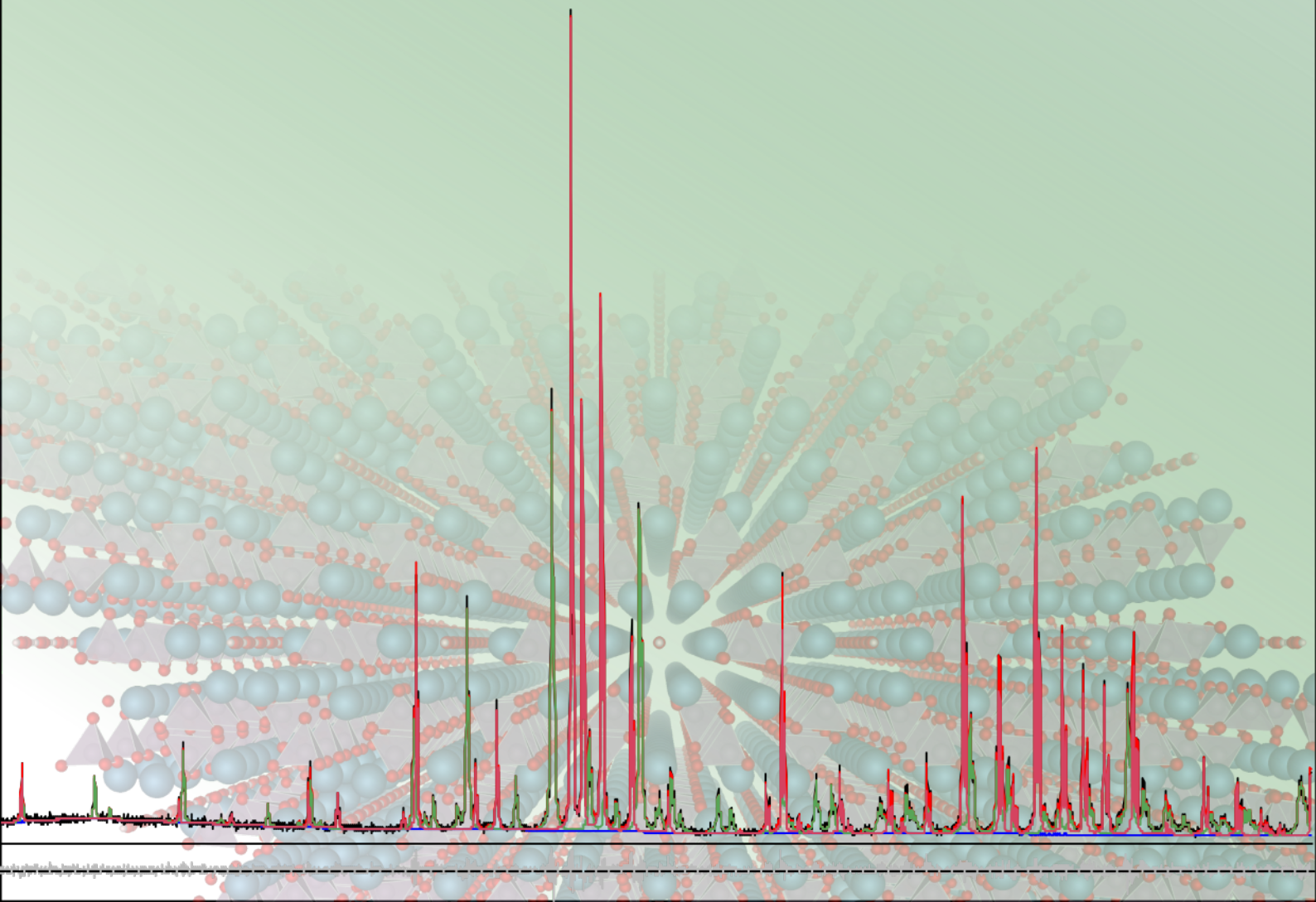
Profex User Manual

Version 4.3

Part 3: User Interface

Nicola Döbelin

January 25, 2021



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https://www.profex-xrd.org

Contents

1 Main Window

The program's main window features a menu bar and several tool bars to access all functions and settings (Fig. 1). The central area of the main window is occupied by the plot area, and optionally one or several text editors, which are accessible by tabs at the top of the plot area. The plot area cannot be closed, but text editors can be closed by clicking the close button on their tab.

The central area is surrounded by several dockable windows showing additional information and giving access to more features. These dockable windows can be closed and opened from the „Window" menu. They can also be re-arranged (Fig. 2) by clicking on the title bar showing the window's name, and dragging it to another location. Dockable windows can be stacked on top of each other to hide less frequently used windows, or detached from the main window, e. g. to be placed on another screen, or closed.

1.1 User Interface Elements

The following list explains the elements of the user interface shown in Fig. 1 in more detail.

1 Menu and tool bars give access to most features, as well as the program's preferences. All menu items are explained in section 2.

2 Projects list lists all open projects and the refinement status. Selecting a project from this list will make it the current project and show it in the central plot area. A right-click menu gives access to more functions. Several projects can be selected for various actions, but only one project can be the current project.

3 Plot options lists all scans loaded in the plot area. The „Show" checkbox can be used to show/hide certain scans to customize the appearance of the plot. A right click menu is available for direct access to certain functions.

4 Convergence progress shows the goodness of fit values R_{wp}. R_{exp} and χ^2 of the running refinement. A right click menu gives access to more functions. Clicking on the graph with the left mouse button toggles between two predefined zoom states.

5 Refinement protocol shows output generated by the refinement backend.

6 Plot area displays raw or refined scans, and opens text editors for control files, results files, structure files, or generic text files.

7 File tabs give access to all open files of a project. Files can be closed by clicking the $\otimes$ icon. Note that the first tab showing the graph cannot be closed. Double-clicking a tab synchronizes all other open projects to show the same type of file.

8 Reference structure tool bar allows to select reference structures to display *hkl* indices, as well as to start scanning and indexing new structure files. See section 1.5 for more information.

9 Sample displacement tool bar shows the current amount of vertical sample displacement resulting in horizontal shift of the diffraction pattern. The buttons allow toggling between 0 and the refined value.

10 Search-match This module allows to configure the search-match parameters (select database, instrument, refinement parameters) and shows the score list after the search-match process completes.

11 Global Parameters and GOALs shows a summary table of refined global parameters. Listing EPS parameters can be configured in the program's preferences dialog.

12 Status bar shows various information such as mouse cursor coordinates on the graph, and the wavelength used to transform 2θ angles to d values.

(not shown) Context help shows the context help text when pressing „F1" on a keyword in a control file.

(not shown) Local Parameters and GOALs shows a summary table of refined local parameters. The parameters shown here can be customized in the program's preferences dialog.

(not shown) Chemical composition shows the bulk chemical composition of all crystalline phases, calculated from refined crystal structures and phase quantities.

(not shown) Peak integrals shows the currently defined peak integrals.

(not shown) Peak detection Shows list of peaks detected by the peak detection function („Run → Peak detection").

1.2 Dockable windows

All windows arranged around the central plot and editor area (no. 2–5, 10, 11 in Fig. 1) can be rearranged or closed to match the user's preferences. They are called dockable windows, because they can be docked to different areas of the main window. Some examples are shown in Fig. 2 and explained below:

Moving: Grab the dockable window at it's title bar (e. g. the bar (green rectangles on Fig. 2) and drag it to a different location. If the window can be docked, the area will be highlighted.

Stacking: Drag the dockable window onto another dockable window. The dragged window will be stacked on top. Tab buttons will automatically appear to give access to both windows. Unlimited numbers of windows can be stacked.

Detaching: Drag a window outside of the main window and release it when no dockable area is highlighted. The window is now detached from the main window and floating freely on the screen. Use this configuration to place windows on a second screen. Detached windows can also be stacked. Drag the detached window back into the main window to dock it.

Closing / Opening: Dockable windows can be closed by clicking on the close button (x) in the title bar. To open it again, use the menu „Window" in the main window's menu bar.

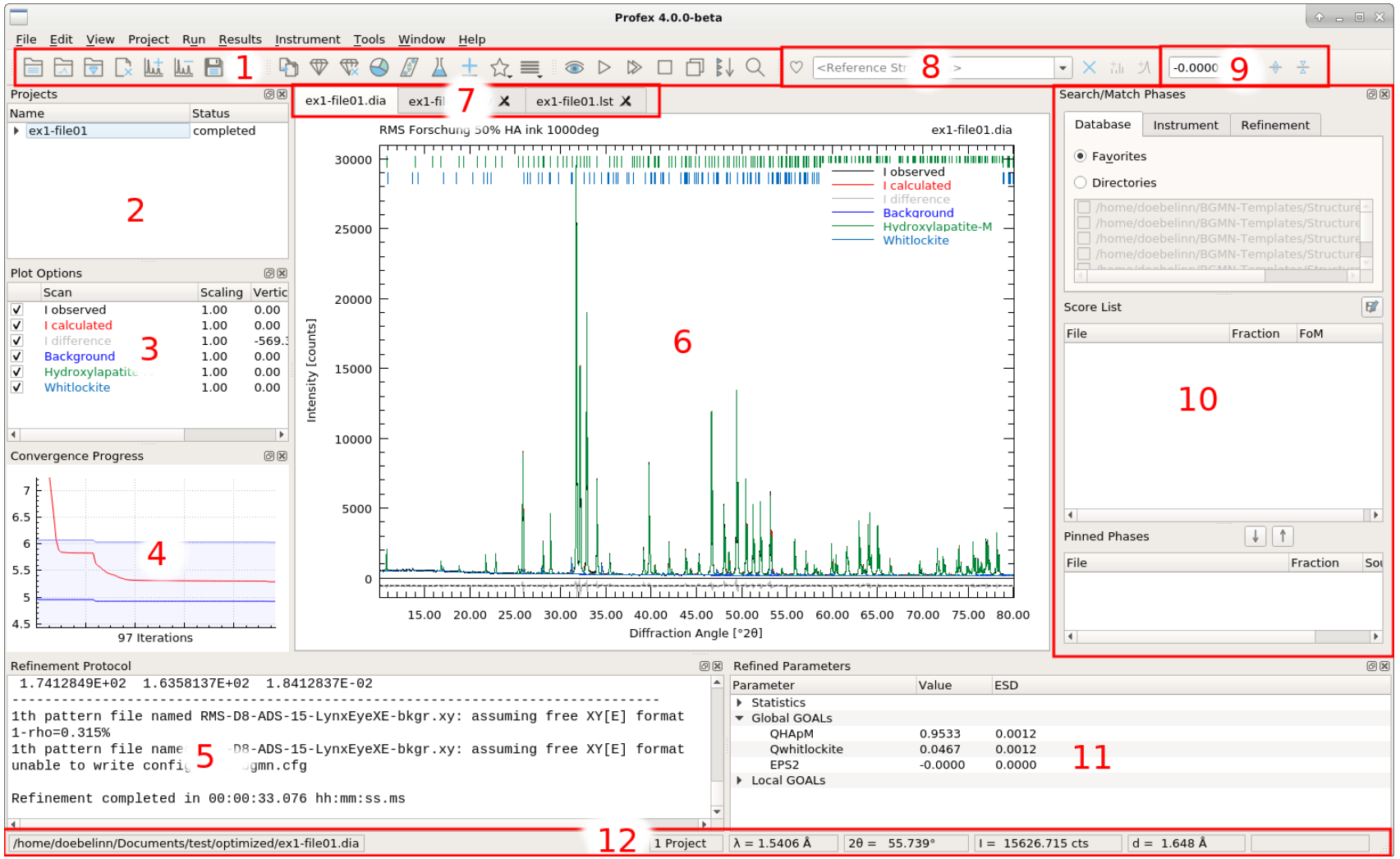


Figure 1: The Profex main window. Elements 1–12 are described in section 1.1.

1.2.1 Projects

This list shows all open projects and their current status. Click on a project to view it in the plot and editor area. Most actions from the menu and toolbar will apply to the currently shown project. Each project item can be expanded to show additional information (project type, sample ID, file path).

Projects can be edited while another project is refining. Multiple projects can be refined at a time, but refinement may be slow depending on CPU power and number of CPU cores.

Running a batch refinement (see section 2.5) will allow to refine several projects in a sequence, rather than parallel.

Several projects can be selected with the mouse by holding the Control or Shift keys. Some actions such as closing, batch refining, results export, etc. will be applied to all selected projects.

Mouse context menu actions are described below:

Start refinement Starts the refinement of the current project.

Close selected projects Closes all selected projects.

Export project data Exports the information shown in the Projects list of all open projects to a CSV file.

Expand all Expands the sub-items of all open projects.

Collapse all Collapses the sub-items of all open projects.

1.2.2 Plot options

This list shows all scans loaded in the currently shown project. To change the scans' drawing style (color, line style, line width), refer to the graph preferences discussed in section 3.3.

If a scan is clicked on with the mouse, it is set to active, as indicated by the symbol ,,A" shown next to the checkbox. Clicking it again will deactivate the scan. Active scans are shown in bolder line width than inactive scans. Only one scan can be set to active at a time. The active scan can be scaled by holding the middle mouse button and moving the mouse vertically. Clicking with the right mouse button will reset the scale. If a rescaled scan is deactivated, it will not be reset by a right mouse click anymore, until it is activated again. The only purpose of activating scans is to visually highlight them and to allow mouse scaling. Currently there is no other functionality related to scan activation.

Visibility of each scan can be changed by checking or unchecking the box in front of the scan name. For refined scans Profex distinguishes between main scans (usually I_{obs}, I_{calc}, I_{diff}, and the background curve), as well as phase patterns. All phase patterns can be toggled on or off at once by using the function ,,View $\rightarrow$ Show/Hide phase patterns". This change is persistent and applies to all open projects. It is a convenience function for easy showing or hiding all phase patterns, but

the same result can be obtained by manually checking or unchecking all phase patterns of all open projects.

hkl tick marks are considered as part of phase patterns. Showing/hiding a phase pattern will also show or hide the phase's *hkl* lines. By using the functions in „View → Plot" (see section 2.3), drawing of *hkl* lines and phase patterns can be controlled separately. This allows to draw either no phase information, *hkl* lines only, phase patterns only, or both.

Double-clicking on a scan parameter (name, scale factor, vertical or horizontal offset) allows to edit the parameter directly. The changes will not be persistent, as they will get lost after closing the scan file or running a refinement. They will, however, be preserved when exporting the scans to ASCII, GNUplot, SVG, or PNG format.

Clicking on a scan with the right mouse button will allow to export an individual scan to a different file format. See part 2 of the user manual for a list of supported file formats.

Scans can be added or removed to the project by the functions „File → Insert Graph File…" and „File → Remove Scan…". However, as soon as the main graph file is reloaded, for example automatically during a refinement, and added or removed scans will be reset and only the content of the reloaded file will be shown.

1.2.3 Refinement protocol

This windows shows the output of the Rietveld refinement backend.

1.2.4 Chemical composition

The „Chemical composition" dock window shows the refined chemical composition of the sample. This information is only available for BGMN, but not for other Rietveld refinement backends. Part 2 of the user manual explains in more detail how to use the chemical composition table.

Clicking with the right mouse button allows to copy the table to the clipboard. It can be pasted to a spread sheet program. The semicolon character „;" is used as a field separator.

1.2.5 Context Help

This window shows the context help, which can be accessed by placing the mouse cursor on a keyword in a control file, and pressing „F1". Context help is available for BGMN, but may not be available for other Rietveld refinement backends (see section 2.11).

