SUNBIM User's Guide (v 4.0)

SUNBIM v.4.0: a suite of programs for the supra- and sub-molecular X-ray imaging of nano and bio materials with SAXS, WAXS, GISAXS and GIWAXS techniques

Table of Contents

1 General Introduction

1.1 The aim of this manual

This manual describes the windows and menus of SUNBIM (Supramolecular & SUbmolecular Nano & Bio Materials X-ray IMaging) to allow users, dealing with SAXS, WAXS, GISAXS and GIWAXS data, to navigate and make informed choices within the program. It does not teach or instruct the user on recommended practices for data-reduction and analysis. To practice with each tool please download tutorial movies from this link.

1.2 What SUNBIM does

SUNBIM is a suite of integrated programs which, through a user friendly Graphical User Interface, is optimized to perform:

i. q-scale calibration and 2D→1D folding on SAXS/GISAXS/WAXS/GIWAXS data, also including possible eccentricity corrections for WAXS/GIWAXS data;
ii. background evaluation and subtraction, denoising and deconvolution of the primary beam angular divergence on SAXS/GISAXS profiles;
iii. indexing of 2D GISAXS frames and extraction of 1D GISAXS profiles along specific cuts;
iv. scanning microscopy in absorption and SAXS contrast: collection of transmission and SAXS data, in a mesh across mm^2 area, organization of the as-collected data into a single composite image of the transmitted intensity values or 2D SAXS frames, analysis of the composed data to derive the absorption map and/or the spatial distribution and orientation of nano-scale structures over the scanned area.

1.3 MATLAB: the underlying language of SUNBIM

SUNBIM is developed in MATLAB language and it is distributed through the website (after a valid registration). It is free of charge for academic, by accepting a license agreement during the software setup, as a stand-alone executable program for MS WINDOWS (a self-extracted executable setup file, 32 and 64 bit, is included at the distribution). The package uses MATLAB Compiler Runtime Library (free of charge and included in the distribution package).

1.4 Acknowledgements

The authors would like to thank the FIRB 2009/2010 project RINAME - Rete integrata per la Nano Medicina (RBAP114AMK_006), the project N-CHEM - Nanomax-integrable sensors for pathological biomarkers diagnosis, the European project NANoREG - A common European approach to the regulatory testing of Manufactured Nanomaterials (GA nr. FP7-310584) and the PRIN 2012 project NOXSS - X-ray Single Shots of Nano Objects (MD.P04.006.006).
Rocco Lassandro is acknowledged for technical support in the XMI-LAB.

2 Getting Started

2.1 Installing SUNBIM

2.1.1 WINDOWS

Double click on the executable setup file available on the website. The installation package is released in two versions: one that directly includes the MATLAB libraries, and another that downloads them from the web.

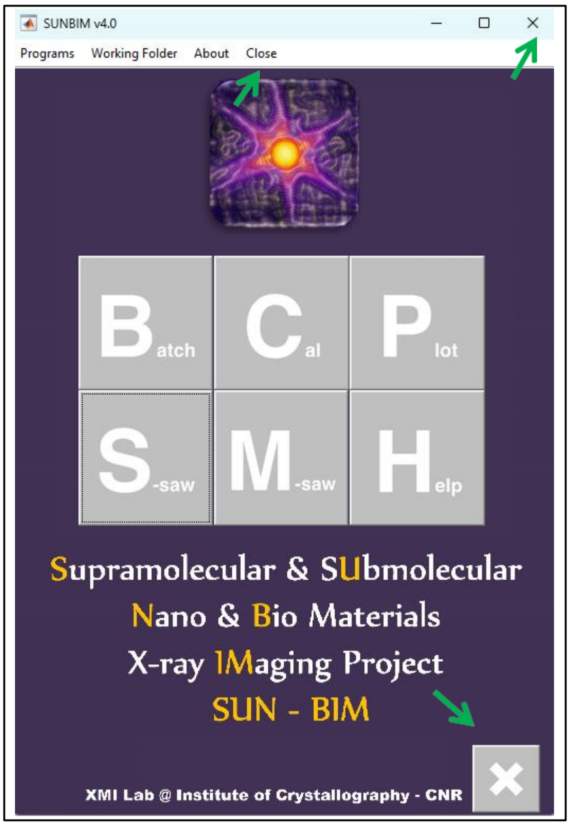
After accepting license agreement, follow the instruction to install SUNBIM on your machine. It will create an icon on your desktop to launch the software and a "C:\SunbimTemp" folder which will be used to uncompress MCR library (MCR_CACHE_ROOT path is defined as windows system variable).

2.1.2 MacOS

Double click on the .dmg setup file available on the website. The installation package is released in two versions: one that directly includes the MATLAB libraries, and another that downloads them from the web.

Follow the instruction to install SUNBIM on your machine. It will create an icon on your desktop to launch the software and a "C:\SunbimTemp" folder which will be used to uncompress MCR library (MCR_CACHE_ROOT path is defined as windows system variable).

2.2 Starting and stopping SUNBIM



Start SUNBIM double clicking the SUNBIM icon on your desktop. After a while (the time to uncompress MCR library and SUNBIM codes written in MATLAB framework) the SUNBIM main menu will open. During execution, a Windows Command Shell (console) window will also open. This allows you to monitor any errors or malfunctions of the program.

