

*Introduction to the programs of
the
FullProf Suite*

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Web site for the *FullProf Suite*

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

Or go to the ILL web site: <http://www.ill.eu>

Look for “users and science”, “groups and instruments”
“diffraction”, “software”, ...

The programs of the *FullProf Suite* are available for the
following platforms:

Windows, Linux and MacOS (Intel)

Web site:

<http://www.ill.eu/sites/fullprof/index.html>

FullProf Suite

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

[Introduction](#) · [What's new](#) · [Programs](#) · [Downloads](#) · [Examples & Tutorials](#) · [Support](#) · [References](#)

Name:	Version date:	Platform:	File size	Link:
FullProf_Suite Windows	Aug - 2008	Windows 9X/NT/2k/XP/Vista	33,234,165	Download
FullProf_Suite Linux	Aug - 2008	Linux - PC	34,623,623	Download
FullProf_Suite Mac	Aug - 2008	Mac OS - Intel	37,758,982	Download

INSTALLATION OF THE FULLPROF SUITE FOR WINDOWS

Download the package, which is an executable file (installer), in a temporary directory and run it. Follow the indications of the installer and pay attention not to use, for holding the files, directories with blanks or non ASCII character in their names

INSTALLATION OF THE FULLPROF SUITE FOR Mac OS AND/OR LINUX

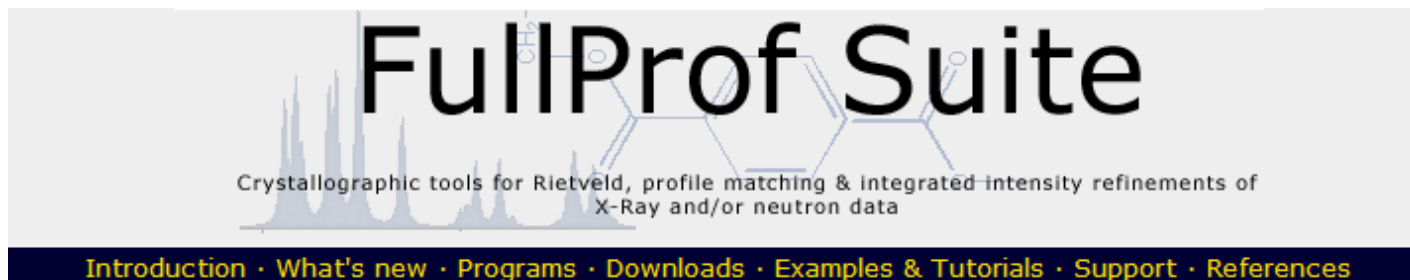
Download the file of the version you wish to install in your system from the WEB page of the FullProf Suite. The steps to follow are the following:

General Mode (for all the users of the system)

- 1.- Activate the super-user mode
- 2.- Create a directory in which you want to hold the programs of the FullProf_Suite.
For instance: /Applications/FullProf_Suite in Mac OS or
/usr/local/bin/FullProf_Suite in some Linux systems
- 3.- Copy the file FullProf_Suite_XXXNN_OP.tgz (XXX=Month NN=year, OP=Lin or Mac) in the directory just created in step 2

Web site:

<http://www.ill.eu/sites/fullprof/index.html>



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Available items in Catalogs section:

Name:	Description:	File size	Link:
FullProf Manual	Users' Guide of FullProf	1,769,341	Download

Available items in Tutorials section:

Name:	Description:	File size	Link:
Atlanta-doc	PDF-docs of a School in Atlanta	2,171,360	Download
ECM-21-Workshop	PDF-docs of ECM-21 Workshop	1,055,669	Download
Exercises-dat	Data files, FullProf exercises	54,250	Download
Exercises-pcr	PCR filese, FullProf exercises	35,608	Download
HoCu_Tutorial	Tutorial magnetic structure	1,130,682	Download
KTb3F12_Tutorial	Tutorial magnetic structure	501,244	Download
Microstructural_effects	Documents about microstructure	544,914	Download
pcr_dat	Data and PCR files	824,597	Download
size-sph	Notes about size effects	14,298	Download
sr_oxalate	Simulated annealing in FullProf	30,958	Download

Available items in Examples section:

Name:	Description:	File size	Link:
FullProf examples	A set of PCR examples files to run on FullProf program	546,446	Download

Programs of the FullProf Suite

FP_Suite_Toolbar: Program for accessing the whole set of the FullProf Suite.

WinPLOTTR / WinPLOTTR-2006: Programs for visualising powder diffraction patterns. Fitting independent peaks (CW and TOF), interface for FullProf and many of the programs of the FullProf Suite

FullProf : **Crystal and magnetic structure refinement**, powder/single crystals, polarised neutrons, constant wavelength, TOF, energy dispersive, multiple patterns, simulated annealing for **solving crystal and magnetic** structures (integrated and profile intensities).

EdPCR: Editor of the FullProf input control file

Fourier/GFourier and Bond_Str/GBond_Str. Fourier and distance/angle calculations.

SuperCell/K_Search: Program for searching propagation vectors

BasIREPS: Program for calculating basis functions of irreducible representations of space groups. Useful for determining magnetic structures .

Fp_Studio: Program for visualising crystal and magnetic structures

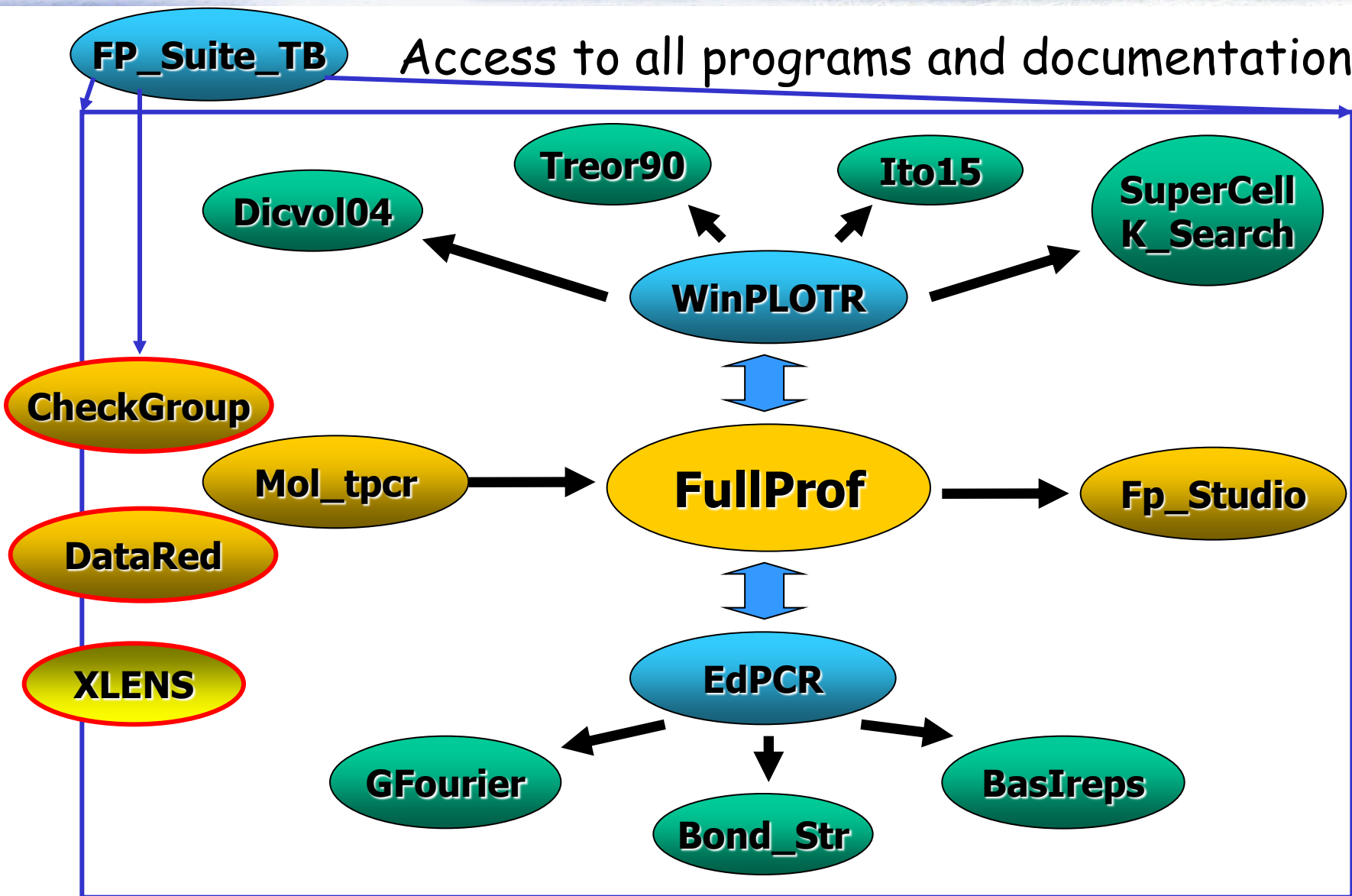
Check_Group: Program for getting the space group (powders and single crystals)