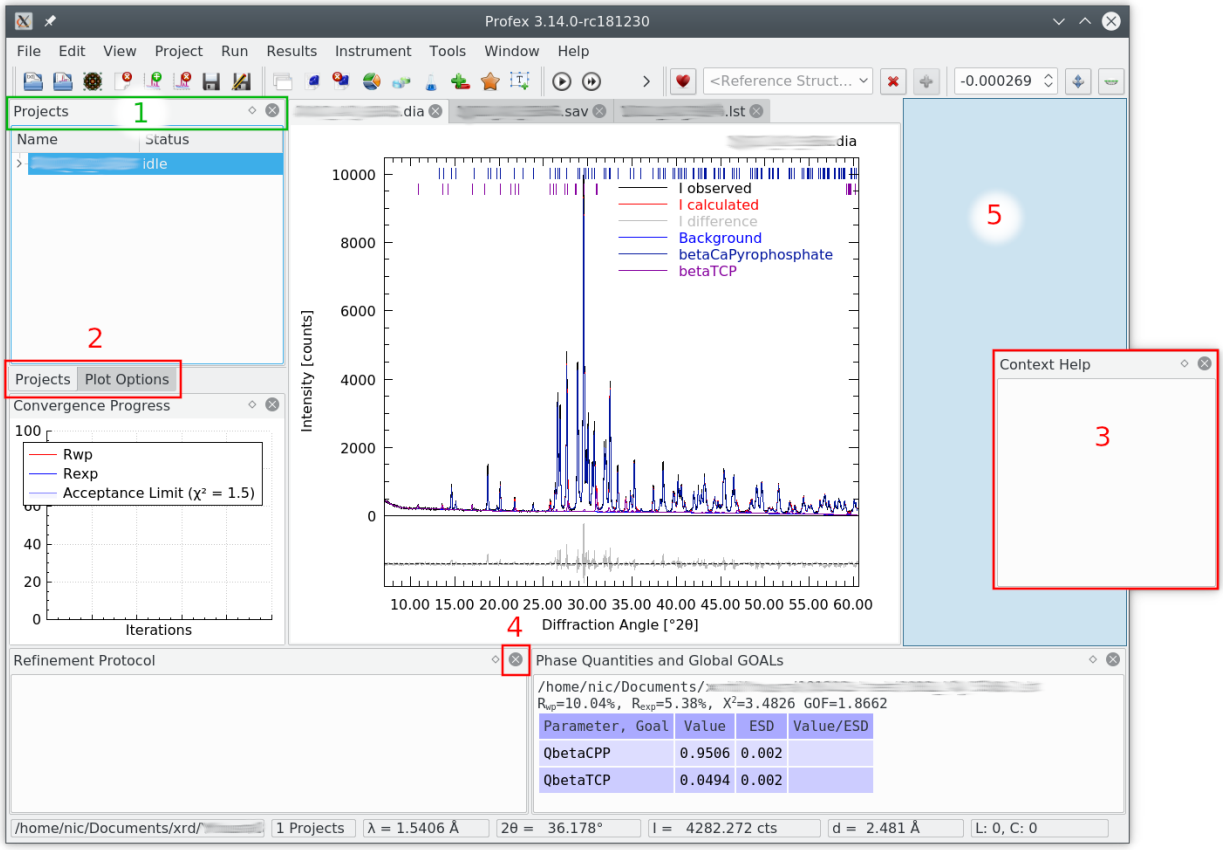
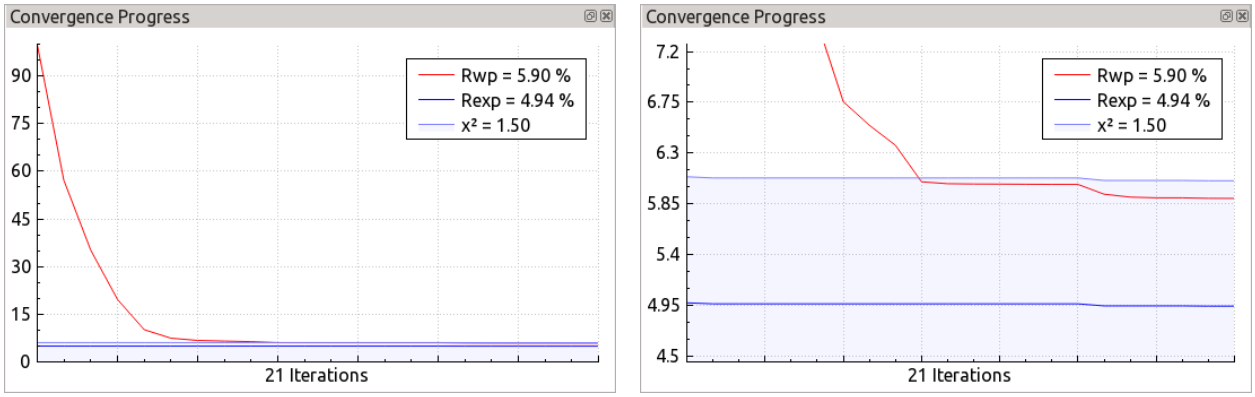


Figure 2: Many elements of the user interface can be re-arranged by grabbing the title bar (1) and dragging the window to a different place (2 stacked; 3 detached from the main window; 4 closed). The green rectangle (1) shows the title bar that can be grabbed with the mouse to rearrange the windows. To attache a floating window to the main window, grab it by the title bar and move it close to the edge of the main window, until a dock indicator (5) appears.

1.2.6 Convergence Progress

The „Convergence Progress" window shows a live graph of R_{wp}, R_{exp}, and an acceptance limit for χ^2. R_{wp} starts at 100 % and converges towards R_{exp} as the refinement progresses. The χ^2 acceptance limits marks the level at which the goodness of fit can be considered acceptable. The value can be configured in the „Limits" page of the preferences dialog. For optimum goodness of fit R_{wp} reaches R_{exp}.

Clicking with the right mouse button allows to toggle the legend visibility, and to export the graph data to text files or PDF files. Clicking with the left mouse button toggles the y-axis scaling between full scale (0–100 %) and zoomed in on the latest values (Fig. 3). In unzoomed state the scroll wheel can be used to zoom vertically into the graph.



(a) Full-scale y-axis.

(b) Zoomed y-axis.

Figure 3: Convergence progress dialog.

1.2.7 Peak integrals

A detailed description of how to use the „Peak intergrals" feature is given in part 2 of the user manual. The „Peak integrals" window shows a table with all integrals, starting with the name of the range in the first column, followed by the start and end angle. These parameters can be adjusted by changing the values in the table. The ranges can be renamed, and both angles can be adjusted. The following columns show the integrated intensity of all scans in the project. Depending on the state of the button „Subtract linear background" on the right, the integrated intensity includes the background or not.

The button „Apply ranges to all open projects" adds all defined ranges to all other open projects. If the other projects had integral ranges, these ranges will be cleared first. A dialog to select the projects receiving the intgral ranges is shown before applying the ranges.

The button „Paste data from clipboard" is a convenient way to define ranges in a spreadsheet program or in a text editor and apply to Profex. For example to create 5 ranges at specific angles, use a text editor and enter the ranges in the format „Name;Start Angle;End Angle", separated either by ; or by a tabulator, and angles be given in °2θ:

```
Range 1;10.00;11.00
Range 2;12.00;12.75
Range 3;25.75;26.25
Range 4;29.50;30.25
Range 5;45.10;45.90
```

Alternatively, create this list in a spreadsheet program. Then copy the list to the clipboard and click the button „Paste data from clipboard" in Profex. The new ranges will be appended to the list.

1.2.8 Peak list

This list shows all peak positions determined by the ,,Peak detection" function. More information on how to use peak detection is given in part 2 of the user manual. If peak detection is executed several times, a new *hkl* dataset will be created and appended to the plot each time. In order to display the *hkl* data of a certain dataset in the table, select it from the box ,,hkl list".

Peaks selected with the mouse will be highlighted in the scan. Selected peaks can be deleted by clicking ,,Remove selected line". To clear the selection and highlighting in the graph, click ,,Clear selection".

The entire *hkl* list can be exported to a text file by clicking ,,Save list to CSV file".

1.2.9 Search-Match

The Search-Match window allows to control the search-match parameters, and it displays the results of the phase matching. Details on how to use search-match are described in part 2 of the user manual.

1.2.10 Refined parameters

This window shows a summary of the refined parameters. The data is extracted from the *.lst file. In addition to data found in the *.lst file, the fit parameters χ^2 and GoF are shown in the ,,Statistics" group.

The values shown in the ,,Global GOALs" and ,,Local GOALs" groups can be configured by the user. The process is described in Section 3.4.9.

1.2.11 Peak fitting

The peak fitting module allows to fit individual peaks or groups of peaks with mathematical functions. This is useful to determine peak parameters such as the center position, peak width, or integrated intensity, as well as to deconvolute overlapping peaks. Functions can be selected from a predefined set of equations as described in section 5.4. Detailed information on how to use peak fitting is given in part 2 of the user manual.

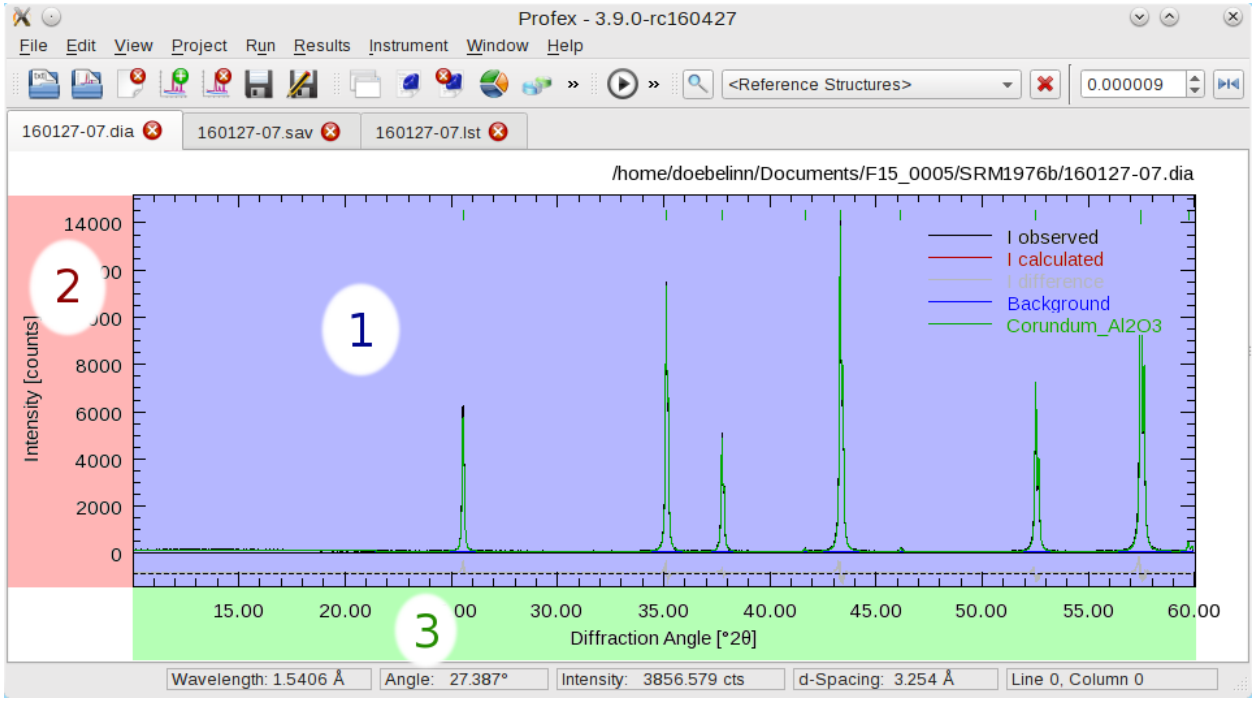


Figure 4: The plot area is divided into several regions interacting with the mouse cursor: 1 central data area, 2 left margin area, 3 bottom margin area.

1.3 The Plot Area

The plot area is the central area of the main window. It shows the loaded scans. Some appearance options can be configured in the preferences dialog as described in section 3.3. Visibilities of the legend, *hkl* indices, and phase patterns can globally be switched on or off in the menu „View → Plot", as described in section 2.

Scans from different graph files can be added to the plot area by the function „File → Insert Graph File…". Several files can be selected at a time. To remove a specific scan, select it in the dock window „Plot Options" and click „File → Remove scan…". When starting a refinement, the project's main graph file will automatically be reloaded and all added or removed scans will be reset to the main graph file's content.

The plot area interacts with mouse and key events. A summary of mouse and keyboard commands can be displayed by pressing the „Shift" key or selecting „Help → Mouse and keyboard commands". The plot area is divided into several segments (Fig. 4): The central data area shows the scans, *hkl* indices, and legend. The left margin area showing the y-axis labels. The bottom margin area shows the x-axis labels. The top margin area shows the file name. The right margin area is currently unused. The central area, left margin area, and bottom margin area interact in different ways with the mouse cursor.

1.3.1 Central Data Area

Moving the mouse cursor: The cursor position will be displayed in the status bar at the bottom of the main window. The horizontal and vertical position will be shown in degrees 2θ and counts or counts per second, depending on the unit of the y-axis (see section 3). Additionally, the horizontal position will also be shown as d value in $\AA$. The wavelength is used to calculate d values. If no wavelength information is found in the scan file, Profex will use the default wavelength specified in the preferences (see section 3).

Hovering the mouse pointer on a *hkl* index line at the top of the plot will show a tool tip displaying the phase name, *hkl* Miller indices, and the texture factor.

Left Mouse Button – Zooming: Use the left mouse button and drag the mouse to zoom into the plot.

Alternatively use the mouse scroll wheel to zoom horizontally to the location of the mouse cursor, or hold the Ctrl key and use the scroll wheel to zoom vertically to the location of the mouse cursor.

Hold the Ctrl key and left mouse button to move the zoomed scan.

Hold the Shift key and left mouse button to create a peak integral range.

Right Mouse Button – Unzooming: Click the right mouse button in the data area to view the entire scan range.

„c" Key – Cross hair cursor: Press the „c" key on the keyboard to activate a cross hair cursor (Fig. 5). Press „c" again to disable it.

„n" Key – Counting noise cursor: Press the „n" key on the keyboard to show or hide a cursor indicating a range of

$$\pm\sqrt{Intensity[counts]}$$

This range represents the Poisson-distributed statistical counting noise and allows to evaluate mismatches between I_{obs} and I_{calc}, for example at the tips of peaks (Fig. 5).

When moving to the difference curve, the noise cursor will show the counting noise at the intensity of the first scan (e. g. I_{obs}) at the same 2θ position.

„s" Key – Spectral line cursor: Press the „s" key to show or hide a cursor showing lines at the position of $K\alpha_1$, $K\alpha_2$, and $K\beta$. The $K\alpha_1$ line will be drawn at the position of the mouse cursor (Fig. 5). Positions for $K\alpha_2$ and $K\beta$ lines will be calculated from the d value at the cursor position. If no wavelength is available, the default wavelength specified in the preferences dialog will be used (see section 3). For monochromatic synchrotron radiation this feature is meaningless. Use the cross hair cursor instead.

Additionally, peaks from characteristic Tungsten radiation ($WL\alpha_1$ and $WL\beta$) can be shown by activating the option „Show characteristic Tungsten lines with spectral line cursor" in the preferences dialog (section 3). This allows to inspect the diffraction pattern for Tungsten

contamination lines caused by aging X-ray tubes. The relative intensities of Tungsten lines [4] are $WL\alpha_1$ (100 %), $WL\beta_1$ (49.4 %), $WL\beta_2$ (20.2 %). $WL\beta_2$ is not shown.

„h" Key – Help dialog Press the „h" key to show a tooltip with information on keyboard and mouse commands.

Double Click – Load reference structure: Double click with left mouse button will load the reference structure with it's strongest peak closest to the double click position. This is a very simplistic way for phase identification, however, it can be very efficient and useful in some situations. Note that only indexed structure files are considered. Refer to section 1.5 for more information on indexing of references structure files. Also note that the strongest peak of the reference structure indices depends on the instrument configuration used for indexing (fix or variable divergence slit) and may therefore not be at the location of the currently processed scan.

Middle Mouse Button – Scale reference lines: Hold the middle mouse button and move the mouse vertically to scale the intensity of reference lines. Dragging the lines below the line of zero counts allows comparing peaks in the difference curve.

Double Click + Ctrl – List of coordinates: Hold the Ctrl key and double click with the left mouse button to copy the coordinates of the mouse cursor to the refinement output console. From there the coordinates can be copied and pasted to another program for further processing.

1.3.2 Left Margin Area

Right Mouse Click: Opens the context menu:

Scale Linear: Sets the scaling of the y-axis to linear. The change is only temporary, i. e. the setting in the preferences dialog is not affected. Other open projects and projects opened after changing the y-axis scaling will still use the scaling specified in the preferences dialog. To permanently change the scale, it must be changed in the preferences dialog.

Scale Sqrt: Sets the scaling of the y-axis to $\sqrt{counts}$. The change is volatile (see above).

Scale Log10: Sets the scaling of the y-axis to $log_{10}(counts)$. The change is volatile (see above).

Zoom to Baseline: Sets the zoom range from the baseline (0 counts for linear and square root scaling, 1 count for log10 scaling) to the maximum intensity. It essentially hides the difference curve. This feature is convenient for square root or log10 scales, for which the difference curve tends to dominate the display.

Zoom to minimum intensity: Sets the zoom range from the minimum intensity found in any of the scans (except for the difference curve) to the maximum intensity. This is particularly useful for log 10 scaling, which tends to over-represent the white space between 0 and the background.

Reset Y-Axis Zoom: Resets the zoom of the y-axis to show the full angular range. The zoom state of the horizontal axis is maintained.

1.3.3 Bottom Margin Area

Right Mouse Click: Opens the context menu:

Reset X-Axis Zoom: Resets the zoom of the x-axis to show the full angular range. The zoom state of the vertical axis is maintained.