Warning: do not close this window, otherwise the program will terminate.

Stop SUNBIM by closing the SUNBIM main menu window by means of one of these procedures:

1. click the closing button of the window
2. select "Close" option from the menu
3. click the closing button on the right bottom of the window

After that, a dialog will open asking if you really want to close SUNBIM, including the running sub-programs. By choosing "Yes" all the opened sub-programs will be closed.

3 SUNBIM sub-programs

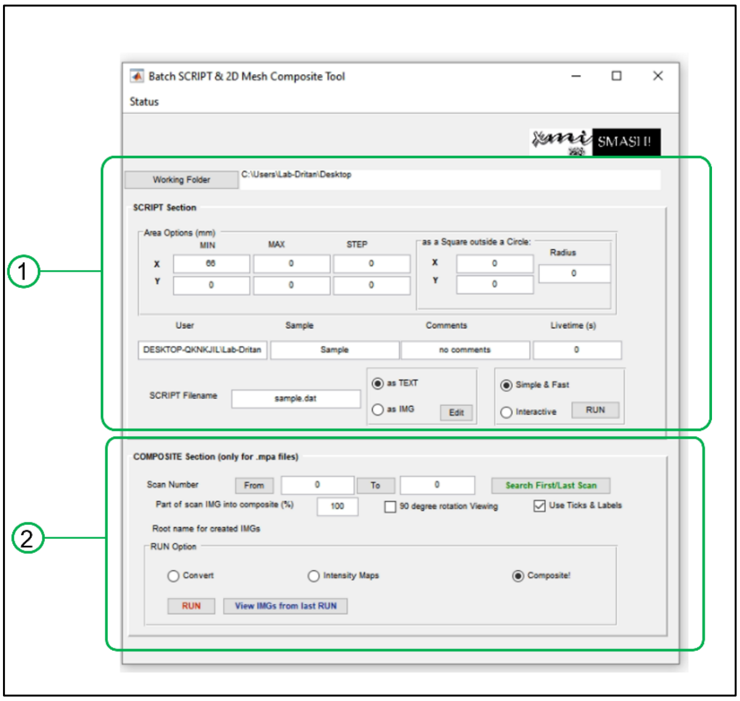
Users can interact with SUNBIM through several sub-programs/windows. From the main SUNBIM window you can access to different sub-windows, depending on your aims. The list of the sub-menu is the following:

- Batch Script & 2D Mesh Composite window
- Calibration window
- One-D Data Analysis Manager window
- S-SAWANA (Single Scan SWAXS Data Analysis) window
- M-SAWANA (Multi Scan SWAXS Data Analysis) window
- Help window (this document)

In the following, a brief gallery of these windows will be shown, followed by a more detailed presentation of available menus.

3.1 Batch Script & 2D Mesh Composite window

To open Batch Script & 2D Mesh Composite window click on "Batch" icon or select "Batch Script & 2D Mesh Composite" from the "Programs" menu of the main SUNBIM window. This is a dedicated GUI to prepare batch script files (ASCII files), to run a sequential acquisition of 2D frames (in scanning mode). It has been written for a specific RIGAKU instrument [1] but can be adapted, upon request to the developers, for other SAXS instruments.



The Batch Script & 2D Mesh Composite window is divided in 2 main sections:

1) *Script Section*, to prepare script;
2) *Composite Section*, to compose the acquired data into a single map.

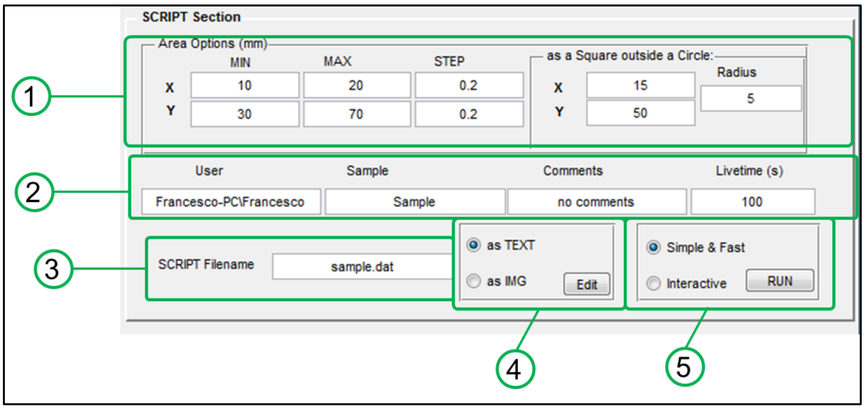
The Script Section is explained in more details in this section, whereas Composite Section will be described in 3.5.1 section. Please note that in this window the composite can only be performed for .mpa files (Rigaku). For other file types, it is necessary to use the dedicated Composite Section directly.

Hint: Before to start, use "Working Folder" to select the working folder where the script will be stored.

The Menu contains the "Status" command for opening and saving Batch Script & 2D Mesh Composite status previously saved. If accidently the Batch Script & 2D Mesh Composite Window has been closed, a temporary "Status" file is automatically created, which can be recalled when the Batch Script & 2D Mesh Composite Window is re-started from the SUNBIM main menu. In fact, when user opens Batch Script & 2D Mesh Composite for the second time, the software will ask the user if he wants to recover the last used status or not.