Datared/GDatared: Program for single crystal data reduction

Mol_tpcr: console utility for creating Rigid body groups

External programs: **DICVOL04, TREOR90, ITO, XLENS**

FullProf Suite



Toolbar of the FullProf Suite

File: Select working directory

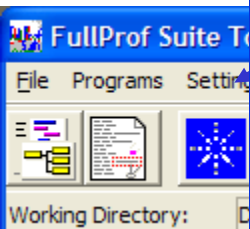
Run Programs



Edit current file

Charge PCR or recognised files

Setting of the Toolbar



Settings for FullProf Suite Toolbar

FullProf Suite Programs

FullProf:

WinPlotr:

General Programs

Editor: **My favourite text editor**

Browser:

PDF Viewer:

PS Viewer:

External Programs

Program 1:

Label Program:

Program 2:

Label Program:

Program 3:

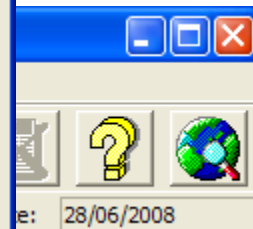
Label Program:

Program 4:

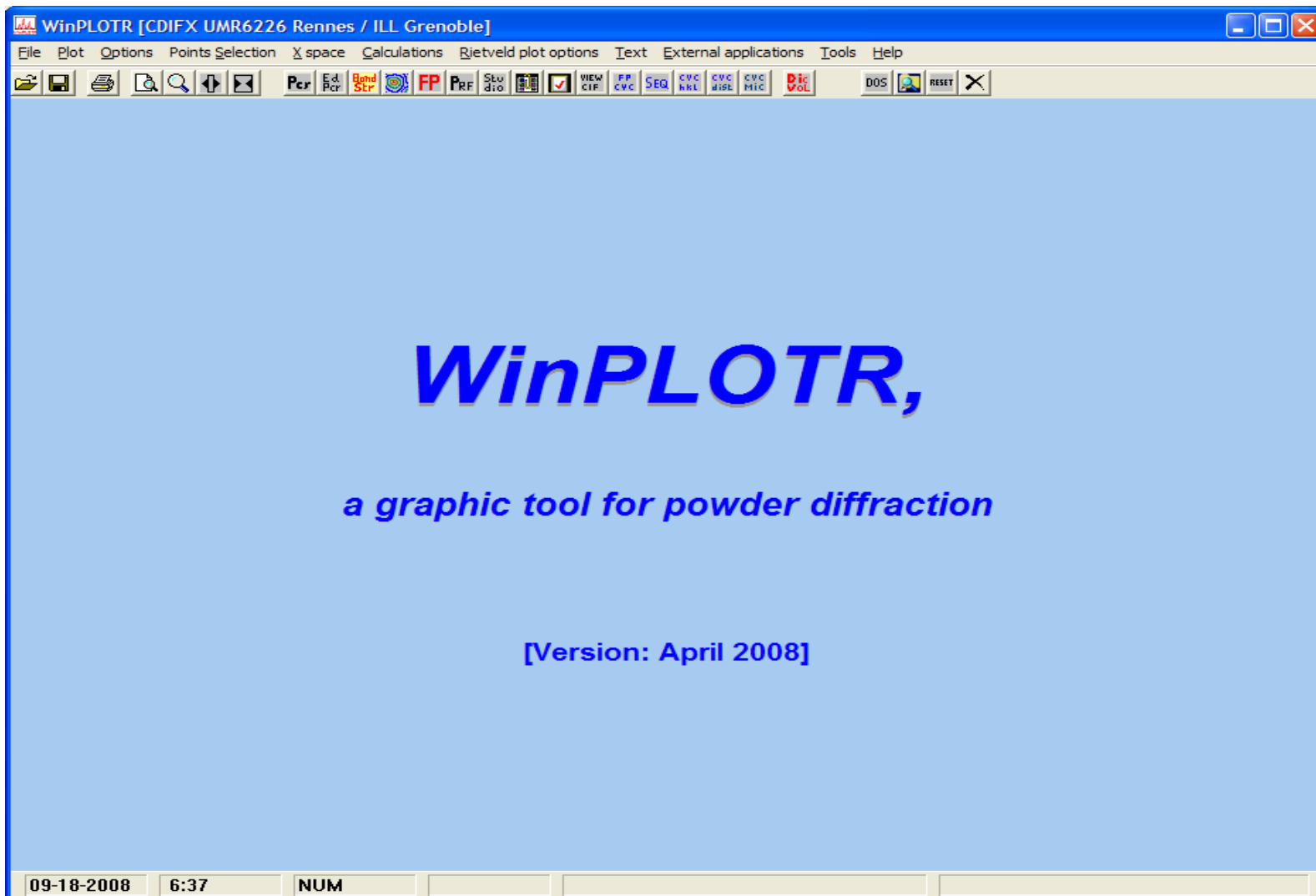
Label Program:

