Past and Future of the FullProf Suite. Current Options to define the magnetic structure models in FullProf

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Outline

1: Short descriptions of magnetic structures

2: Magnetic structure factors

3: different options existing in FullProf

4: Past and Future of the FullProf Suite

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1: Short descriptions of magnetic structures

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THE MOST ELEMENTARY WAY OF DESCRIBING A COMMENSURATE MAGNETIC STRUCTURE

Ignoring symmetry (except the translation symmetry), a list of all the atoms within the unit cell, with their fractional coordinates, thermal displacement parameters and occupation probabilities, as well as the attached magnetic moments describes completely the crystal and magnetic structure. This is a description in *P*1

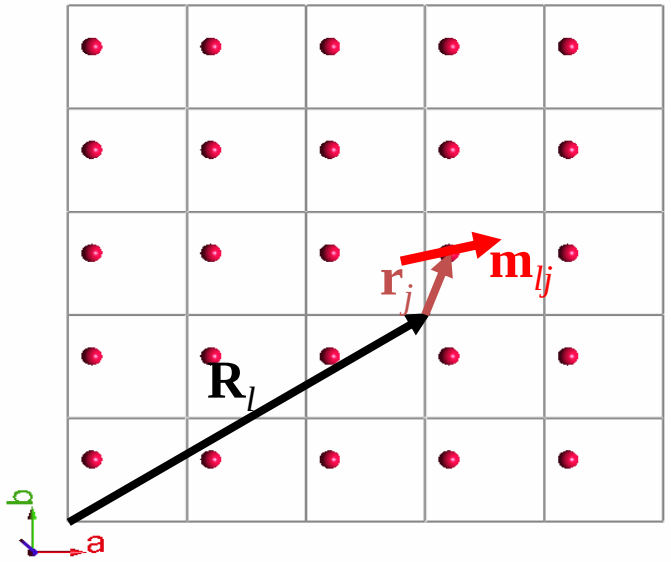
Unit cell: *a*, *b*, *c*, α, β, γ

$$\{\mathbf{r}_j = x_j\mathbf{a} + y_j\mathbf{b} + z_j\mathbf{c} \quad B_j, O_j \quad j = 1,2,...n\} \qquad \textit{crystal} \quad +$$

$$\{\mathbf{m}_j = m_{xj}\mathbf{a}/a + m_{yj}\mathbf{b}/b + m_{zj}\mathbf{c}/c \quad j = 1,2,...n\} \quad \textit{magnetic structure}$$

Notice that the magnetic moments in Bohr magnetons are referred to the frame:
U=(**a**/a, **b**/b, **c**/c) = ($\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$)

FORMALISM OF PROPAGATION VECTORS



This formalism allows the description of magnetic structures (commensurate and incommensurate) using the crystallographic unit cell of the paramagnetic state

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{kj}} \; exp\{-2\pi i \mathbf{k}\mathbf{R}_l\}$$

$$\mathbf{R}_{lj} = \mathbf{R}_l + \mathbf{r}_j = l_1\mathbf{a} + l_2\mathbf{b} + l_3\mathbf{c} + x_j\mathbf{a} + y_j\mathbf{b} + z_j\mathbf{c}$$

Necessary condition for real $\mathbf{m}_{lj}$ $\quad \mathbf{S}_{-\mathbf{kj}} = \mathbf{S}_{\mathbf{kj}}^{*}$

General expression used in **FullProf** $\quad \mathbf{S}_{\mathbf{kj}} = \frac{1}{2}(\mathbf{R}_{\mathbf{kj}} + i\mathbf{I}_{\mathbf{kj}})\exp\{-2\pi i\phi_{\mathbf{kj}}\}$

Only six parameters are independent. The writing above is convenient when relations between the vectors **R** and **I** are established (e.g. when |**R**|=|**I**|, or **R** . **I** =0)

FORMALISM OF PROPAGATION VECTORS

Another convention (Used in Superspace formalism)

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{M}_{\mathbf{kj}} \; exp\left\{-2\pi\, i\mathbf{kR}_{lj}\right\}$$

$$\mathbf{M}_{\mathbf{kj}} = \frac{1}{2}(\mathbf{M}_{\mathbf{kj}}^{\cos} + i\mathbf{M}_{\mathbf{kj}}^{\sin})$$

For a single pair (k,-k) and its harmonics:

$$\mathbf{m}_{lj} = \sum_{n} \mathbf{M}_{n\mathbf{kj}}^{\sin} \sin(2\pi\, n\mathbf{kR}_{lj}) + \mathbf{M}_{n\mathbf{kj}}^{\cos} \cos(2\pi\, n\mathbf{kR}_{lj})$$

$$\mathbf{m}_{lj} = \mathbf{m}(x_4) = \sum_{n} \mathbf{M}_{n\mathbf{kj}}^{\sin} \sin(2\pi\, nx_4) + \mathbf{M}_{n\mathbf{kj}}^{\cos} \cos(2\pi\, nx_4)$$

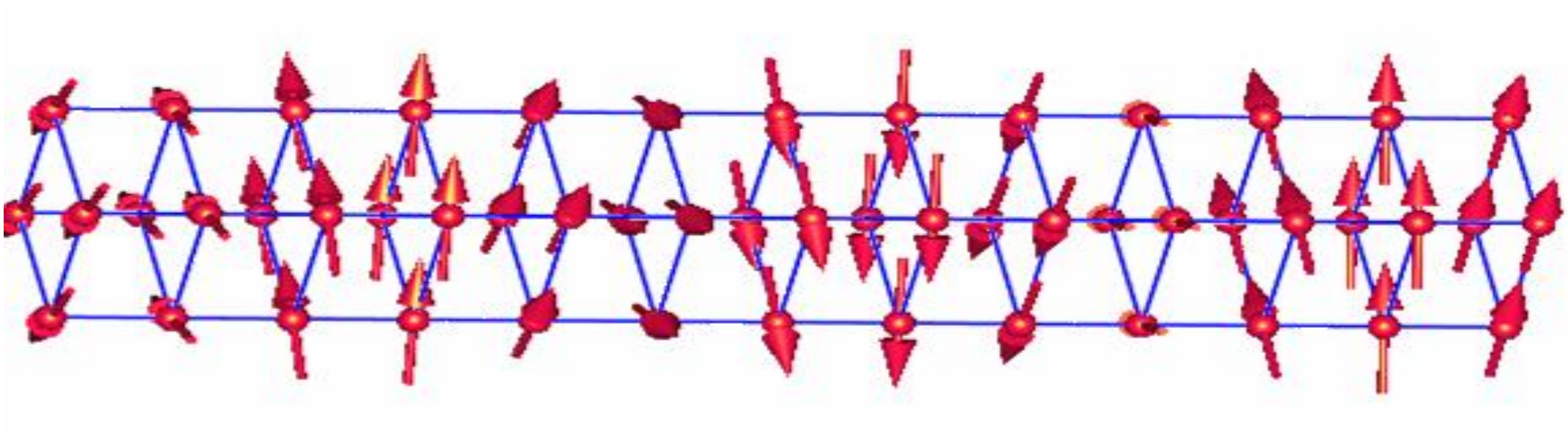
FORMALISM OF PROPAGATION VECTORS

A magnetic structure is fully described by:

i) Wave-vector(s) or propagation vector(s) $\{\mathbf{k}\}$.

ii) Fourier components $\mathbf{S}_{\mathbf{k}j}$ (6 components) for each magnetic atom j and wave-vector $\mathbf{k}$.

Or equivalently the vectors $\mathbf{M}_{\mathbf{k}j} = \frac{1}{2}(\mathbf{M}_{\mathbf{k}j}^{\cos} + i\mathbf{M}_{\mathbf{k}j}^{\sin})$



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Magnetic Bragg Scattering

Intensity (non-polarised neutrons)

$$I_{\mathbf{h}} = N_{\mathbf{h}} N_{\mathbf{h}}^{*} + \mathbf{M}_{\perp \mathbf{h}} \cdot \mathbf{M}_{\perp \mathbf{h}}^{*}$$

Magnetic interaction vector

$$\mathbf{M}_{\perp \mathbf{h}} = \mathbf{e} \times \mathbf{M}(\mathbf{h}) \times \mathbf{e} = \mathbf{M}(\mathbf{h}) - \mathbf{e}\,(\mathbf{e} \cdot \mathbf{M}(\mathbf{h}))$$

$$\mathbf{h} = \mathbf{H} + \mathbf{k} \quad \Leftarrow \text{Scattering vector} \qquad \mathbf{e} = \frac{\mathbf{h}}{h}$$

Magnetic Structure Factor: k-vectors

We use of the **reciprocal unit cell of the paramagnetic state + k-vectors** for indexing the magnetic Bragg reflections

$$\mathbf{M(h)} = p\sum_{j=1}^{n} O_j f_j(\mathbf{h}) T_j \sum_s \mathbf{S}_{\mathbf{k}js}\, exp\{2\pi i[(\mathbf{H}+\mathbf{k})\{S|\mathbf{t}\}_s \mathbf{r}_j]\}$$

j : index running for all n magnetic atom sites in the magnetic asymmetric unit

s : index running for all atoms of the orbit corresponding to the magnetic site j (s=1,… p_j). Total number of atoms: N = Σ p_j

$\{S|\mathbf{t}\}_s$ Symmetry operators of the propagation vector group or a subgroup

If no symmetry constraints are applied to S_k, the maximum number of parameters for a general incommensurate structure is 6N (In practice 6N-1, because a global phase factor is irrelevant)

Magnetic Structure Factor: Basis Vectors of *irreps*

The fundamental hypothesis of the Representation Analysis of magnetic structures is that the Fourier coefficients of a magnetic structure are linear combinations of the basis functions of the irreducible representation of the propagation vector group $\mathbf{G_k}$ or the full group **G** or a subset of the star (e.g. **k**, **-k**).

$$\mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C^{\nu}_{n\lambda} \mathbf{S}^{\mathbf{k}\,\nu}_{n\lambda}(js)$$

$$\mathbf{M}(\mathbf{h}) = p\sum_{j=1}^{n} O_j f_j(\mathbf{h}) T_j \sum_{n\lambda} C^{\nu}_{n\lambda} \sum_{s} \mathbf{S}^{\mathbf{k}\,\nu}_{n\lambda}(js) exp\{2\pi i\, \mathbf{h}_s \mathbf{r}_j\}$$

Magnetic structure factor in terms of basis vectors of irreducible representations and refinable coefficients $C^{\nu}_{n\lambda}$