3.1.1 Script Section

The Script Section allows user to define the area to scan with the possibility to skip one or more *ARs* areas (Avoid Region). The scanning area can be visualized as image as well as text file (batch script file).



1. Area Options: user can decide the area size defining minimum and maximum in X and Y and the step of the scanning grid; moreover user can define a square area defining the center and the radius of a circle containing the square area.
2. User can fill these fields to add some information on the script file as:
   - User name
   - Sample name
   - Comments about the experiment
   - Live time of the single data acquisition (mandatory)
3. Define the name of the script file (mandatory) in ".dat" format (text)
4. This option allows to visualize scanning area as an editable text or as image
5. Select "Simple & Fast" and then click "RUN" to create the batch script file. If "Interactive" option is selected, and then "RUN" is clicked, a window will open where the area is visualized and it is possible to interactively draw the scanning area and/or the avoid some areas. In "Interactive" mode it is possible to merge several scannig/avoid areas into the same file or to split them into different one.

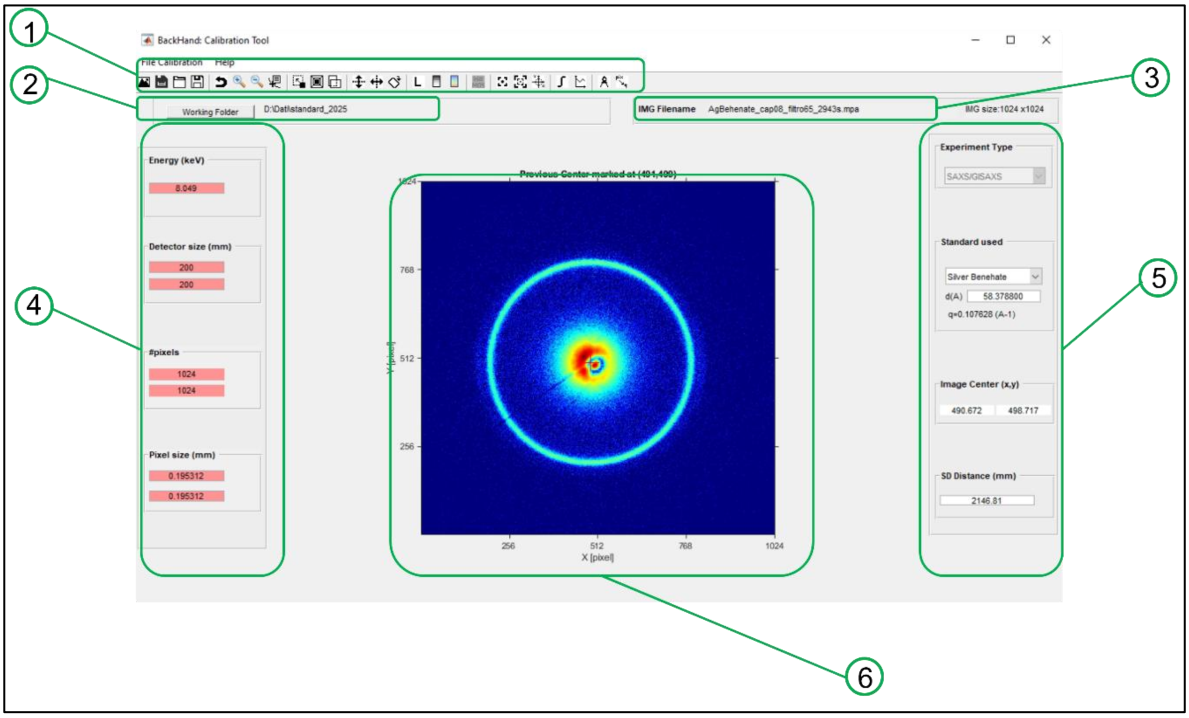
For more details how to use the "Script Section", please check the video tutorial: **BatchScript_4.0.mp4**

References

[1] Altamura, D., Lassandro, R., De Caro, L., Siliqi, D., Ladisa M. & Giannini, C. (2012). *J. Appl. Cryst*. **45,** 869–873.

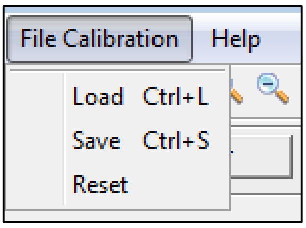
3.2 Calibration window

To open Calibration window click on the "Cal" icon or select "Calibration" from the "Programs" menu of the main SUNBIM window.



1) Menu and toolbar
2) Working Folder selection
3) File Name of the calibration image
4) General information about the:
    - Energy beam (in keV)
    - Detector size (in mm)
    - Number of the pixel of the image loaded for calibration
    - Pixel size of the image/detector (in mm)
5) Experimental Information:
    - Experiment type (SAXS/GISAXS or WAXS/GIWAXS)
    - Standard used for calibration (Silver Benehate, Silicon or others)
    - Image Center in (x,y) coordinate
    - Sample-to Detector Distance (in mm)
6) The loaded image

3.2.1 Menu and toolbar



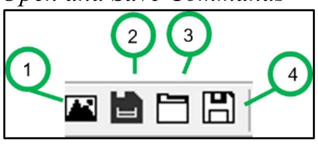
They contain commands for opening and saving calibration files, opening images to use for calibration and all the commands useful to perform calibration. The "File Calibration" menu contains the options for reading and writing files. User can load a calibration file previously created after the calibration procedure. Moreover, he can save a new calibration file (".mat") after the calibration procedure is completed, to use it for S-SAWANA or M-SAWANA analysis. The "Reset" command resets all the fields of the Calibration Window to restart the entire procedure.

