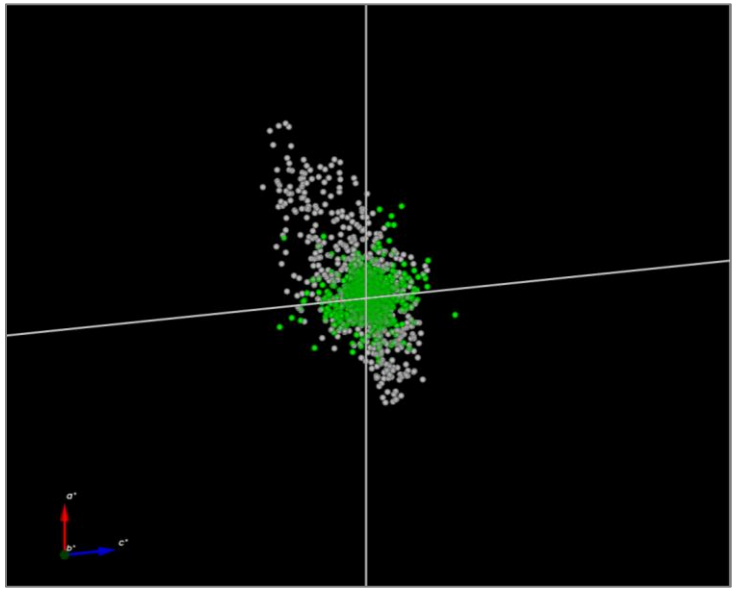
Peak search



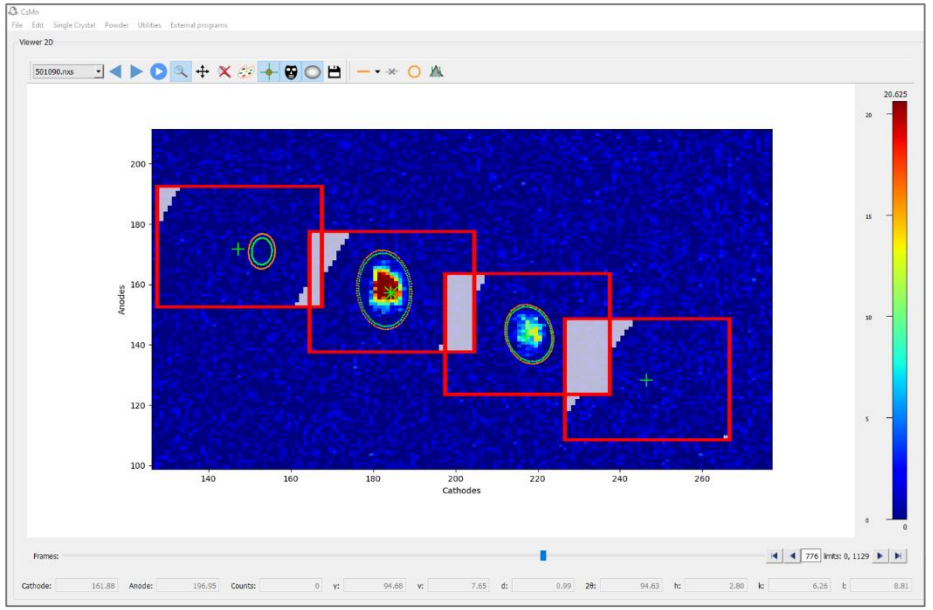
UB Matrix



Refinement



Integration

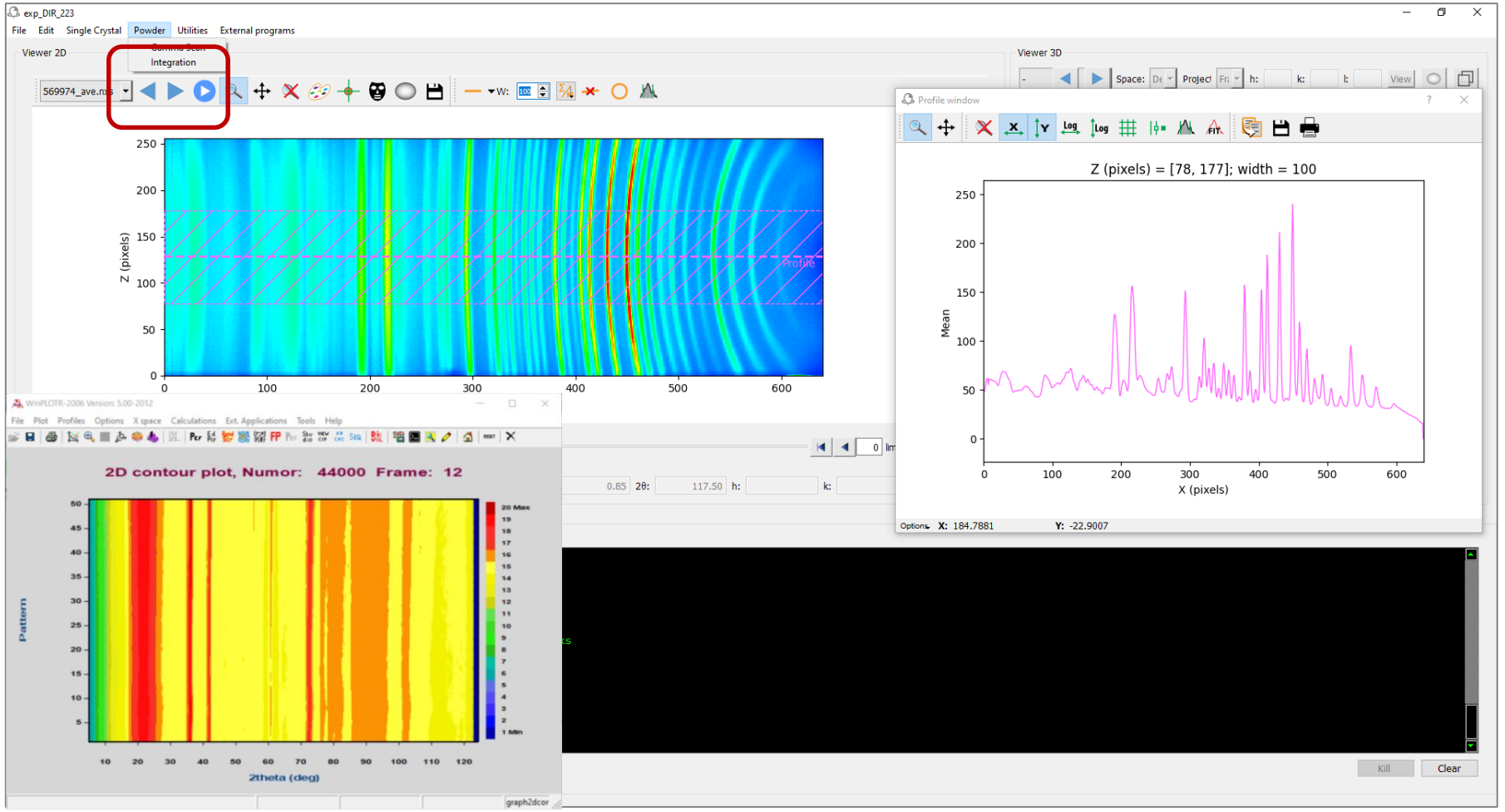


E

NEUTRONS FOR SOCIETY

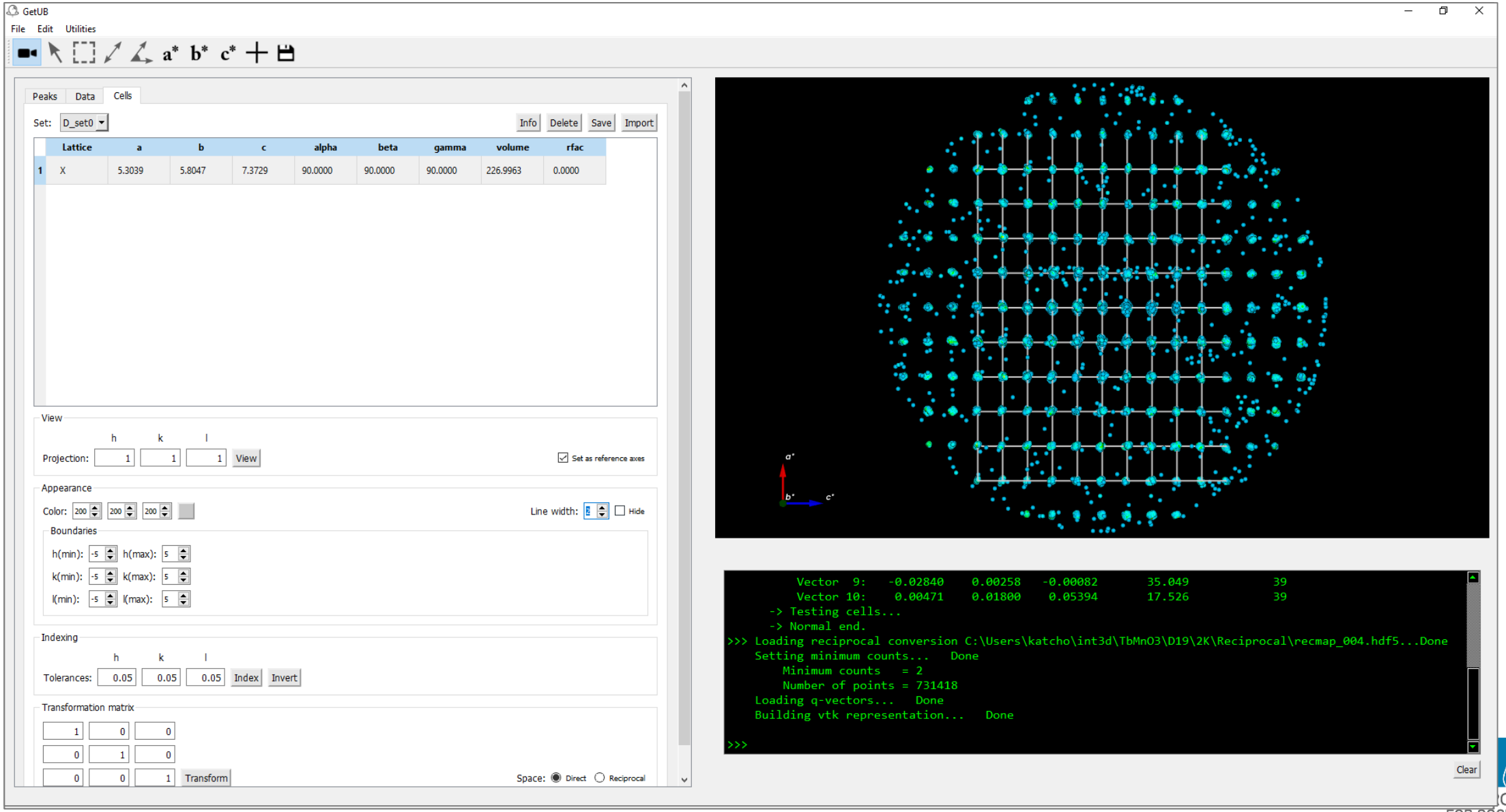
Other Capabilities of Int3D