Magnetic Space Groups: conventional approach

The use of Shubnikov groups implies the use of the **magnetic unit cell** for indexing the Bragg reflections

$$\mathbf{M}_{\perp} = \mathbf{e}\times\mathbf{M}\times\mathbf{e} = \mathbf{M} - \mathbf{e}\,(\mathbf{e}\cdot\mathbf{M}) \qquad I \propto \mathbf{M}_{\perp}^{*}\mathbf{M}_{\perp}$$

Magnetic structure factor (without symmetry):

$$\mathbf{M}(\mathbf{H}) = p\sum_{m=1}^{N_{mag}} \mathbf{m}_m f_m(H)\exp(2\pi i\mathbf{H}\cdot\mathbf{r}_m)$$

Using magnetic space group symmetry, we consider n independent magnetic sites labelled with the index μ. The index s labels the representative symmetry operators of the Shubnikov group: $\mathbf{m}_{\mu s} = \det(h_s)\,\delta_s\, h_s\, \mathbf{m}_{\mu}$ is the magnetic moment of the atom at sublattice s of site μ.

$$\mathbf{M}(\mathbf{H}) = p\sum_{\mu=1}^{n} O_\mu f_\mu(H) T_\mu \sum_s \det(h_s)\,\delta_s\, h_s\, \mathbf{m}_\mu exp\{2\pi i[(\mathbf{H}\{h|\mathbf{t}\}_s \mathbf{r}_\mu]\}$$

The free parameters of the structure are the atom positions and magnetic moments: $\mathbf{r}_\mu$, $\mathbf{m}_\mu$

Magnetic Structure Factor: Symmetry Modes

Using the cell basis of the subgroup of the paramagnetic state group and considering displacive and magnetic modes from the representation analysis one can write the position of the atoms and the magnetic moments of the asymmetric unit as:

$$\mathbf{r}_{\mu} = \mathbf{r}_{\mathbf{0}\mu} + \mathbf{u}_{\mu} = \mathbf{r}_{\mathbf{0}\mu} + \sum_{\tau,m} A_{\tau,m}\ \boldsymbol{\varepsilon}_{(\tau,m|\mu)}$$

$$\mathbf{m}_{\mu} = \sum_{\tau,m} M_{\tau,m}\ \boldsymbol{\kappa}_{(\tau,m|\mu)}$$

The structure factor can be written in terms of the amplitudes of displacive and magnetic modes ($A_{\tau,m}, M_{\tau,m}$) through the (normalized) basis vector ($\boldsymbol{\varepsilon}_{(\tau,m|\mu)}, \boldsymbol{\kappa}_{(\tau,m|\mu)}$) of the irreducible representations (τ) contributing to the final symmetry

$$\mathbf{M}(\mathbf{H}) = p\sum_{\mu=1}^{n} O_{\mu} f_{\mu}(H) T_{\mu} \sum_{s} \det(h_s)\,\delta_s\, h_s \sum_{\tau,m} M_{\tau,m}\ \boldsymbol{\kappa}_{(\tau,m|\mu)} exp\{2\pi i[(\mathbf{H}\{h|\mathbf{t}\}_s(\mathbf{r}_{\mathbf{0}\mu} + \sum_{\tau,m} A_{\tau,m}\ \boldsymbol{\varepsilon}_{(\tau,m|\mu)})]\}$$

The free parameters of the structure are the amplitudes: $A_{\tau,m}, M_{\tau,m}$

Magnetic Structure Factor: Superspace formalism

Let us consider a general case with d propagation vectors $\mathbf{k}_p$, a Bragg reflections is indexed like:

$$\mathbf{h} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^* + \sum_{p=1}^{d} m_p\mathbf{k}_p$$

The integer indices $(h_1, h_2, h_3, m_1, \ldots m_d) = (h_1, h_2, \ldots h_{3+d})$ may be considered as the coordinates in the reciprocal space of a $(3+d)$D superspace.

In real space the magnetic moments can be written as a very general Fourier series as:

$$\mathbf{m}_{jl} = \mathbf{m}_j(\bar{x}_4, \bar{x}_5, .., \bar{x}_{3+d}) = \sum_{n_1=-m_1}^{m_1} \ldots \sum_{n_d=-m_d}^{m_d} \mathbf{T}_j^{(n_1,..,n_d)} \exp[-2\pi i\{n_1, n_2 \ldots n_d\}\cdot\mathbf{r}_I^j]$$

$$\mathbf{m}_j(\bar{x}_4, \bar{x}_5, .., \bar{x}_{3+d}) = \sum_{n_1=0}^{\infty} .. \sum_{n_d=0}^{\infty} \mathbf{M}_{\cos j}^{(n_1,..,n_d)} \cos[2\pi(n_1\bar{x}_4 + .. + n_d\bar{x}_{3+d})] + \mathbf{M}_{\sin j}^{(n_1,..,n_d)} \sin[2\pi(n_1\bar{x}_4 + .. + n_d\bar{x}_{3+d})]$$

Where $\bar{x}_{3+p} = t_p + \mathbf{k}_p\bar{\mathbf{r}}_{jl} = t_p + \mathbf{k}_p(\mathbf{R}_l + \mathbf{r}_j^0) = t_p + \boldsymbol{\sigma}_{1p}\bar{x}_1 + \boldsymbol{\sigma}_{2p}\bar{x}_2 + \boldsymbol{\sigma}_{3p}\bar{x}_3$

are the components of the vector $\mathbf{r}_I^j$. The initial phase t_p is arbitrary and may be taken as zero.

A point in superspace has coordinates: $\mathbf{r}_S^j = (x_{S1}^j, x_{S2}^j, \ldots x_{S3+d}^j) = (\mathbf{r}_E^j, \mathbf{r}_I^j)$

Magnetic Structure Factor: Superspace formalism

An operator in superspace has the form:

$$\hat{g}_S = \{g_S, \delta \,|\, \mathbf{t}_S\} \quad \Rightarrow \quad g_S = \begin{pmatrix} \mathbf{g} & \mathbf{0} \\ \mathbf{H}_g & \mathbf{E}_g \end{pmatrix} \qquad \mathbf{t}_S = (t_1, t_2, \ldots t_{3+d}) = (\mathbf{t}, t_4, \ldots, t_{3+d}) = (\mathbf{t}, \mathbf{t}_I)$$

Where **g** is the 3×3 rotational part of the parent 3D operator, $\mathbf{H}_g$ is a d×3 matrix and $\mathbf{E}_g$ is a d×d integer matrix with zeros and ones, verifying the relations:

$$\boldsymbol{\sigma}\mathbf{g} = \mathbf{E}_g\boldsymbol{\sigma} + \mathbf{H}_g$$

where $\boldsymbol{\sigma}$ is a d×3 matrix containing as rows the components of the propagation vectors. The parameter δ is equal to 1 if the operator is un-primed and -1 if it is primed. These matrices are determined by the action of the 3D operators of the parent paramagnetic space group on the propagation vectors.

The action of the symmetry operators in the magnetic moment of an atom with internal coordinates $\mathbf{r}_I^j$ is given by the equation:

$$\mathbf{m}_k[\mathbf{r}_I^k] = \mathbf{m}_k[\mathbf{H}_g\mathbf{r}_0^j + \mathbf{E}_g\mathbf{r}_I^j + \mathbf{t}_I] = \delta det(\mathbf{g})\mathbf{g}\,\mathbf{m}_j[\mathbf{r}_I^j]$$

This equation is the basis for obtaining the constraints on the amplitudes $\mathbf{M}_{\cos j}^{(n_1,..,n_d)}, \mathbf{M}_{\sin j}^{(n_1,..,n_d)}$ for the site j. The program **FullProf** calculates the magnetic structure factor applying these equations when the complete list of operators are obtained from the provided generators.

Magnetic Structure Factor: Superspace formalism

Writing $\mathbf{T}_j^{(n_1,..,n_d)} = \mathbf{T}_j^{[n]} = \frac{1}{2}(\mathbf{M}_{\cos j}^{[n]} + i\mathbf{M}_{\sin j}^{[n]})$

The general expression of the magnetic structure factor in 3D when the underlying crystal structure is not modulated is:

$$\mathbf{M}(\mathbf{h}_s) = p\sum_j O_j f_j(\mathbf{h}) e^{-B_j|h/2|^2} \sum_{\hat{g}} \delta det(\mathbf{g})\mathbf{g}\mathbf{T}_j^{[n]\mathbf{E}_g} \exp\{2\pi i(\mathbf{H}(\mathbf{g}\mathbf{r}_0^j + \mathbf{t}_g) + [n](\mathbf{H}_g\mathbf{r}_0^j + \mathbf{t}_I))\}$$

In which $\mathbf{h}_s = (\mathbf{H}, [n])$ are the integer indices of the reflection; $\mathbf{g}$, $\mathbf{H}_g$ and $\mathbf{E}_g$ are the submatrices of a general superspace operator and $\mathbf{t}_s = (\mathbf{t}_g, \mathbf{t}_I)$ is the translational part of the operator.

We have used the notation $[n] = (n_1, n_2 \ldots n_d)$ as a d-dimensional vector characterizing the satellite reflections. The application of the submatrix $\mathbf{E}_g$ transforms $[n]$ into another set of indices $[n']$ that are equal, or opposite, to a provided set of $\mathbf{T}^{[m]}$, and we can apply the constraint $\mathbf{T}^{[-m]} = \mathbf{T}^{[m]*}$. For calculating the symmetry constraints on $\mathbf{T}^{[m]}$ for a particular atom position one has to apply the equations:

$$\mathbf{T}_j^{[n]\mathbf{E}_g} = \sum_{\hat{g}} \delta det(\mathbf{g})\mathbf{g}\mathbf{T}_j^{[n]\mathbf{E}_g} \exp\{2\pi i(\mathbf{H}(\mathbf{g}\mathbf{r}_0^j + \mathbf{t}_g) + [n](\mathbf{H}_g\mathbf{r}_0^j + \mathbf{t}_I))\}$$

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DIFFERENT OPTIONS FOR DESCRIBING THE MAGNETIC MODEL

Steps for determining magnetic structures with NPD (1)

1: **Collect a NPD pattern of the sample in the paramagnetic state** ($T > T_N$ or T_C). Refine the crystal structure using the collected data and get all the relevant structural and profile parameters. Use FULLPROF and WINPLOTR for doing this task.