Hint: If accidently the Calibration Window has been closed, a temporary calibration file is automatically created, which can be recalled when the Calibration Window is re-started from the SUNBIM main menu. In fact, when the user opens the Calibration Window for the second time, the software will ask him if he wants to recover the last used status or not.

The "Help" menu connects user to the tutorial link where he finds also this manual.

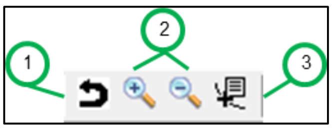
The "Calibration Toolbar" contains all the commands for the calibration procedure. It is divided in groups, according to their purpose. Specific icons and tooltip strings explain to user the aim of each commands.

Open and Save Commands



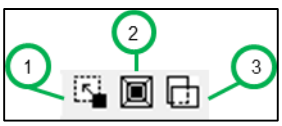
1. Open a new image to perform calibration. When a new image has been loaded, a dialog will ask the user for what kind of experiment he wants to perform the calibration: SAXS/GISAXS or WAXS/GIWAXS.
2. Export Image as .tiff
3. Load a previously created calibration ".mat" file (see before).
4. Save a calibration ".mat" file.

Basic Commands



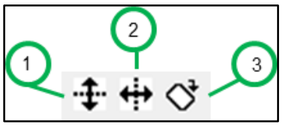
1. Reset all the image changes performed during the calibration procedure.
2. Zoom In and Zoom Out on the image (toggle button).
3. Data Cursor (toggle button): turn on full-window crosshairs that follow your pointer. Turns on (x,y) coordinate window on the left bottom of the image that shows the current pointer position in terms of each image's axes coordinates: pixels or q-coordinates (the latter option is available if the calibration procedure has been already performed).

Shift and Pad Commands



1. Shift the image along x or y axis. Choose this option if the image of the sample is not correctly centered. The command circularly shifts the elements of the image matrix.
2. Pad the image along x or y axis. Choose this option if the image of the sample is not centered. The command creates a zero pad (zero intensity pixels frame) before or after (selected by user) the size of the image along the selected axis.
3. Transpose the image matrix (toggle button).

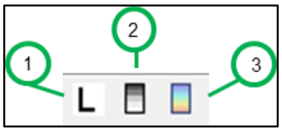
Flip and Rotate Commands



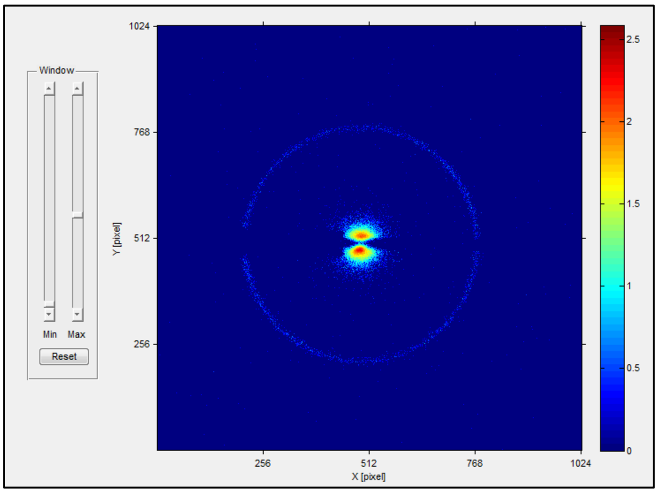
1. Flip Up-Down the image (toggle button).
2. Flip Left-Right the image (toggle button).
3. Rotate the image: a dialog window will ask user the rotation angle in degree. The rotation of the image is performed clockwise or anti-clockwise (using positive or negative value for the angle) about the image center.

Hint: Note that the rotation tool only rotates the pattern, not the frame. Therefore, if a 90° rotation is needed, the image should be first transposed and then flipped up or down, in order to have the whole frame rotated and not to have the pattern cut by the frame.

Image Color Options



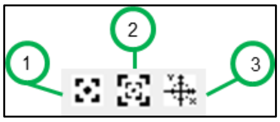
1. Change the intensity scale of the image from logarithmic (default) to linear (toggle button).
2. Change the color map of the image from RGB (default) to gray scale (toggle button).
3. Insert a lateral color bar. Choose this function if you want to change the range of the color map of the image (toggle button).



