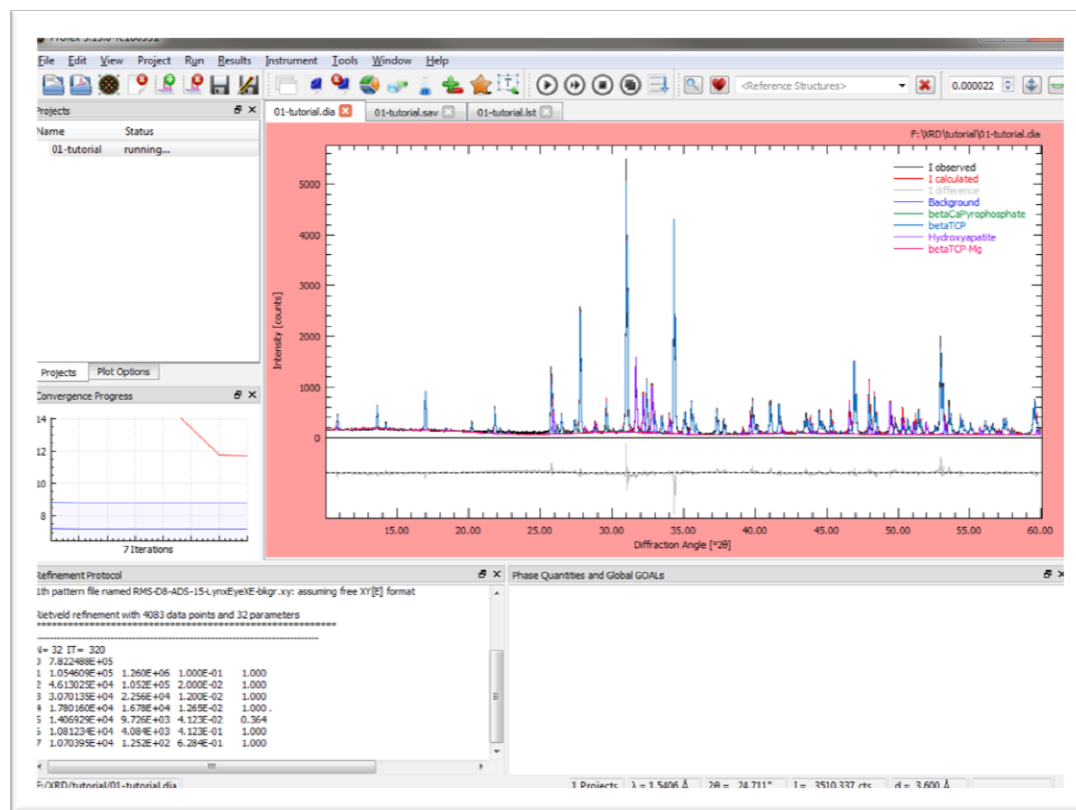


PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

New features in Profex 3.13

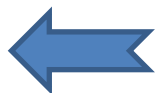
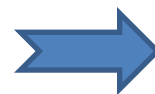


PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

```
% SampleID:  
% Theoretical instrumental function  
VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq  
% Wavelength  
LAMBDA=CU  
% Phases  
STRUC[1]=betaCPP.str  
STRUC[2]=betaTCP.str  
STRUC[3]=Hydroxylapatite.str  
STRUC[4]=betaTCP-Mg.str  
% Measured background  
UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy  
RU=10  
% Measured data  
VAL[1]=01-tutorial.xy  
% Minimum Angle (2theta)  
WMIN=10  
% Maximum Angle (2theta)  
% WMAX=60  
% Result list output
```

F7



```
% SampleID:  
% Theoretical instrumental function  
VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq  
% Wavelength  
LAMBDA=CU  
% Phases  
STRUC[1]=betaCPP.str  
% STRUC[2]=betaTCP.str  
STRUC[2]=Hydroxylapatite.str  
STRUC[3]=betaTCP-Mg.str  
% Measured background  
UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy  
RU=10  
% Measured data  
VAL[1]=01-tutorial.xy  
% Minimum Angle (2theta)  
WMIN=10  
% Maximum Angle (2theta)  
% WMAX=60  
% Result list output
```

Comment / Uncomment lines using the F7 key

Remaining structures and parameters will
automatically be re-numbered

PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

F4 key opens file manager

The screenshot shows the Profex 3.13.0-rc180531 software interface. The main window displays a plot of Intensity [counts] versus Diffraction (2θ) for 'Serie 2_Tag 1 (15.04.2015) ND / 5% CPP'. The plot shows a series of sharp peaks on a noisy baseline. The y-axis ranges from 0 to 6000, and the x-axis ranges from 5.00 to 30.00. The status bar at the bottom indicates 'F:\XRD\tutorial\01-tutorial.raw' and '1 Projects λ = 1.54'.