2: **Collect a NPD pattern below the ordering temperature**. Normally additional magnetic peaks appear in the diffraction pattern. It is important to make a refinement by fixing all the structural parameters, without putting a magnetic model in the PCR file, in order to see clearly the magnetic contributions to the diffraction pattern. Get the peak positions of the additional peaks using WINPLOTR-2006 and save them in a format adequate to the program K-SEARCH.

3: **Determine the propagation vector(s)** of the magnetic structure by using the program K-SEARCH or by trial and error with an additional phase in the PCR file treated in Le Bail Fit (LBF) mode (no magnetic model). If there are no additional peaks and only an additional contribution to the nuclear peaks is observed, the magnetic structure has as propagation vector **k** = (0, 0, 0).

DIFFERENT OPTIONS FOR DESCRIBING THE MAGNETIC MODEL

Steps for determining magnetic structures with NPD (2)

4: Once the propagation vector is determined, use the program BASIREPS in order to get the basis vectors of the *irreps* of the propagation vector group G_k. In the case of *irreps* with dimensions higher than 1, the user has to select the appropriate combination of basis vectors because BASIREPS does not make an analysis of the isotropy groups as a function of the order parameters. For selecting the appropriate symmetry few options are available:

4-1: ***Commensurate structure***: With the help of BASIREPS, one can determine the Shubnikov group and the appropriate magnetic symmetry operators, or, alternatively, use directly the basis vectors of the *irreps*. Another option is to use the Bilbao Crystallographic Server to obtain mCIF files that can be converted to templates of PCR files for the possible Shubnikov groups. It is also possible to use ISODISTORT to obtain directly a template of a PCR file for working directly with displacive and magnetic symmetry modes. By default, ISODISTORT uses the standard setting that may be very different from the parent-related setting, which is preferred by experimentalists. This can be changed easily before generating the template.

4-2: ***Incommensurate structure***: One can directly use the output of BASIREPS for constructing a model of incommensurate magnetic structure using the basis vectors or complex Fourier coefficients. Other options are those that allows working with particular forms of magnetic structures (conical structures, real space description of multi-helical structures, etc.)

Steps for determining magnetic structures with NPD (3)

4-3: ***Incommensurate structure in superspace***: If the superspace approach is preferred, the best option currently available for working with FULLPROF is to obtain from ISODISTORT a magnetic CIF files that can be converted to PCR by using the program MCIF_TO_PCR. The best way of working is to generate the superspace group using a setting related to the parent paramagnetic space group without changing the origin. The adequate symbol of the superspace group can be easily obtained from symbol of the parent group (or one of its subgroups) and looking at the internal translations of the symmetry operators.

5: Solve the magnetic structure by using the symmetry information obtained in step 4 using trial and error methods (5-1) or the simulated annealing (SAnn) procedure (5-2) implemented in FULLPROF.

5-1: **In the first case one has to modify the PCR file used in step 2 by adding an additional magnetic phase** by putting `Jbt=1` (magnetic phase with Fourier coefficients/magnetic moments referred to the unitary basis along the unit cell axes), `Irf=-1` (only satellites will be generated). The best way to create such additional magnetic phase is to copy it from an already existing PCR file similar to that of the current case and modify it using the symmetry information obtained in step 4. Run FULLPROF fixing nearly all parameters, except the magnetic moments or the coefficients of the basis functions, and check in the plots if the calculated magnetic peaks have intensities close to the observed ones. If not, change the magnetic model (use another representation or other magnetic symmetry operators) and try again. In some cases this is enough to solve the magnetic structure. In case this does not work use the method described in 5-2.

Steps for determining magnetic structures with NPD (4)

5-2: **In the second case one has to modify the PCR file used in step 2 by adding an additional phase in LBF mode** (as for one of the options in step 3). This additional phase has no atoms and we have to put `Jbt`=2, `Irf`= -1 and `Jview`=11. The nuclear phase has to be treated with fixed scale factor and structural parameters. This allows getting the purely magnetic reflections in a separate file that can be used by FULLPROF in SAnn mode.

6: Refine the magnetic structure using the Rietveld method implemented in FULLPROF. Once the magnetic model gives a calculated powder diffraction pattern close enough to the observed one, we start the refinement phase. If we use the trial and error method (5-1) the refinement step is just the continuation of the previous step. If the simulated annealing method (5-2) was used we have to translate the final solution, stored in an automatically generated PCR file, to the file for treating directly the powder diffraction profile.

DIFFERENT OPTIONS FOR DESCRIBING THE MAGNETIC MODEL

(1) Standard Fourier (all kind of structures) coefficients refinement with $\mathbf{S}_k$ described with components along {**a**/a, **b**/b, **c**/c} (**`Jbt = 1,10`**), or in spherical coordinates with respect to a Cartesian frame attached to the unit cell (**`Jbt = -1, -10`**).

(2) Time reversal operators, presently only for **k**=(0,0,0) (**`Jbt = 10 + Magnetic symmetry`** keyword after the symbol of the SPG) (obsolete)

(3) Shubnikov Groups in BNS formulation (**`Jbt = 10 + Isy=2`**). Whatever magnetic space group in any setting. The PCR file may be generated from an mCIF file.

(4) Real space description of uniaxial conical structures (**`Jbt = 5`**) (symmetry is ignored)

DIFFERENT OPTIONS FOR DESCRIBING THE MAGNETIC MODEL

(5) Real space description of multi-axial helical structures with elliptic envelope
(**Jbt = -1, -10 + (More=1 & Hel = 2)**)

(6) Refinement of $C_{n\lambda}^{\nu}$ coefficients in the expression:

$$\mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{\mathbf{k}\,\nu}(js)$$

Jbt = 1 and Isy=-2

(7) Refinement of the magnetic structure using symmetry modes (commensurate):
Jbt = -6 and Isy=2

(8) Refinement of the magnetic structure using superspace groups:
Jbt = 7 and Isy=2

DIFFERENT OPTIONS FOR DESCRIBING THE MAGNETIC MODEL

The documentation for using the different options in FULLPROF is scattered in the old manual and the document `fp2k.inf`

Se also the document:

Magnetic structure analysis and refinement with FullProf.pdf

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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 * * *

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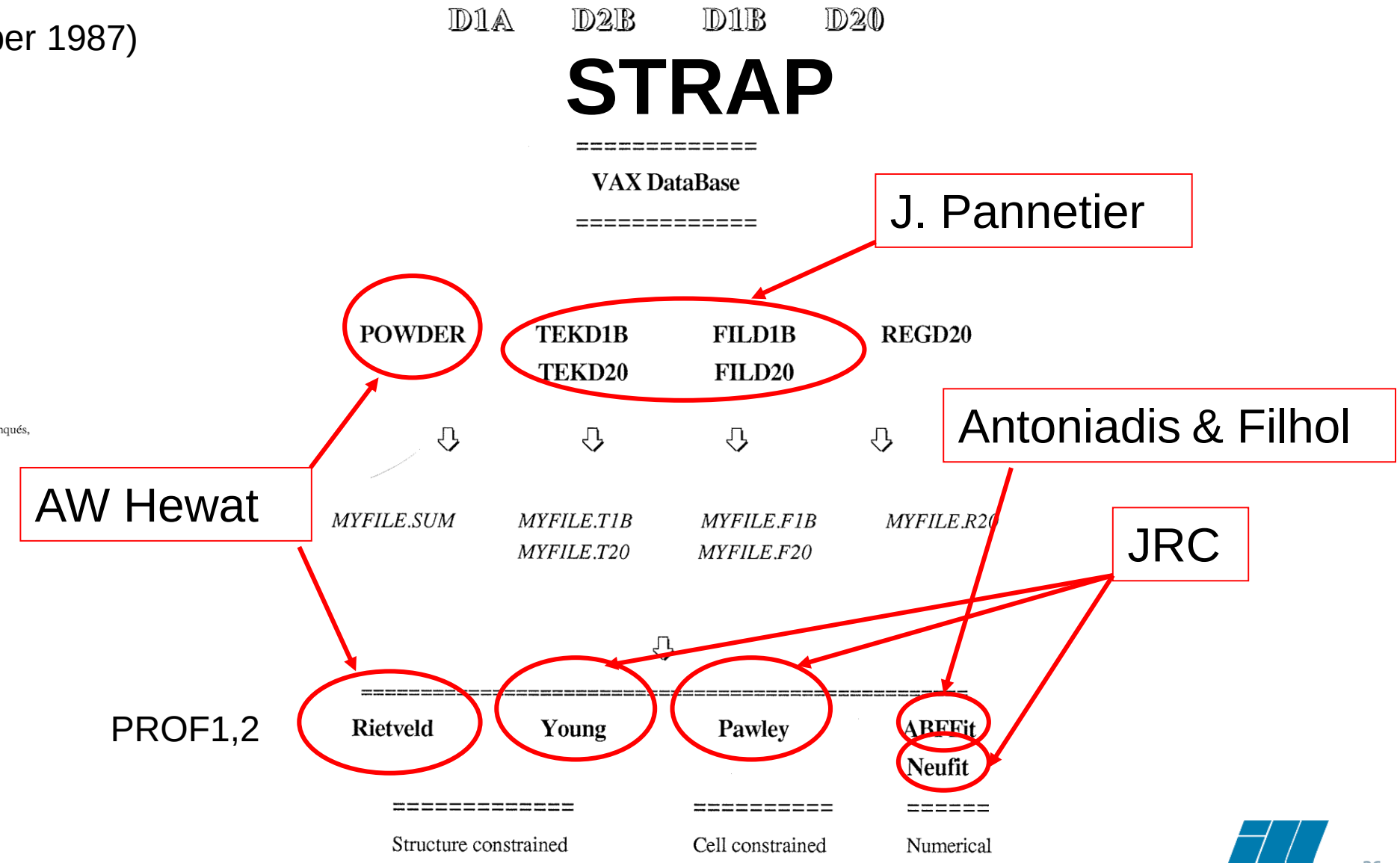

History of FullProf: From 1988 to 1992 @ILL

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)**

~ 30 years ago!

THE REFERENCE PAPER OF FULLPROF

Recent advances in magnetic structure determination by neutron powder diffraction

Physica B 192, 55 (1993)

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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 EARLY DEVELOPMENT OF FULLPROF

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**).

