First FullProf School 2025:

Diffraction data analysis of energy materials

Introduction to the FullProf Suite

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NEUTRONS FOR SOCIETY

Outline

1. History of the FullProf Suite Development.
2. Programs of the FullProf Suite.
3. Live Presentation of the FullProf Suite

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2. Programs of the FullProf Suite.
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Ancestors of FullProf: From 1967 to 1986

PREF & PROFLS
Hugo Rietveld -1967,1969 Petten

Language: Algol, Fortran

PREF & PROFLS
Alan Hewat - 1973 Harwell

Uij added, Fortran

PREF & PROFLS
Von Dreele - 1973 Oxford

Bigger structures & X-rays (didn't work!)

DBW2.9 -1981-1994
Young & Wiles - 1973 Oxford

X-ray profiles, Young & Wiles rewrite a single program, Sakthivel (DBWS)

TOFPREF & TOFLS
Von Dreele - 1982 RAL

Neutron TOF, IPNS adopted by Rotella for VAX

GSAS
Larson & Von Dreele - 1982 -1986

LPHM- Hunter % Howard -Australia
Phillips – Instrument package
Might be other descendants from DBW/DBWS

FullProf – J. Rodriguez-Carvajal –France

Hugo Rietveld family of programs

From B Von Dreele slide

THE EARLY DEVELOPMENT OF FULLPROF: 1988 - 1992

Reorganization of the Fortran 77 code of DBW (include files, more modular subroutines)

Anisotropic broadening due to strains and size effects

Introduction of **magnetic structures** and the formalism of propagation vectors.

Refinement without structural model as replacement of the Pawley program (**Le Bail fit**).

History of FullProf: From 1988 to 1992 @ILL

Still @ILL … but moving to the LLB

The first public version of FullProf was presented in a Satellite of XV IUCr congress in Bordeaux on powder diffraction (1990), in which Le Bail fits and conventional treatment of commensurate magnetic structures were implemented.

J. Rodriguez-Carvajal, "FullProf: A Program for Rietveld Refinement and Pattern Matching Analysis," Abstract of the Satellite Meeting on Powder Diffraction of the XV Congress of the IUCr, Toulouse, France, 1990, p. 127

Later I implemented 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 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): Recent advances in magnetic structure determination by neutron powder diffraction**

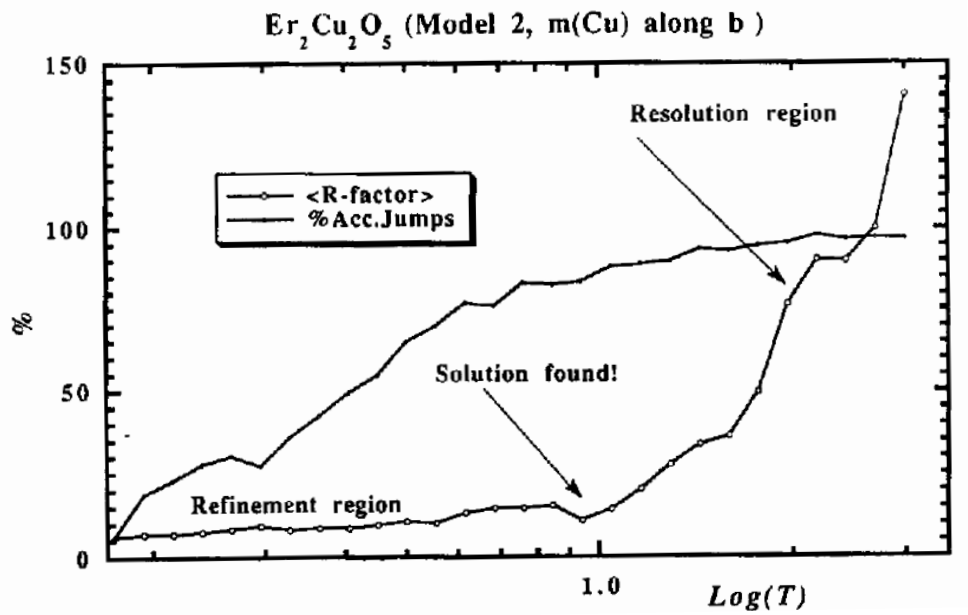
The reference paper of FullProf

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

First description of some features of the program **FullProf**

Description of the program **MagSan** for determining commensurate magnetic structures using Simulated Annealing (later included in **FullProf** for general structures)

begin
  Initialize (set to zero useful quantities, do preliminary calculations)
  $\tau = 1$
  do
    do
      Perturb the system:
      $\Omega_{old} \rightarrow \Omega_{new}$, $\Delta = E(\Omega_{new}) - E(\Omega_{old})$
      if $\Delta \leq 0$ then accept, else
        if $\exp(-\Delta/T_\tau) >$ random[0,1] then accept
      if accept then **Update** (replace Ω_{old} by Ω_{new})
    until **equilibrium is approached closely enough** (Ncyc)
    $T_{\tau+1} = f(T_\tau)$ (decrease temperature, usually $T_{\tau+1} = qT_\tau$, $q \simeq 0.9$)
    $\tau = \tau + 1$
  until **stop criterion is true** (maximum τ, convergence, low % accepted. . .)
end