Data reduction of powder data (D19)



Other Capabilities of Int3D

Raw data in reciprocal space

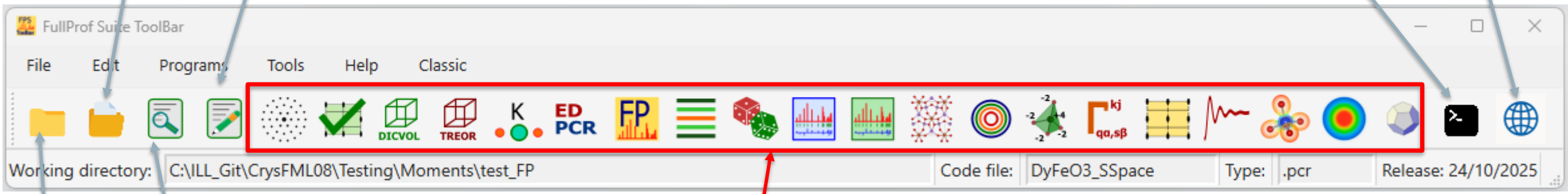


Load a file in the Toolbar

Show result files for editing

Web page

Terminal



Edit the loaded file

Look for Working Directory

Programs acting on files: Codefile.Type
From left to right:
gDataRed, CheckGroup, DICVOL, TREOR90, k_Search, EdPCR, FullProf, Faults, GLOpSAnn, WinPLOTR, WinPLOTR-2006, FullProf_Studio, gFourier, BondStr, BasIreps, Crystallographic Calculator, MolPDF, VESTA, Dysnomia, Brillouin