On the left side, there is a 'Projects' panel with a table showing the current project:

Name	Status
01-tutorial	idle

Below the projects panel is a 'Convergence Progress' plot showing 'Iterations' on the x-axis (0 to 100) and a y-axis representing progress (0 to 100). The plot shows a series of peaks that increase in height as iterations progress.

At the bottom left, the 'Refinement Protocol' panel displays 'Phase Quantities and Global GOALS' with a table of parameters:

Parameter, Goal	Value	ES
betaCPP/sum	0.0448	0.0
betaTCP/sum	0.6393	0.0
HAp/sum	0.1913	0.0
betaTCPMg/sum	0.1246	0.0

On the right side, a file manager window is open, showing the contents of the 'F:\XRD\tutorial' directory. The window lists various files and folders, including '01-tutorial.dia', '01-tutorial.lst', '01-tutorial.par', '01-tutorial.raw', '01-tutorial.sav', '01-tutorial.xy', 'betaCPP.str', 'betaTCP.str', 'betaTCP-Mg.str', 'Hydroxylapatite.str', 'RMS-D8-ADS-15-Ly...', and 'RMS-D8-ADS-15-Ly...'. The status bar at the bottom of the file manager indicates '14 Elemente'.

A blue arrow points from the 'F4' key icon to the file manager window, indicating that pressing the F4 key opens the file manager.

PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

Base Line

Scan: Serie 2_Tag 1 (15.04.2015) ND / 5% CPP

Algorithm: Golotvin-Williams

Parameters

Data smoothing M: 3

Window Size N: 10

Noise Multiplier n: 1.00

Sampling steps: 20

Sensitivity: 3

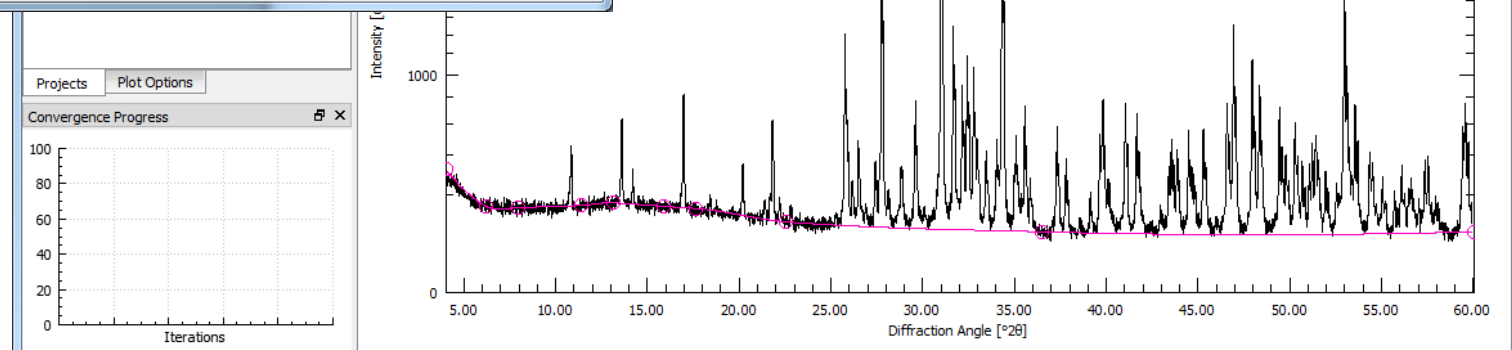
Last Point: Last match

Interpolation: Akima Spline

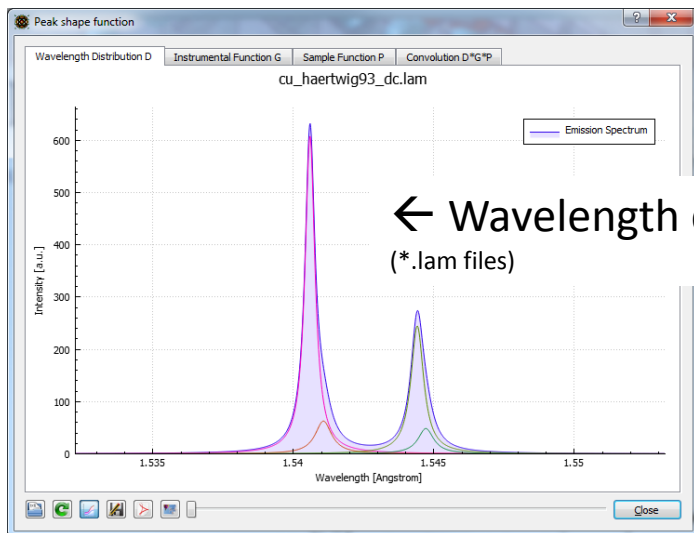
	2theta	Intensity
1	4.00000	317.00
2	6.21742	154.71
3	7.95706	150.57
4	11.41183	158.71
5	13.15146	168.14
6	15.87117	155.29
7	17.61081	147.29
8	22.53569	104.00
9	36.52628	76.43
10	60.01136	76.43