☐ Toolbar always on TOP

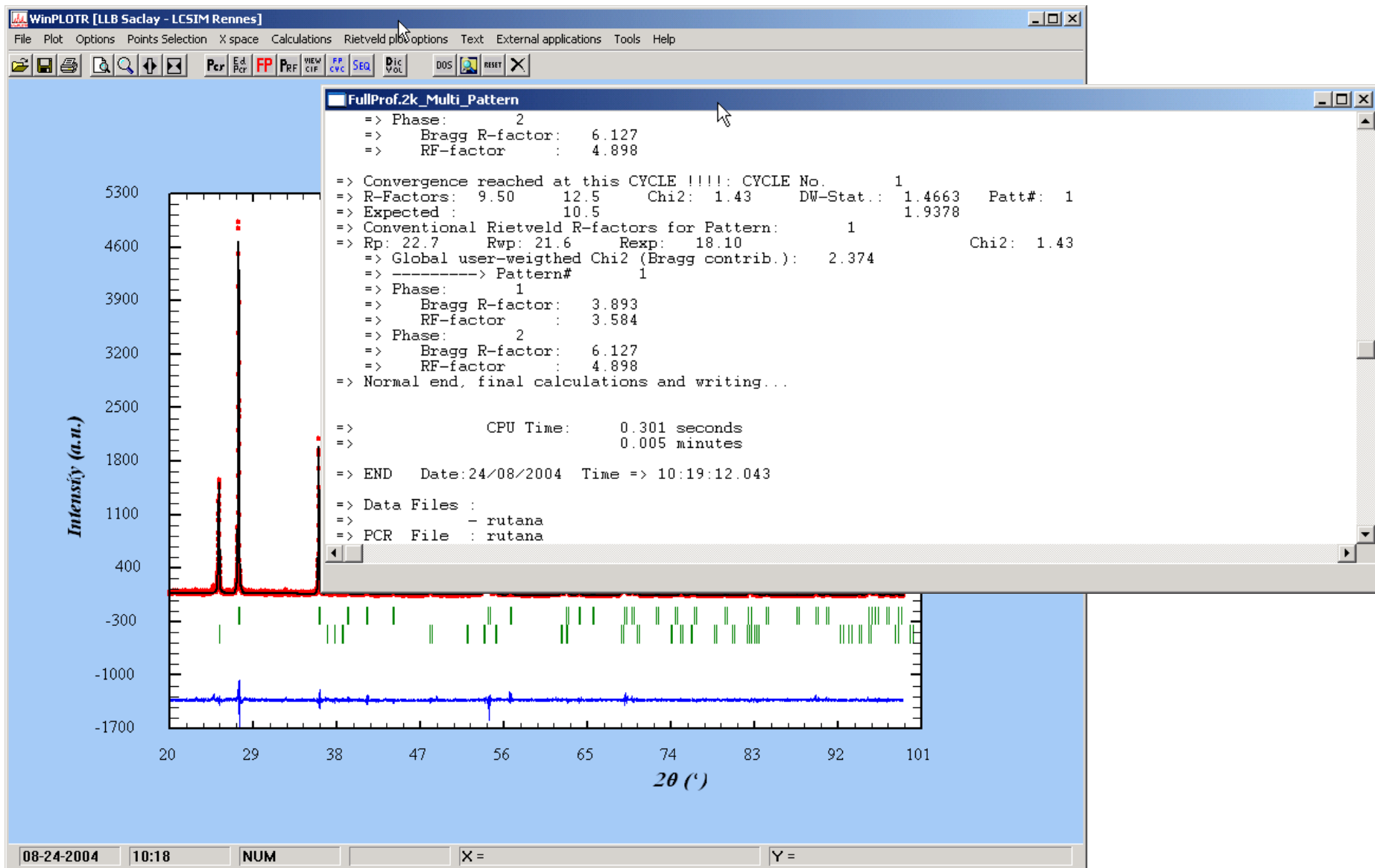
Prefix for console programs



WinPLOTTR: program to access the whole FullProf Suite



Running FullProf from WinPLOTR



WinPLOTR: reading the X-ray and neutron diffraction patterns, running indexing programs, fitting peaks, etc

Basics operations for configuring WinPLOTR

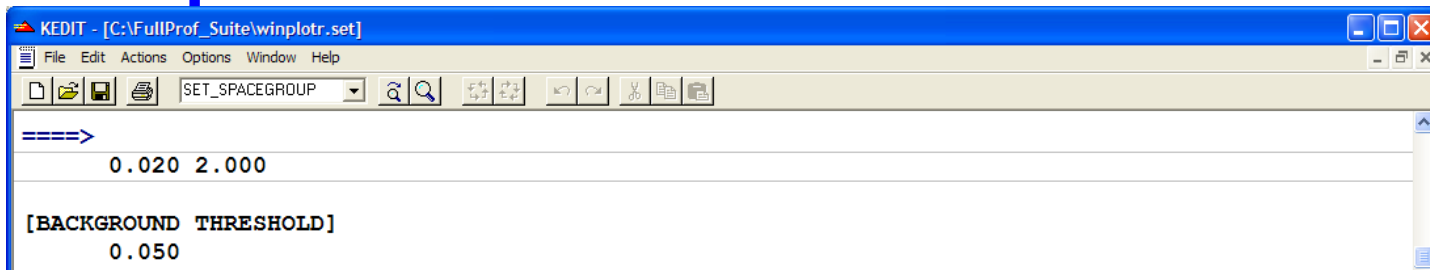
The file WinPLOTR.set

Accessing general applications, Explorer, Acrobat reader, ...

- 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
- 5: Making individual peak fits
- 6: Exporting a background file
- 7: Invoking other programs

Configuration of WinPLOTR

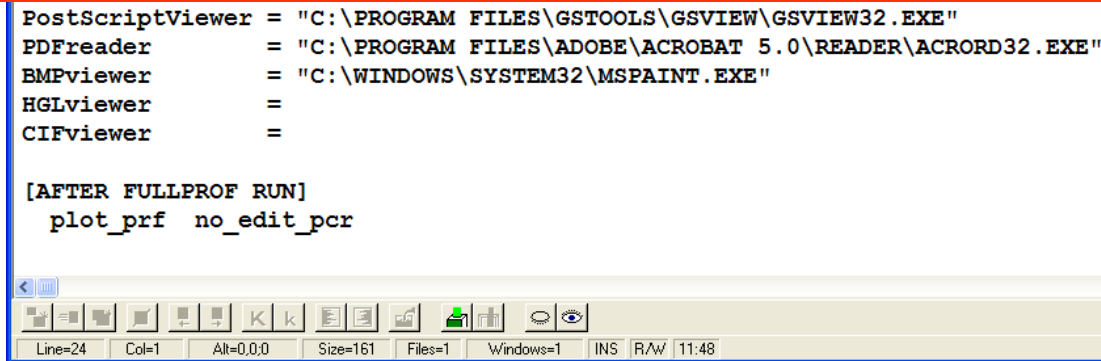
File: winplotr.set



```
KEDIT - [C:\FullProf_Suite\winplotr.set]
File Edit Actions Options Window Help
[Icons] SET_SPACEGROUP [Icons]
====>
0.020 2.000
[BACKGROUND THRESHOLD]
0.050
```


Not needed for WinPLOTR-2006!

The preferences can be selected using the mouse, and can be saved locally or globally!



```
KEDIT - [C:\FullProf_Suite\winplotr.set]
File Edit Actions Options Window Help
[Icons]
PostScriptViewer = "C:\PROGRAM FILES\GSTOOLS\GSVIEW\GSVIEW32.EXE"
PDFreader = "C:\PROGRAM FILES\ADOBE\ACROBAT 5.0\READER\ACRORD32.EXE"
BMPviewer = "C:\WINDOWS\SYSTEM32\MSPAINTE.EXE"
HGLviewer =
CIFviewer =
[AFTER FULLPROF RUN]
plot_prf no_edit_pcr
[Icons]
```

FullProf Suite for Windows, Linux and MacOS



WinPLOTR-2006 Version: 0.50

File Plot Profiles Options X space Calculations Ext. Applications Tools Help

Single refinement Sequential refinements

Buttons for running FullProf

WinPLOTR-2006

*a Powder Diffraction graphic tool
for Windows, Linux and MacOS*

Version: 0.50 April - 2008

Copyright (c) 2002-2005, JGP - JRC

Profiles: 0 Phases: 0 23/6/2006 1:35:29

My Computer

GIOT-BiCa-3D...

securite au travail.pps

y-2004, JRC-LLB)
ations of Space Groups
axial vector properties

Browse...

Brillouin Zone Label: X

Atoms in unit cell

y/a z/a

none

start

D:\Docs\Conferences...

Czech_Crystallograph...

Orlando_Mag_b.ppt

WinPLOTR-2006 Versi...