The early development of FullProf
The middle of the nineties

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

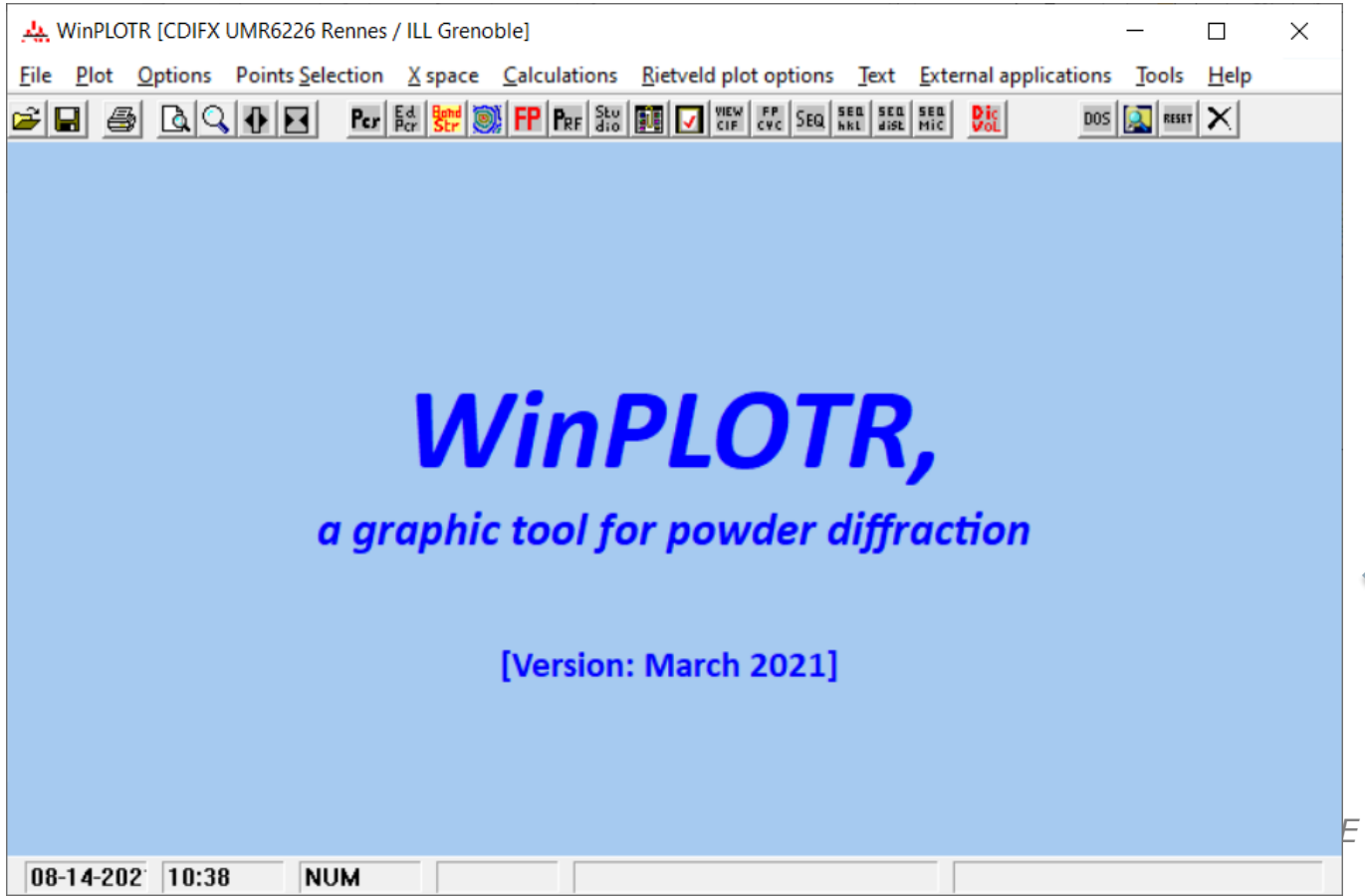
Rewriting the code (C++ or Fortran 90?), 1995-1996 ... Finally a subset (ELF) of Fortran 90 for FullProf.

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

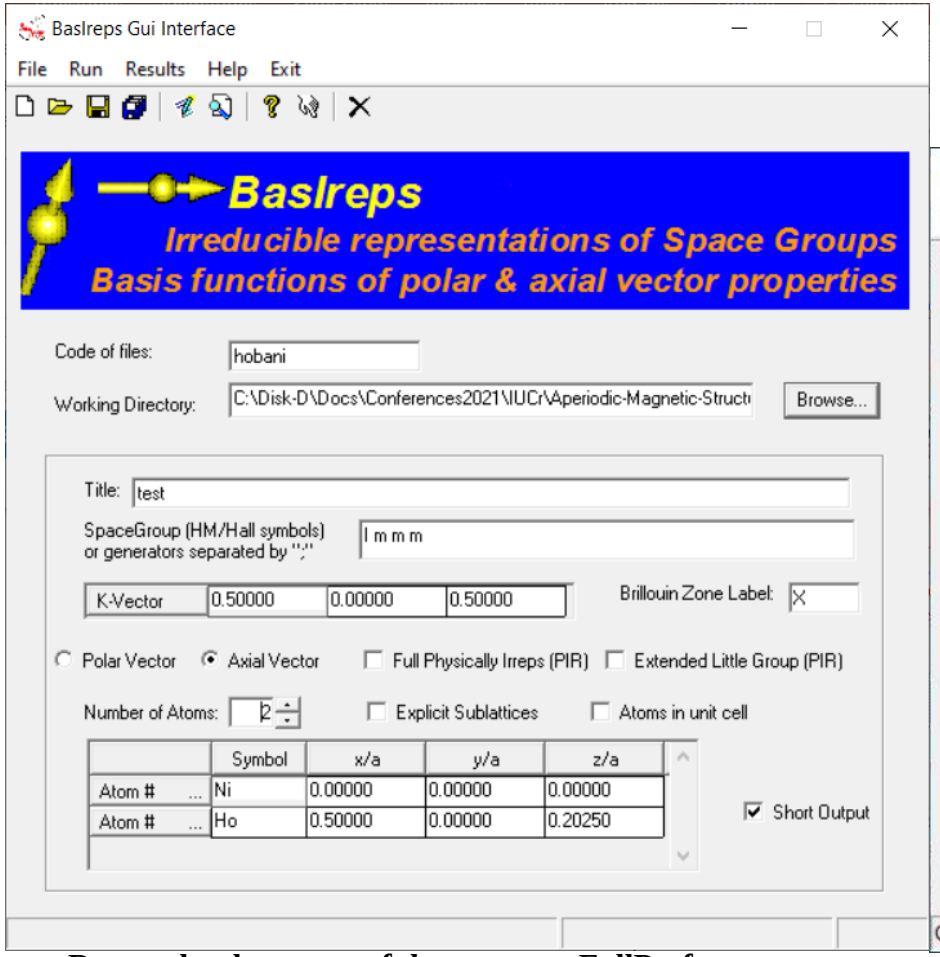


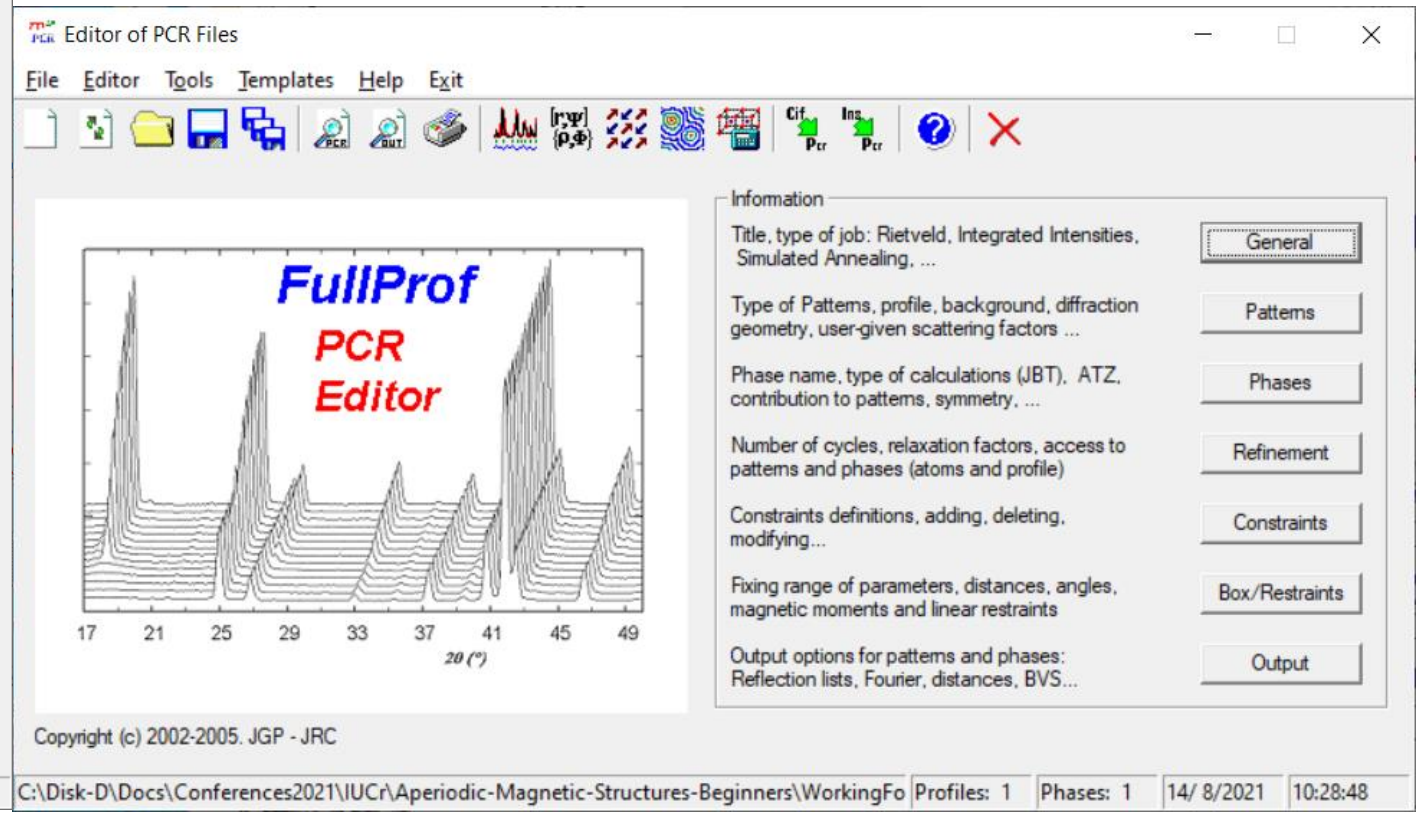
- Visualization of powder patterns
- Peak search, background generation
- Fitting capabilities
- Run FullProf from WinPLOTR
- Interoperability with other programs: BondStr, DICVOL, TREOR, etc.