1.3.4 Stacking Scans

All scans in the plot area, originating from a single graph file or combined from several graph files using „File → Insert Graph File…", can be stacked vertically and/or horizontally. Offsets can be adjusted by „View → Increase vertical displacement", „View → Decrease vertical displacement", „View → Displace left", and „View → Displace right". All displacements can be reset by „View → Reset Displacement". An initial offset will be applied, which can be reduced incrementally by calling the function moving the scans in the opposite direction. The following commands were used to create the graphs shown in Figs. 6a and 6b:

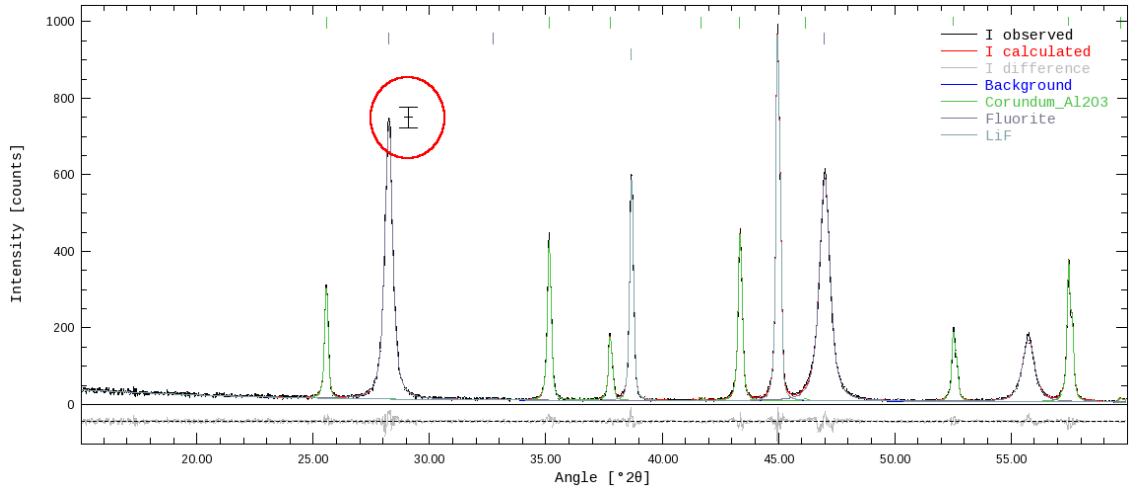
1. „View → Increase vertical displacement" to stack the scans vertically at regular intervals of the maximum intensity of the strongest scan (Fig. 6a).
2. „View → Decrease vertical displacement" was called several times to reduce – not reset – the vertical offset, followed by „View → Displace right" to stack the scans to the right (Fig. 6b).

A special vertical offset will be applied when calling „View → **Decrease** vertical displacement" **first**. In that case, positive vertical stacking will be applied, but instead of regular intervals, each scan will be displaced to the maximum intensity of the previous scan (Fig. 6). This will avoid large gaps above scans with low maximum intensity, however, it can also be confusing with scans of very low intensity (e. g. amorphous samples or the background curve). In the latter case, applying a regular stacking interval by calling „View → **Increase** vertical displacement" may be preferred.

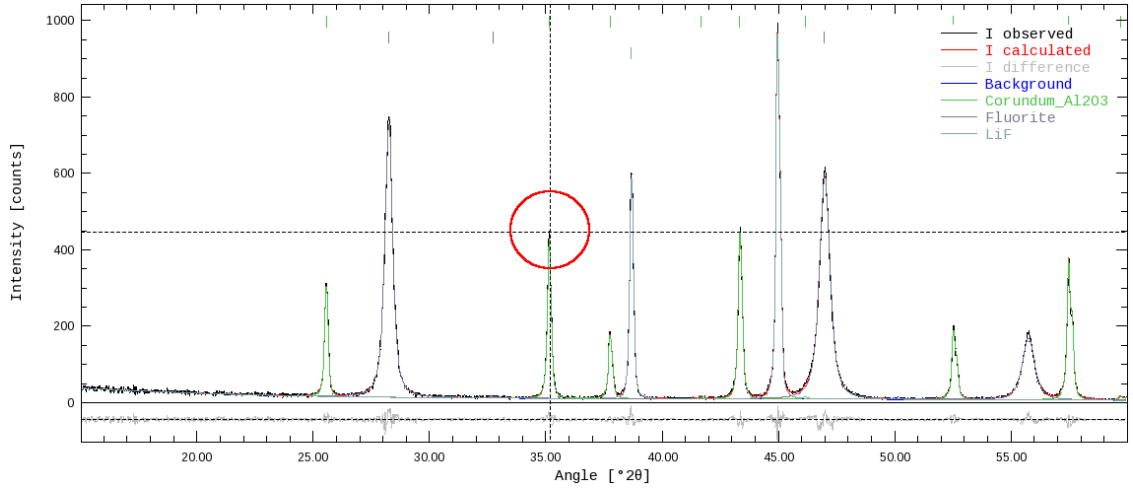
1.4 Text Editors

Text editors can show any kind of text files, including control files, list files, structure files, or any generic text file. For control files and list files they will show syntax highlighting for better representation.

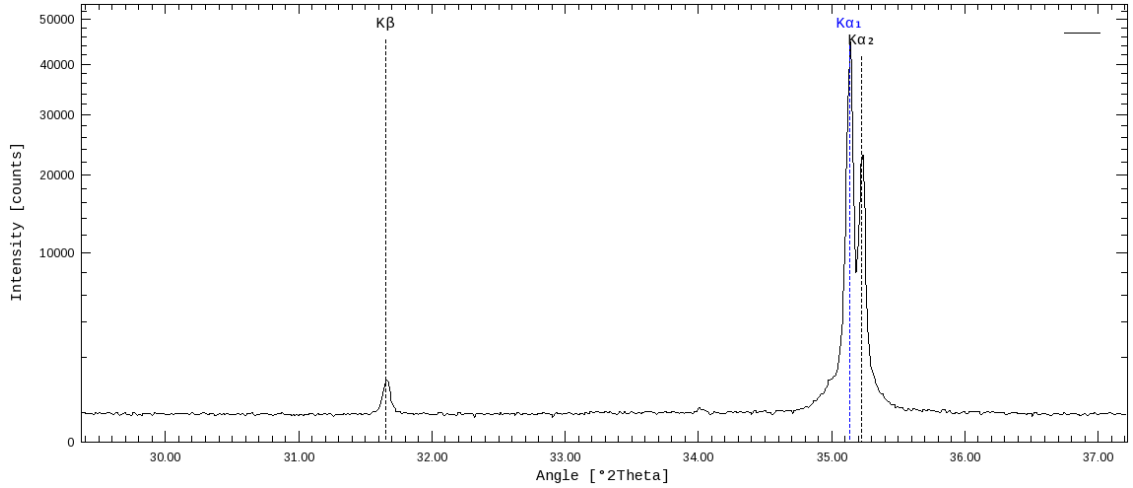
Besides the standard actions for text editors, such as copy, paste, undo, redo, and selection, the context menu shown by clicking with the right mouse button has some special features for control and structure files.



(a)

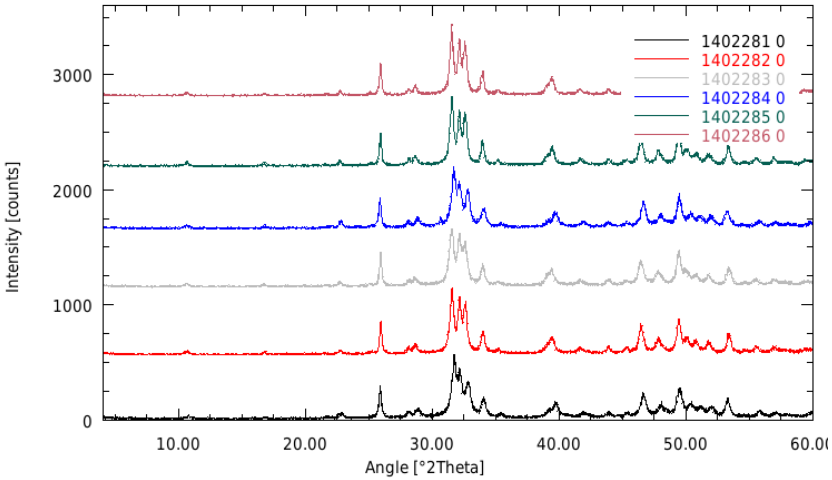


(b)

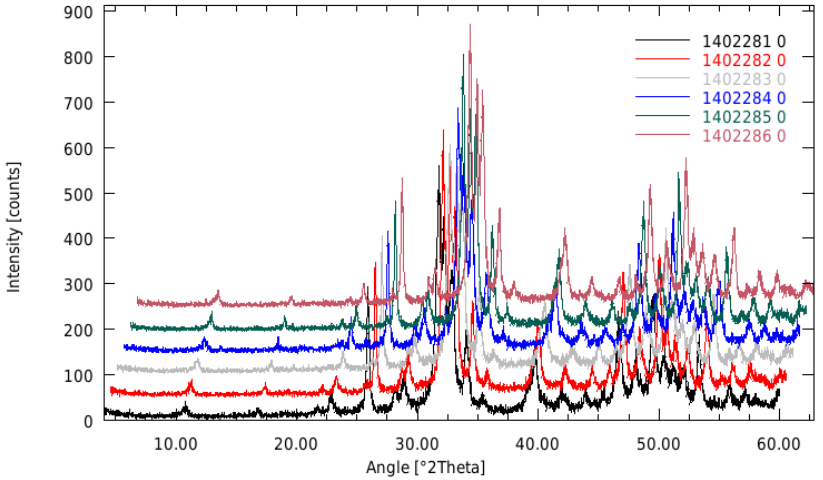


(c)

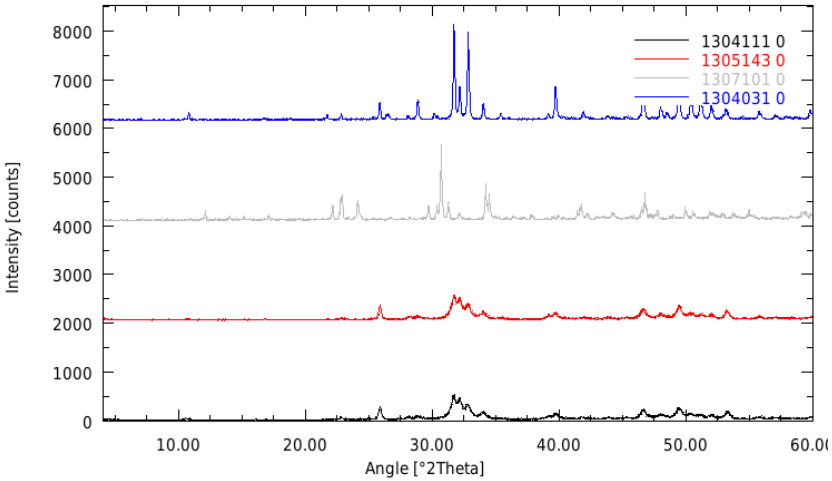
Figure 5: Different cursors of the plot area: (a) counting noise cursor, (b) cross hair cursor, (c) spectral lines cursor.



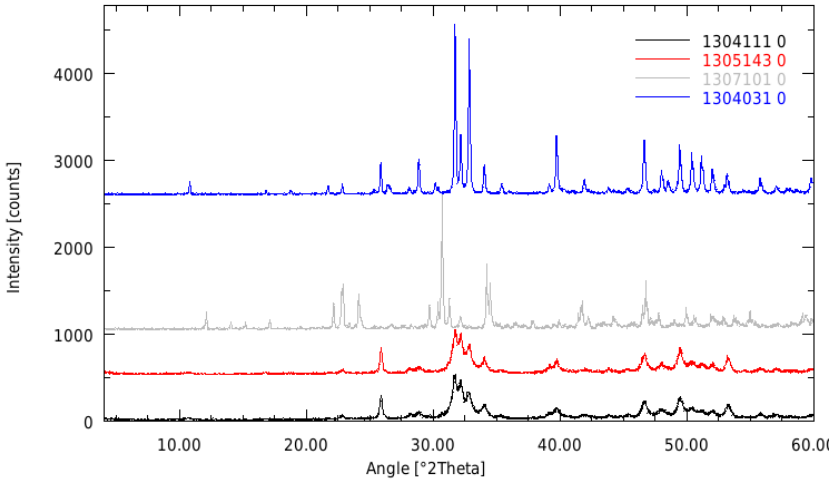
(a) Vertically stacked



(b) Vertically and horizontally stacked



(c) Regular offset



(d) Adaptive offset

Figure 6: Stacked scans.

1.4.1 Control File specific features

Open File: When placing the cursor on a file name and clicking with the right mouse button, the context menu will show the action „Open File" at the bottom. Depending on the file type, the file will be opened as a scan file (VAL[n], DIAGRAMM), or as a text file (STRUC[n], STRUCOUT[n], SimpleSTRUCOUT[n], RESOUT[n], PDBOUT[n], FCFOUT[n]).

Note that if the file name contains spaces or underscores, the full file name must be selected with the text cursor before right-clicking. Else the file name will not be recognized correctly.

Add <output> file: When placing the cursor on a STRUC[n] file line and clicking the right mouse button, the context menu will offer to add various structure output files. The refined crystal structure will be written to these files at the end of the refinement. They may be useful for import into other programs, e. g. for structure visualization or publication in databases or papers. The output file names will be set to `<phaseName>-<projectBasename>.ext` so as to create unique file names and prevent accidential overwriting of output files from other projects in the same directory. The formats offered are STRUCOUT[n], SimpleSTRUCOUT[n], RESOUT[n], PDBOUT[n], and FCFOUT[n]. Please refer to the BGMN documentation for more information about the file formats.

1.4.2 Control and Structure File specific features

When placing the cursor on a parameter and clicking with the right mouse button, the context menu will offer the following actions:

Fix Parameter: This will set the parameter under the mouse cursor to be fixed (i. e. not refined).

Refine Isotropically: This will release the parameter under the mouse cursor for isotropic refinement. Reasonable lower and upper limits will be applied by default.

Refine Anisotropically: This will release the parameter under the mouse cursor for anisotropic refinement. A reasonable upper limit will be applied by default. Note that if the parameter cannot be refined anisotropically (e. g. unit cell parameters, fractional coordinates, etc.), choosing anisotropic refinement will set the parameter to isotropic refinement, but without any lower and upper limits.

Refinement states of parameters can also be toggled with the keys F5 and F6. If clicked on a parameter supporting anisotropic refinement, the refinement state will be changed in the following order:

F5: `anisotropic` → `isotropic with limits` → `fix`

F6: `fix` → `isotropic with limits` → `anisotropic with upper limit`

If the parameter does not support anisotropic refinement, the refinement state will be changed in this order:

F5: `isotropic without limits` → `isotropic with limits` → `fix`

F6: `fix` → `isotropic with limits` → `isotropic without limits`

Reasonable default limits will be used in all cases. If the toggled parameter is an `EPSn` parameter in the control file, the numbering of `PARAM[n]` will be updated automatically if necessary.

1.5 Tool bars

All functions shown in the main toolbar, project toolbar, and refinement toolbar are also accessible in the menu bar and are described in detail in section 2. Toolbars can be re-arranged by dragging the left end to another position, or shown / hidden by right-clicking on a toolbar and checking or unchecking the toolbar in the context menu.

Elements of the reference structure toolbar are only visible if at least one project is loaded. They are not accessible through a menu, only by the toolbar buttons:

Reference structures: A menu allowing to select a reference structure from all STR files found in the structure database directory. If selected, the STR file's *hkl* lines will be shown in the graph. This is a generic way of phase identification. When using the „Add Phase" dialog while a reference structure is displayed, this structure file will be pre-selected in the „Add Phase" dialog.

If STR files have not been indexed before, *hkl* indices will be calculated on the fly when the structure is selected. On modern computers, this only takes a second or two. Afterwards the *hkl* positions will be buffered and will be available instantly next time the same structure is selected. The buffer can be cleared as described in section 3.4.5. Note that the double-click function described in section 1.3 is only available for indexed reference structures.

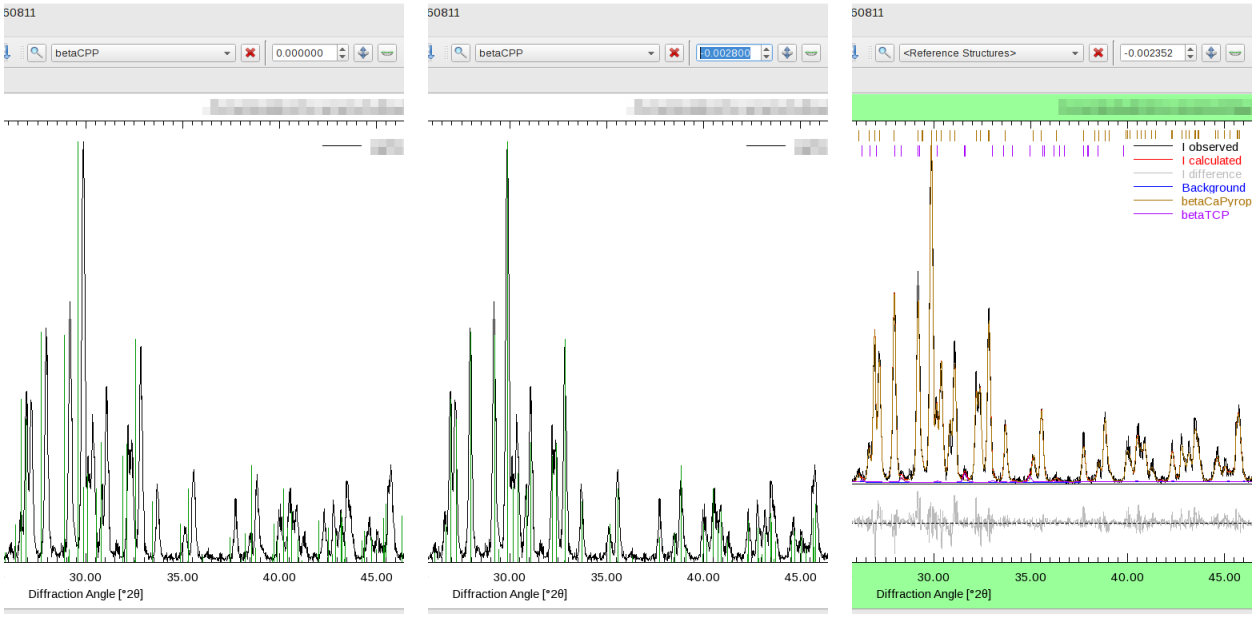
The reference structure menu is editable. When clicking on the menu and starting to type the name of a phase, auto-completion will propose the best matching phase. Press Enter to accept the proposed phase.