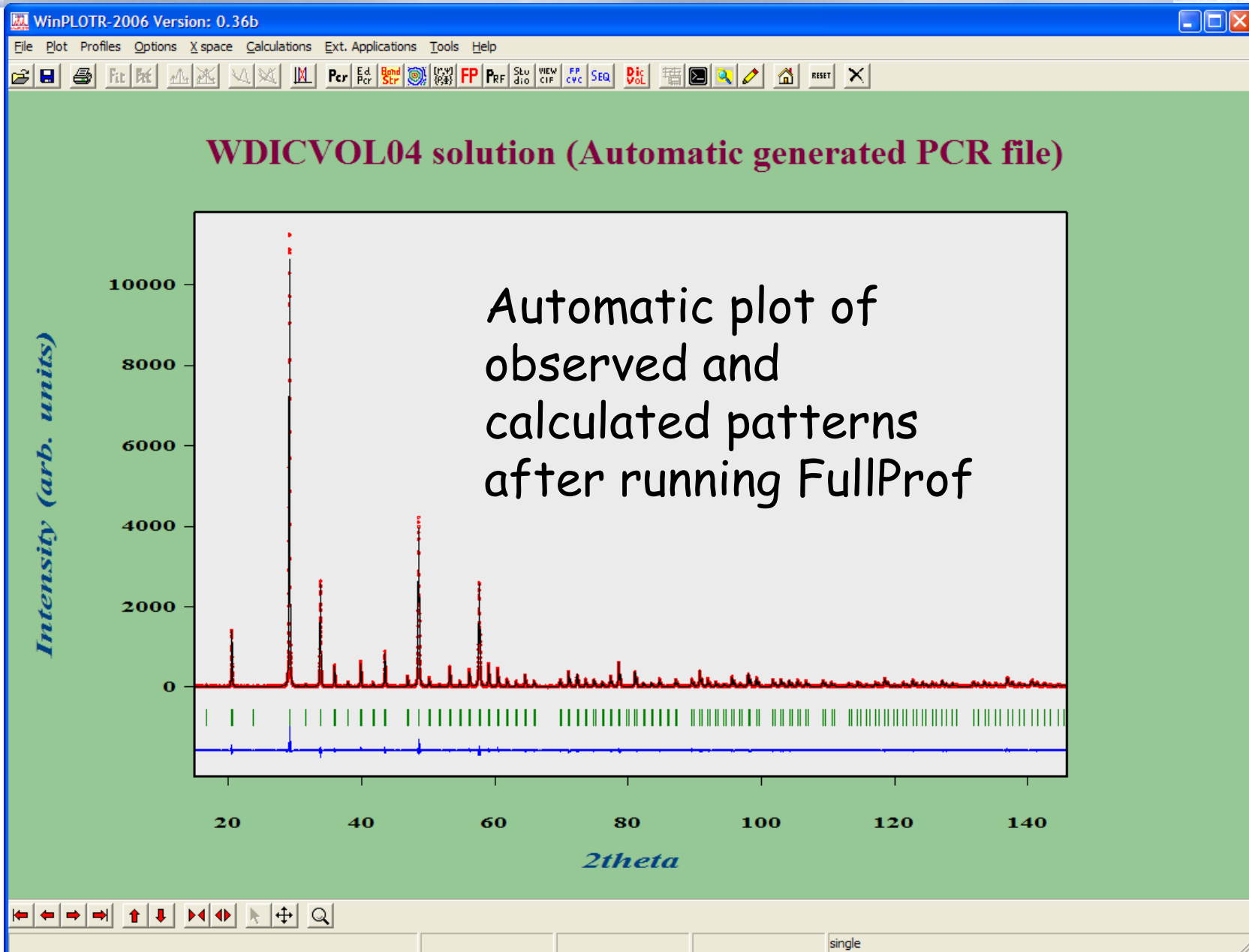
Bond_Str GU-Interface

FpStudio Ver-1.0

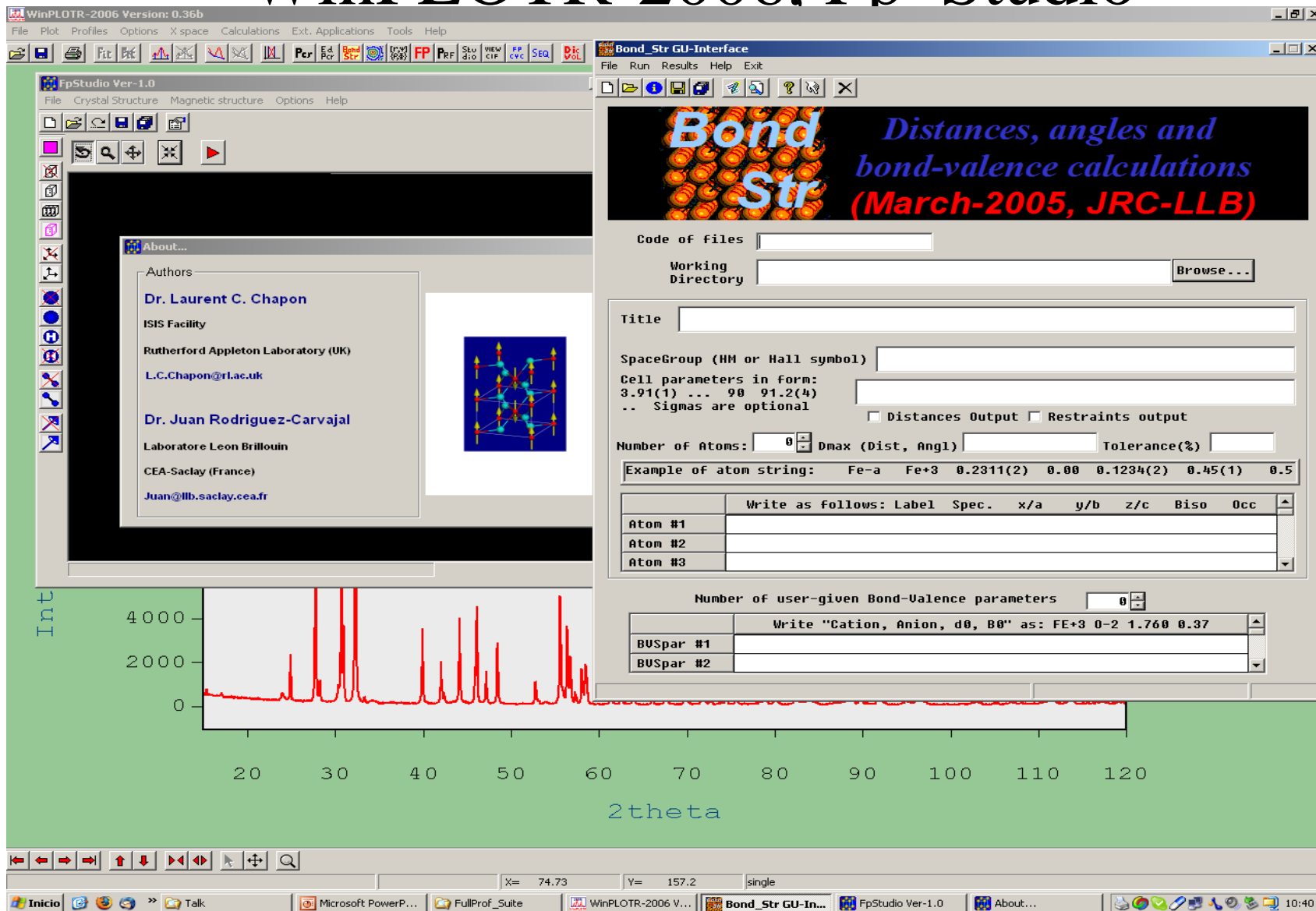
BasIreps Gui Interface

Editor of PCR Files

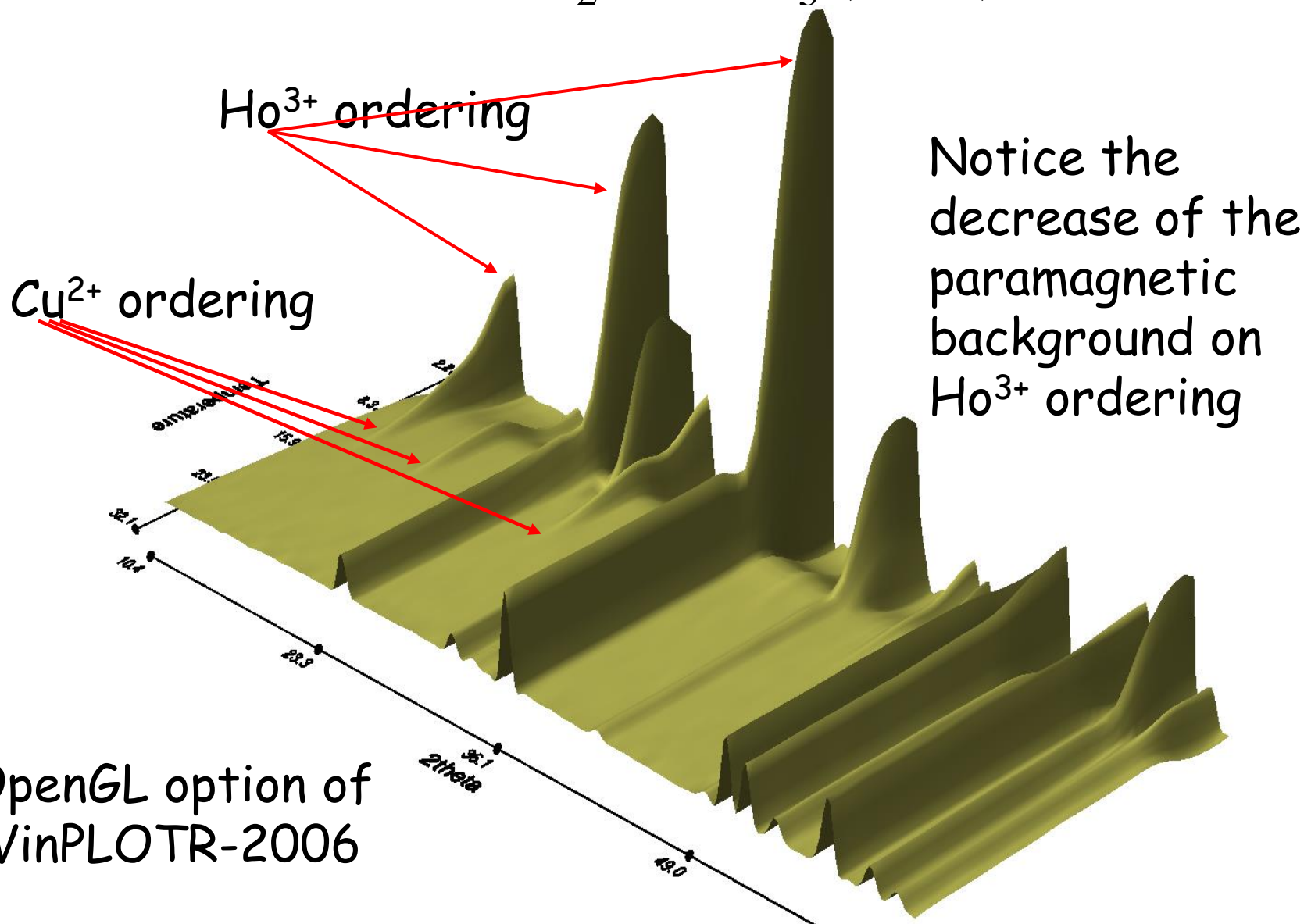
1:41 AM



FullProf Suite: Bond_Str, WinPLOTR-2006, Fp Studio



Magnetic ordering of Ho and Cu ions in $\text{Ho}_2\text{BaCuO}_5$ (D1B)