WAMOS Command

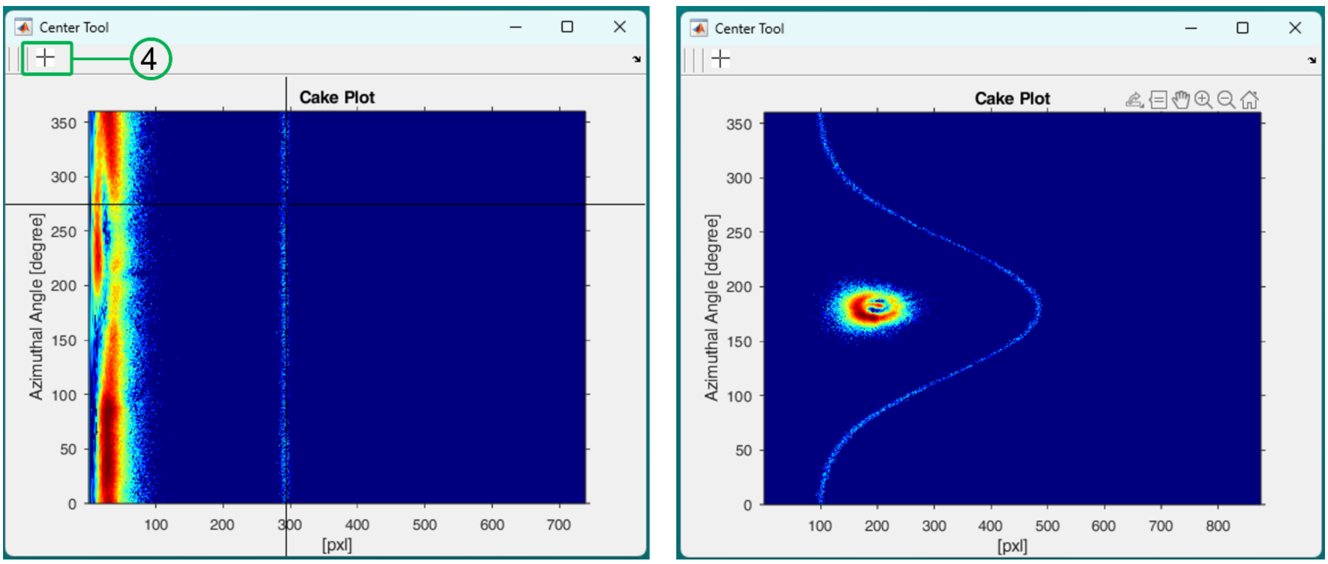
Choose this command if you want to perform the "WAxs Maximum cOnformal geometry Script (WaMOS)" procedure. This option performs a high-throughput online automatic data-folding procedure specifically studied for WAXS data. For this reason the button is only enabled if user deals with WAXS or GIWAXS data. The detector tilt (eccentricity) and rotation are determined by either a Hankel Lanczos singular value decomposition or a deterministic phase space (tilt-rotation plane) spanning [1]: while the former one relies on a linear algebra scheme, applied to the azimuth-radius data matrix inversion, the latter approach is a brute-force search.

Center Searching Commands

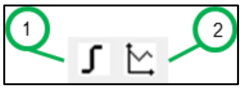


1. Guess the center of the beam over the image. User can select among four methods to guess center: manually (click one point directly on the center), or, automatically with triangulation (select three points along a specific diffraction ring) or waves method [2] or radon geometry [3,4]. When center has been found, the field "Image Center" on the right side of the "Calibration Window" (see figure in 3.2) is uploaded.
2. Automatically refine the center position (inside a cubic box 3x3x3 pixels). Choose this option to refine the center beam position using an automatic algorithm after selecting a point on the ring.
3. Transforms the image from Cartesian to polar coordinates (Cake Plot): transforms the rings into straight and vertical lines. Choose this option to check the correctness of the beam center.
4. Push button 4 to activate crosshair and check the correctness of the beam center.

Hint: Image in polar coordinates for a correct beam center (left) and for a not correct beam center (right).



Radial Integration Commands

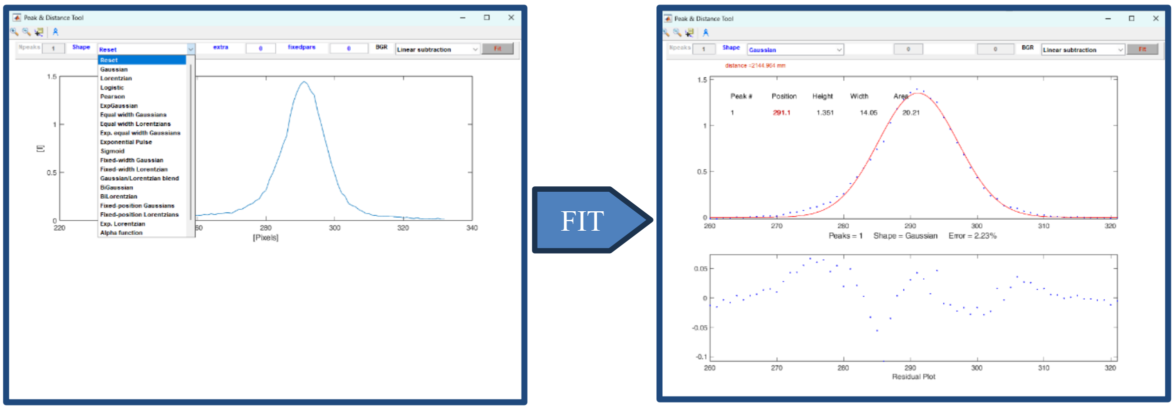


1. Perform radial integration. Use this function after you found the beam center. Radial integration button asks user to select a pixel range for the integration by clicking two points on the image.
2. Plot the performed radial integration.