SOURCE

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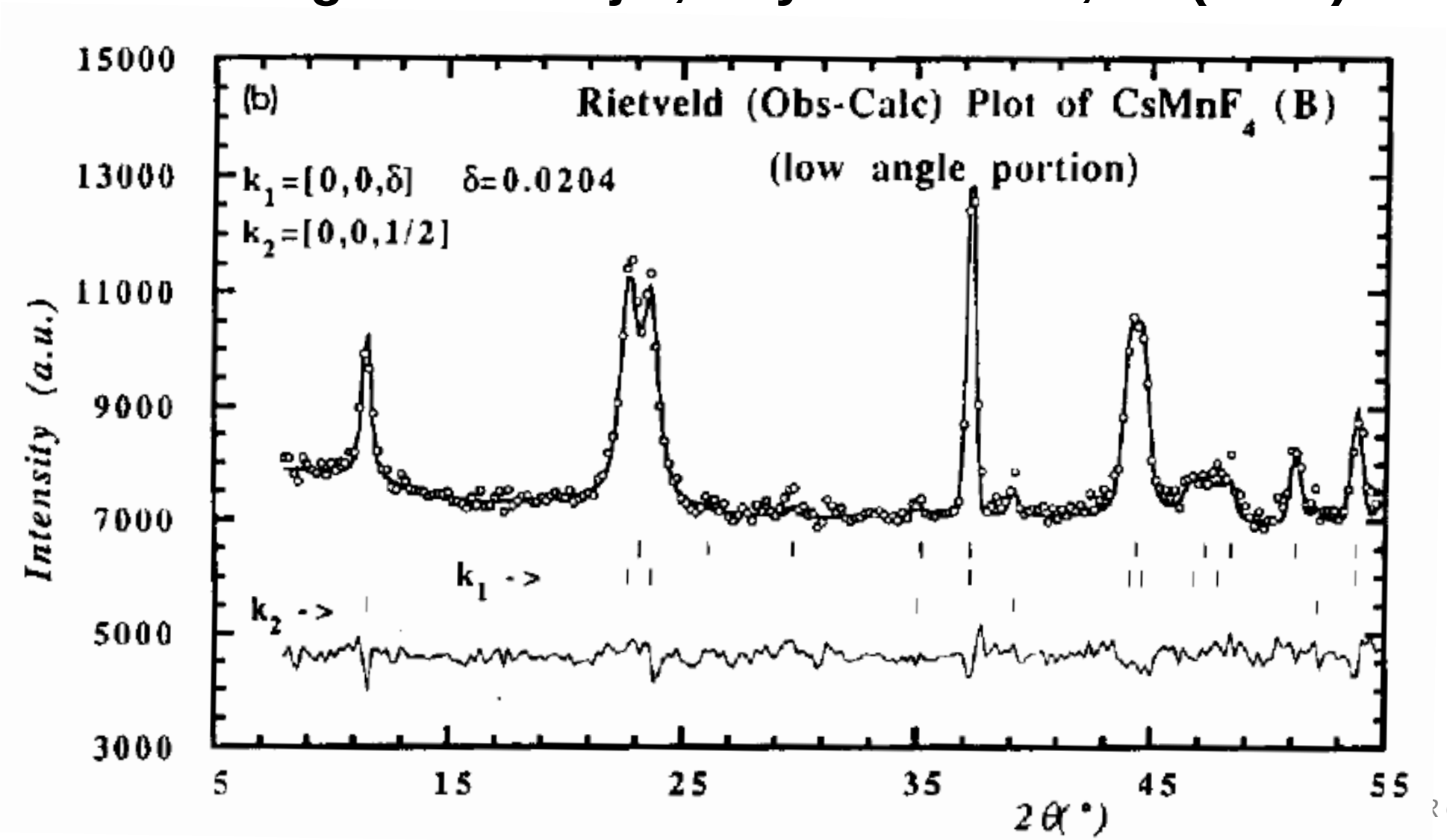
The reference paper of FullProf

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



The early development of FullProf
The middle of the nineties

Rigid bodies, special form factors … (1992 … 1995)