How to use the FullProf Suite: **Old way**

➔ **Open WinPLOT**

➔ A button on **WinPLOT** gives access to **EdPCR**

➔ Within **EdPCR** you have access to a series of programs of the **FullProf_Suite**

➔ **BasIreps**: Irreducible representations of space groups

➔ **GFourier**: Fourier maps

➔ **FullProf_Studio**: visualization Xtal & Magnetic Structures



Execute WinPLOT

How to use the FullProf Suite: **New way**

➔ **Open the ToolBar and select Working Directory**

➔ **Select the working file (normally a PCR file)**

➔ **When running a program it tries to use the code of the charged file for obtaining the input file**

➔ **Access to WinPLOTTR, EdPCR, Bond_Str, DicVOL, DataRed, CheckGroup, XLENS, etc**

➔ **BasIreps: Irreducible representations of space groups**

➔ **GFourier: Fourier maps**

➔ **FullProf_Studio: visualization Xtal & Magnetic Structures**



A program for analysis of diffraction patterns: *FullProf*

- A program for :
 - Simulation of powder diffraction patterns
 - Pattern decomposition \Rightarrow 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, 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

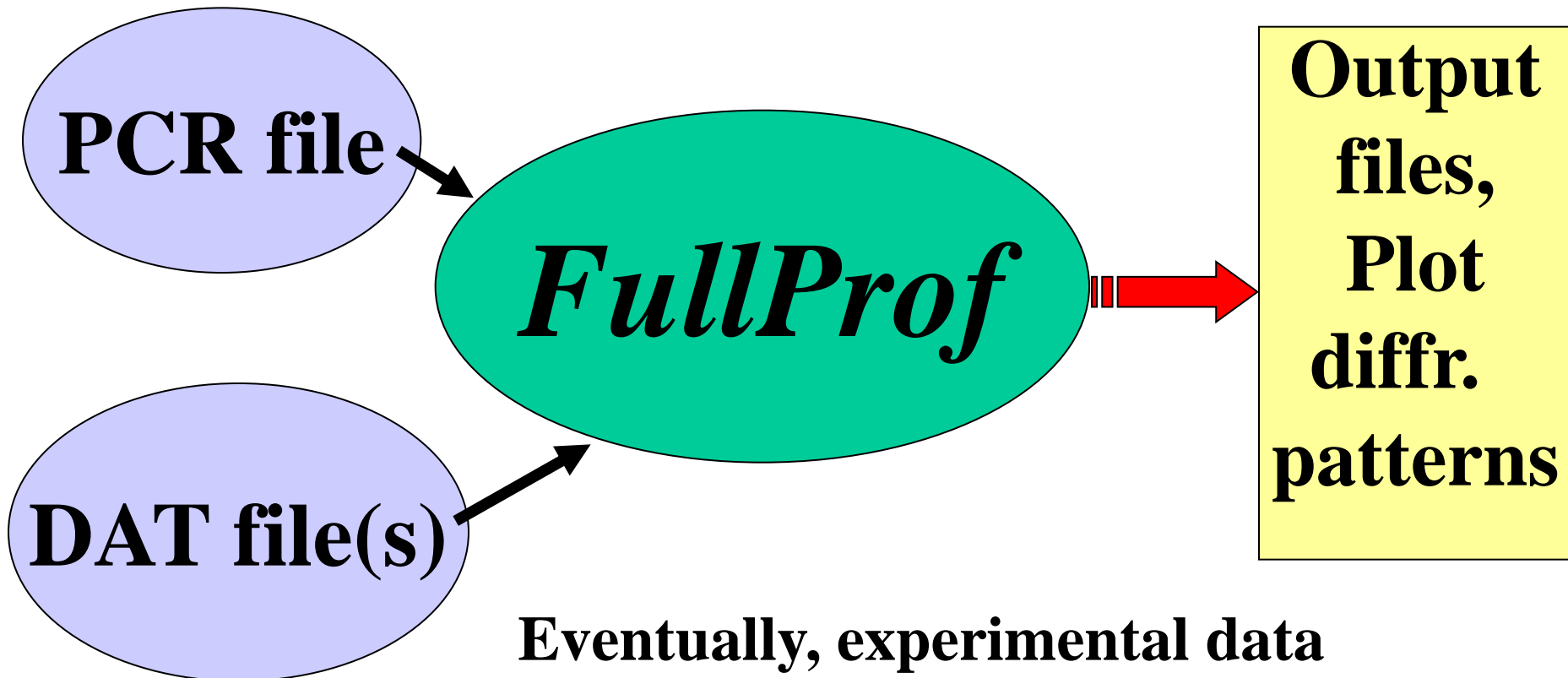
Inside the programs of the FullProf Suite

- **The programs are written in Fortran 95**
- **All of them are based in CrysFML: a series of Fortran 95 modules constituting a mathematical and crystallographic library.**
- **GUIs completely separated from the calculation kernels.**

How works *FullProf*

Minimal input:

Input control file (extension ‘*.pcr*’): PCR-file
Model, crystallographic/magnetic information





The PCR file: steep learning curve

DAT file(s)



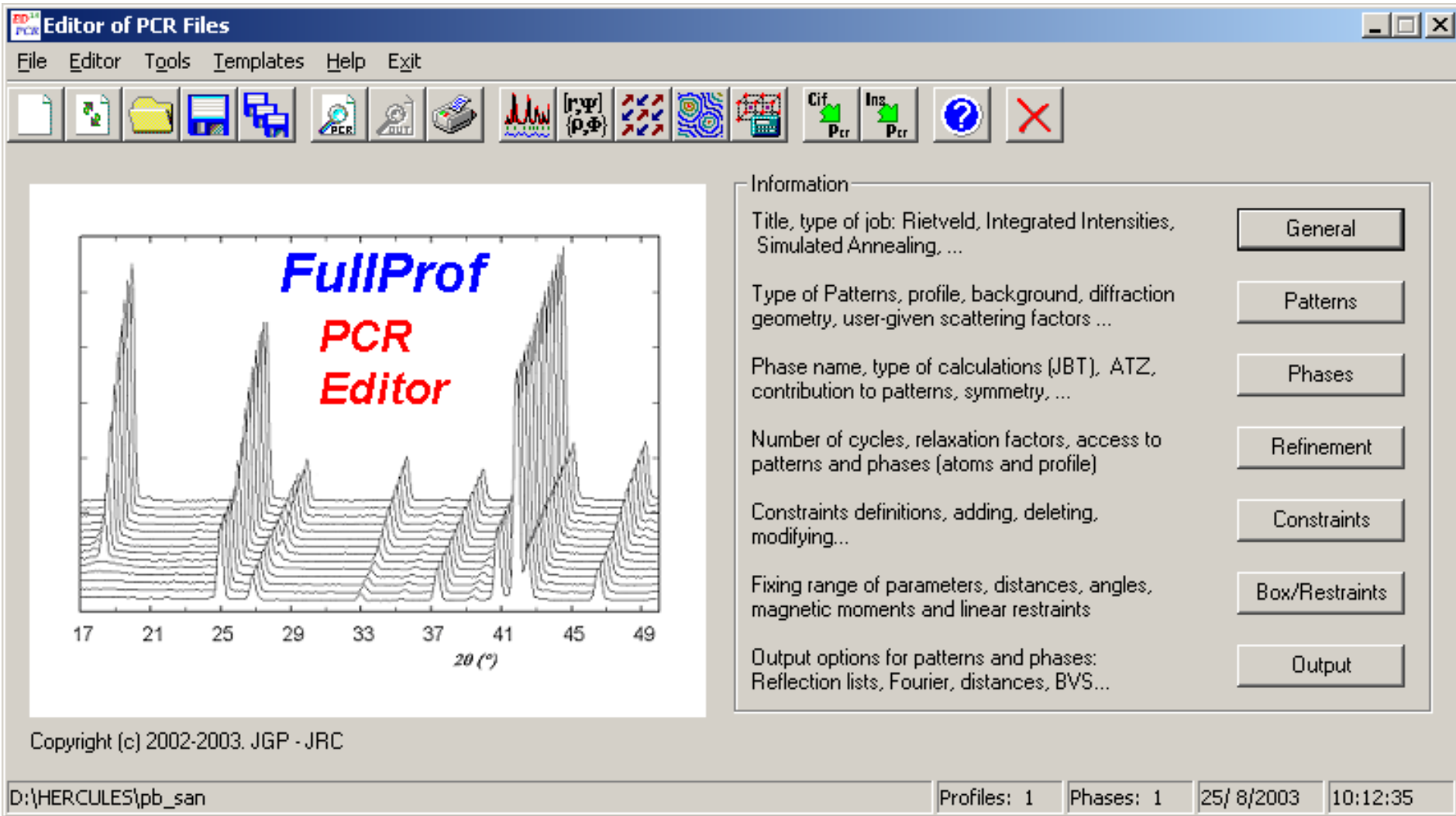
Format depending on the instrument, usually simple