Sample-to-Detector distance Command

1. From Peak Position to Sample-to-Detector (SD) distance: pushing this button a new window is opened, and a procedure to calculate the SD distance can be performed: the radially integrated profile can be fitted with a list of standard functions (Gaussian, Lorentzian, Logistic, Pearson and more) and background subtracted (linear subtraction, quadratic subtraction, flat baseline correction). User can choose the range of the radial integration to perform the best fit. An automatic algorithm finds the peak, estimates the error and calculates the peak position. As a result, the SD distance is calculated and uploaded in the corresponding field of the "Calibration Window" (see figure in section 3.2).

   Hint: if after the fitting procedure the peak position is not correct, user can manually select the peak position so that the SD distance is nevertheless calculated.



2. Change image coordinates from pixels coordinates to reciprocal q-coordinates (toggle button). Choose this function after the SD distance calculation has been correctly performed.

For more details how to use the "Calibration" tool, please check the video tutorial **Calibration_4.0.mp4**

3.2.2 General information

On the left of the Calibration window, a panel of general information about the energy used for the experiment, the detector and pixel sizes (in mm) and the number of the pixels of the loaded image is displayed. If no image is loaded user can edit each of the fields, whereas if an image is loaded "number of pixels" fields show the effective number of the pixels of the image and is so disabled. Detector size, number of pixels and pixel size fields are connected together, in order to calculate each correct value when one of them is manually changed.

3.2.3 Experimental Information

On the right of the Calibration window, the user can manage with experiment type selection, the standard used for the experiment, the image center and the sample-to-detector (SD) distance. If no image is loaded, all the fields are enabled; otherwise, only the choice of the standard used is enabled. This is because the experiment type is defined by the user just after loading the image; moreover image center and SD distance are calculated during the calibration procedure.

Hint It is very important to remark that if no image is loaded, Calibration window allows the user to save a valid calibration file if:

- "energy", "detector size" or/and "number of pixels" or/and "pixel size", and "SD distance" fields are correctly edited with known values
- "experiment type" and "standard used" are correctly selected.

References

[1] Cervellino, A., Giannini, C., Guagliardi, A. & Ladisa, M. (2006). *J. Appl. Cryst*. **39**, 745-748.

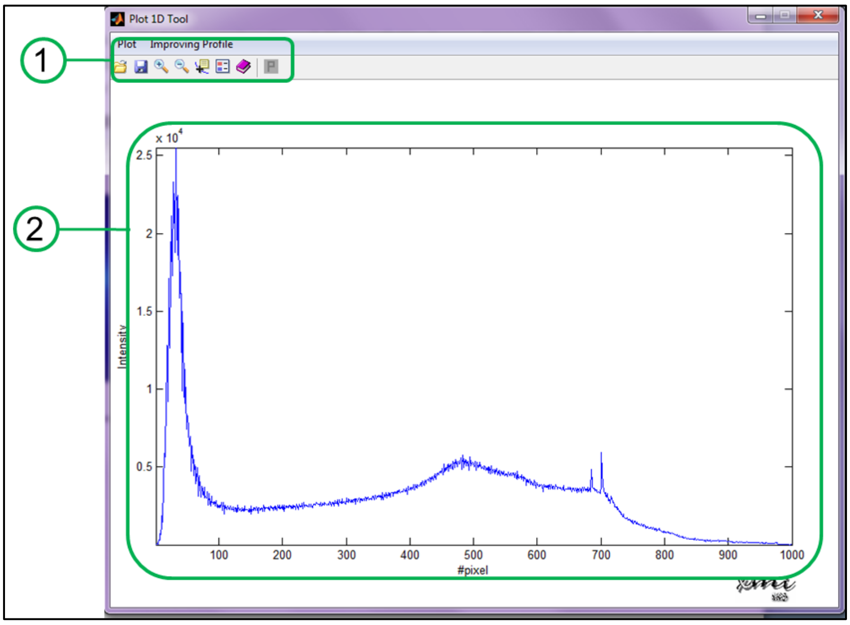
[2] Landau, L.D. & Liftshitz, E.M. (1987). "Fluid mechanics" Course of theoretical physics, vol 6, second edition, Pergamon Press, Ch.1, par 12, 32-35.

[3] Radon, J. (1986). *IEEE Trans Med Imaging*. 5(4):170-6.

[4] Barbano, P.E.; Fokas, A.S.; Kastis, G.A. (2009)"Analytical reconstructions for PET and spect employing L1- denoising", Digital *Signal Processing, 2009 16th International Conference*, 1 - 5

3.3 One-D Data Analysis Manager window

To open One-D Tool window click on "Plot" icon or select "One-D Data Analysis Manager" (Single scan SWAXS and Data Analysis window)" from the "Programs" menu of the main SUNBIM window or select "1D profile" from the "Integration" menu in the S-SAWANA window (see next section).