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

The early development of FullProf

The end of the nineties to the new century





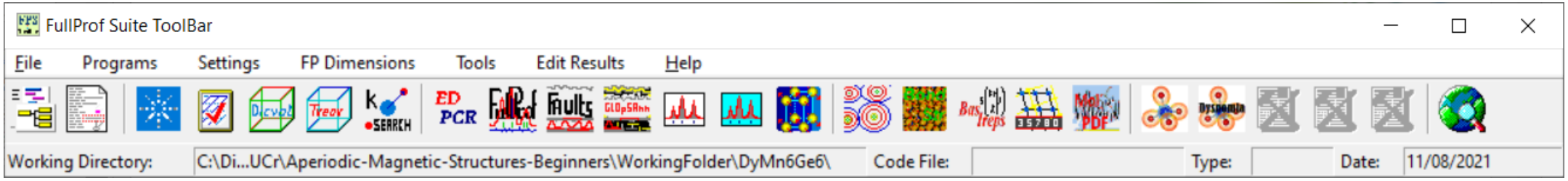
Recent developments of the program FullProf
Juan Rodríguez-Carvajal
Commission for Powder Diffraction, IUCr, Newsletter **26**, 12-19 (2001).

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

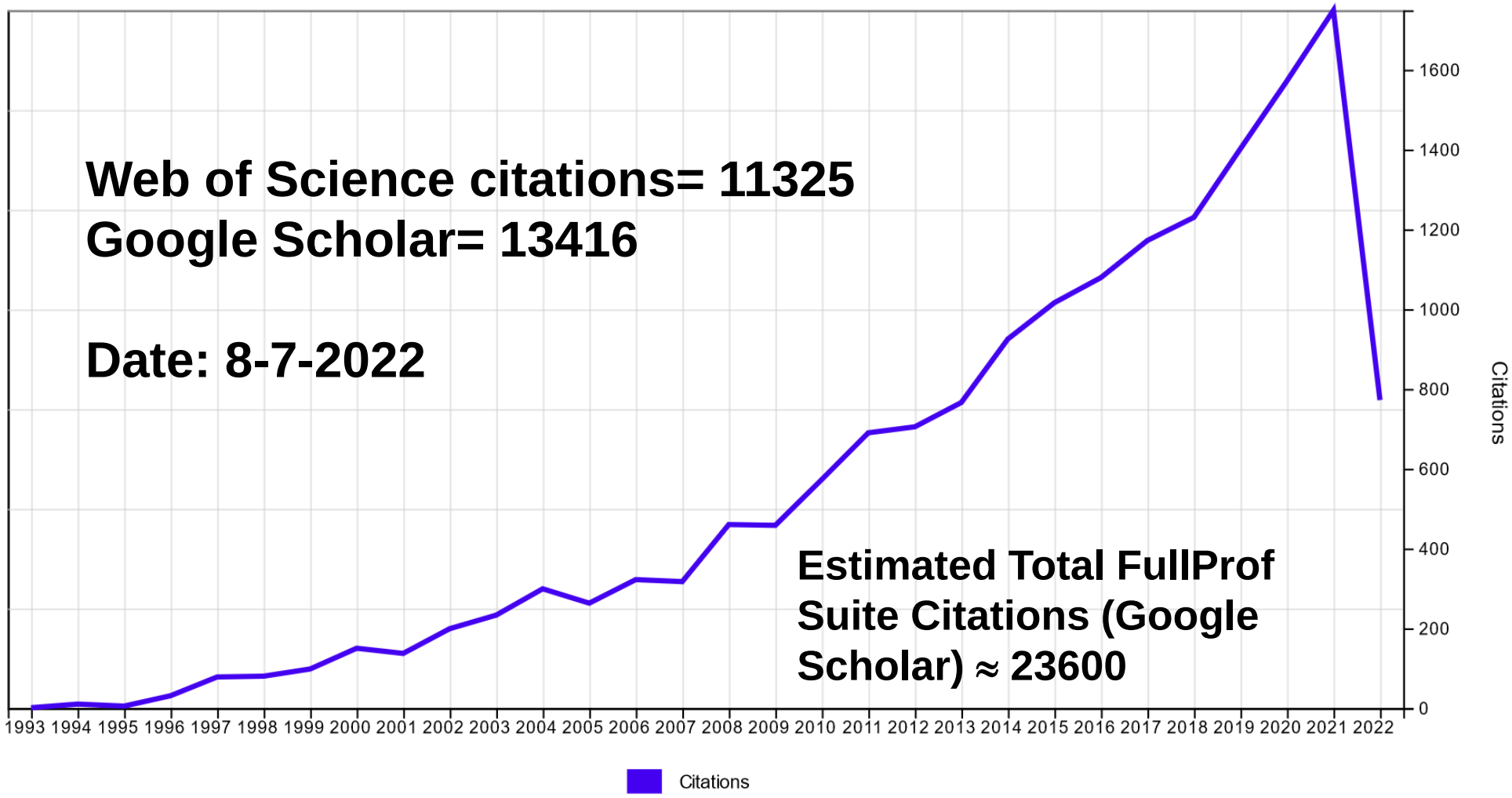


- Development of **FullProf Studio** (L.C. Chapon)
- Development of **GBondStr/BondStr** (J. González-Platas)
- Development of the new **WinPLOTR-2006** (O. Baltuano)
- During the first decade of the new century the **FullProf Suite** was continuing developed and largely distributed through the Internet

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).

PHYSICA B PAPER CITATIONS OVER TIME



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

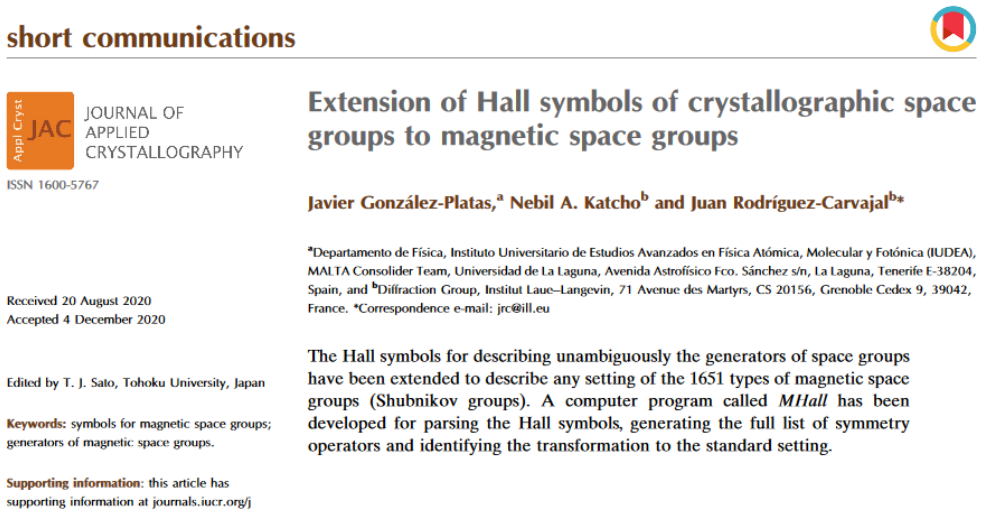
CrysFML written using the latest Fortran standard.

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

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[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

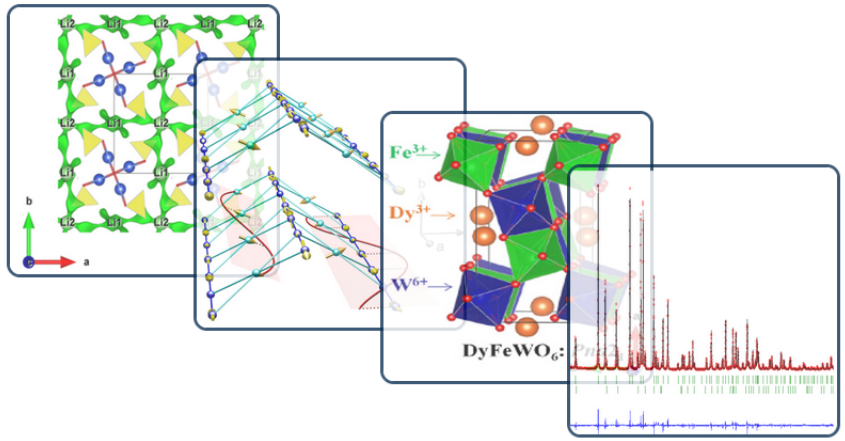
https://www.ill.eu/sites/fullprof/nebil/

Most Visited | Getting Started | Seguir una carta, un C... | OMG Big Ass Latina H... | Other Bookmarks

The FullProf Suite — Home | Updates | Programs | Downloads | References

FullProf Suite

Crystallographic tools for Rietveld, profile matching and integrated intensity refinements of X-ray and / or neutron data