PCR file

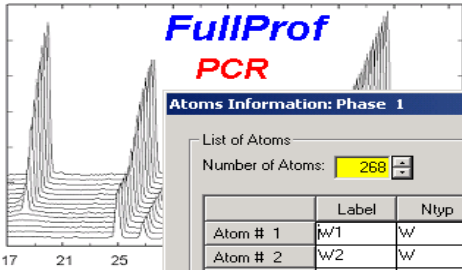


- ➔ **Many variables and options**
- ➔ **Complex to handle**
- ➔ **Hint: copy an existing (working) PCR-file and modify it for the user case, or...**
- ➔ **USE the new GUI: EdPCR**

A GUI for *FullProf*: EdPCR



GUI using Winteracter: <http://www.winteracter.com>



Copyright (c) 2002-2004. JG

Information

Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...

Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...

Phase name, type of calculations (IRT), ATZ

Atoms Information: Phase 1

List of Atoms

Number of Atoms: 268

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	W1	W	0.35526	0.27012	-0.03009	0.00000	1.00000	Anisotropic
Atom # 2	W2	W	0.40583	0.18486	0.04721	0.00000	1.00000	Anisotropic
Atom # 3	W3	W	0.58689	0.20667	-0.01618	0.00000	1.00000	Anisotropic
Atom # 4	PD1	PD	0.43553	0.08081	-0.01926	0.00000	1.00000	Anisotropic

Anisotropic Thermal Factors / Form Factors

	B11	B22	B33	B12	B13	B23
Atom # 1	0.00357	0.00219	0.00048	-0.00035	-0.00028	-0.00009
Atom # 2	0.00388	0.00209	0.00041	-0.00040	-0.00012	-0.00015
Atom # 3	0.00335	0.00215	0.00043	-0.00019	-0.00014	-0.00016
Atom # 4	0.00467	0.00211	0.00054	-0.00032	-0.00033	-0.00021

Special Form Factor

#	SASH-Type	Matrix	i=1	i=2	i=3	N. Coeff.	Indices	#1	#2	#3	#4	#5	#6
1	Spherical												
2	Spherical												
3	Spherical												

Refine Positions

Refine B_iso

Refine B_aniso

Fix All

Global 1.00

aded regions

Phase 6 P

Prop. Vectors

6 7

Unit Weights

Micro-Absorption

Reduction factor of number of data points: 0

Profile

HKL Shifts

Micro-Structure

Further Parameters

OK

Cancel

GUI for *BasIreps*

BasIreps Gui Interface

File Run Results Help Exit

Code of files:

Working Directory:

BasIreps (May-2004, JRC-LLB)
Irreducible representations of Space Groups
Basis functions of polar & axial vector properties

Title:

SpaceGroup (HM/Hall symbols) or generators separated by ",":

K-Vector: Brillouin Zone Label:

☒ Polar Vector ☐ Axial Vector

Number of Atoms:

☐ Explicit Sublattices ☒ Atoms in unit cell

	Symbol	x/a	y/a	z/a
Atom # 1	Tb3+	0.00000	0.00000	0.50000
Atom # 2	Tb4+	0.00000	0.50000	0.25000

Code of files

Title

k-vector

Axial/polar

Number of atoms

Working directory

Space group symbol or generators

Brillouin Zone label

Atoms in Unit Cell

Atoms positions

Example of *BasIreps* output: *.bsr

```

+++++
=> Basis functions of Representation IRrep( 1) of dimension  2 contained 3 times in GAMMA
+++++

```

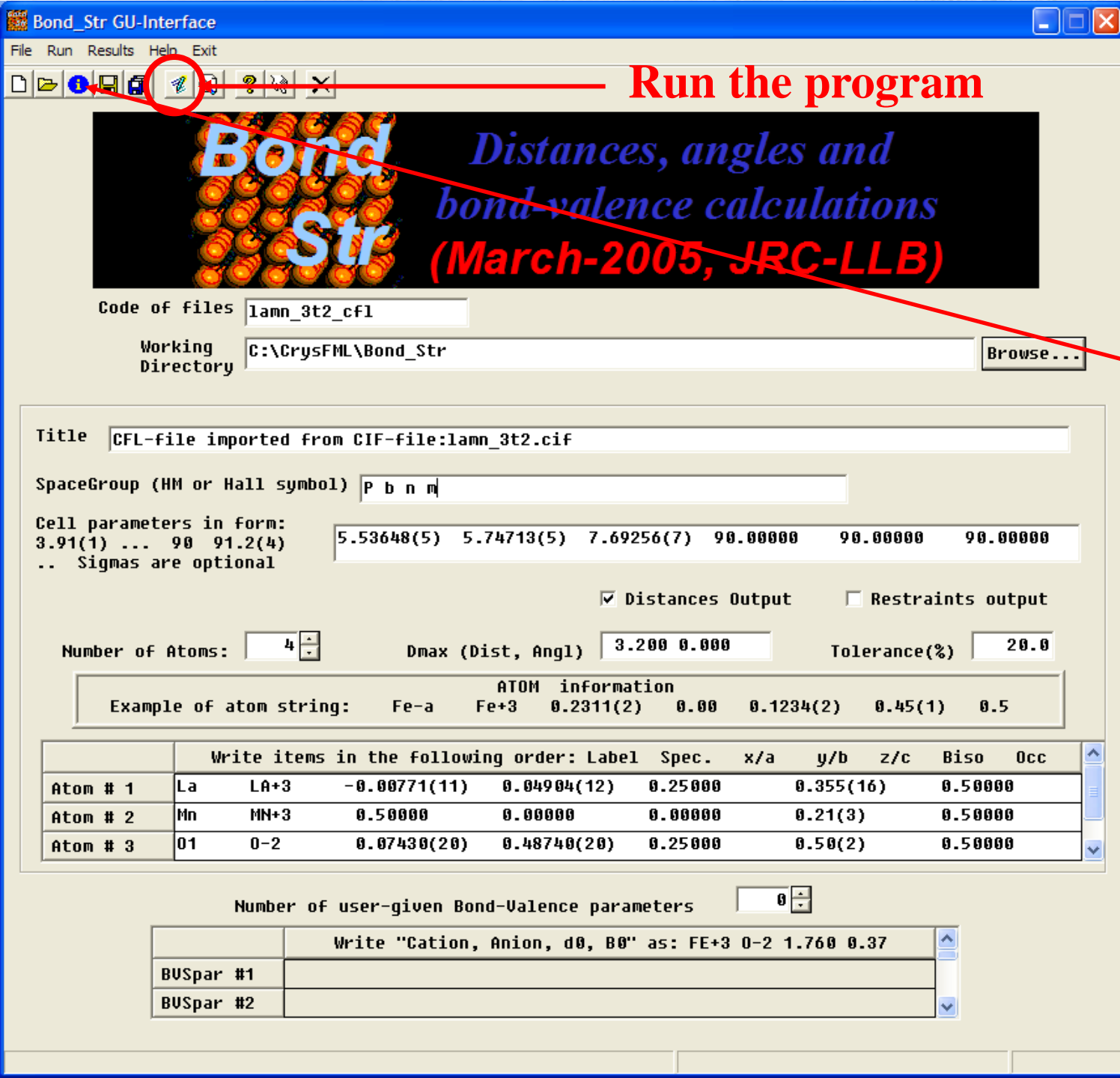
SYMM	x,y,z	-x+1/2,-y,z-1/2	y+3/4,-x+1/4,-z+3/4	-y+1/4,x+1/4,-z+3/4
Atoms:	Cu_1	Cu_2	Cu_3	Cu_4
1:Re	(1 0 0)	(0 0 0)	(0 -1 0)	(0 -1 0)
Im	(0 0 0)	(-1 0 0)	(0 0 0)	(0 0 0)
2:Re	(0 1 0)	(0 0 0)	(1 0 0)	(1 0 0)
Im	(0 0 0)	(0 -1 0)	(0 0 0)	(0 0 0)
3:Re	(0 0 1)	(0 0 0)	(0 0 -1)	(0 0 1)
Im	(0 0 0)	(0 0 1)	(0 0 0)	(0 0 0)
4:Re	(-1 0 0)	(0 0 0)	(0 0 0)	(0 0 0)
Im	(0 0 0)	(-1 0 0)	(0 1 0)	(0 -1 0)
5:Re	(0 1 0)	(0 0 0)	(0 0 0)	(0 0 0)
Im	(0 0 0)	(0 1 0)	(1 0 0)	(-1 0 0)
6:Re	(0 0 1)	(0 0 0)	(0 0 0)	(0 0 0)
Im	(0 0 0)	(0 0 -1)	(0 0 -1)	(0 0 -1)

```

----- LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....
General expressions of the Fourier coefficients Sk(i) i=1,2,...nat