Append OK Cancel

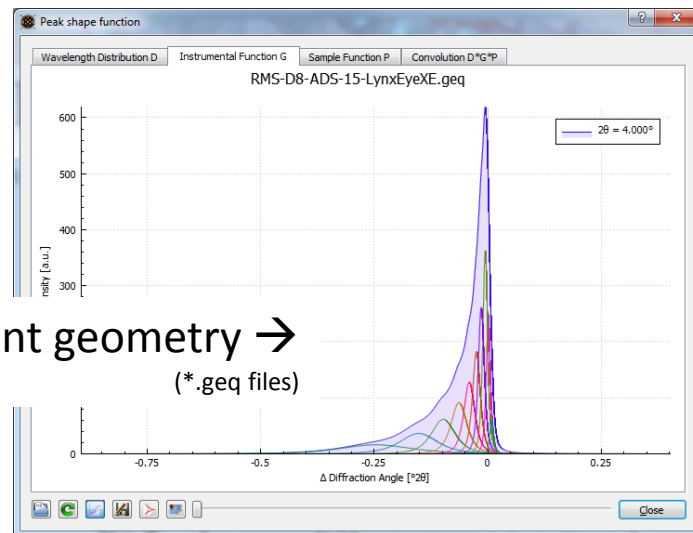
Manually add a base line



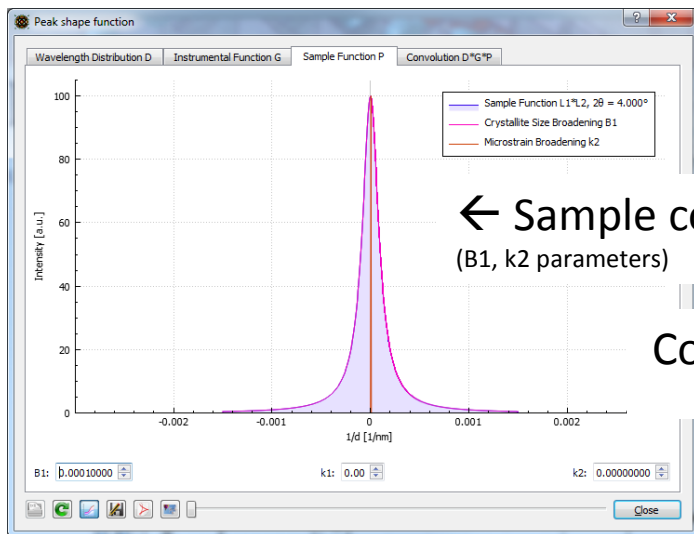
Visualization of peak profile contributions:



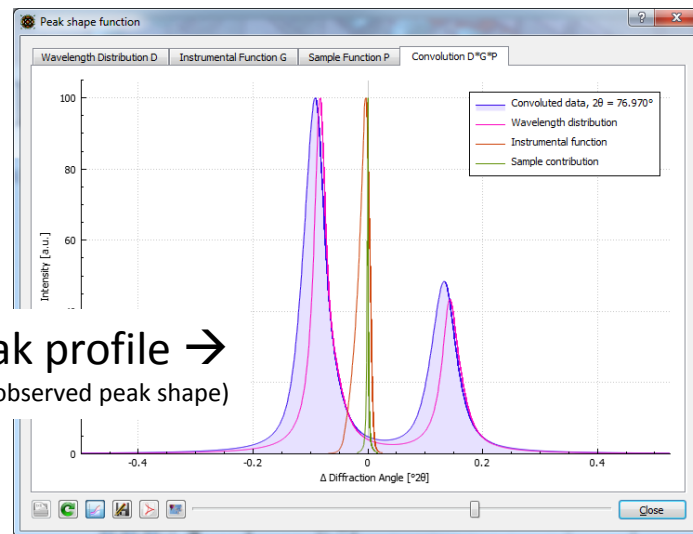
← Wavelength distribution
(* .lam files)