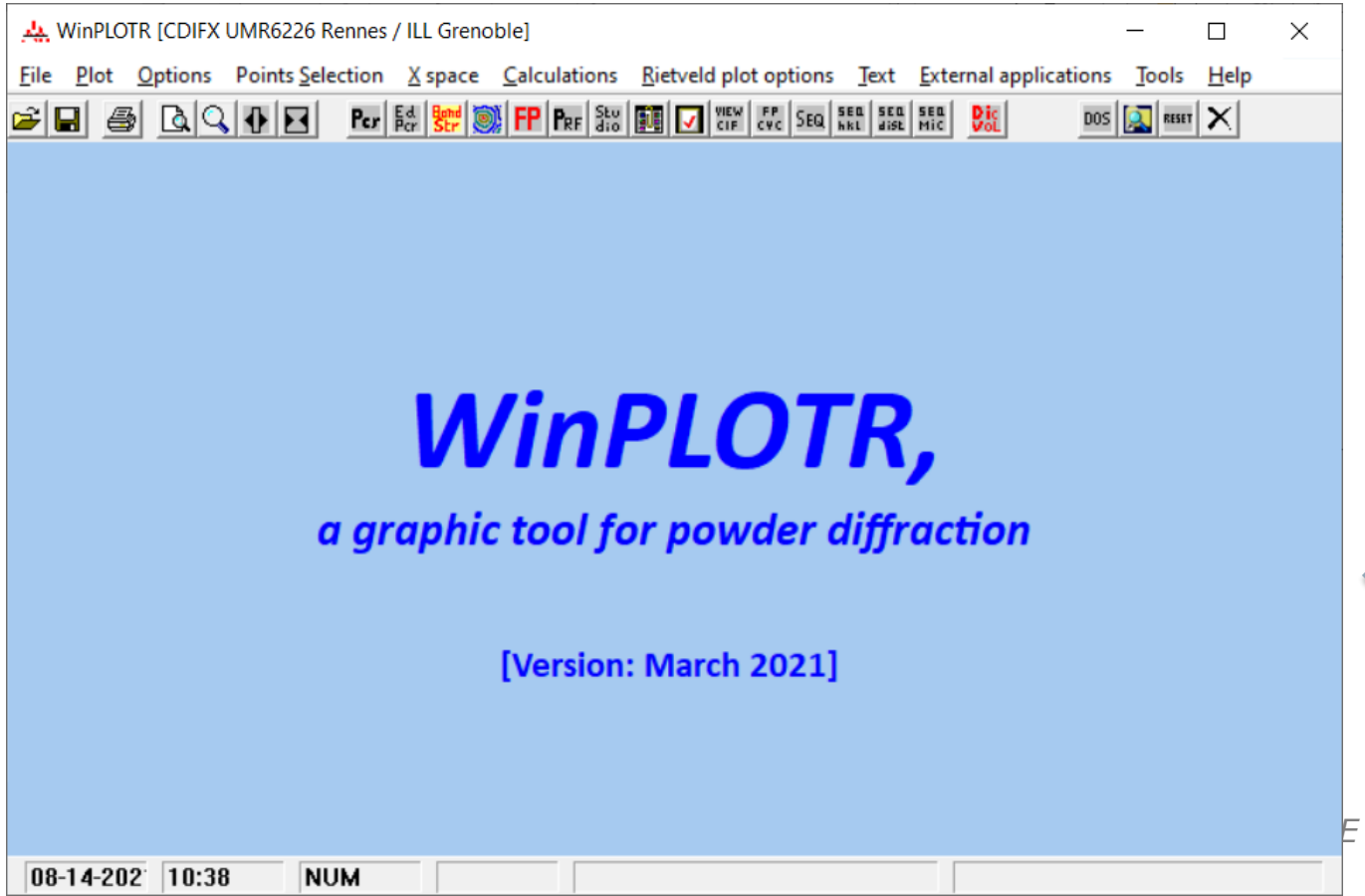
Rewriting the code (C++ or Fortran 90?), 1995-1996 ... Finally a subset (ELF) of Fortran 90 for FullProf.

Suppression of old code, commons, creation of modules, starting the development of CrysFML (subset of Fortran 90: F), time of flight neutron diffraction, multiple patterns, single crystal refinements.