Reset reference structure: This button will reset the reference structure dropdown menu and hide reference *hkl* lines. After resetting, no structure will be pre-selected in the „Add Phase" dialog anymore.

Search and index new reference structures: Pressing this button will scan the structure database directory for new STR files and index all new files. The reference structures become immediately available in all projects.

Favorites: If clicked, only the phases flagged as favorite will be displayed in the dropdown menu. Important: Double-clicking on a peak in the graph to select the nearest reference structure will only search among the favorite structures if this button is clicked.

Height displacement of the sample surface and misaligned detectors cause a shift of the measured reflections in 2θ. This may cause confusion, because the peak positions and d values differ from the true value and *hkl* reference lines. Phase identification would become more difficult as double-clicking on the strongest peak would load a wrong reference structure. Sample height errors can



(a) (b) (c)

Figure 7: Sample height displacement results in a shift of the peaks in 2θ. The reference peaks no longer match the shifted measured peaks (a). Manually correcting for the shift aligns the reference peaks (b). After refinement, the refined shift is automatically applied (c).

be corrected using the spin box and buttons in the reference structure toolbar as described below (Fig. 7).

Spin box `EPS2`: Changing the value from 0.0 to a positive or negative value will shift *hkl* lines and the mouse cursor coordinates accordingly. The spin box shows the BGMN variable `EPS2` in radians. The effective sample height displacement Δ can be calculated from `EPS2` and the instrument radius R as follows:

$$\Delta = \frac{R \cdot EPS2}{2}$$

Δ and R have the same unit, e. g. millimeters. After a successful refinement, the correct refined value for `EPS2` will be applied automatically in order to center *hkl* tick marks and reference lines on the peaks. Internally Profex also reads the refined values for zero-offset (`EPS1`) and penetration depth (`EPS3`) and applies the corresponding angular corrections. But in contrast to `EPS2` these values cannot be controlled by the user.

Button „Set angular corrections to refined values”: Pressing this button will reset all angular corrections (`EPS1`, `EPS2`, `EPS3`) to the refined values read from the refinement results file (*.lst).

Button „Set angular corrections to zero”: Pressing this button will reset all angular corrections (`EPS1`, `EPS2`, `EPS3`) to 0.0.

2 Menu Structure

2.1 File

Open Text File... (Ctrl+O) Opens a file in a text editor. If a project with the same name as the text file's base name is already open, the file is opened in this project. Else a new project is created.

If the text file is a control or results file, Profex will automatically locate all other control and results files of the same project, as well as the scan file, and open them, too. Non-existing files are ignored.

BGMN structure files (*.str) are always opened in the currently shown project, regardless of the project name.

Open Raw Scan File... (Ctrl+G) Opens a scan file in a new project. If a control and/or results file with the same base name is found, Profex will open it, too. The file dialog will only show file format filters for raw data files.

Open Refinement Project... (Ctrl+R) Opens a previously created refinement project. The file dialog will only show file format filters for refinement output files.

Open Project Archive A project backup created with „Project → Save Project backup" can be extracted and opened. The archive will be extracted in a sub-folder named after the archive file.

Insert Scans... (Ctrl+I) Inserts scans from one or more graph files into an existing project. The additional scans will only be displayed in the project's graph view. Other files, such as the control file, will not be modified. If no project is available, a new one will be created, based on the name of the first selected graph file. Inserted scans will be discarded when the project's graph file is reloaded, e. g. during a refinement.

Remove Scan... Removes the scan selected in the „Plot Options" window from the graph view. No other files will be modified. Removed scans will be restored when the project's graph file is reloaded, e. g. during a refinement.

Save (Ctrl+S) Saves the current file under the same file name. This function only works for text files.

Save file as... (Shift+Ctrl+S) Saves the current file under a new file name. A file dialog is shown to ask for the file name, location, and file format.

Save all text files in all projects (Ctrl+Alt+S) Saves all modified text files (control and structure files) in all open projects. This function can be used after calling „Edit → Copy control file", because the newly created control files will only be created in text editors, but not yet saved to disk. Calling this function will save them to disk all at once.

Recent Graph Files Shows a list of recently opened graph files.

Recent Text Files Shows a list of recently opened text files. For scan files, different output formats can be selected. Scans can be saved as raw data for further processing, or images.

Print (Ctrl+P) Prints the currently shown text or graph file. Printing options may differ depending on the platform and device driver.

Print all Graphs (Shift+Ctrl+P) Prints the graphs of several open projects at once. A project selection dialog will be shown first. By default all open projects are selected. If the graphs are printed to a PDF file, one file containing all graphs will be created.

Export all Graphs to SVG Creates SVG (vector graphics) files of several projects. A project selection dialog will be shown first. By default all open projects are selected. Each graph will be saved to an individual SVG file.

Close Project (Ctrl+W) Closes the current project. If a refinement is running, a message will ask for confirmation before aborting the refinement.

Close All Projects Closes all open projects. If one or more refinements are in progress, a warning will be displayed and no project will be closed.

Import Structure File... Opens a dialog to convert CIF files (*.cif) or ICDD XML files (*.xml) to BGMN structure files (*.str). See part 2 of the user manual for more information on how to export CIF files. CIF files can be obtained from various databases. ICDD XML files can be exported from the ICDD PDF-4+ graphical user interface using „Save PDF card as...".

Scan Batch Conversion... Opens a dialog for batch conversion of graph files. All currently opened project scans will be added to the batch list by default. More files can be added or deleted in the dialog. More details on how to use batch conversion are given in part 2 of the user manual.

Scan batch refinement script... This function creates a script file to run a list of refinements outside of Profex. This is useful to refine a large number of files on a remote system, for example on a high-performance cluster. Supported output formats are Bash scripts for unix systems (Linux, Mac OS X) and Windows CMD files.

Quit (Ctrl+Q) Quits the application.

2.2 Edit

Undo (Ctrl+Z) Reverts the last change in the currently shown text file.

Redo (Shift+Ctrl+Z) Restores the last undone change in the currently shown text file.

Cut (Ctrl+X) Cuts the selected text and keeps it in the clipboard. This action only works on text editors, it has no effect on the graph display.

Copy (Ctrl+C) Copies the selected text to the clipboard. On graph displays a pixel image of the graph is copied to the clipboard. The resolution can be specified in the preferences (section 3.3.4).

Paste (Ctrl+V) Pastes the content of the clipboard. This action only works on text editors, it has no effect on the graph display.

Copy Control File Copies the current project's control file to other projects and adapts all input and output file names to match the projects' base names. A dialog will allow to select which projects' control file shall be modified. Existing control files will be overwritten.

Note that this function does not check whether referenced structure files are actually present in all project directories. It only manages control files, but not structure files.

Insert Text Block Inserts the selected pre-defined text block to the current text editor at the cursor's position. If a graph is shown, this action will do nothing. Text blocks can be configured in the preferences dialog.

Reset File Reverts the current project's control file to the state before the last refinement. This function is only used for the Fullprof.2k backend, but not for BGMN, because BGMN usually does not modify STR and SAV files.

Find and Replace... (Ctrl+F) Searches a string in a control or structure file, and replaces it. If „use Regular Expression" is checked, the „Find" keyword will be interpreted as a regular expression pattern.

Find in Files Searches a string in all or a specific type of all open text files. The search string is interpreted as a regular expression pattern. If a capture is specified, only the capture will be displayed in the match list. Else the entire matching line will be displayed.

Preferences... Opens the program's preferences dialog. All preference options are discussed in detail in section 3.

2.3 View

Set Zoom Range... Opens a dialog to zoom the graph to precise upper and lower limits for angle and intensity. After closing the range dialog, a project selection dialog is shown to apply the zoom range to multiple projects.

Reset Zoom Range... Resets the zoom range. A project selection dialog is shown to reset multiple projects at a time.

Reset margin color Resets the color of the graph margin to idle color. This is useful for taking screenshots after completed refinements.

Show/Hide Phase Patterns (Ctrl+0) Activates or deactivates visibility of all phases. This option applies to all open projects. It only checks or unchecks the visibility boxes of all phase patterns in the Plot Options list for convenient displaying or hiding of all phases. Individual phases can be shown or hidden by selecting or un-selecting the „show" option in the Plot Options list. More information is given in section 1.2.2.

Plot Configure the visibility of the following elements on the plot:

Legend Shows or hides the plot legend.

hkl Indices Shows or hides the *hkl* index tick marks at the top of the plots.

Increase Vertical Displacement (Ctrl+Up) Applies a regular vertical offset to all scans. The initial offset will correspond to the maximum intensity of the strongest scan. When called again, this function will increase the previous offset by a constant value.

Decrease Vertical Displacement (Ctrl+Down) Reduces the vertical offset of all scans by a constant value. If no vertical offset exists, an initial adaptive offset will be applied, with a vertical displacement of each scan corresponding to the maximum intensity of the scan below.

Displace left (Ctrl+Left) If no horizontal offset exists, it will apply a horizontal offset to the left to all scans. If an offset to the left exists, the offset will be increased by a constant value. If an offset to the right exists, the offset will be reduced by a constant value.

Displace right (Ctrl+Right) If no horizontal offset exists, it will apply a horizontal offset to the right to all scans. If an offset to the right exists, the offset will be increased by a constant value. If an offset to the left exists, the offset will be reduced by a constant value.

Reset Displacement (Ctrl+Space) Resets all horizontal and vertical offsets.

2.4 Project

Add / Remove Phase... (F8) Opens a dialog to create or manage a control file. New phases can be added or existing phases can be removed from the refinement. If no control file exists yet, a new one will be created. In that case, the correct instrument configuration file must be selected. The option to create a default control file is automatically activated or deactivated, depending on whether or not a control file already exists.

If a phase is activated in the Reference Phase box, it will be pre-selected in the Add Phase list.

If a default control file is created despite an existing control file, the existing one will be overwritten, any previously added modifications or phases will be lost.

Selected structure files and instrument configuration files will be copied from the structure and device database directory to the project directory. Files already existing in the destination directory will be skipped. If the option ,,overwrite existing files" is checked, existing structure files will be overwritten with the file copied from the structure file database. A detailed description of the structure file handling is given in part 2 of the user manual and in section5.1.

When removing a phase from the control file, the structure file can optionally be deleted. Deleting structure files may cause problems with other projects stored in the same directory and accessing the same structure files.

Add amorphous peak A special structure file is added to the current project with just one wide peak modelling the bump caused by amorphous phases. The center position of the peak can be entered in a dialog. Note that this amorphous phase cannot be used to quantify the amorphous content, it only improves the refinement of the background curve.

Open all project STR files (Ctrl+F8) Opens all BGMN structure files (*.str) referenced in the current project's control file (*.sav) in new pages.

Close all project STR files (Ctrl+F7) Closes all BGMN structure files (*.str) shown in the current project.

Edit all project STR files Opens a dialog allowing to modify the refinement state of all (or a selection of) STR files used in the current project.

Set Internal Standard Allows to define one refined phase as internal standard phase with a given quantity. The calculation of phase quantities will be changed to apply the internal standard correction, and the standard phase will no longer be shown in the summary table.

Unset Internal Standard Reverts the internal standard calculation of refined phase quantities. All phases will be shown in the summary table in quantities normalized to the sum of all phases.

Refinement Presets Lists all refinement presets to create refinement control files. Select one of them to apply the preset to the current project. More information on refinement presets is given in part 2 of the user manual.

Save as Refinement Preset... Creates a new refinement preset from the currently loaded project. More information on refinement presets is given in part 2 of the user manual.

Save Project Backup (Ctrl+B) Creates a ZIP compressed archive of the current project. The file name is determined automatically as `projectBasename-YYYYMMDD-hhmm.zip`. It will be stored inside the current project's working directory. The archive includes the raw data file, all instrument files, structure files, and output files of the project.

Save Project Backup As...(Ctrl+Shift+B) Creates a ZIP compressed archive of the current project. The file name and path can be selected by the user. The archive includes the raw data file, all instrument files, structure files, and output files of the project. The ZIP archives can be stored as a backup or shared with other users, as they contain all project relevant data.

Edit Excel Export Opens a dialog to configure the export of refinement results to Excel. This option is only available on Windows.

2.5 Run

Run Search-Match Runs the phase searching and matching process. The process can be configured in the „Search/Match phases" window (Window → Search/Match phases). A detailed description on how to use search-match is given in part 2 of the user manual.

Run Refinement (F9) Starts the refinement of the currently shown project.

Run Batch Refinement (F10) Starts a batch refinement of several open projects. A project selection dialog will be shown first to select all or a selection of projects to be scheduled. If this function is called while a batch is already running, all selected projects will be scheduled and appended to the running batch.

Abort Current Refinement (Shift+F9) Aborts refinement of the currently shown project. In batch refinement mode all projects scheduled for batch refinement will be unscheduled. If the currently shown project is not running but scheduled, it will be unscheduled but the remaining batch refinement will not be interrupted. In either case refinements started outside of the batch will not be interrupted.

Abort All Refinemet (Shift+F10) Aborts all running projects and batches. If more projects than the currently shown one are affected, the user will be asked for confirmation.

Run peak detection Starts the peak detection process using EFLECH. Results are displayed in the window „Peak List" (Window → Peak List). A detailed description of peak detection is given in part 2 of the user manual.

Follow Active Refinement When processing a batch refinement, activate this function to always raise the currently refining project. If a project refinement has completed, the next scheduled project will automatically be raised. This allows to monitor the batch refinement on screen. The function can be toggled on and off at any time, also during a running batch. It is automatically deactivated as soon as the user selects a text editor of any open project, so as to avoid automatically raising a different project while a text file is being edited or read.

2.6 Results

Export Global Parameters and GOALs (Ctrl+E) Exports the global parameters and goals (e. g. phase quantities) to a semicolon separated spread sheet (*.csv). Part 2 of the user manual provides more information on results export.

Export Local Parameters and GOALs (Shift+Ctrl+E) Exports the local parameters and goals (e. g. structural parameters) to a semicolon separated spread sheet (*.csv). Part 2 of the user manual provides more information on results export.

Export refined chemical composition... Writes the calculated chemical composition to a semicolon separated spread sheet (*.csv). Part 2 of the user manual provides more information on results export.

Export Peak Integrals Exports all peak integral data to a semicolon separated spread sheet (*.csv). Part 2 of the user manual provides more information on results export.

Export CIF file from LST file This function reads LST files of all open projects and writes crystal structure information to CIF files. One CIF file will be created for each crystal structure found. The file will be stored in the project directory. Information on saved files is shown in the refinement protocol console. Part 2 of the user manual provides more information on results export.

Export CELL file from RES file This function reads RES files of all open projects and writes crystal structure information to CELL files for the software Castep [5]. One CELL file will be created for each crystal structure found. The file will be stored in the project directory. Information on saved files is shown in the refinement protocol console. If no RES file is available for a

specific phase, a tag `RESOUT[n]=filename.res` must be added to the control file (*.sav) and the refinement must be repeated.

Generate report A report of the current refinement results is generated. The resulting HTML file can be viewed in a web browser and printed from there. Part 2 of the user manual provides more information on creating refinement reports.

Export to Excel (Windows only) Exports the results of the current project to excel according to the export configuration in „Project → Edit Excel Export". On platforms other than Windows, this option is not available.

2.7 Instrument

New Configuration... Read some hardware information from Bruker RAW V4, Bruker BRML V5, and PANalytical XRDML files to create a BGMN instrument configuration file from scratch. Other raw data formats are not supported. Usually several variables required by BGMN will not be available from the raw data files and will thus have to be entered manually. See part 2 of the user manual for more information on creating instrument configuration files. This feature is experimental.

Edit Configuration... Opens a dialog to process BGMN instrument configurations. See part 2 of the user manual for more information on creating instrument configuration files.

Edit Current Configuration... Opens the instrument configuration file used in the current project in an editor. If the configuration file (*.sav) is not found in the current project directory, the file will be searched in the devices repository. If found, a copy will be created in the project directory and opened in the dialog.

Show Peak Shape... Opens a dialog that calculates the theoretical peak shapes for a selected instrument configuration file.

2.8 Tools

Browse BGMN Space Groups... Opens a dialog to browse space groups and atomic positions supported by BGMN. The dialog reads the file SPACEGRP.DAT, which is part of the BGMN software distribution.

Browse Atomic Scattering Factors... Opens a dialog to browse atomic scattering (form) factors supported by BGMN. The dialog reads the file AFAPARM.DAT, which is part of the BGMN software distribution.

Calculate Absorption Coefficients A dialog opens that allows to calculate linear and mass absorption coefficients for phases and samples. If a refinement project is loaded, the dialog will use the refined phases to compute absorption coefficients for each phase based on its chemical composition, and for the sample based on the phase quantities. However, phases can also be manually added and removed in order to compute absorption coefficients for arbitrary compositions.

Process DIA files (coming soon)

Scan Math The tool „Scan Math" allows to perform calculations on the intensities of all scans loaded in a project. Expressions must be entered in Java Script syntax [6, 7]. A detailed description of the Scan Math dialog is given in part 2 of the user manual.