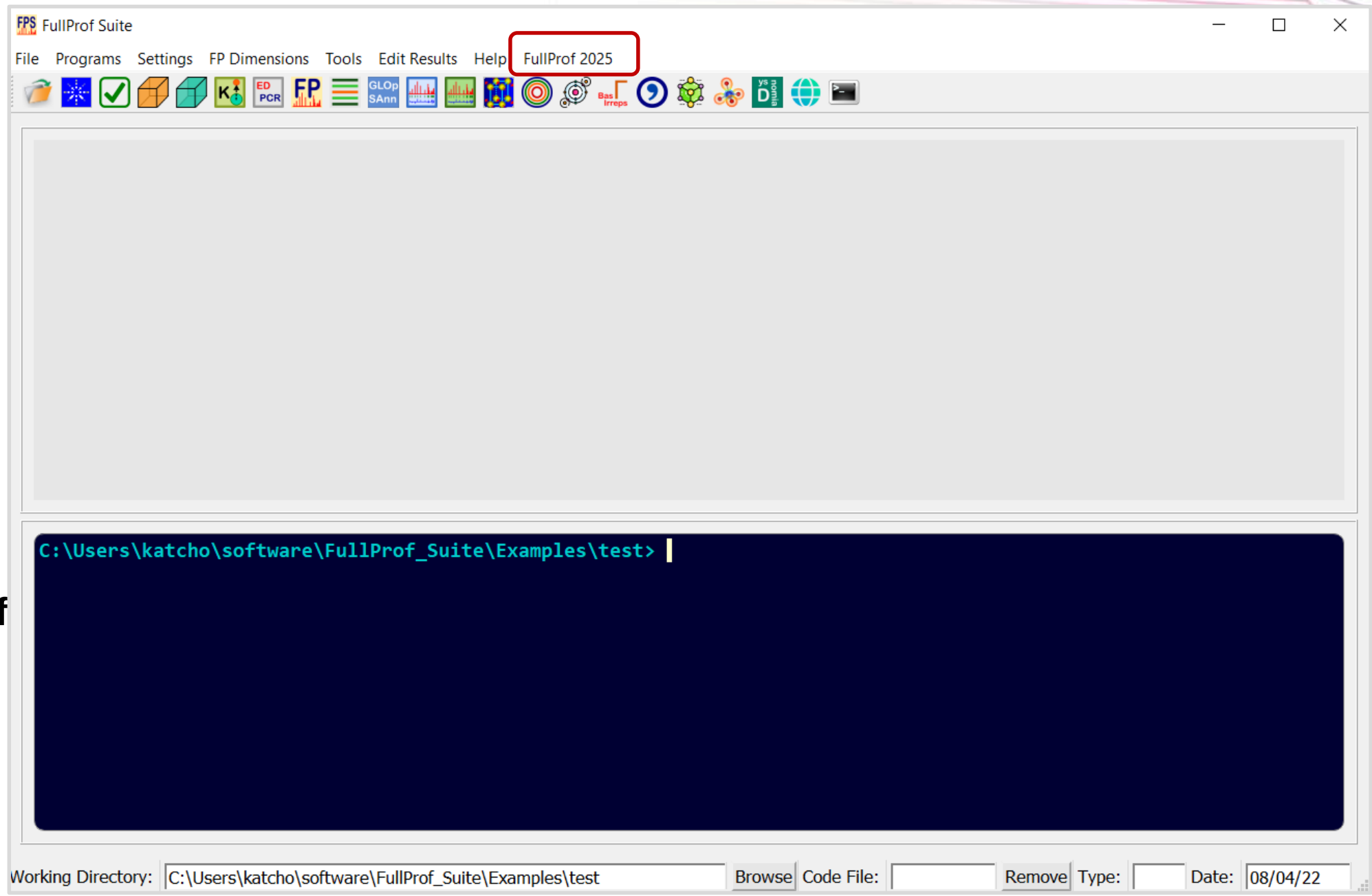


Download the latest release version of FullProf

FullProf upgrading

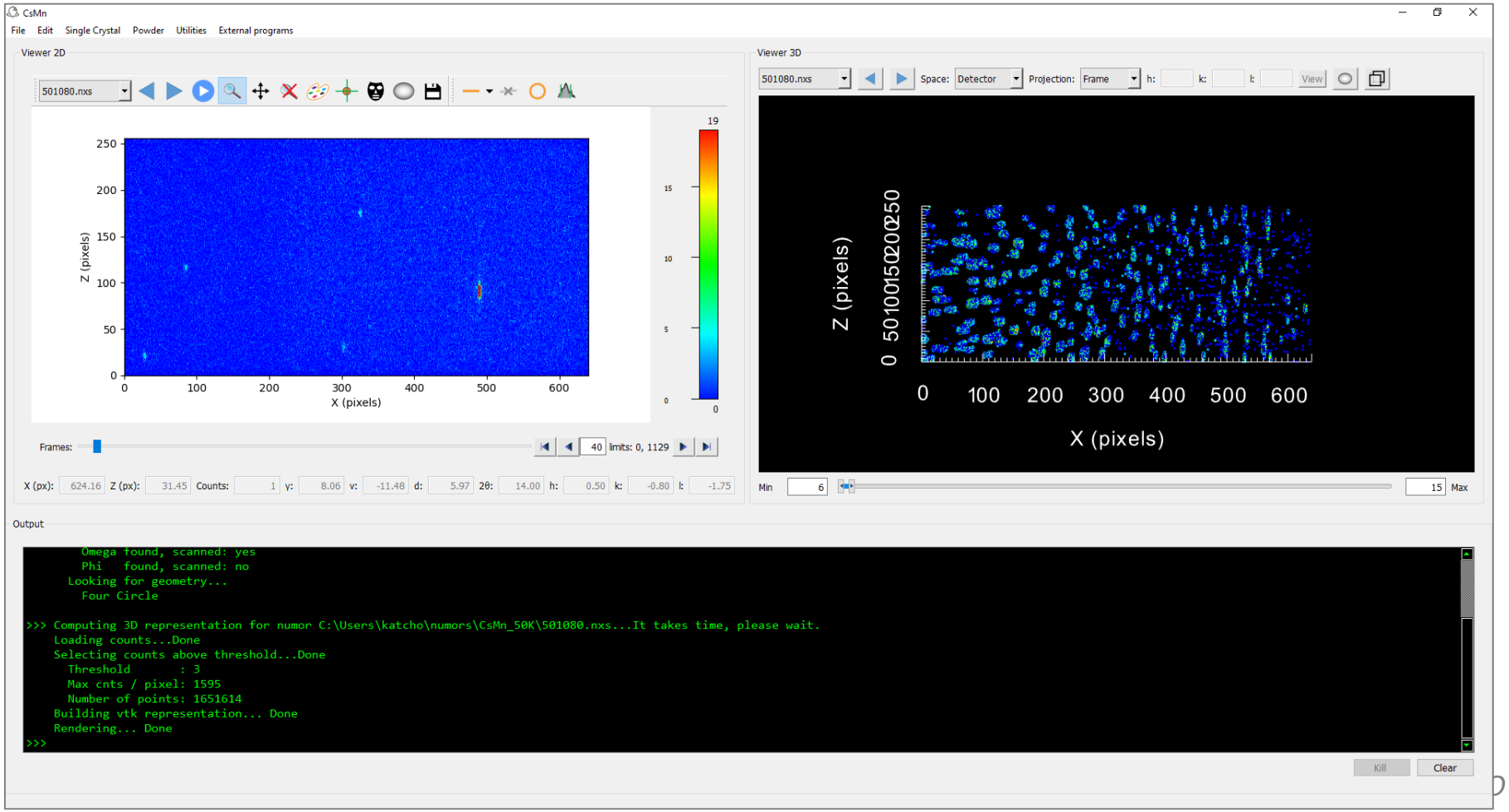
Classic

FullProf 2025

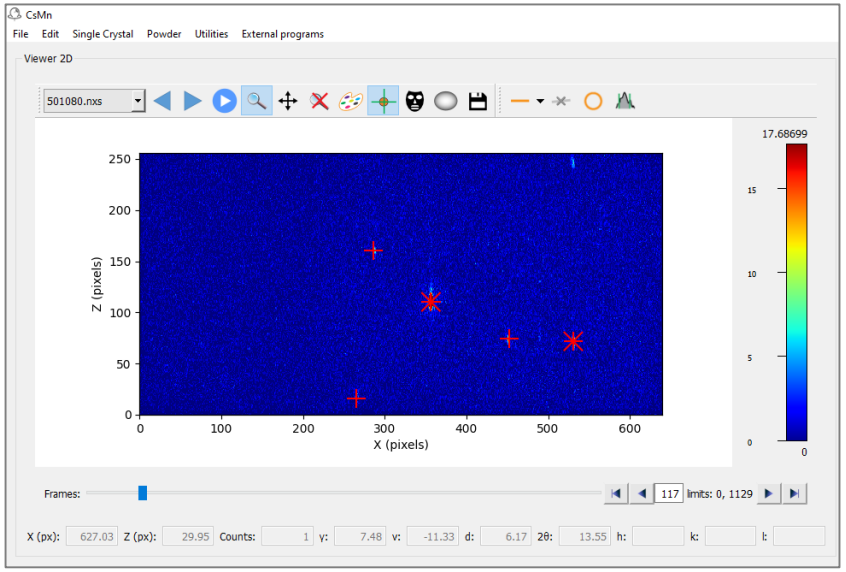


The future GUI for FullProf Suite will be similar to that of the Int3D GUI

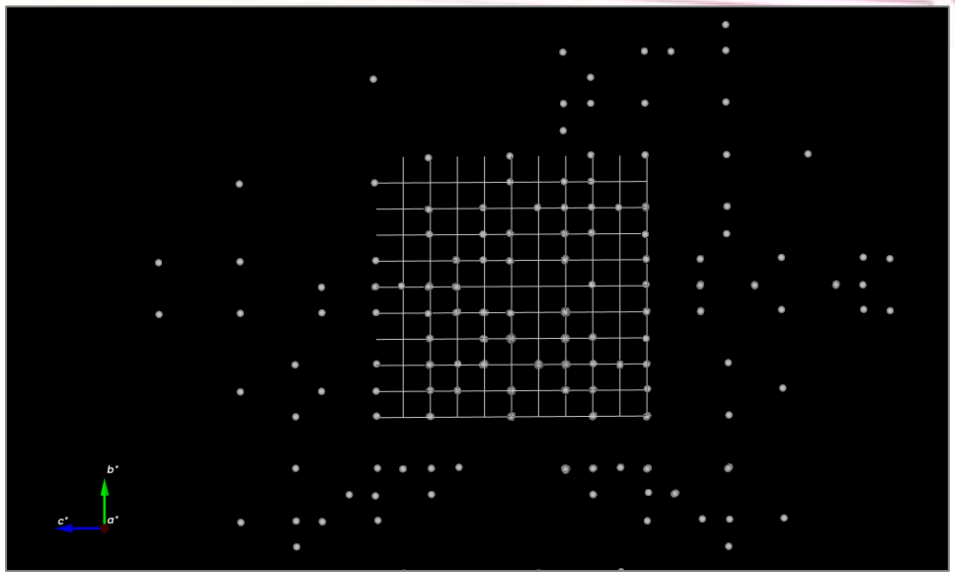
The GUI consists of a **menu bar**, a **2D viewer** (left), a **3D viewer** (right) and a **terminal** (bottom)