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

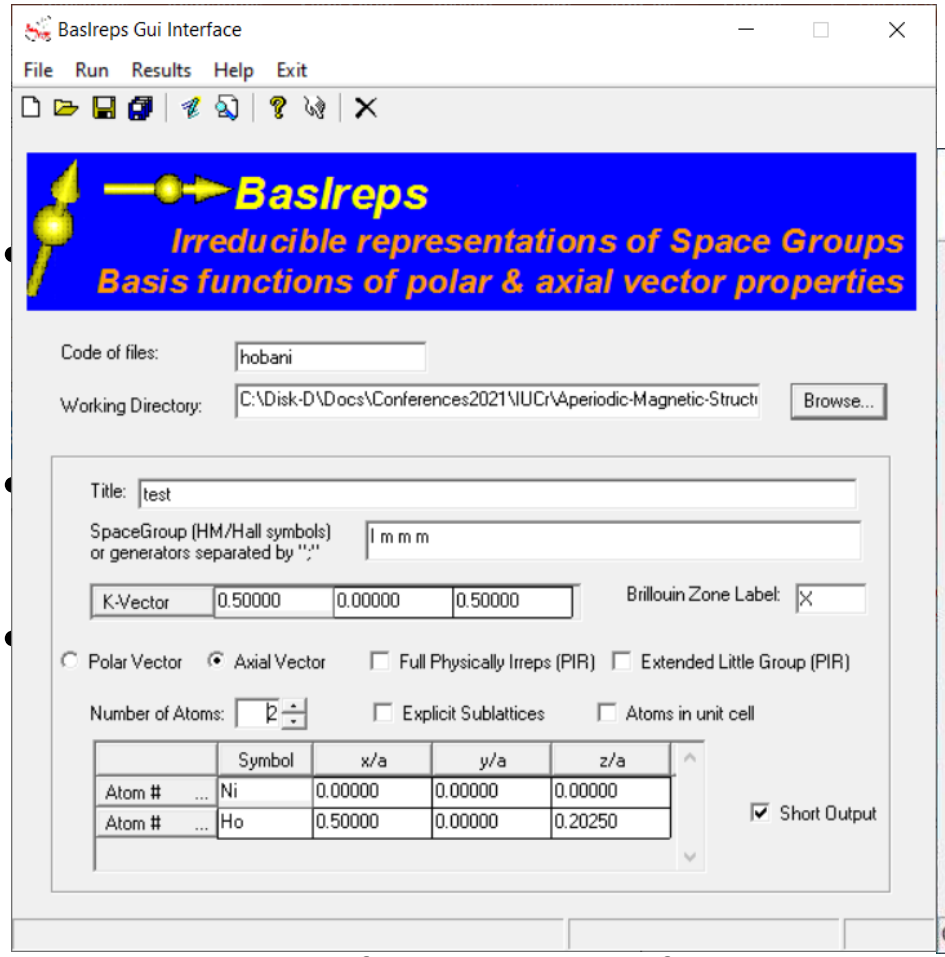


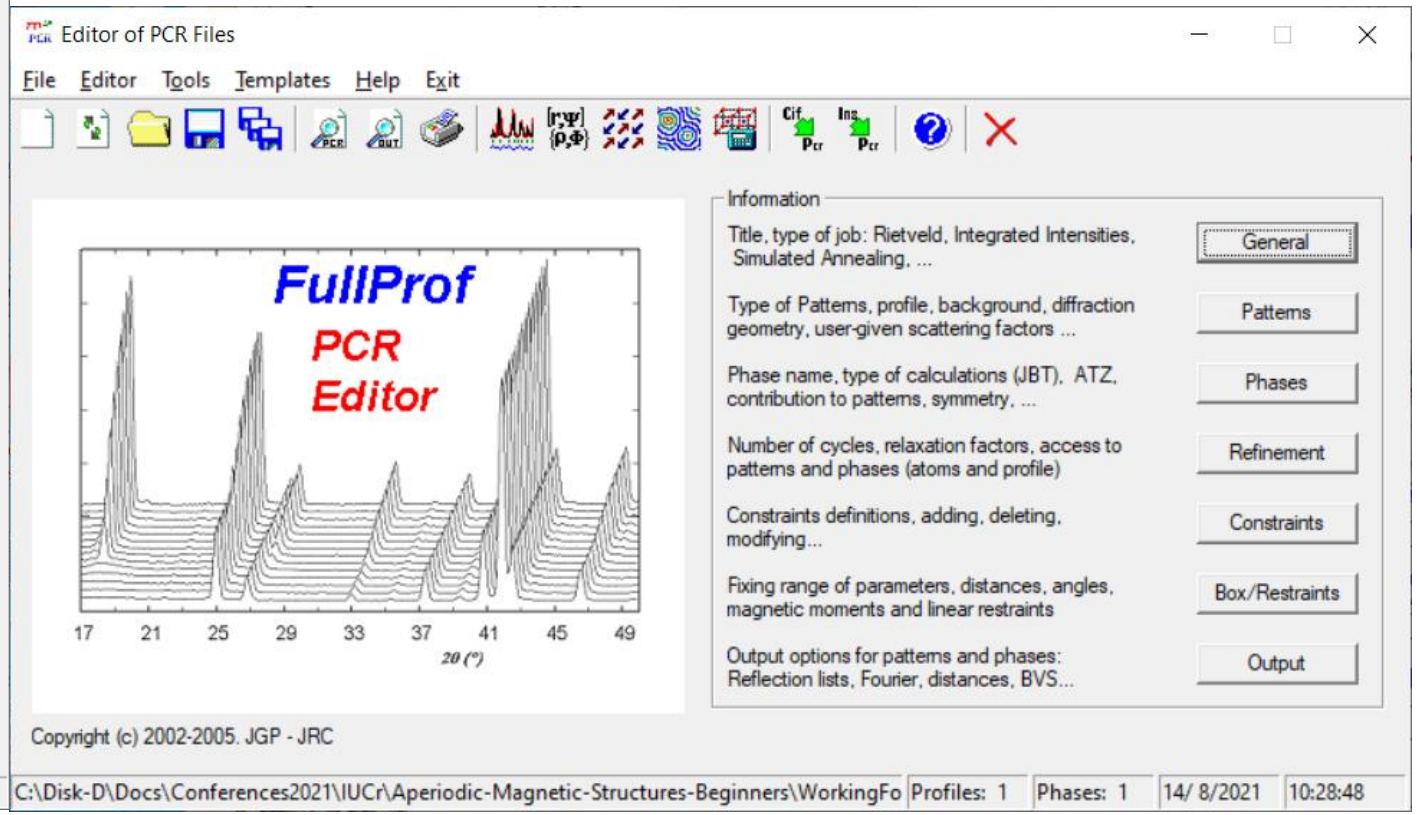
- Visualization of powder patterns
- Peak search, background generation
- Fitting capabilities
- Run FullProf from WinPLOTR
- Interoperability with other programs: BondStr, DICVOL, TREOR, etc.