Add Baseline... Opens a dialog to calculate a baseline (background curve) for a certain scan in the project. Part 2 of the user manual provides more information on baselines.

Electron density maps Opens a dialog to compute electron density maps from *.fcf and *.res output files. See part 2 of the user manual for more information on electron density maps.

Index Reference Structures Searches the structure file repository and indexes new structure files. Entries of files no longer found in the repository are removed from the database.

2.9 Locations

Current Project Opens a file manager at the directory of the currently shown project.

Structure Repositories This menu lists all structure repository directories configured in the Profex preferences. Selecting a repository opens a file manager at the selected location.

Device Repositories This menu lists all device repository directories configured in the Profex preferences. Selecting a repository opens a file manager at the selected location.

Preset Repositories This menu lists all preset repository directories configured in the Profex preferences. Selecting a repository opens a file manager at the selected location.

2.10 Window

Projects Shows or hides the Projects list window.

Plot Options Shows or hides the Plot Options window.

Refinement Protocol Shows or hides the Refinement Protocol window.

Chemical composition Shows or hides the table showing the refined chemical composition in oxide form.

Context Help Shows or hides the context help display.

Convergence Progress Shows or hides the window showing a graph with R_{wp} and R_{exp} values during a refinement.

Peak Integrals Shows or hides the peak integral window.

Peak List Opens a table with all refined peak parameters read from the BGMN *.par file.

Search/Match phases Opens the Search/Match module for phase identification.

Refined parameters Shows or hides the summary window for refinement statistics and refined parameters and goals.

Peak Fitting Opens the module for non-linear curve fitting.

2.11 Help

Context Help... (F1) Shows the context help of the keyword under the text cursor. The „Context Help" window („View" menu) must be shown to display the context help.

BGMN Variables... Opens a web browser showing the BGMN variables documentation page.

Mouse and Keyboard Commands Shows a dialog with mouse and keyboard commands for plot windows.

About Profex... Shows information about Profex. The button „Copy system information to clipboard" copies the system information as well as the content of the log file to the clipboard. It can be pasted in text format to other programs. This information can be helpful for support requests. All information is encoded in plain text. Users are requested to carefully review the content and delete any critical personal or technical information prior to sharing the information with the Profex developers.

3 Preferences

3.1 General

Icon theme Select the icons used by Profex. Three options are availble:

Light: A plain monochrome icon set to be used with a light desktop theme.

Light color: A bi-color icon set to be used with a light desktop theme.

Dark: A plain monochrome icon set to be used with a dark desktop theme.

Toolbar Layout Select how icons and text in Profex' toolbars are shown. „Follow Style" will match the system-wide style used by the operating system.

Restore open projects If checked, Profex will load all previously open graph files upon program start. If unchecked, Profex will not load any projects or files at program start.

Default Project Type For file formats not specific for either BGMN or Fullprof.2k, this option determines which type of project will be created when such a file is opened. The file type is identified by the file extension.

File extensions can also be associated with either of the two backends by adding the extension either to the list of „File Extensions associated with BGMN" or „File Extensions associated with Fullprof".

Number of CPU cores used by BGMN Specifies how many parallel threads will be used by the refinement backend (only available for BGMN). „Automatic" will use all available logical CPU cores.

Number of parallel batch refinements Defines the number of refinements running in parallel in a batch refinement. If this number is greater than 1, the number of threads used for each project will be divided by the number of parallel refinements to avoid over-saturating the CPU.

File Extensions associated with Fullprof These file types will always be opened as Fullprof projects, regardless of the default project type. Enter the extension in small letters without asterisks and periods, separated by a space character. Example: `pcr dat sum prf`

File Extensions associated with BGMN These file types will always be opened as BGMN projects, regardless of the default project type. Enter the extension in small letters without asterisks and periods, separated by a space character. Example: `sav lst dia str`

Default Wavelength This wavelength, given in Å, is used for scan files not containing any information about the wavelength.

Always use default Wavelength If checked, Profex will ignore the wavelength read from the scan file and always use the default wavelength to calculate d values from diffraction angles. Use this option with care. Any wavelength information read from raw data files will be ignored if this option is checked.

3.2 Text Editors

Font Sets the font of the text editor and refinement protocol window.

Syntax highlighting Select the color set used for syntax highlighting by the text editors. Four options are available:

Automatic: Selects an appropriate theme for light and dark desktop themes.

Light mode: Selects a highlighting theme with dark colors that are easily readable on a light background.

Dark mode: Selects a highlighting theme with light colors that are easily readable on a dark background.

Off: Turns syntax highlighting off. The font is black on light desktop themes, and white on dark themes.

3.3 Graphs

3.3.1 Appearance

Use AntiAliasing for Graphs (slow!) Uses anti aliasing to draw the plots. If checked, lines look smoother but also wider. Drawing will be slower if checked.

Show characteristic Tungsten lines with spectral line cursor When using the spectral line cursor (1.3), additional lines will be shown for characteristic Tungsten radiation ($WL\alpha_1$ and $WL\beta_1$). This allows to inspect the diffraction pattern for Tungsten contamination lines caused by aging X-ray tubes.

Show major grid lines Show or hide vertical and horizontal grid lines at the positions of major tick marks. Major grid lines will be drawn as medium dashed lines.

Show minor grid lines Show or hide vertical and horizontal grid lines at the positions of minor tick marks. Minor grid lines will be drawn as light dotted lines.

Show complete file name If checked, the file name of the graph file will be shown with the absolute path in the top right corner of the graph display. If unchecked, only the file name without file path will be shown.

Display Line Width Width in pixels of all lines (plots, axes, tick marks) of the graph on computer screens. If plot lines are too fine (e. g. on high-resolution displays) increase this value.

Symbol Size Size of the measured data points when not using solid lines (e. g. dots or crosses) in pixels.

Y-axis Scaling Scaling of the y-axis. Options are linear, logarithmic with a base of 10 (log10), or square root (sqrt).

Y-axis unit Shows the y-axis unit either in counts, or in counts per second (cps). Counts per second may not be available, depending on the file format of the loaded scan. If the time per step is not available, Profex will fall back to the unit ,,Counts" and assume a counting time of 1 second per step.

Only the display of scans will be affected by the choice of the unit. Internally, all calculations and file format conversions will be performed in ,,Counts". As a consequence, when converting a format supporting ,,Counts per second" (such as XRDML) to a format not supporting it (such as ASCII XY), the displayed unit may change from [cps] to [counts].

Multi-Scan Files Select whether multi-range files will be shown as individual scans, as the sum of all ranges, or as the average of all ranges.

Create Thumbnail If checked, a thumbnail picture of the refined plot will be created at the end of the refinement. This file is stored in the project directory with the name `project-basename_tn.png`. It allows easy browsing of refined projects. The width of the picture can be specified in pixels. The height is calculated from the displayed aspect ratio.

Use margin colors If activated, the margin of the graph will change color to indicate the refinement status. By default, the color for idle projects is white, for refining (active) projects red, and for completed projects green. The colors can be customized.

Idle Select the color of the graph's margin in idle state. Usually white is the preferred option.

Active Select the color of the graph's margin in active state (during refinements). The default is light red. If no color change is preferred, select the same color as for idle state.

Complete Select the color of the graph's margin in complete state (after convergence of refinements). The default is light green. If no color change is preferred, select the same color as for idle state. The margin color can be set back to idle color by clicking ,,View $\rightarrow$ Reset margin color".

3.3.2 Fonts

Font Title Select the font of the file name at the top-right of the graph.

Font Axis Labels Select the font of the graph axis labels.

Font Tick Marks Select the font of the graph tick marks.

Font Legend Select the font of the graph legend.

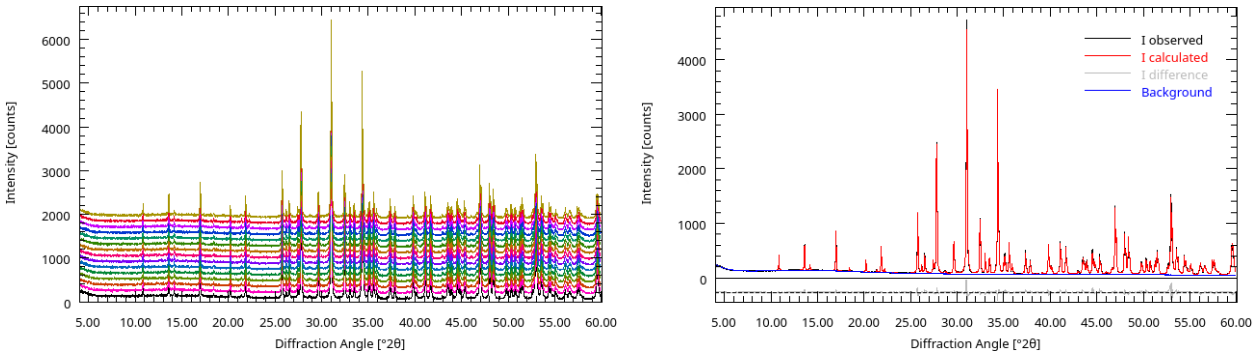


Figure 8: Randomly generated scan colors (left) used for multi-scan files. Standardized colors for refined projects (right).

3.3.3 Scan Styles

Color Customize the list of colors to be used to draw scans by double-clicking on the color cell. If more scans are loaded than colors are available from the list, a random color will be created and added to the list. The first color defaults to black, all following colors are randomly generated. They can be changed manually later on. Line widths can be changed on the Graph's Appearance page.

Point Style Select the style to draw scans. „Solid" draws the scan as a solid line. „Points" draws a dot at the measured position, „Cross" draws a cross at the measured position. Symbol sizes of crosses and points can be changed on the Graph's General Appearance page.

\+ Add another color to the color list.

− Remove the currently selected color from the list.

Standard colors Multiple scans can be loaded either from a raw data file containing more than one scan, or from a refined project containing one raw data scan (Iobs), as well as several calculated scans (Icalc, Idiff, background). Multi-scan files use the colors specified in the color list above. However, separate colors can be used for refined projects. These standard colors override the colors in the list above as soon as Profex detects a refined project. This is helpful to use pretty colors for multi-scan files, but the *defacto* standardized colors for Iobs (black), Icalc (red), Idifference (grey), and background (blue). An example for the two different modes is shown in Fig. 8.

3.3.4 Print and Export

Print: Line Width Width in points of all lines (plots, axes, tick marks) of the graph on printouts. This value should usually be greater than the display line width. It has to be matched to the printer device driver by printing test plots.

Print: Font Scale Factor The font size on printouts can be scaled. Use values greater than 1.0 if the font is too small, and smaller than 1.0 if the font size is too large. The value has to be matched to the printer device driver by printing test plots.

ASCII Data Export: Field Separator Enter the field separator used when exporting data to ASCII text files. Only non-alphanumeric characters are allowed. Common choices are the semicolon (;), comma (,), space ( ), or tab.

Raster Export: Width Width of the exported image in pixels.

Raster Export: Height Height of the exported image in pixels.

SVG Export: Font Scale Factor Adjusts the font scale on SVG graphs. Increase the value if the font is too small, or decrease if the font is to large.

3.4 BGMN

3.4.1 Backend Configuration

BGMN executable Selects the BGMN executable file. This file is part of the BGMN installation. It is called `BGMN.EXE` on Windows, and `bgmn` on Mac OS X and Linux.

MakeGEQ executable Selects the MakeGEQ executable file. This file is part of the BGMN installation. It is called `MakeGEQ.EXE` on Windows, and `makegeq` on Mac OS X and Linux.

Geomet executable Selects the Geomet executable file. This file is part of the BGMN installation. It is called `GEOMET.EXE` on Windows, and `geomet` on Mac OS X and Linux.

Teil executable Selects the Teil executable file. This file is part of the BGMN installation. It is called `TEIL.EXE` on Windows, and `teil` on Mac OS X and Linux.

Eflech executable Selects the Eflech executable file. This file is part of the BGMN installation. It is called `EFLECH.EXE` on Windows, and `eflech` on Mac OS X and Linux.

Convert raw scans to XY format If checked, raw scan files will be converted to ASCII XY free format (*.xy) prior to starting the refinement.

This option must only be disabled if the raw file format is directly supported by the BGMN backend (e. g. *.val, *.rd).

Spectral line cursor shows all wavelengths from BGMN *.lam file By default Profex uses a hard-coded table of characteristic wavelengths to display the spectral lines of $K\alpha_1$, $K\alpha_2$, and $K\beta$ with the spectral line cursor. The primary wavelength is read from the scan file (raw data file or refined profile), and all related secondary wavelengths are found in the hard-coded table. If this option is checked, Profex will try to locate the *.lam file specified in the BGMN refinement control file using the keyword `LAMBDA=`, and read all wavelengths specified there.

The radiation spectrum in the *.lam file is often modeled by overlapping Lorentzian curves. It is therefore not unusual to use 4 or more emission lines with slightly different wavelength,

widths, and intensities to model $K\alpha_1$ and $K\alpha_2$ with realistic emission line profiles. If additionally $K\alpha_3$ satellites and $K\beta$ are modeled, even more emission lines are required. The emission spectrum described in the *.lam file can therefore be relatively complex, and displaying all lines with the spectral line cursor can lead to a cluttered plot display. For most users using conventional X-ray tubes with characteristic radiation spectra, with or without $K\beta$ filters or monochromators, leaving this option unchecked is recommended.

If the *.lam file was not specified, cannot be found, or cannot be parsed, Profex falls back to the internal hard-coded table of characteristic wavelengths, just as if this option was unchecked.

Any comment trailing the emission line parameters will be used to label the line. For example, to add line labels to the file „cu_bergmann83.lam", which is part of the Profex-BGMN-Bundle distribution:

```
% Cu-K-alpha doublet as measured in october 1983 by J. Bergmann
ILAM=4 TITEL=CU_vom_Oktober_1983
0.401939 6.49098 0.0010981
0.266445 6.49013 0.0019875
0.167844 6.47504 0.0012544
0.163773 6.47400 0.0017246
```

add comments to each data line:

```
% Cu-K-alpha doublet as measured in october 1983 by J. Bergmann
ILAM=4 TITEL=CU_vom_Oktober_1983
0.401939 6.49098 0.0010981 % CuKa1 (1)
0.266445 6.49013 0.0019875 % CuKa1 (2)
0.167844 6.47504 0.0012544 % CuKa2 (1)
0.163773 6.47400 0.0017246 % CuKa2 (2)
```

Now the emission lines will be labelled as „CuKa1 (1)", „CuKa1 (2)" etc. when activating the spectral line cursor. *.lam files with parametrized intensities are also supported, as for example the default „cu.lam" file distributed with the Profex-BGMN-Bundle package:

```
% Berger CuK1,2,3 + Kb XPERT BERN
ILAM=6
0.01586*ifthenelse(ifdef(alpha3ratio),(alpha3ratio)/0.01586,1) 6.51571 0.00783 % CaKa3
0.56768*ifthenelse(ifdef(alpha2ratio),(1-alpha2ratio)/0.64369,1) 6.49099 0.00092 % CuKa1 (1)
0.07601*ifthenelse(ifdef(alpha2ratio),(1-alpha2ratio)/0.64369,1) 6.48905 0.00126 % CuKa1 (2)
0.25107*ifthenelse(ifdef(alpha2ratio),(alpha2ratio)/0.35631,1) 6.47496 0.00109 % CuKa2 (1)
0.08688*ifthenelse(ifdef(alpha2ratio),(alpha2ratio)/0.35631,1) 6.47366 0.00130 % CuKa2 (2)
0.00249*ifthenelse(ifdef(betaratio),(betaratio)/0.00249,1) 7.18206 0.00151 % CuKb
```

Normalize quantity goals to 100 % Normally quantity goals are normalized to 1.0:

```
sum=betaTCP+betaCPP
GOAL[1]=betaTCP/sum
GOAL[2]=betaCPP/sum
```

If this option is checked, the goals will be normalized to 100 %:

```
sum=betaTCP+betaCPP
GOAL[1]=100*betaTCP/sum
GOAL[2]=100*betaCPP/sum
```

Create report after refinement If checked, a refinement report in HTML format will be created automatically after the refinement. The report can be customized as shown in part 2 of the user manual, and viewed in a web browser.

3.4.2 Repositories

Structure File Repositories Specifies the location where BGMN structure files (*.str) are stored. Several directories can be entered. Sub-directories will be scanned for *.str files automatically. Double or redundant entries will be ignored.

Device File Repositories Specifies the locations where BGMN instrument files (*.sav, *.ger, *.geq, *.tpl) are stored. Several directories can be entered.

Preset Repositories Specifies the locations where refinement preset files (*.pfp) are stored. Several directories can be entered.

3.4.3 Peak detection

Search for new peaks If checked, the detection process is allowed to add new peaks to the list. This option should always be activated.

Eliminate obsolete peaks Allows the process to remove peaks from the list if they become obsolete later in the peak search.

Allow RP=2 Allows the process to use profile function RP=2 (no peak broadening).

Allow RP=3 Allows the process to use profile function RP=3 (Lorentzian broadening B1 only).

Allow RP=4 Allows the process to use profile function RP=4 (Lorentzian broadening B1 and squared Lorentzian broadening B2).

Allow increment of profile function If checked, the process is allowed to automatically step the profile function up to RP=3 or RP=4 if peak broadening is detected.

Allow reduction of profile function If checked, the process is allowed to automatically step the profile function down to RP=3 or RP=2 if no peak broadening is detected.