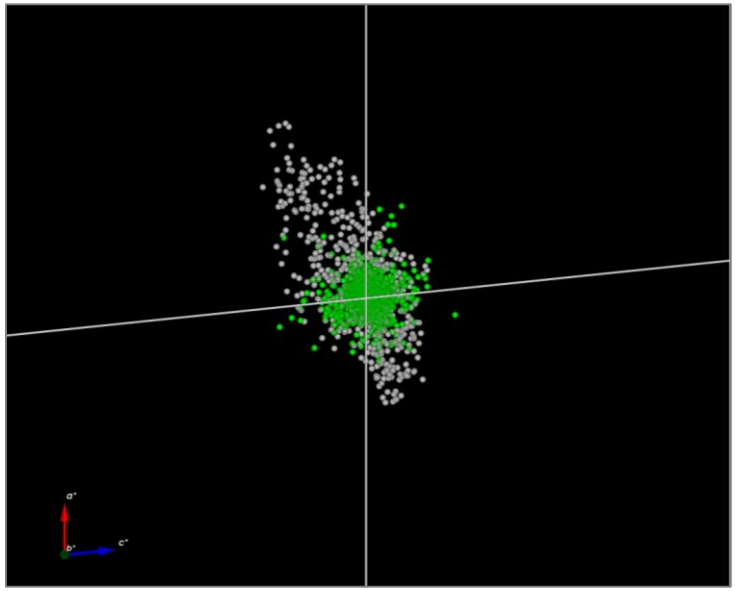
Peak search



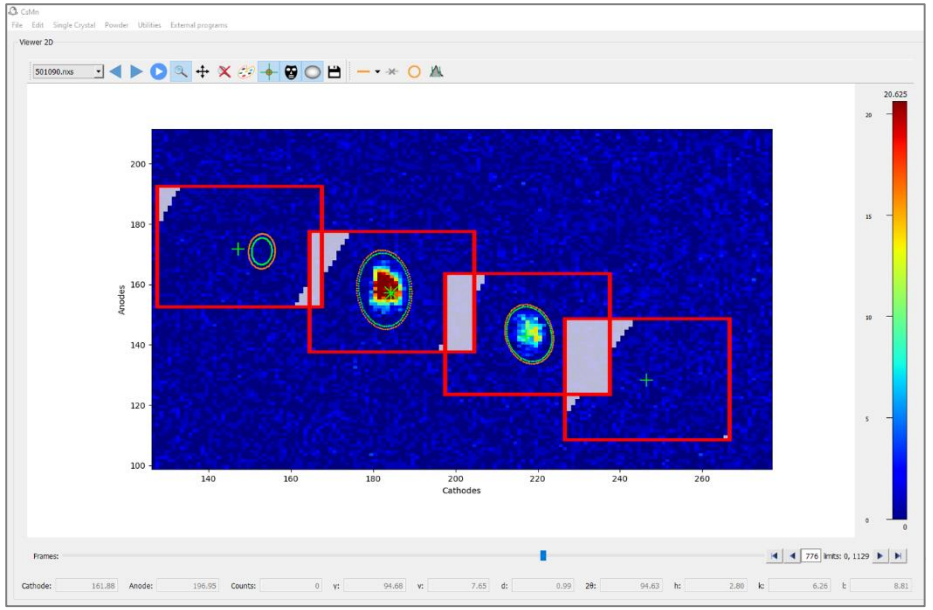
UB Matrix



Refinement



Integration

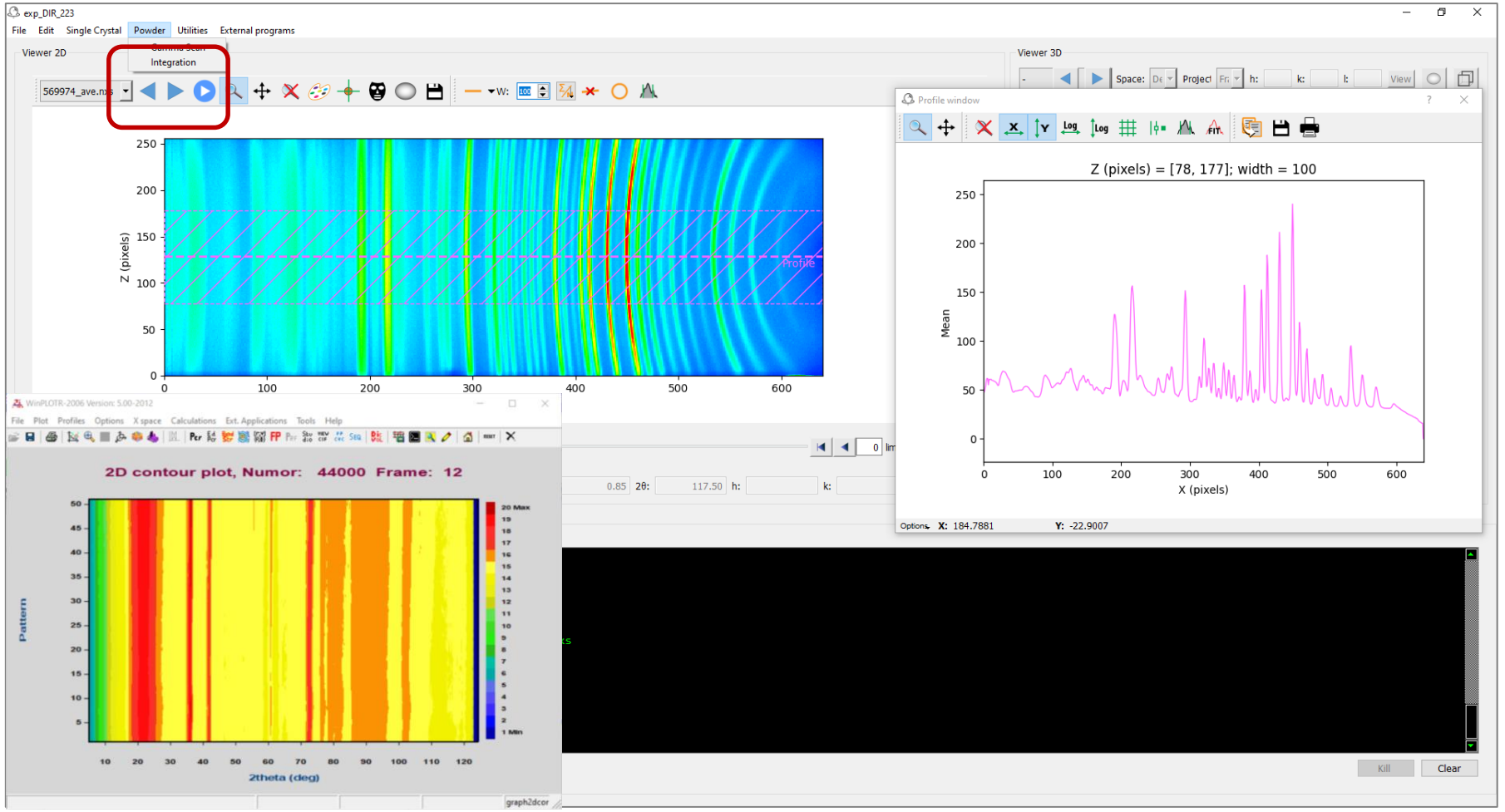


E

NEUTRONS FOR SOCIETY

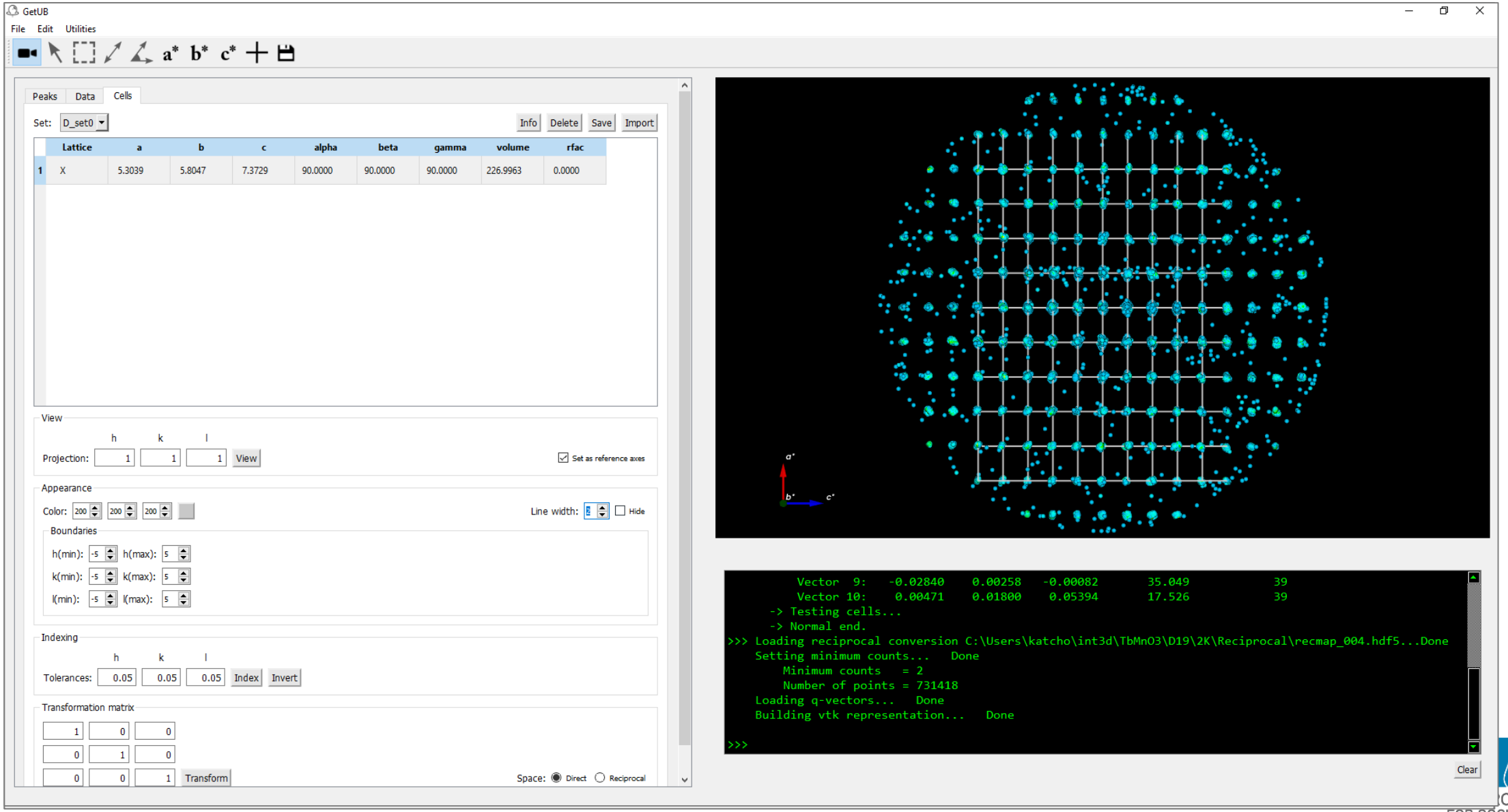
Other Capabilities of Int3D

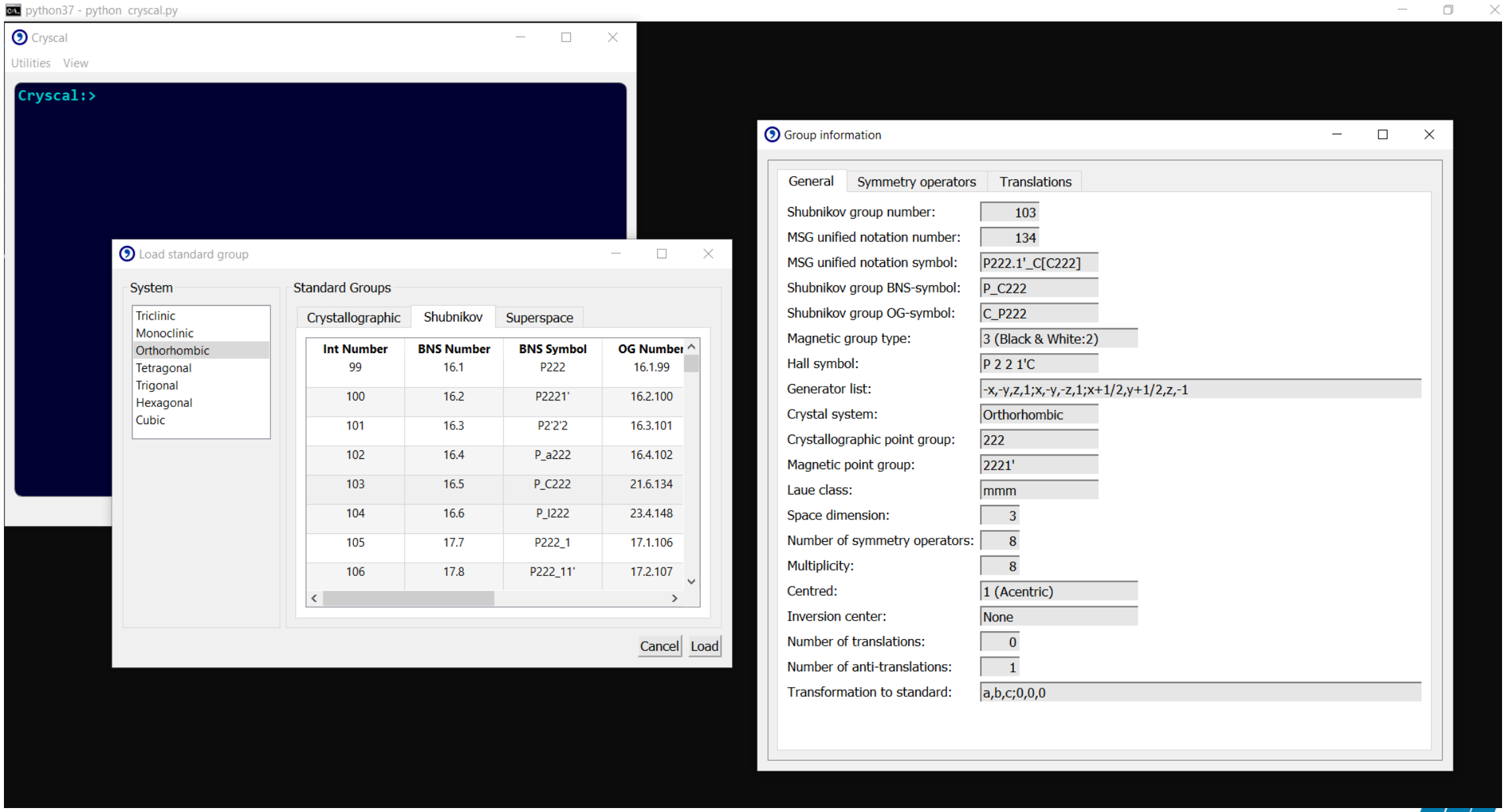
Data reduction of powder data (D19)

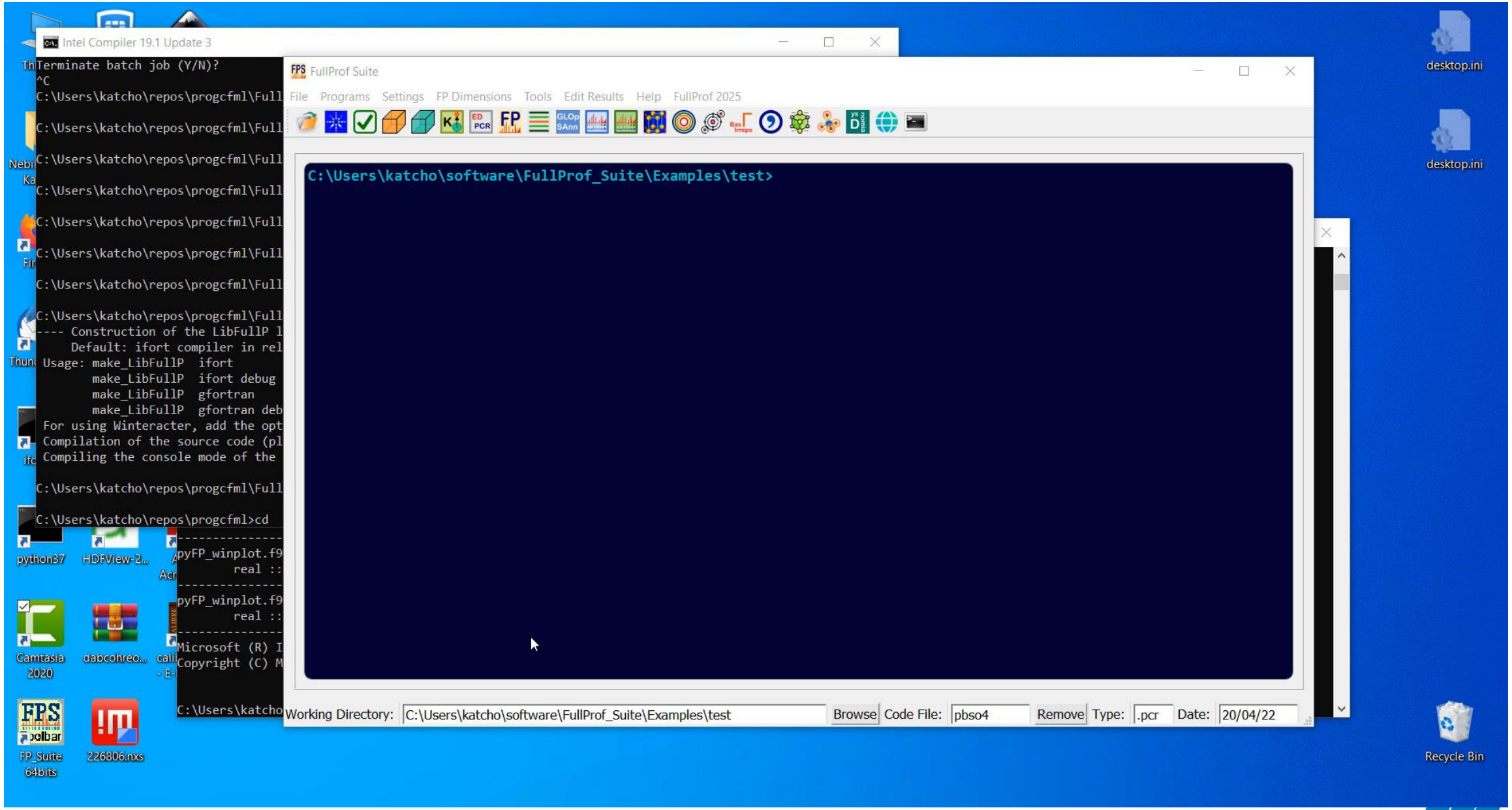


Other Capabilities of Int3D

Raw data in reciprocal space




python37 - python cryscal.py
Cryscal
Utilities View
Cryscal:>
Load standard group
System
Triclinic
Monoclinic
Orthorhombic
Tetragonal
Trigonal
Hexagonal
Cubic
Standard Groups
Crystallographic
Shubnikov
Superspace
Int Number
BNS Number
BNS Symbol
OG Number
99 16.1 P222 16.1.99
100 16.2 P2221' 16.2.100
101 16.3 P2'2'2 16.3.101
102 16.4 P_a222 16.4.102
103 16.5 P_C222 21.6.134
104 16.6 P_I222 23.4.148
105 17.7 P222_1 17.1.106
106 17.8 P222_11' 17.2.107
Cancel
Load
Group information
General
Symmetry operators
Translations
Shubnikov group number: 103
MSG unified notation number: 134
MSG unified notation symbol: P222.1'_C[C222]
Shubnikov group BNS-symbol: P_C222
Shubnikov group OG-symbol: C_P222
Magnetic group type: 3 (Black & White:2)
Hall symbol: P 2 2 1'C