A recent version of WinPLOTR that works only in Windows and it is a 32 bit application. It 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).

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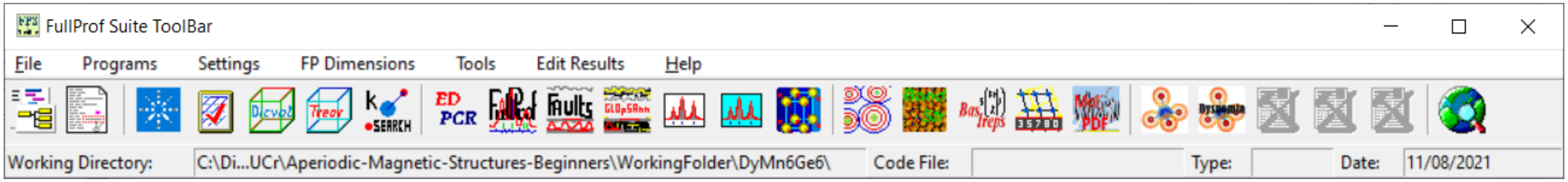
The early development of FullProf
The new century: CrysFML and FullProf 2k



- Development of **FullProf Studio** (L.C. Chapon)
- Development of **GBondStr/BondStr** (J. González-Platas)
- Development of the new **WinPLOTR-2006** (J. González-Platas, O. Baltuano)
- During the first decade of the new century the **FullProf Suite** was continuing to be 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).

Outline

1. History of the FullProf Suite Development.

2. **Programs of the FullProf Suite.**

3. Live Presentation of the FullProf Suite

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**
- **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)**