Simplify background Search for a simplified background polynome during the fit.

3.4.4 Search-Match

Penalty Weighing Coefficients

Unit Cell (a) A value > 1.0 increases the penalty for phases with mismatching unit cell parameters. A value of 0.0 disables the penalty function for unit cell mismatches. The default value of 1.0 applies a moderate penalty.

Weight Fraction (b) A value > 1.0 increases the weight of GEWICHT in the computation of the figure of merit. A value of 0.0 disables GEWICHT from the computation of the figure of merit. The default value of 1.0 applies a moderate weight to GEWICHT.

Crystallite Size (c) A value > 1.0 increases the penalty for phases with small crystallite sizes. A value of 0.0 disables the penalty function for small crystallite sizes. The default value of 1.0 applies a moderate penalty. This parameter only takes effect if the refined $B1$ value is greater than the penalty threshold for $B1$.

Micro-strain (d) A value > 1.0 increases the penalty for phases with micro-strain. A value of 0.0 disables the penalty function for micro-strain. The default value of 1.0 applies a moderate penalty. This parameter only takes effect if the refined $k2$ value is greater than the penalty threshold for $k2$.

Penalty Thresholds

Crystallite size (B1) The penalty function for small crystallite sizes only takes effect if the refined $B1$ value exceeds the threshold specified here.

Micro-strain (k2) The penalty function for micro-strain only takes effect if the refined $k2$ value exceeds the threshold specified here.

Duplicates

Unit cell axes (nm) Specifies the range in which unit cell parameters are considered to be equivalent. Phases with unit cell parameters differing less than the range specified here are considered duplicates.

Unit cell angles ($^\circ$) Specifies the range in which unit cell angles are considered to be equivalent. Phases with unit cell angles differing less than the range specified here are considered duplicates.

3.4.5 Reference Structures

Automatically select best matching reference phase When opening a graph file, automatically search and select the reference phase with it's strongest peak at the position of the scan's highest intensity. This is the same as double clicking at the strongest peak just after loading the scan file. Note that only indexed reference structures will be considered.

Automatically index new structure files If checked, Profex will scan the structure file directory for new structure files each time Profex is started and the first project is loaded.

If not checked, new structures will only be indexed when „Tools → Index structure database" is clicked manually.

Structures will not be available for double-click phase identification as long as they have not been indexed.

Draw hkl reference lines from background curve if available If this option is checked, Profex will use a scan with name „background" to draw the base of the *hkl* reference lines on. If no such scan is found or this option is unchecked, the *hkl* lines will be drawn from the zero line.

Color of Reference hkl Lines Color of the *hkl* lines when selecting a reference structure from the Reference Structures box.

Clear *hkl* index buffer Clears the buffer file with structure file *hkl* indices. Profex must be restarted for this to take effect. All structure files will be re-indexed either automatically, or when selected from the Reference Structures box.

***hkl* reference line range** Specifies the upper 2θ angle for *hkl* indices to be calculated. Larger ranges will require more time to index. The range may be smaller or larger than scan file ranges.

3.4.6 Favorites

Select reference structure files to be shown in the „Add / Remove Phase" and the reference structure dropdown menu when the „Favorites" filter is applied.

3.4.7 Refinement Limits

On this page the upper and lower limits automatically added by Profex to refined parameters are specified. These limits are used when creating BGMN structure files (*.str) from CIF or ICDD XML structure files, or when toggling the refinement state of parameters.

Unit Cell Parameters Specifies the upper and lower limits of unit cell parameters. The value is a fraction of the unit cell parameter specified in %. It is therefore independent of the setting of `UNIT`.

Fractional Coordinates Upper and lower limits of fractional coordinates released for refinement. The unit of this value is in fractional coordinates and thus independent of the parameter `UNIT`. Example: Releasing the coordinates of the following atom for refinement with a limit of 0.05:

```
E=SI Wyckoff=f x=0.25 y=0.5 z=0.1234 TDS=0.02
```

will result in (without line break):

```
E=SI Wyckoff=f PARAM=x=0.25_0.20^0.30 PARAM=y=0.5_0.45^0.55
               PARAM=z=0.1234_0.0734^0.1734 TDS=0.02
```

B1 Specifies the upper limit for B1. The lower limit is always 0.0.

k2 Specifies the upper limit fo k2. The lower limit is always 0.0.

TDS Specifies the upper limit for atomic displacement parameters TDS. No unit conversion is applied. When changing the `UNIT` from `UNIT=NM` to `UNIT=ANGSTROEM` in the control file, the TDS limit must be changed accordingly (multiplied by 100). The lower limit is always 0.0.

χ^2 **acceptance limit** Draws an additional line on the convergence display graph at the χ^2 value specified here. This is just a visual aid to quickly verify if the fit has reached an acceptable convergence. Values can be chosen freely. Recommended values are in the range of 1.2–1.5.

Reset Resets all limits to reasonable default values:

Unit cell parameters	= 1.00%
Fractional coordinates	= 0.05
B1	= 0.010
k2	= 0.00010
TDS	= 0.020
χ^2 acceptance limit	=1.50

3.4.8 GOAL Management

Manage Phase Quantification GOALs If this option is checked, a GOAL to compute relative phase quantities will be added by Profex when a new phase is added with the „Add / Remove Phase" dialog. When removing a phase using the „Add / Remove Phase" dialog the corresponding quantification GOAL will be removed.

Custom GOALs not identified as quantification GOALs will be preserved and appended to the list of quantification GOALs.

Note that the syntax of GOALs written by Profex changed with version 3.12.0, as described below.

GOAL syntax format The syntax used by Profex to define phase quantification GOALs changed with Profex version 3.12.0. The previous syntax („simple") is still available for compatibility reasons, but the new syntax („extended") provides some more flexibility. The syntax version only affects writing new GOALs. Reading old projects using the simple syntax will work even if this option is set to „extended" format.

The simple syntax used in Profex 3.11 and older defines the sum of all phases and divides each GOAL by the sum in order to obtain relative phase quantities normalized to 1.0:

```
sum=Calcite+Aragonite
GOAL[1]=Calcite/sum
GOAL[2]=Aragonite/sum
```

When adding another phase „corundum" and declaring it as an internal standard with a phase content of 10 wt-%, the GOALs section is re-written as follows:

```
ISTD=Corundum
ISTDQ=0.1000

sum=ISTD*(1-ISTDQ)/ISTDQ
Amorph=1-(Calcite+Aragonite)/sum
GOAL[1]=Calcite/sum
GOAL[2]=Aragonite/sum
GOAL[3]=Amorph
```

Using the new extended GOALs syntax, intermediate variables will be used, and the first example code looks as follows:

```
sum=Calcite+Aragonite
QCalcite=Calcite/sum
QAragonite=Aragonite/sum
GOAL[1]=QCalcite
GOAL[2]=QAragonite
```

Instead of `Calcite/sum`, the GOAL is now called `QCalcite`, using the prefix „Q". The prefix is a character prepended to the phase name. The denominator for phase normalization is called „sum".

Adding 10 wt-% corundum and using it as an internal standard will change the GOALs section as follows:

```
ISTD=corundum
ISTDQ=0.1000

sumabs=ISTD*(1-ISTDQ)/ISTDQ
QabsCalcite=Aalcite/sumabs
QabsAragonite=Aragonite/sumabs
```

```
QabsAmorph=1-(Calcite+Aragonite)/sumabs
GOAL[1]=QabsCalcite
GOAL[2]=QabsAragonite
GOAL[3]=QabsAmorph
```

This time the GOAL name prefix is „Qabs" and the denominator is „sumabs". Prefixes and denominators can be customized as described below.

If the option „Also add GOALs for relative phase quantities" is activated, GOALs for relative and absolute phase quantities will be written when using an internal standard. In that case, the GOALs section the last example above will look as follows:

```
ISTD=Corundum
ISTDQ=0.1000

sum=Calcite+Aragonite+Corundum
QCalcite=Calcite/sum
QAragonite=Aragonite/sum
QCorundum=Corundum/sum

GOAL[1]=QCalcite
GOAL[2]=QAragonite
GOAL[3]=QCorundum

sumabs=ISTD*(1-ISTDQ)/ISTDQ
QabsCalcite=Aalcite/sumabs
QabsAragonite=Aragonite/sumabs
QabsAmorph=1-(Calcite+Aragonite)/sumabs

GOAL[4]=QabsCalcite
GOAL[5]=QabsAragonite
GOAL[6]=QabsAmorph
```

Now it becomes apparent that the new syntax allows easier identification of relative and absolute phase quantity GOALs. The prefix for relative quantities could also be set to „Qrel" in order to obtain GOAL names `QrelCalcite` and `QabsCalcite` for even easier reading.

Relative Phase Quantity GOALs: GOAL name prefix Set the prefix used to label quantification GOALs when not using an internal standard. Only alphanumeric characters are allowed (a–z, A–Z, 0–9). Default is „Q".

Relative Phase Quantity GOALs: Denominator variable Set the name of the denominator variable used to calculate quantification GOALs when not using an internal standard. Default is „sum".

Absolute Phase Quantity GOALs: GOAL name prefix Set the prefix used to label quantification GOALs when using an internal standard. Only alphanumeric characters are allowed (a–z, A–Z, 0–9). Default is „Qabs".

Absolute Phase Quantity GOALs: Denominator variable Set the name of the denominator variable used to calculate quantification GOALs when using an internal standard. Default is „sumabs".

Absolute Phase Quantity GOALs: Also add GOALs for relative phase quantities When checked, both relative and absolute phase quantities will be calculated when using an internal standard. If not checked, only absolute quantities will be calculated. This option only affects projects using an internal standard.

3.4.9 Summary Table

Global Parameters and GOALs

Show warnings for values below detection and quantification limit If activated, Profex will show a warning for phase quantities getting small relative to their ESD. For example, if the limit of quantification (LOQ) is defined as 0.25, the variation coefficient (ESD / value) must be smaller than 25 %, or, in other words, the refined value must be greater than 4 · its ESD. Else a warning „< LOQ" will be shown in the summary table. More information can be found in part 2 of the user manual.

Variation coefficient for LOQ: Defines the threshold for „< LOQ" (below limit of quantification) warnings. Typical values are 0.25 if the refined value must be at least four times its ESD in order to be quantifiable, or 0.10 if it must be at least 10 times greater than its ESD. This variable can also be set in the control file (*.sav), see section 4. Values read from the control file override values specifiec in the preferences dialog. More information can be found in part 2 of the user manual.

Variation coefficient for LOD: Defines the threshold for „< LOD" (below limit of detection) warnings. Typical values are 0.50 if the refined value must be at least twice its ESD in order to be detectable, or 0.33 if it must be at least three times greater than its ESD. This variable can also be set in the control file (*.sav), see section 4. Values read from the control file override values specifiec in the preferences dialog. More information can be found in part 2 of the user manual.

Minimum ESD (ignore ESDs below) = For phase quantities approaching 0.0, the ESD also approaches 0.0. Such phases appear to be detectable and quantifiable even at infintesimally small quantities, but in fact it is an artifact of the ESD computation. In order to avoid this, a minimum ESD can be specified here. Refined ESDs below this value will be ignored and hard set to the minimum ESD. Typical values are 0.05 wt-%. Set this value to 0.00 to use all refined ESD values, regardless of how small they are. More information can be found in part 2 of the user manual.

Listed GOALs A list of global GOAL names that will be read from the BGMN list file (*.lst) and shown in the summary table for global parameters and goals. If the text field is empty, all global GOALs will be shown. This text field supports regular expression patterns. For example, instead of listing all EPS*n* values separately:

```
EPS1
EPS2
EPS3
EPS4
```

one can use a regular expression to list all refined EPS values:

```
^EPS[1-4]$
```

or alternatively:

```
^EPS\d$
```

Regular expressions are useful to identify GOALs describing a phase quantity. Quantity GOALs managed by Profex always have a unique name ending on `/sum`. A regular expression pattern describing GOAL names of type `<any name>/sum` can thus be used to list only phase quantity GOALs. The following pattern only matches GOALs with names ending on `/sum`:

```
^[^\/]+\/sum$
```

For the new GOALs syntax used in Profex 3.12 and newer, quantification GOALs use prefixes „Q" or „Qabs" (both are customizable) instead of the denominator. These GOALs are captured with the following expressions:

```
^Q\S+$
^Qabs\S+$
```

Numerous tutorials on regular expressions can be found on the internet.

Reset Pressing this button erases the text field with global parameters and GOALs and inserts a default set of parameters.

Local Parameters and GOALs

Listed GOALs Enter the parameters to be read from the local parameters and goals section in the BGMN list file (*.lst) and shown in the summary table for local parameters and goals. The text field supports regular expression patterns. For example, instead of listing all unit cell parameters separately:

```
A
B
C
ALPHA
BETA
GAMMA
```

one could use a regular expression pattern

```
^A|B|C|ALPHA|BETA|GAMMA$
```

or alternatively:

```
^[A-C]$
^ALPHA|BETA|GAMMA$
```

However, with regular expression patterns the parameters may be listed in arbitrary order. Regular expressions are particularly useful for GrainSize results. Printing all refined GrainSizes is achieved by the following pattern:

```
^GrainSize\(\d,\d,\d\)$
```

Reset Pressing this button erases the text field with local parameters and GOALs and inserts a default set of parameters.

3.5 Fullprof

Fullprof Executable Specifies the path to the Fullprof executable `fp2k.exe`.

Structure files directory Specifies the location of the directory with structure template files.

Device files directory Specifies the location of the directory with device template files.

Stop on convergence Normally Fullprof aborts the refinement when convergence criteria are reached. Checking this option forces Fullprof to always perform the number of refinement cycles specified with the parameter `Ncy`.

Divergence slit angle As Fullprof expects all scans to be measured with a fixed divergence slit setting, Profex will attempt to convert scans measured with automatic or variable divergence slit. The slit opening in degrees specified here is the opening the scans will be converted to. A value less than 1.0 degree is recommended.

3.6 Chemical Composition

The chemical composition page allows to edit the oxide forms and their molecular weights used to calculate the elemental composition of the sample. Elements with empty molecular weight, or with molecular weight of 0.0 g/mol, will be ignored. It is recommended to leave the oxide and molecular weight cells of oxygen (element No. 8) empty to suppress display of oxygen as a separate element in the chemical composition results table.

A dialog to select the oxide form and automatically calculate the corresponding molecular weight can be opened by double-clicking on the element symbol (left column).

Double-clicking an oxide cell (middle column) or molecular weight cell (right column) allows to enter oxide names and molecular weights directly by bypassing the dialog mentioned above.

Element, Oxide, and Molecular Weight table This table holds the oxide formula and oxide molecular weight for each element. Edit the values by double clicking a cell. Double clicking an element cell will open a dialog to determine oxides and their molecular weight. Double clicking any other cell allows direct input of oxide formulas and values.

Reset Resets the table to the internal default values. All customizations will be lost.

3.7 Text Blocks

On this page text blocks can be managed. See part 2 of the user manual for more information on how to use text blocks. Click the + button to create a new text block, then enter the text in the editor. All changes will be saved automatically when closing the preferences dialog. Click − to delete the current text block. The block will be deleted permanently when closing the preferences dialog with the ,,OK" button. Close the dialog with ,,Abort" if the text block was deleted accidentally.

4 Profex-specific Control File Variables

Profex reads some additional variables from BGMN control files (*.sav) that are not mandatory for the BGMN refinement backend. Some of them are only parsed by Profex and ignored by BGMN, and some of them are used for specific calculations of GOALs.

4.0.1 Refinement Control Files (*.sav)

sum This variable is used to compute relative phase quantities normalized to 100 %. Normally it holds the sum of the `GEWICHT` variables of all phases. If one phase is set as an internal standard, the `sum` variable is used for the normalization to the internal standard quantity. `sum` is automatically managed by Profex if phases are added, removed, or set and unset as internal standard.

ISTD Holds the phase name of the internal standard phase. It is only present if an internal standard has been defined. It is added and removed by Profex if an internal standard is set or unset.

ISTDQ Holds the phase quantity of the internal standard phase normalized to 1.0 (not to 100 %). It is only present if an internal standard has been defined. It is added and removed by Profex if an internal standard is set or unset.

LOQ Relative standard deviation (ESD / value) considered as the limit of quantification (LOQ). This value will override the value set in the preferences dialog. It will only be parsed if the option „Show warnings for values below detection and quantification limit" is set active in the preferences dialog. If the ratio `ESD / value` of a refined phase quantity exceeds `LOQ`, it will be highlighted in the summary table and a warning „< LOQ" will be shown.

LOD Relative standard deviation (ESD / value) considered as the limit of detection (LOD). This value will override the value set in the preferences dialog. It will only be parsed if the option „Show warnings for values below detection and quantification limit" is set active in the preferences dialog. If the ratio `ESD / value` of a refined phase quantity exceeds `LOD`, it will be highlighted in the summary table and a warning „< LOD" will be shown.

MINESD Sets the minimum ESD that is considered realistic for refined phase quantities. This variable overrides the value set in the preferences dialog „Minimum ESD (ignore ESDs below) =".

SampleID: A custom sample ID string can be entered to add random sample information to the refinement. Profex is able to extract sample ID information from some raw data formats, such as Bruker *.raw and *.brml. In that case it will add the SampleID tag automatically when the BGMN control file (*.sav) is created. SampleIDs are also exported to CSV tables when using the results export features.