Brillouin

Appearance | k-vectors

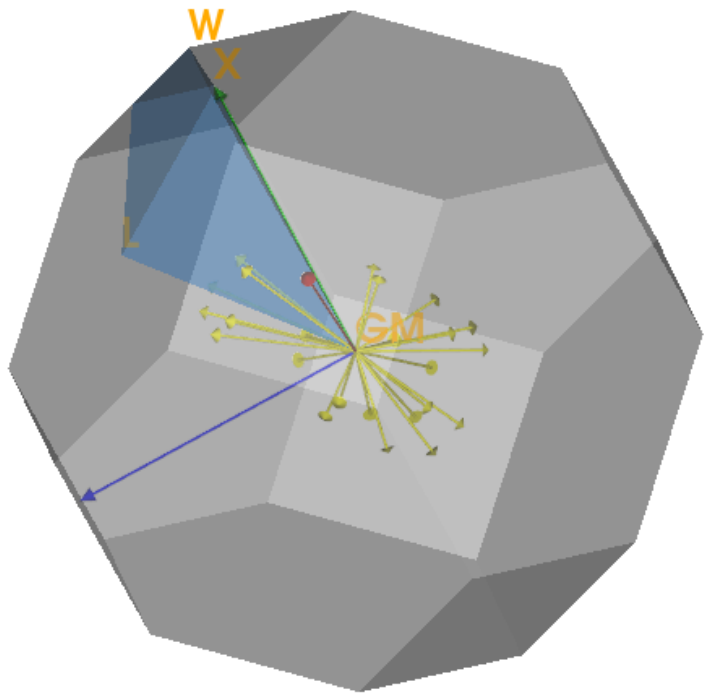
	a	b	c	α (°)	β (°)	γ (°)	
Conventional cell:	5.0000	5.0000	5.0000	90.0000	90.0000	90.0000	Default