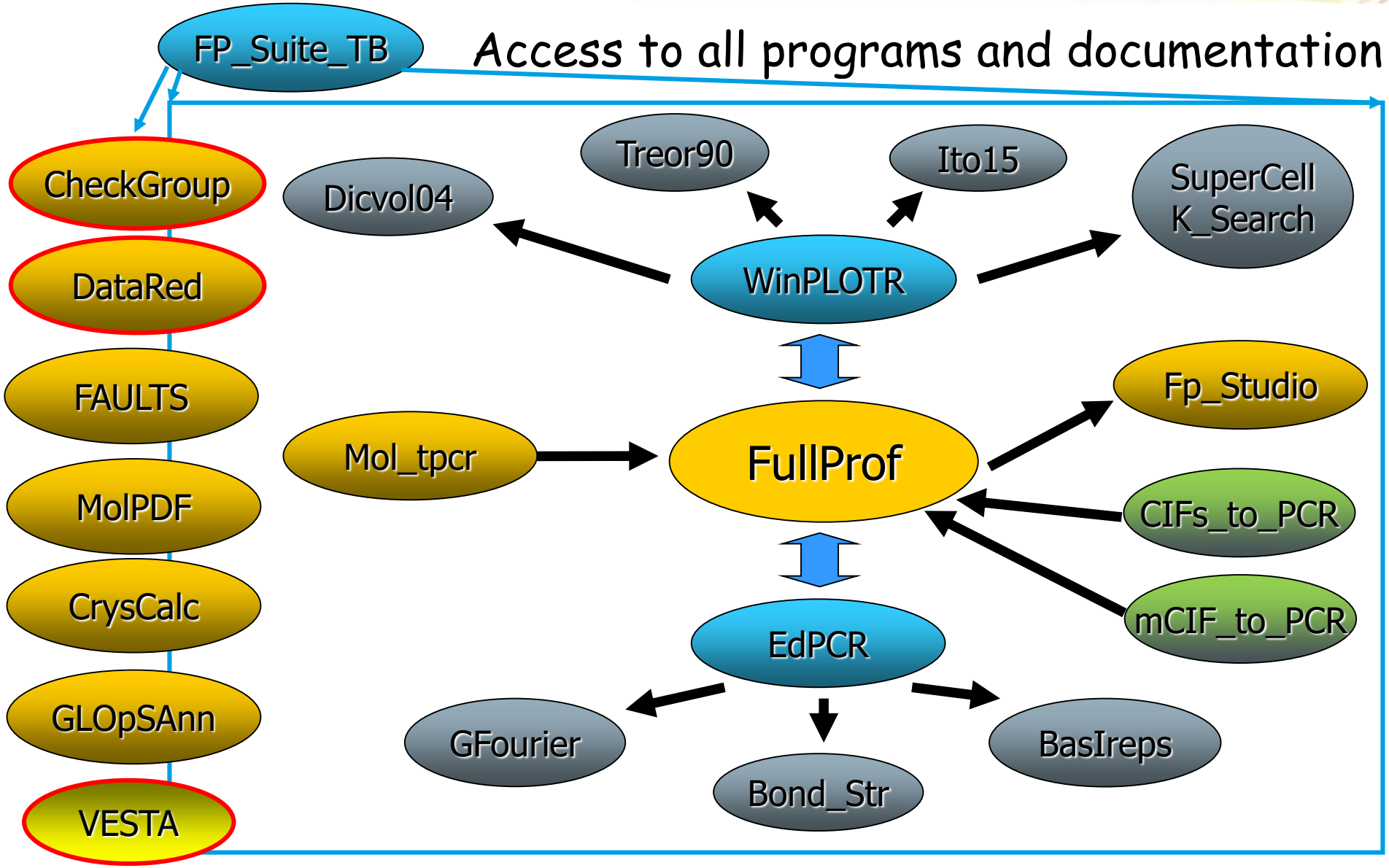
The PCR file

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**

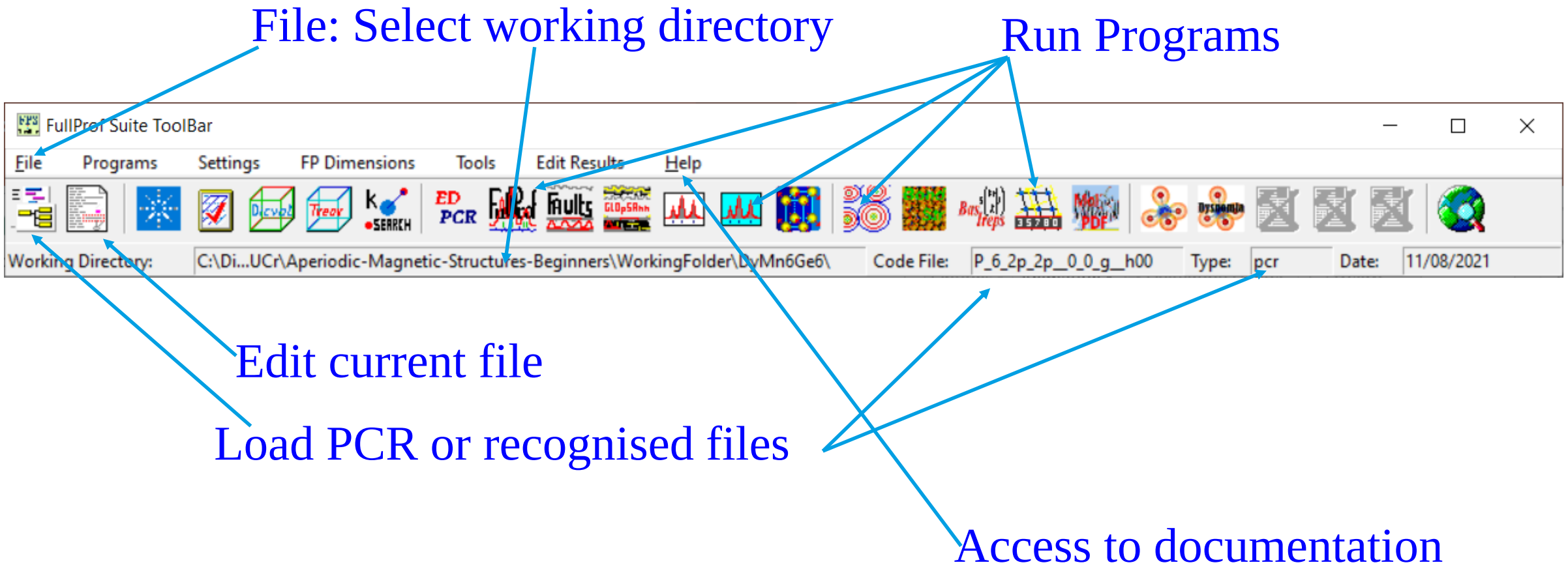
It may be produced from the scratch by using **EdPCR**