Example:

```
% SampleID: Sample No 160810-01, room temperature
```

Note that all comment signs (also at the beginning of the line) will be ignored. Profex will extract the string following `SampleID:` regardless of comment signs. In the example above, the extracted sample ID string will be `Sample No 160810-01, room temperature`.

Warning: Avoid semicolons (;) in the sample ID string. This character is used as a field separator in the CSV results tables. Using it in the sample ID will confuse the layout of the CSV tables.

4.0.2 Instrument Configuration Files (*.sav)

`ZTSTRETCH` The width of the raytraced profiles will be scaled by this value or function prior to profile interpolation. This can be helpful for unconventional goniometer setups, when the fundamental parameters are unknown or unable to accurately describe the profile.

Instead of a constant scale factor, a `zweiTheta` dependent function can be specified in JavaScript syntax. The value for `zweiTheta` is read in degrees.

For example, to increase the profile width with increasing diffraction angle 2θ following a $\tan(2\theta)$ characteristic, use the following equation:

```
ZTSTRETCH=1+Math.tan(Math.PI*zweiTheta/180.0)
```

For more information on the JavaScript syntax, refer to [6, 7].

5 Technical Information

5.1 Scan File Conversion

In contrast to the BGMN Rietveld backend, which only supports a limited number of scan file formats natively, Profex reads a wide and growing list of file formats. When running a refinement on a scan file format not supported by BGMN, Profex will by default automatically convert the file in the background and modify the control file accordingly. This section describes the conversion process and the settings allowing the user to control the conversion.

Automatic scan file conversion can be switched on and off in the preferences dialog by checking or unchecking the option „Edit → Preferences... → BGMN → Convert raw scans to XY format". Scan file handling by Profex will be different depending on this setting. Unless conversion is not desired for specific reasons, users are strongly advised to activate this option.

It is a surprisingly complex task to determine the correct file name of a project's raw scan (VAL$[n]$ keyword in the control file). The possible scenarios to be considered are manifold. Profex has sophisticated routines to determine the best guess for a VAL file name under all circumstances. These routines are illustrated in Figures 10–13.

In principle, when creating a new project, a raw scan file as obtained from the instrument is opened and a new control file is created either by using the „Add a new phase" dialog or the „Copy control file" function. Either way the loaded raw scan file determines the location and the base name of the project, and all input and output file names in the control file will automatically be set to this scan's file base name. The scan file name to be read by the BGMN Rietveld backend is specified with the `VAL[n]=ScanFile.xxx` line in the control file. The scan file name is given by the project name, as described above, but the file format and extension is determined by Profex automatically, depending on the raw scan format and the setting of „Edit → Preferences... → BGMN → Convert raw scans to XY format". If a format natively supported by BGMN is detected, the file will be used without conversion. If the format is not supported, the behavior will depend on the setting „Convert raw scans to XY format": If active, the file will be converted to *.xy format and the VAL$[n]$ file entry will be adapted accordingly. If inactive, no conversion will be done and it is in the user's responsibility to guarantee correct file names and formats. See Fig. 9 for more explanations.

However, the processes described above represent relatively simple scenarios, when the raw scan file is opened and the format and file name are known. In many situations it determining the correct file name is not as straight-forward. The following situation represents a worst case: A DIA file is opened, conversion to *.xy is inactive, and the control file is created from another project using the „Copy control file" feature. Normally, when a DIA file exists, a control file should also exist with a valid VAL$[n]$ entry. However, when sharing or moving DIA files, or when the base name of the DIA and control file do not match, it may still occur that a DIA file is present but the corresponding control file cannot be located. Trying to find the correct raw scan file used to create die DIA file is difficult in such a situation:

1. The control file copied over from another project contains input and output file names (VAL, DIAGRAMM, OUTPUT, etc.) of the source project. All file names must be changed to the destination project. The VAL file name found in this control file must not be used.
2. The displayed scan is a DIA file, which cannot be used as input file.
3. Converting the DIA file to *.xy is not allowed.
4. There is no reference to the raw scan in any of the available files.
5. In that case, Profex will scan the directory of the DIA file for a raw scan file in a format natively supported by BGMN. But there is no guarantee that such a file is found.

This is one of many scenarios when finding the correct VAL file name is not trivial. However, the complex processes illustrated in Figures 10–13 cover most situations, and if no solution can be found, a warning will be issued.

If the raw scan format (here: xrdml) is not natively supported by BGMN, Profex will change the VAL[n] file name to *.xy and convert the file automatically.

```
working directory
├── scan_1.sav
├── scan_1.xrdml
├── structure_1.str
├── instrument.sav
├── instrument.geq
└── instrument.ger
```

```
% Input files
VAL[1]=scan_1.xy
VERZERR=instrument.geq
LAMBDA=CU
STRUC[1]=structure_1.str
% Output files
LIST=scan_1.lst
OUTPUT=scan_1.par
DIAGRAMM=scan_1.dia
...
```

If conversion to *.xy is deactivated, VAL[n] will be the raw scan file. If it is not supported natively by BGMN (e. g. xrdml), refinement will not start.

```
working directory
├── scan_1.sav
├── scan_1.xrdml
├── structure_1.str
├── instrument.sav
├── instrument.geq
└── instrument.ger
```

```
% Input files
VAL[1]=scan_1.xrdml
VERZERR=instrument.geq
LAMBDA=CU
STRUC[1]=structure_1.str
% Output files
LIST=scan_1.lst
OUTPUT=scan_1.par
DIAGRAMM=scan_1.dia
...
```

Natively supported file formats (here: Seifert val) do not require conversion to *.xy. Profex will use the raw scan file name for the VAL[n] entry, regardless of the state of the „Convert raw scans to XY" setting.

```
working directory
├── scan_1.sav
├── scan_1.val
├── structure_1.str
├── instrument.sav
├── instrument.geq
└── instrument.ger
```

```
% Input files
VAL[1]=scan_1.val
VERZERR=instrument.geq
LAMBDA=CU
STRUC[1]=structure_1.str
% Output files
LIST=scan_1.lst
OUTPUT=scan_1.par
DIAGRAMM=scan_1.dia
...
```

Figure 9: Some examples for working and failing VAL[n] file scenarios.

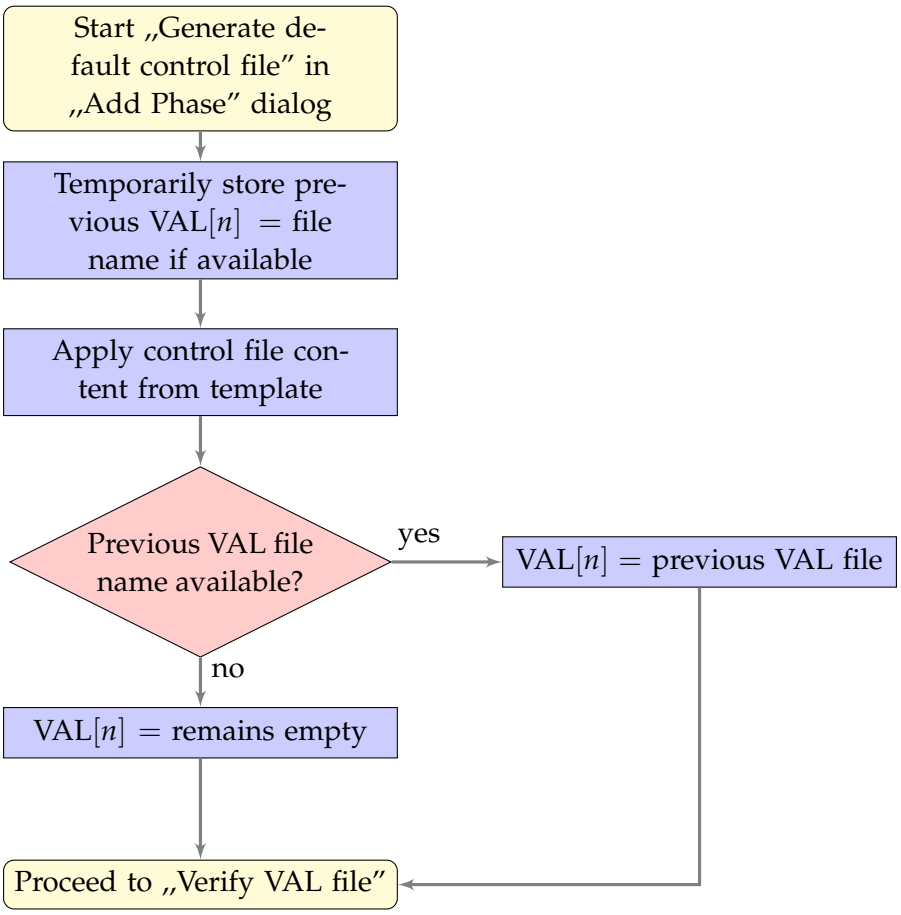


Figure 10: VAL file handling when calling the „Add Phase" dialog and activating the option „Generate default control file" to create a control file from a template file.

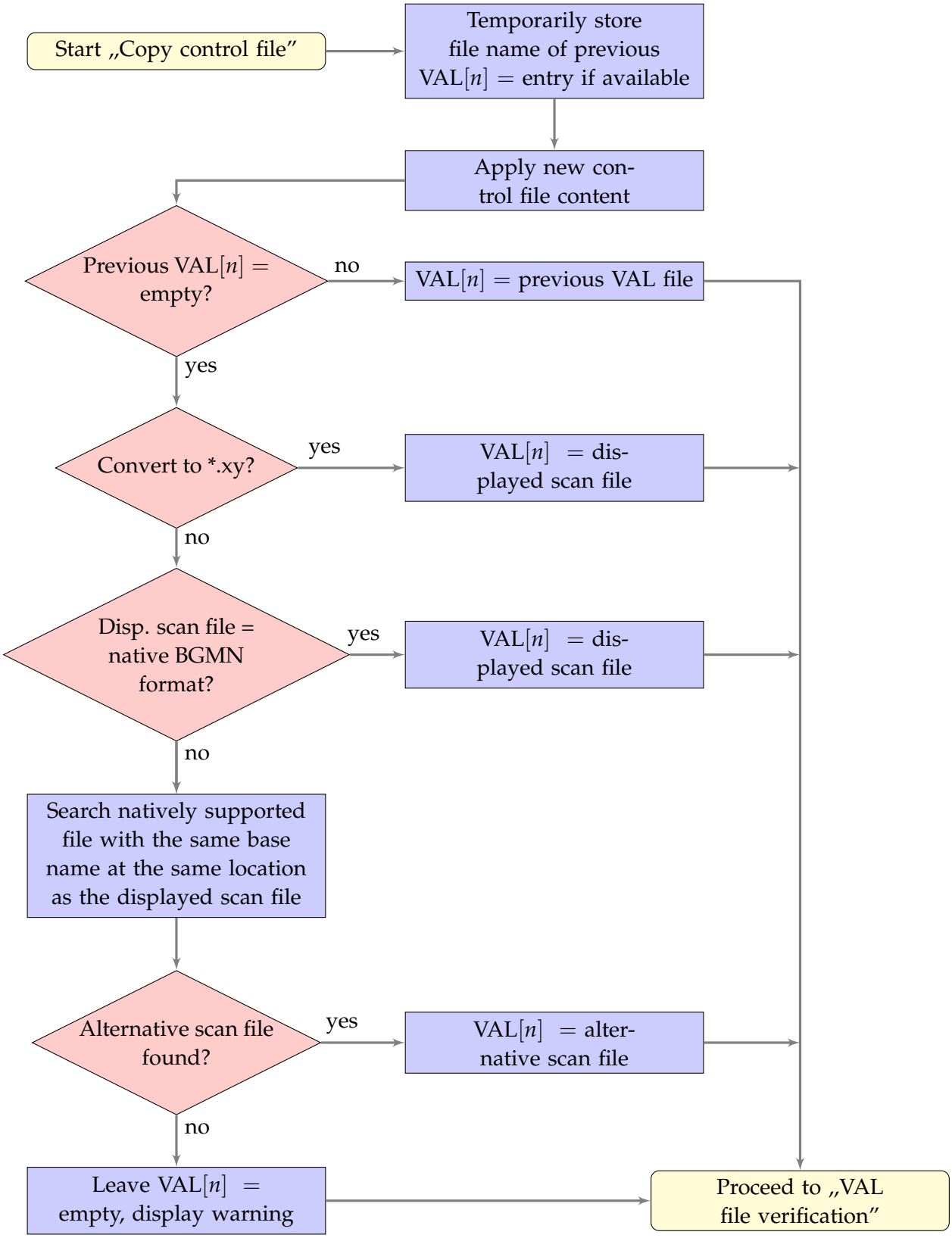


Figure 11: VAL file name handling when using the „Copy control file” function.

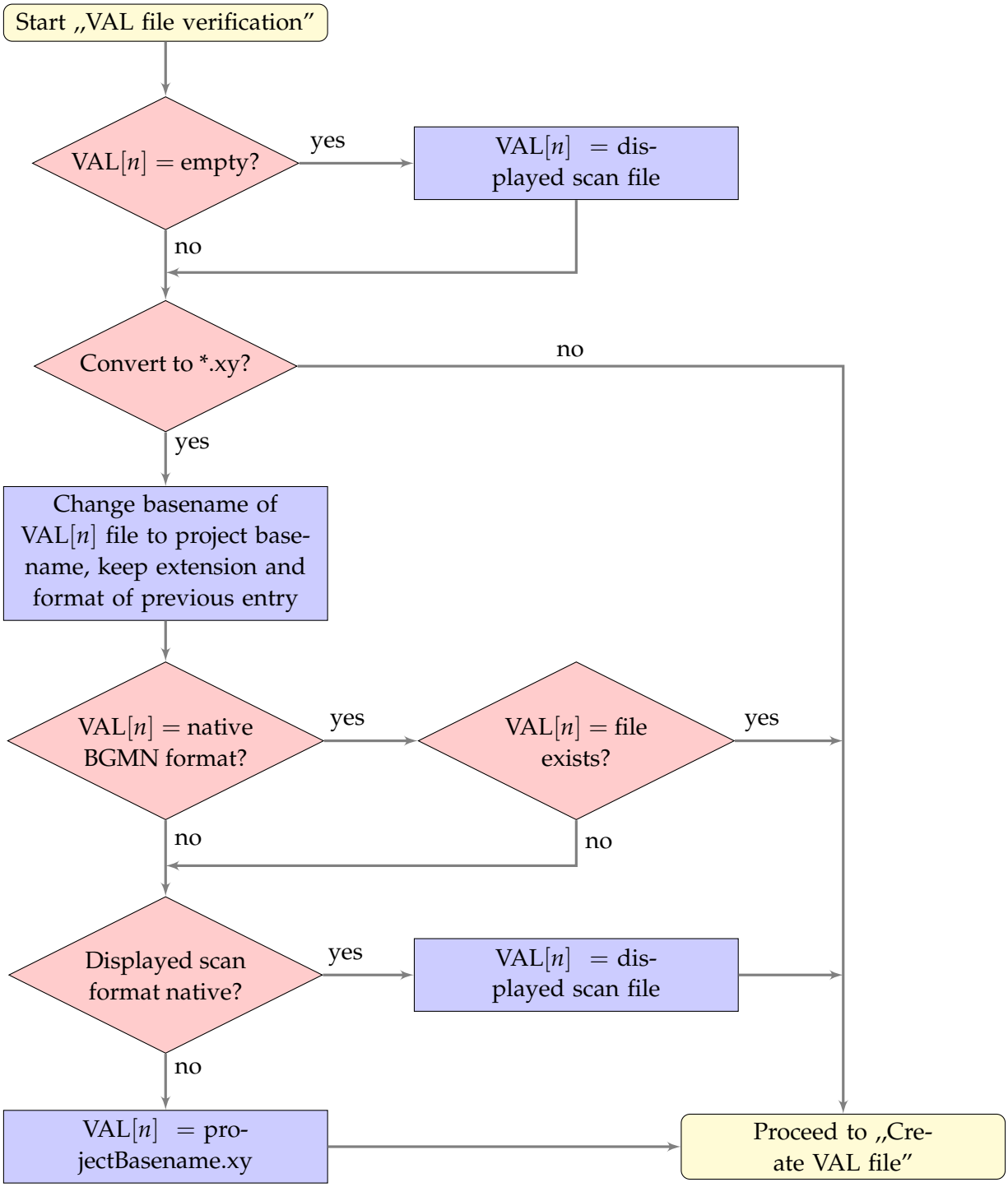


Figure 12: Automatic verification of a VAL[n] file entry in the SAV control file. This function is called at several occasions when modifying the control file content. E. g. after creating a default control file, or after applying a control file from another project.