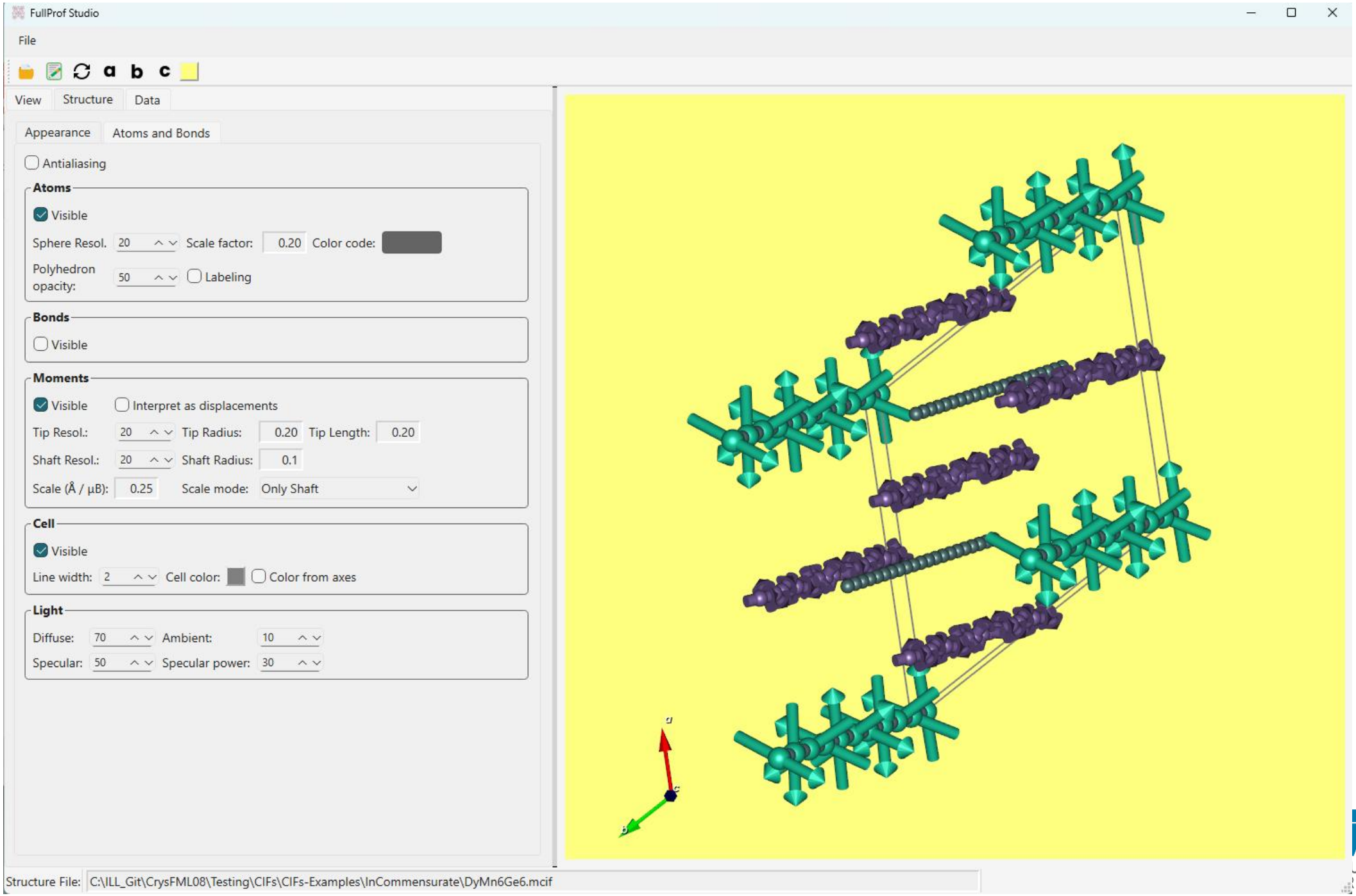
Space group: 219: F -4 3 c Draw

Label	Axes	x	y	z
GM	Conventional	0.0000	0.0000	0.0000
	Primitive	0.0000	0.0000	0.0000
L		0.5000	0.5000	0.5000
		0.5000	0.5000	0.5000
W		0.5000	1.0000	0.0000
		0.5000	0.2500	0.7500
X		0.0000	1.0000	0.0000
		0.5000	0.0000	0.5000

	kx	ky	kz			
k-vector (CDML):	0.25	0.5	0.123	Conventional	Reduce to 1BZ	Add -k	Compute star

Arm	Axes	x	y	z
1	Conventional	0.3115	0.1865	0.3750
	Primitive	0.3115	0.1865	0.3750
2		-0.3115	0.0635	-0.1250
		-0.3115	0.0635	-0.1250
3		0.1885	-0.1865	0.1250
		0.1885	-0.1865	0.1250
4		-0.1885	-0.0635	-0.3750
		-0.1885	-0.0635	-0.3750
5		0.3750	0.3115	0.1865
		0.3750	0.3115	0.1865
6		0.1865	0.3750	0.3115




FullProf Studio
File
a
b
c
View
Structure
Data
Appearance
Atoms and Bonds
Antialiasing
Atoms
Visible
Sphere Resol. 20
Scale factor: 0.20
Color code:
Polyhedron opacity: 50
Labeling
Bonds
Visible
Moments
Visible
Interpret as displacements
Tip Resol.: 20
Tip Radius: 0.20
Tip Length: 0.20
Shaft Resol.: 20
Shaft Radius: 0.1
Scale (Å / μB): 0.25
Scale mode: Only Shaft
Cell
Visible
Line width: 2
Cell color:
Color from axes
Light
Diffuse: 70
Ambient: 10
Specular: 50
Specular power: 30
Structure File: C:\ILL_Git\CrysFML08\Testing\CIFs\CIFs-Examples\InCommensurate\DyMn6Ge6.mcif

Live presentation of the FullProf Suite

Toolbar
WinPLOTR-2006
Etc …


science campus
THANK YOU!