PRESENTATION OF THE FULLPROF SUITE

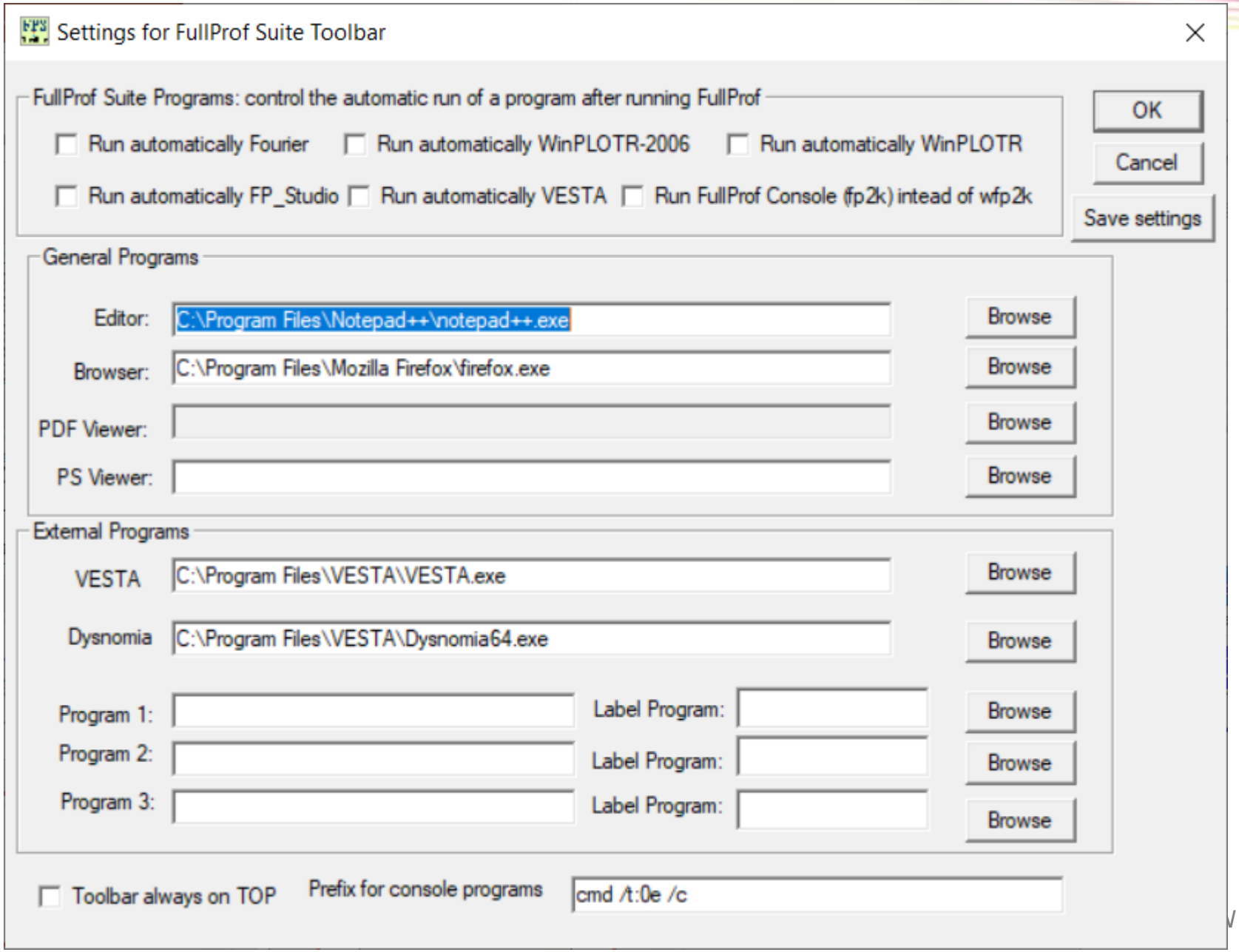


Other utilities:
MHall
TOF_fit_LM
. . .