Generator list: -x,-y,z,1;x,-y,-z,1;x+1/2,y+1/2,z,-1
Crystal system: Orthorhombic
Crystallographic point group: 222
Magnetic point group: 2221'
Laue class: mmm
Space dimension: 3
Number of symmetry operators: 8
Multiplicity: 8
Centred: 1 (Acentric)
Inversion center: None
Number of translations: 0
Number of anti-translations: 1
Transformation to standard: a,b,c;0,0,0


Intel Compiler 19.1 Update 3
Terminate batch job (Y/N)?
^C
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---- Construction of the LibFullP l
Default: ifort compiler in rel
Usage: make_LibFullP ifort
make_LibFullP ifort debug
make_LibFullP gfortran
make_LibFullP gfortran deb
For using Winteracter, add the opt
Compilation of the source code (pl
Compiling the console mode of the
C:\Users\katcho\repos\progcfml\Full
C:\Users\katcho\repos\progcfml>cd
FullProf Suite
File Programs Settings FP Dimensions Tools Edit Results Help FullProf 2025
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Working Directory: C:\Users\katcho\software\FullProf_Suite\Examples\test
Browse
Code File: pbso4
Remove
Type: .pcr
Date: 20/04/22
desktop.ini
desktop.ini
python37
HDFView-2...
Camtasia 2020
FP_Suite 64bits
226806.nxs
Recycle Bin


science campus
THANK YOU!