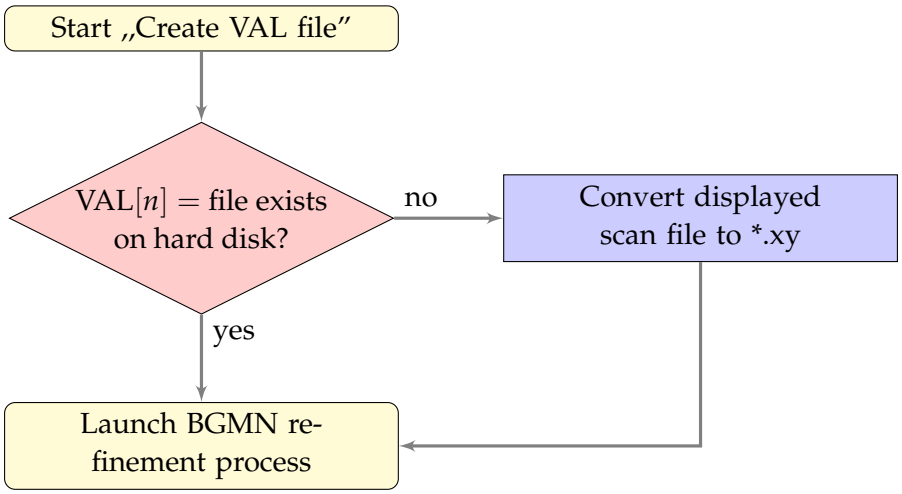


Figure 13: Immediately before running the refinement process, Profex checks whether the VAL file referenced in the control file exists on the hard disk. If not, a *.xy file will be created from the currently displayed scan file.

5.2 Refinement Presets

Preset files store data in XML format. Their storage location can be configured in „Edit → Preferences... → BGMN → Configuration → Presets directory". When opened in a text editor, the file must have the following structure:

```
<?xml version="1.0" encoding="UTF-8"?>
<preset name="anyName">
    <device MD5hash="..." RelativePath="...">myInstrument.geq</device>
    <device MD5hash="..." RelativePath="...">myInstrument.ger</device>
    <device MD5hash="..." RelativePath="...">myInstrument.sav</device>
    <template MD5hash="..." RelativePath="...">myTemplate.tpl</template>
    <structures>
        <structure MD5hash="..." RelativePath="...">myPhaseA.str</structure>
        <structure MD5hash="..." RelativePath="...">myPhaseB.str</structure>
        <structure MD5hash="..." RelativePath="...">myPhaseC.str</structure>
    </structures>
    <other>
        <textfile MD5hash="..." RelativePath="...">background.xy</textfile>
        <textfile MD5hash="..." RelativePath="...">description.txt</textfile>
        <binaryfile MD5hash="..." RelativePath="...">report.docx</binaryfile>
    </other>
</preset>
```

At least one `<device>` and `<template>` node must be present. If one of them is missing, applying the preset will abort. If more than one template node is present, all but the first will be ignored. An arbitrary number of `<structure>` and `<other><...file>` nodes may be present. All paths can either be absolute or relative to the location of the preset file. Device and template files do not need to have the same file name. It is possible to use different template files with the same device file.

Files specified in

```
<other>
    <textfile>...</textfile>
</other>
```

and

```
<other>
    <binaryfile>...</binaryfile>
</other>
```

tags will be copied to the project directory. These tags can be used for arbitrary files, such as descriptions, background scans, raw data, report files etc. It is important to specify whether the file is stored in text or binary format. For text format files Profex will convert the line endings

to the target platform to maintain platform independence. Binary files will be copied without modification. If unsure, use `<binaryfile>`, as the copied file will not be modified.

Note that custom profile functions („Edit → Preferences… → BGMN → STR File Handling") will not be applied when using presets, as it would undermine the purpose of reproducing precisely defined refinement scenarios.

A typical file structure of a preset named „scenarioA" is shown below:

```
Presets
└─ scenarioA
   ├─ scenarioA.pfp
   ├─ instrA.geq
   ├─ instrA.ger
   ├─ instrA.sav
   ├─ scenarioA.tpl
   ├─ phaseA.str
   ├─ phaseB.str
   └─ instrA-bkgr.xy
```

The preset file „scenarioA.pfp" references all other files being part of the preset:

```
<!DOCTYPE ProfexPreset>
<preset version="20160910" name="scenarioA">
    <device MD5hash="fc74..." RelativePath="">instrA.geq</device>
    <device MD5hash="0523..." RelativePath="">instrA.ger</device>
    <device MD5hash="c2fb..." RelativePath="">instrA.sav</device>
    <template MD5hash="f089..." RelativePath="">scenarioA.tpl</template>
    <structures>
        <structure MD5hash="1fdb..." RelativePath="">phaseA.str</structure>
        <structure MD5hash="787e..." RelativePath="">phaseB.str</structure>
    </structures>
    <other>
        <textfile MD5hash="cc87..." RelativePath="">
            instrA-bkgr.xy
        </textfile>
    </other>
</preset>
```

The optional node argument `MD5hash` stores a checksum of the file in hexadecimal format. The checksum will be verified each time the preset is applied. In case of a mismatch, a warning is presented informing the user that the file has been modified and offering to cancel or proceed. The optional argument `RelativePath` stores the file's destination path relative to the scan file the preset is applied to.

5.2.1 Source and destination paths

Refinement presets offer some flexibility in terms of referenced file locations (structure, device, other files), both at the source (in the presets directory) and destination (in the project directory) of the preset. The preset file „scenarioA.pfp" will be used as an example. If the file name of, for example, a structure file is specified without a path, the structure file will be searched at the location of the preset file:

```
<structure RelativePath="">
    phaseA.str
</structure>
```

```
Presets
└─ scenarioA
   ├─ scenarioA.pfp
   └─ phaseA.str
```

If the file name is specified with a relative path (here „structures"), it will be searched in a sub-directory starting from the preset file:

```
<structure RelativePath="">
    structures/phaseA.str
</structure>
```

```
Presets
└─ scenarioA
   ├─ scenarioA.pfp
   └─ structures
      └─ phaseA.str
```

It is also possible to specify absolute file paths to locate the structure file. In that case, the structure file will be searched at the absolute path location, regardless of the location of the preset file:

```
<structure RelativePath="">
    C:\Profex-BGMN\Profex\Presets\scenarioA\phaseA.str
</structure>
```

The destination of the structure file (or any other file) is specified by the „RelativePath" argument. It will be used when the preset is applied to a scan file (here „myScan.raw") to specify the location relative to the scan file after the preset has been applied. If no relative path is given, the structure file will be copied to the location of the scan file:

```
<structure RelativePath="">
    phaseA.str
</structure>
```

```
myProject
├─ myScanA.raw
└─ phaseA.str
```

If a relative path is specified, a sub-directory will be created for the structure file:

```
<structure RelativePath="structures">
    phaseA.str
</structure>
```

```
myProject
├─ myScanA.raw
└─ structures
   └─ phaseA.str
```

The relative path of the structure file at the source location will be ignored. The structure file will be copied to the relative path specified as „RelativePath=":

```
<structure RelativePath="destination/phases">
    source/structures/phaseA.str
</structure>
```

```
myProject
├─myScanA.raw
└─destination
  └─phases
    └─phaseA.str
```

There is one exception when the relative path at the source location is not ignored: If no relative path is specified (empty or absent) and the structure file is located in a sub-directory in the preset directory, this sub-directory will be used as a relative path. This is necessary in order to maintain backward compatibility with previous versions of Profex presets:

```
<structure RelativePath="">
    structures/phaseA.str
</structure>
```

```
myProject
├─myScanA.raw
└─structures
  └─phaseA.str
```

Warning: It is possible to specify destination locations of files outside of the project directory:

```
RelativePath="..\structures"
```

This is likely to cause problems by overwriting files used by other projects. It is strongly advised not to specify relative paths outside of the project directory.

5.3 Automatic conversion of thermal displacement parameters

During the conversion from CIF or XML to STR format Profex automatically transforms the thermal displacement parameters to the format supported by BGMN. Depending on the source format, the following conversions are calculated (anisotropic β_{ij} values are not supported by the CIF format.):

Isotropic B: Isotropic B is the format supported by BGMN. However, BGMN uses a different unit than normally provided in the CIF file. Automatic conversion therefore performs the following conversion:

$$B_{iso}[nm^2] = 0.01 \cdot B_{iso}[\mathring{A}^2]$$

Anisotropic B_{ij}: Anisotropic B_{ij} are converted to isotropic B values in the expected unit [8]:

$$B_{iso}[nm^2] = 0.01 \cdot \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* A_i A_j$$

with reciprocal lattice parameters $a^*[\mathring{A}^{-1}]$ and real lattice parameters $A[\mathring{A}]$.

Anisotropic U_{ij}: Anisotropic U_{ij} are converted to U_{equiv} using the expression [8]:

$$U_{equiv} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* A_i A_j$$

with reciprocal lattice parameters $a^*[\mathring{A}^{-1}]$ and real lattice parameters $A[\mathring{A}]$. U_{equiv} is converted to B_{iso} by the following equation.

Isotropic U_{equiv}: Isotropic U_{equiv} values are converted to isotropic B:

$$B_{iso}[nm^2] = 0.01 \cdot 8.0 \cdot \pi^2 \cdot U_{equiv}$$

5.4 Peak fit functions

The peak fitting module supports several polynomial functions for background fitting, and peak functions for peak fitting.

Linear

Type	background
a	constant coefficient
b	linear coefficient

$$f(x) = a + b \cdot x$$

Gaussian

Type	peak
a	center position
b	half width at half maximum
c	intensity

$$f(x) = c \cdot \exp\left(-ln(2) \cdot \left(\frac{x-a}{b}\right)^2\right)$$

Lorentzian

Type	peak
a	center position
b	half width at half maximum
c	intensity

$$f(x) = \frac{c}{1 + \left(\frac{x-a}{b}\right)^2}$$

Pseudo-Voigt

Type	peak
a	center position
b	half width at half maximum
c	intensity
d	shape

$$f(x) = c \cdot \left((1-d) \cdot \exp\left(-log(2) \cdot \left(\frac{x-a}{b}\right)^2\right) + \frac{d}{1 + \left(\frac{x-a}{b}\right)^2}\right)$$

Pearson-VII

Type	peak
a	center position
b	half width at half maximum
c	intensity
d	shape

$$f(x) = \frac{c}{\left(1 + \left(\frac{x-a}{b}\right)^2 \cdot \left(2^{\frac{1}{d}} - 1\right)\right)^d}$$

Split Gaussian

Type	peak asymmetric
a	center position
b_1	half width at half maximum left side
b_2	half width at half maximum right side
c	intensity

$$f(x) = (1-p) \cdot c \cdot \exp\left(-ln(2) \cdot \left(\frac{x-a}{b_1}\right)^2\right) + p \cdot c \cdot \exp\left(-ln(2) \cdot \left(\frac{x-a}{b_2}\right)^2\right)$$

$$p = \begin{cases} 0.0 & \text{if } x \leq a \\ 1.0 & \text{if } x > a \end{cases}$$

Split Lorentzian

Type	peak asymmetric
a	center position
b_1	half width at half maximum left side
b_2	half width at half maximum right side
c	intensity

$$f(x) = (1-p) \cdot \frac{c}{1 + \left(\frac{x-a}{b_1}\right)^2} + p \cdot \frac{c}{1 + \left(\frac{x-a}{b_2}\right)^2}$$

$$p = \begin{cases} 0.0 & \text{if } x \leq a \\ 1.0 & \text{if } x > a \end{cases}$$

Split Pseudo-Voigt

Type	peak asymmetric
a	center position
b_1	half width at half maximum left side
b_2	half width at half maximum right side
c	intensity
d	shape

$$f(x) = (1-p)\cdot c\cdot\left((1-d)\cdot\exp\left(-log(2)\cdot\left(\frac{x-a}{b_1}\right)^2\right)+\frac{d}{1+\left(\frac{x-a}{b_1}\right)^2}\right)$$
$$+p\cdot c\cdot\left((1-d)\cdot\exp\left(-log(2)\cdot\left(\frac{x-a}{b_2}\right)^2\right)+\frac{d}{1+\left(\frac{x-a}{b_2}\right)^2}\right)$$

$$p=\begin{cases}0.0 & \text{if } x\le a\\ 1.0 & \text{if } x>a\end{cases}$$

Split Pearson-VII

Type	peak asymmetric
a	center position
b_1	half width at half maximum left side
b_2	half width at half maximum right side
c	intensity
d	shape

$$f(x) = (1-p)\cdot\frac{c}{\left(1+\left(\frac{x-a}{b_1}\right)^2\cdot\left(2^{\frac{1}{d}}-1\right)\right)^d}$$
$$+p\cdot\frac{c}{\left(1+\left(\frac{x-a}{b_2}\right)^2\cdot\left(2^{\frac{1}{d}}-1\right)\right)^d}$$

$$p=\begin{cases}0.0 & \text{if } x\le a\\ 1.0 & \text{if } x>a\end{cases}$$

Quadratic

Type	background
a	constant coefficient
b	linear coefficient
c	quadratic coefficient

$$f(x) = a + b \cdot x + c \cdot x^2$$

Cubic

Type	background
a	constant coefficient
b	linear coefficient
c	quadratic coefficient
d	cubic coefficient

$$f(x) = a + b \cdot x + c \cdot x^2 + d \cdot x^3$$

Polynomial 4

Type	background
a	constant coefficient
b	linear coefficient
c	quadratic coefficient
d	cubic coefficient
e	quartic coefficient

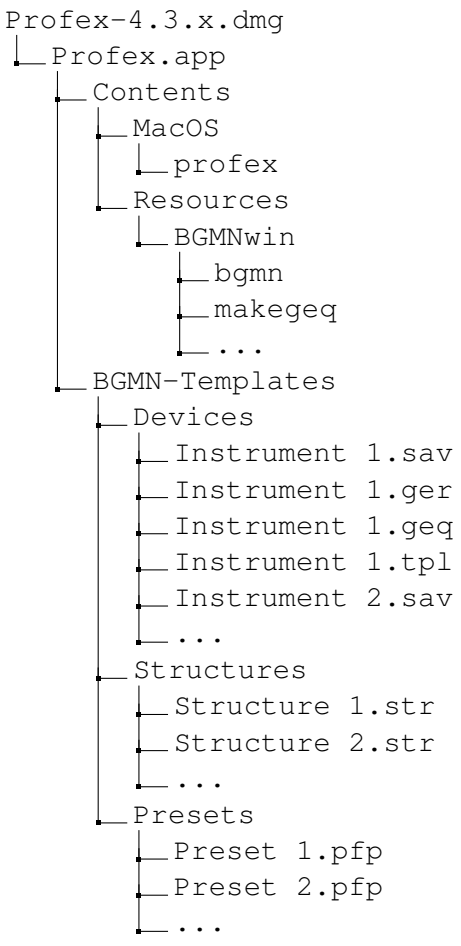
$$f(x) = a + b \cdot x + c \cdot x^2 + d \cdot x^3 + e \cdot x^4$$

5.5 Bundle File Structure

5.5.1 Windows

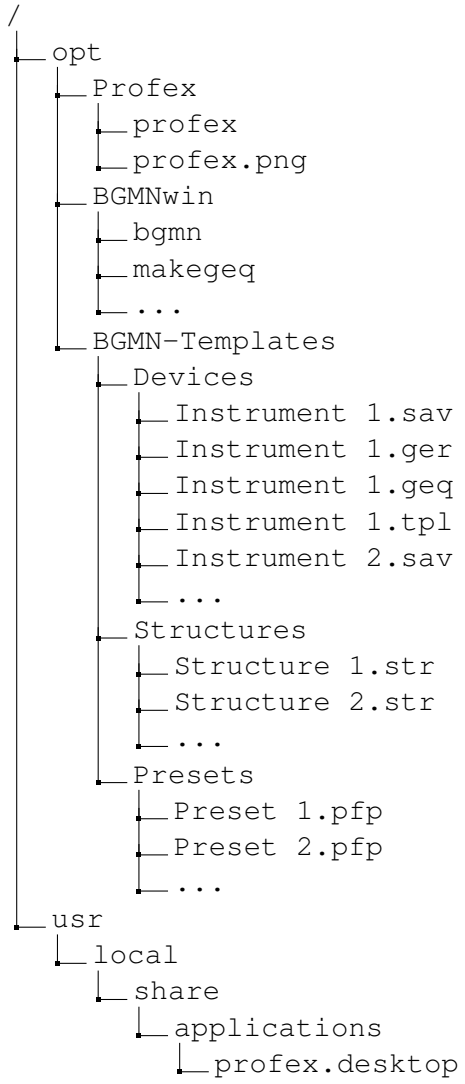
```
Profex-4.3.x.zip
└─Profex-4.3.x
   ├─profex.exe
   ├─...
   ├─BGMNwin
   │  ├─BGMN.EXE
   │  ├─MakeGEQ.EXE
   │  └─...
   ├─Devices
   │  ├─Instrument 1.sav
   │  ├─Instrument 1.ger
   │  ├─Instrument 1.geq
   │  ├─Instrument 1.tpl
   │  ├─Instrument 2.sav
   │  └─...
   ├─Structures
   │  ├─Structure 1.str
   │  ├─Structure 2.str
   │  └─...
   └─Presets
      ├─Preset 1.pfp
      ├─Preset 2.pfp
      └─...
```

5.5.2 Mac OS X


Profex-4.3.x.dmg
Profex.app
Contents
MacOS
profex
Resources
BGMNwin
bgmn
makegeq
...
BGMN-Templates
Devices
Instrument 1.sav
Instrument 1.ger
Instrument 1.geq
Instrument 1.tpl
Instrument 2.sav
...
Structures
Structure 1.str
Structure 2.str
...
Presets
Preset 1.pfp
Preset 2.pfp
...

5.5.3 Linux

No bundles are available for Linux. The program needs to be compiled from source, and BGMN templates can be downloaded from the Profex website. A recommended manual installation us shown below.



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Index