Instrument geometry →
(* .geq files)



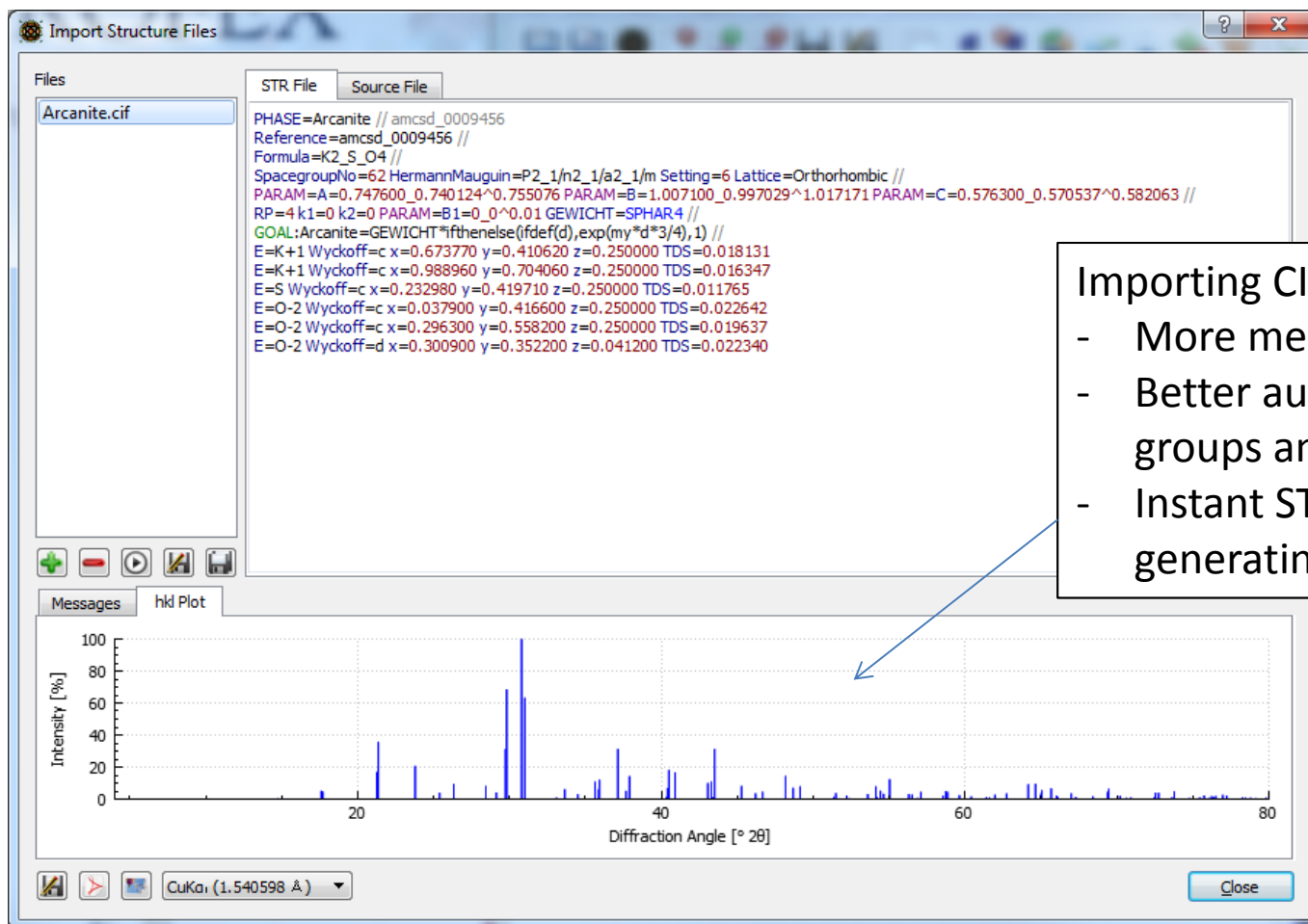
← Sample contribution
(B1, k2 parameters)



Convoluted peak profile →
(observed peak shape)

PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT



Importing CIF files:

- More meaningful error messages
- Better autodetection of space groups and settings
- Instant STR file verification by generating hkl lines

+ many more improvements:

- Open project ZIP archives
- Open multi-scan files as multi-val projects
- Changed behaviour of sample height displacement: Now shifting the measured pattern
- Presets store baselines and peak integrals
- Correct reading of neutron diffraction *.dia files
- Updated FullProf.2k module
- Various bug fixes