```

SYMM x,y,z	Atom: Cu_1	0.0000	0.0000	0.5000
Sk(1): (u-p,v+q,w+r)				
SYMM -x+1/2,-y,z-1/2	Atom: Cu_2	0.5000	0.0000	0.0000
Sk(2): i.(-u-p,-v+q,w-r)				
SYMM y+3/4,-x+1/4,-z+3/4	Atom: Cu_3	0.7500	0.2500	0.2500
Sk(3): (v,-u,-w)+i.(q,p,-r)				
SYMM -y+1/4,x+1/4,-z+3/4	Atom: Cu_4	0.2500	0.2500	0.2500
Sk(4): (v,-u,w)+i.(-q,-p,-r)				



GUI for
Bond_Str

Can read
CIF files

```

Bond_Str Text Editor - [C:\CrysFML\Bond_Str\lamn_3t2_cfl.bvs]
File Edit Search
[Icons]

(01 )-(Mn ) : 1.9680( 2) 0.570( 0)

Coordination number: 4 Eff.Coord. number: 4.00 for atom: 01
Average distance : 2.2304( 5) Distortion: 142.929 xE-04
Predicted distance: 2.0165 Single bond-valence S= 0.500
Valence: -2.000
Sums: 1.994( 2)
Deviation from the Valence Sum Rule (r1,%dev): -0.006 0.277
{r1=Sumj(sij)-Ui, %dev=100abs(r1)/Ui}
Deviation from the Equal Valence Rule (r2): 0.090
{r2=<sij-<sij>rms}

-----
=> Bond-valence and coordination of atom: 02 occupancy: 1.000( 0)
-----

(02 )-(La ) : 2.6496( 11) 0.275( 1)
(02 )-(La ) : 2.6975( 10) 0.242( 1)
(02 )-(La ) : 2.4599( 11) 0.459( 1)
(02 )-(Mn ) : 2.1787( 10) 0.323( 1)
(02 )-(Mn ) : 1.9063( 10) 0.673( 2)

Coordination number: 5 Eff.Coord. number: 5.00 for atom: 02
Average distance : 2.3784( 5) Distortion: 157.256 xE-04
Predicted distance: 2.0990 Single bond-valence S= 0.400
Valence: -2.000
Sums: 1.972( 3)
Deviation from the Valence Sum Rule (r1,%dev): -0.028 1.408
{r1=Sumj(sij)-Ui, %dev=100abs(r1)/Ui}
Deviation from the Equal Valence Rule (r2): 0.158
{r2=<sij-<sij>rms}

=> Lines concerning predicted average distances and single
bond-valence values, as well as the deviations from the
Equal Valence Rule, apply only to those central atoms
having N coordination-atoms of the same chemical species.
(The term 'single bond-valence' refers to the valence value
of a single bond for a regular polyhedron, so S=Valence/N)

=> The Old Global Instability Index (GII) is calculated with the atoms of the asymmetric unit (Num_Atoms).
The normalized GII(a,b,c) below are calculated using the sum over asymmetric unit but multiplying
differences by the multiplicity of the site. N_Atoms_UCell is the total number of atoms in the
conventional unit cell. In all cases the result of the different expressions is multiplied by 100.0

=> Old Global Instability Index ( GII=SQRT{SUM{|BUS-abs(q)|^2}/Num_Atoms} ) = 11.80 /100
=> Normalized GII(a)= SUM {|BUS-abs(q)| *mult} /N_Atoms_UCell = 7.74 /100
=> Normalized GII(b)= SUM {|BUS-abs(q)| *mult/abs(q)}/N_Atoms_UCell = 2.79 %
=> Normalized GII(c)= SQRT{ SUM {|BUS-abs(q)|^2*mult} /N_Atoms_UCell}= 10.63 /100

```

Last minute changes in *FullProf*

Documented in “fp2k.inf”

In this file new features, as well as discovered bugs, of FullProf.2k are periodically documented. For details consult the manual of FullProf. From 10 May 2003, comments on the programs constituting the FullProf suite are also provided.

Juan Rodriguez-Carvajal (Institut Laue-Langevin, Grenoble, France)

>> 29 August 2008: New version of FullProf. Symmetry modes with AMPLIMODES.

- A new version of FullProf has been produced incorporating the possibility for refinement (powder, single crystals, simulated annealing) of amplitudes of symmetry modes. The present version is:

```
*****'  
** PROGRAM FullProf.2k (Version 4.40 - Aug2008-ILL JRC) **'  
*****'
```

- In the present version of FullProf the refinement of a crystal structure can be done in terms of symmetry adapted modes. FullProf uses the output of the program AMPLIMODES from the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/cryst/amplimodes.html>) The free parameters, instead of atom positions, are the amplitudes of symmetry modes. The provided atom positions should not be refined. They are given as a reference of the high symmetry (HS) phase described in the low symmetry (LS) frame.

This option is accessible by putting the variable JBT=6.

The input is exactly the same as for JBT=0, except that no refinement codes are allowed for atom positions. This is taken into account by the program when Aut=1 (automatic mode).

Some useful features in *FullProf*

- ➔ Facilities concerning symmetry, symmetry modes
- ➔ Automatic mode for handling refinement codes and symmetry constraints
- ➔ Rigid body refinements + distances and angles restraints
- ➔ Special form factors, sym. adapted spherical harmonics
- ➔ Simulated Annealing on integrated intensities or profile
- ➔ The treatment of micro-structural effects
- ➔ Different formats of the file containing the Instrumental Resolution Function (FPA)

Constraints: reduce the number of free parameters (rigid body refinements)

Restraints: same number of free parameters + additional observations

How to generate restraints for *FullProf*?