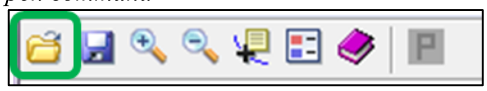


1. Menu and toolbar
2. The loaded graph

3.3.1 Menu and toolbar

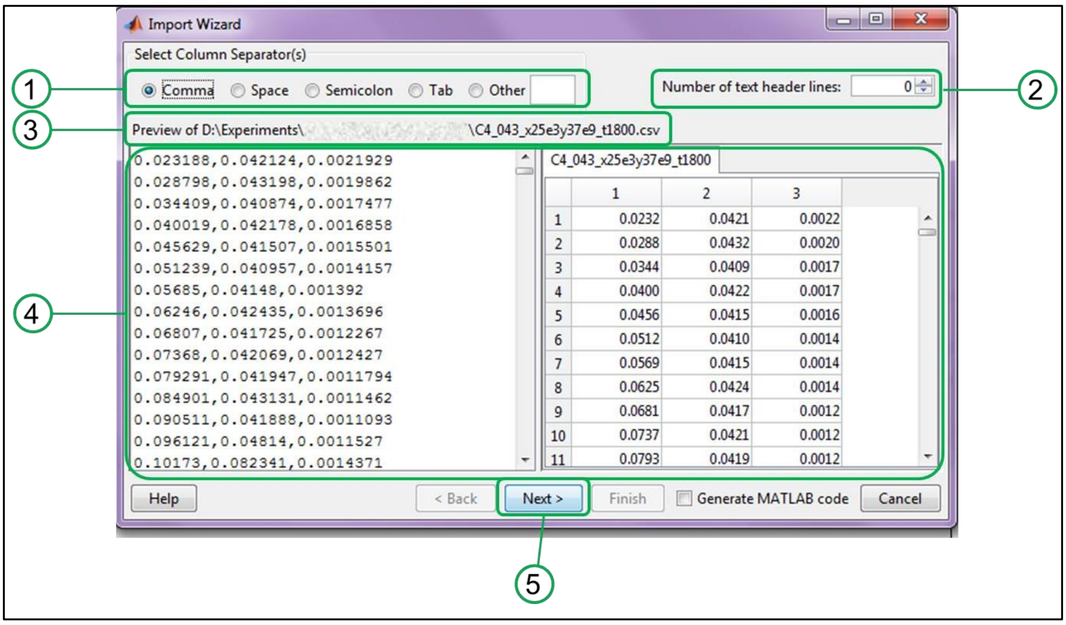
They contain commands for opening and plot one-D data file, to manage graph properties and to perform denoising and deconvolution on the plotted data.

Open command



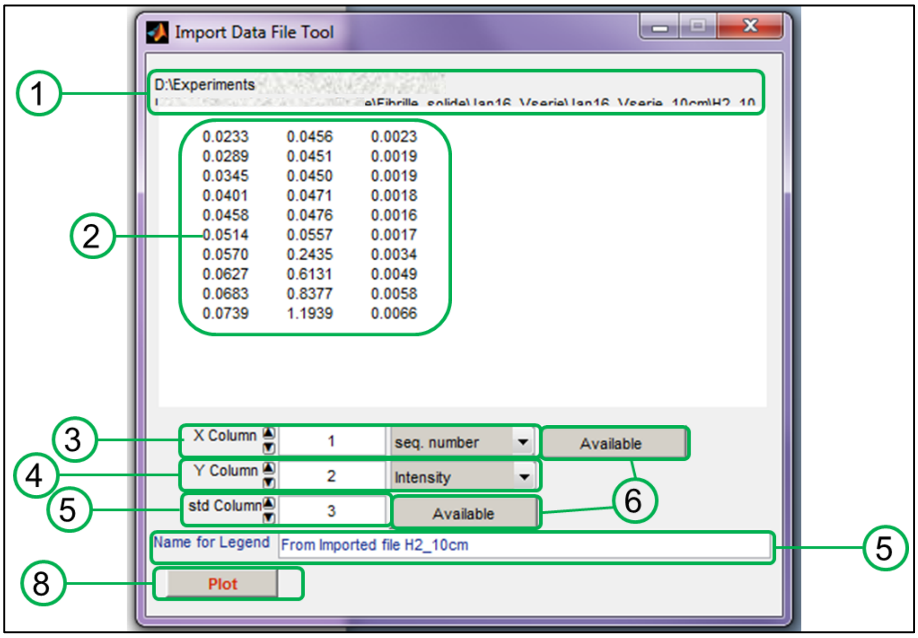
Import an ASCII file or SUNBIM file and open the "*Import wizard*" window.

Import wizard



1. Select the column separator (comma, space, semicolon, tab, other) of the raw data
2. Specify the number of text header lines in your data file
3. File name of the raw data
4. Preview of the raw data file
5. Open the "*Import Data file tool*" window

Import data file tool

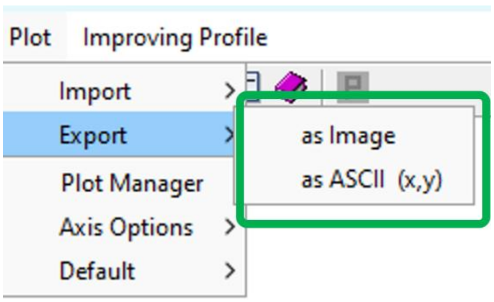


1. File name of the raw data.
2. Preview of the raw data.
3. Set-up X column unit: seq. number, Q(nm-1), Q^2(nm-2), Q(A-1), Q^2(A-2).
4. Set-up Y column unit: Intensity, log(Intensity), 1/Intensity.