PRESENTATION OF THE FULLPROF SUITE



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

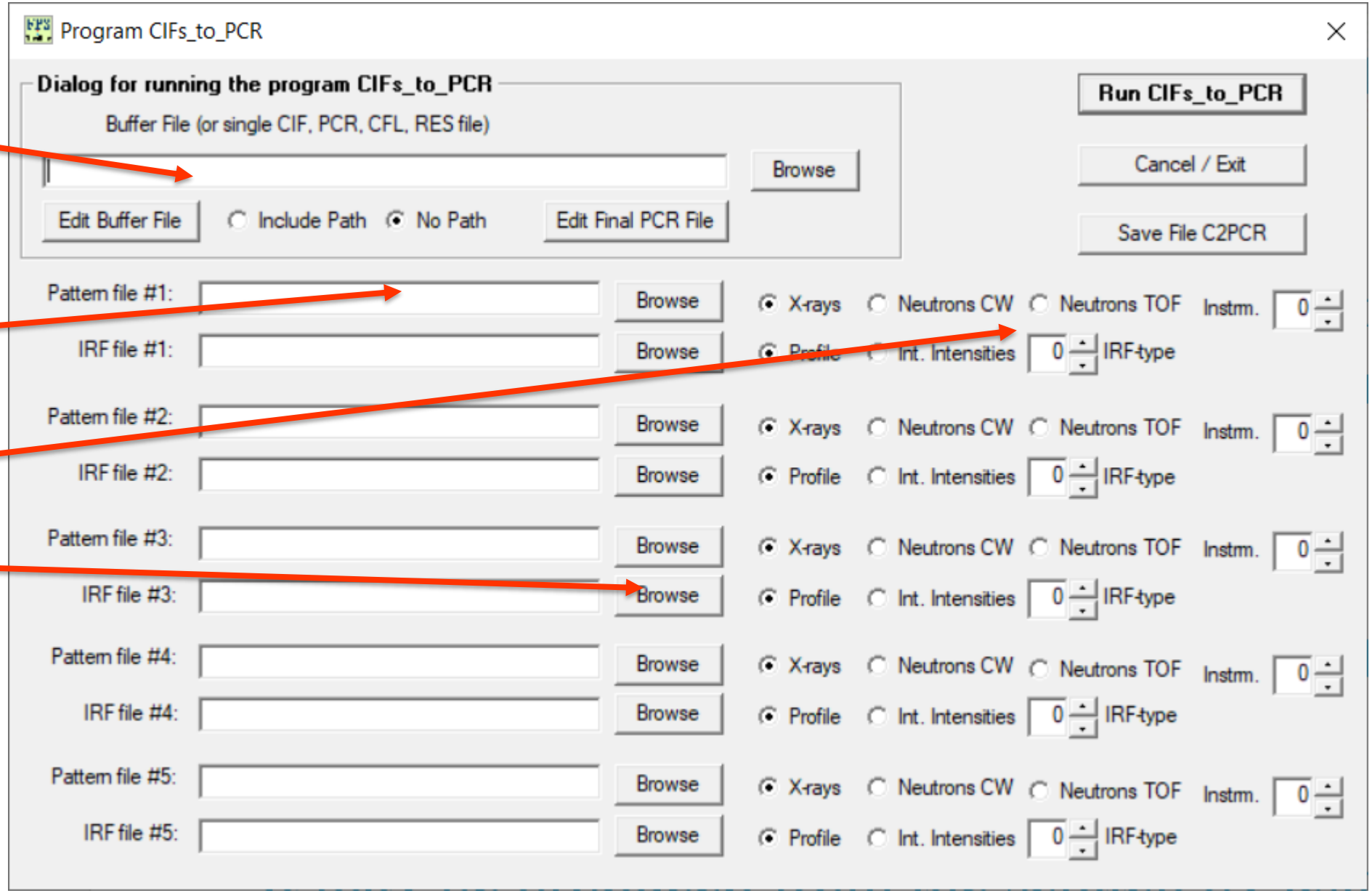
GUI for editing PCR files
Only limited number of options
Shubnikov and superspace groups are not currently available within EdPCR

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



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.

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