Bond_Str GU-Interface

File Run Results Help Exit

Bond Str Distances, angles and bond-valence calculations (March-2005, JRC-LLB)

Code of files

Working Directory

Title

SpaceGroup (HM or Hall symbol)

Cell parameters in form:
3.91(1) ... 90 91.2(4)
.. Sigmas are optional

☒ Distances Output ☐ Restraints output

Number of Atoms: Dmax (Dist, Angl) Tolerance(%)

Example of atom string: Fe-a Fe+3 0.2311(2) 0.00 0.1234(2) 0.45(1) 0.5

	Write as follows: Label Spec. x/a y/b z/c Biso Occ						
Atom # 1	O1	O	0.62500	0.12500	0.24440(20)	0.00000	
Atom # 2	N1	N	0.62500	0.12500	0.31283(13)	0.00000	
Atom # 3	C1	C	0.2018(3)	0.5578(4)	0.34516(14)	0.00000	

Number of user-given Bond-Valence parameters

Write "Cation, Anion, d0, B0" as: FE+3 O-2 1.760 0.37

BUSpar #1

BUSpar #2

1: Calculating distances from FullProf

2: Using Bond_Str importing a CIF file

Both programs generate a file called **CFML_Restraints.tpcr**

How to generate restraints for *FullProf*?

List of possible restraints:

At1	At2	ITnum	T1	T2	T3	DIST	SIGMA
O1	N1	1	0.00000	0.00000	0.00000	1.3393	0.0047
O1	C1	1	0.50000	-0.50000	0.00000	2.2874	0.0045
O1	C1	-2	0.25000	-0.25000	0.50000	3.3163	0.0041
O1	C2	-4	1.00000	-0.25000	-0.25000	3.1481	0.0046
O1	H1	1	0.50000	-0.50000	0.00000	2.5023	0.0051
.

Lines to be pasted into the PCR file

DFIX	1.33935	0.00467	O1	N1
DFIX	2.28738	0.00455	O1	C1_9.545
DFIX	3.31627	0.00413	O1	C1_24.545
DFIX	3.14808	0.00457	O1	C2_6.644
DFIX	2.50228	0.00510	O1	H1_9.545

In CFL format

Rigid body constraints

A utility called *mol_tpcr.exe* can be used to generate a piece of PCR file containing information about a rigid body.

It is possible to generate a CFL file from a CIF, using Bond_Str, and then, doing a minimal editing work, create an appropriate file for *mol_tpcr*

EdPCR allows an easy edition of Rigid Bodies (problem with free atoms!)

Atoms Information: Phase 1

Free Atoms

Number of free Atoms:

	Label	Ntyp	X	Y	Z	B	Occ
Atom #1							
Atom #2							
Atom #3							
Atom #4							

Rigid Block Definition

Number of rigid blocks:

	Name	N. Atoms	X	Y	Z	Theta	Phi	Chi
#1	PI	15	0.65878	0.83502	0.65264	-176.73500	-35.48800	-57.93300
#2	PJ	15	0.89814	0.59798	0.14645	173.65199	-41.87100	-20.48600
#3	PK	15	0.90823	0.84983	0.40316	177.82201	-47.27100	44.15800
#4	PL	15	0.90176	0.85152	0.88187	-2.53700	77.10600	-75.72900

Internal Coordinates

☐ Z Matrix Representation

	Type	R	Theta	Phi	B	Occ
#2	D	3.36743	170.05499	56.65600	8.80577	1.00000
#3	N	1.38667	0.00000	0.00000	3.83061	1.00000
#3	O	2.69269	0.00000	0.00000	3.71433	1.00000
#3	C	1.40761	58.80500	-90.00000	2.83613	1.00000

Buttons: Refine Positions, Refine B_iso, Fix All, Cancel, OK

PCR file generated by EdPCR

```

!-----
!  Data for PHASE number:    1  ==> Current R_Bragg for Pattern#  1:    4.95
!-----
C5H4NO(CH3) ,ESRF 10K
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ      Nvk Npr More
120   0   0 0.0 0.0 1.0   4   0   0   1   0      929.020    0   7   0
!
P 41
!Atom Typ      x      y      z      B      Occ      P6      THETA      PHI      Spc
!  r/xc/rho the/yc/phi phi/zc/z  X0      Y0      Z0      CHI      P16:SAT  DEG  KIND
PI1  N      0.65457  0.83848  0.58247  3.83061  1.00000  1.00000  -176.735  -35.488  0  #CONN C C 0 1.8
      0.00      0.00      0.00      0.00      0.00      0.00      0.00      111.00  121.00
      1.38667   0.000   0.000  0.65878  0.83502  0.65264  -57.933   0.000    1    0
      0.00      0.00      0.00      351.00  361.00  371.00  131.00
PI2  O      0.65070  0.84127  0.51616  3.71433  1.00000      0   0   0      0  #CONN C N 0 1.8
      0.00      0.00      0.00      0.00      0.00      0.00
      2.69269   0.000   0.000
      0.00      0.00      0.00
PI3  C      0.68712  0.76540  0.61290  2.83613  1.00000      0   0   0      0  #CONN O N 0 1.8
      0.00      0.00      0.00      0.00      0.00      0.00
      1.40761  58.805  -90.000
      0.00      0.00      0.00
PI4  C      0.62593  0.90874  0.61882  2.83613  1.00000      0   0   0      0  #CONN D C 0 1.2
      0.00      0.00      0.00      0.00      0.00      0.00
      1.40761  58.805   90.000
      0.00      0.00      0.00
. . . . .

```

Refinement of crystal structures using amplitudes of symmetry modes instead of atom positions in *FullProf*

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[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]

First announcement and pre-registration of a School on this server in 2009

CrystallographyOnline:
International School on
the Use and Applications
of the Bilbao
Crystallographic
Server

Sections

Retrieval Tools

Group-Subgroup
Representations
Solid State
Structure Utilities
Subperiodic
ICSDB

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Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups

Group - Subgroup Relations of Space Groups

SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups

Representing Theory Applications

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Refinement of crystal structures using amplitudes of symmetry modes instead of atom positions in *FullProf*

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Bilbao Crystallographic Server

- CELLSUPER**
10-2007: New version of program CELLSUPER.
- TRANPATH**
7-2007: Minor update and fixes.
- SUPERGROUPS**
6-2007: Added link to Wyckoff Positions splitting.
- SERIES**
1-2007: New version of series of maximal isomorphic subgroups for a given maximum index.
- SIMPLE RETRIEVAL TOOLS**
1-2007: Minor upgrade for GENPOS, WYCKPOS, MAXSUB and SERIES programs.
- HERMANN**
1-2007: New version of program HERMANN.
- SETSTRU**
1-2007: CIF input data, JMOL visualization and minor bugs fixed
- WPASSIGN & EQUIVSTRU**
1-2007: CIF input data and JMOL visualization

Results in text/plain format
Results in text/xml format

Bilbao Crystallographic Server
http://www.cryst.ehu.es

Solid State Theory Applications

SAM	Spectral Active Modes (IR and RAMAN Selection Rules)
NEUTRON	Neutron Scattering Selection Rules
SYMMODES	Primary and Secondary Modes for a Group - Subgroup pair
AMPLIMODES	Symmetry Mode Analysis
PSEUDO	Pseudosymmetry Search in a Structure
DOPE	Degree of Pseudosymmetry Estimation
BPLOT	Pseudosymmetry Search with KPLOT
TRANPATH	Transition Paths (Group not subgroup relations)

Structure Utilities

CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures to lower symmetry Space Group basis.
SETSTRU	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure

Subperiodic Groups: Layer, Rod and Frieze Groups Retrieval Tools

GENPOS	Generators and General Positions of Subperiodic Groups
WPOS	Wyckoff Positions of Subperiodic Groups
MAXSUB	Maximal Subgroups of Subperiodic Groups

Databases

ICSDb	Incommensurate Crystal Structure Database
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For comments, please mail to
cryst@wm.lc.ehu.es

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Tutorials on the FullProf Suite

Tutorial 1

How to extract structure factors from X-ray powder diffraction and solve the structure using direct space methods. A *trivial* example: Y_2O_3

Data: powder diffraction pattern or Y_2O_3

Tutorial 2

Tutorial on Magnetic Structure Determination and Refinement using Neutron Powder Diffraction and FULLPROF

Data: LaMnO₃ at 150K and 50K

PCR file with the crystal structure at 150K

Tutorials on the FullProf Suite

Tutorial 3

How to work with symmetry modes using FullProf and AMPLIMODES.

Two simple examples: CaTiO_3 and LaMnO_3

Data: powder diffraction patterns of CaTiO_3 and LaMnO_3 .

Tutorial 4

How to use restraints and the rigid body description of molecular fragments in the program FullProf.

Data: Sr-oxalate, naphthalene, urea

PCR files