5. Set-up standard deviation (errors) column unit.
   The unit for each X and Y axis can be also chosen by select "Axis options" from the "Plot" menu. In addition from the "Plot" menu it is also possible to choose some frequently used combinations for the unit of X-Y axes, as reported in the following:
   - Absolute scale [I vs q]
   - Logarithmic Scale [log(I) vs q]
   - Double Logarithmic [log(I) vs log(q)]
   - Guinier [log(I) vs q^2]
   - Kratky [I*q^2 vs q]
   - Porod [I*q^4 vs q]
6. Click "Available" if the data file contains the error on the intensity as third column otherwise click "Not available".
7. Write the Name for the legend of the graph.
8. Plot the data contained in the input file.

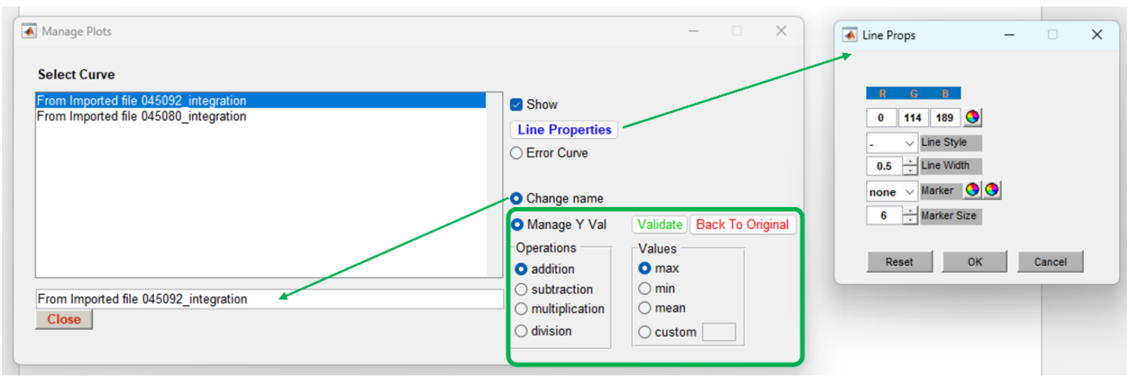
Save command

Save a .tiff image of the plot. Otherwise a selected plot can be saved by select Export as ASCII file (x,y) from the "Plot" menu.



Plot Manager

Select Plot Manager if you want to make changes to the plot(s).



The window allows you to:

1. Change the line properties (color and line style) of the selected profile
2. Display the error curve of the selected profile

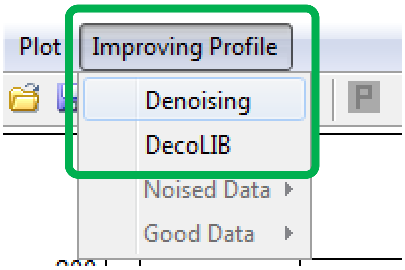
3. Change the name of the profile that will be shown in the legend

4. Apply arithmetic operations to the selected profile (Y values)

Basic commands

1. *Zoom*-in and Zoom-*out* on parts of plot (toggle button)
2. Data cursor (toggle button): clicking the mouse on a plot displays data values of the point clicked
3. Enable or disable legend on the graph
4. Plot manager: it is possible from the manage plots window to select or deselect one or more plots from the graph and the corresponding error curve, to set Line properties for each curve in the graph (color, line style, line width, marker and marker size) and to change the name on the legend reported in the graph.

Denoising and deconvolution



Perform denoising and deconvolution (DecoLIB) of the primary beam angular divergence on SAXS/GISAXS profiles by using the algorithm described in [1,2,3].

For more details how to use the "One-D Data Analysis Manager", please check the video tutorial: "**one_plot_4.0.mp4**"

References

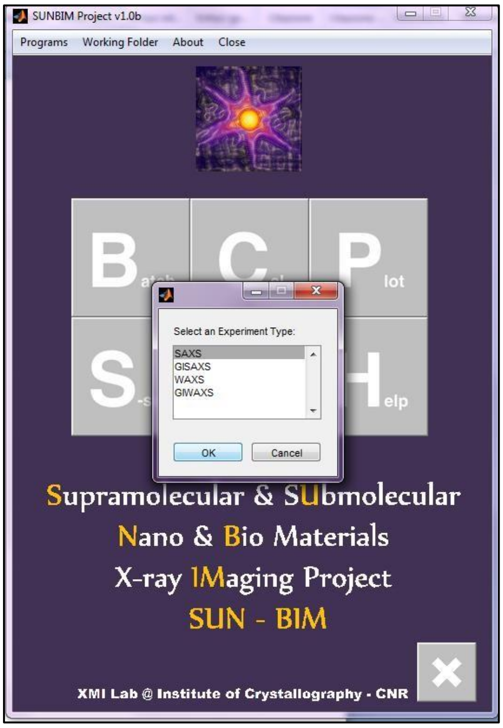
[1] De Caro, L., Altamura, D., Vittoria, F.M., Carbone, G., Qiao, F., Manna L. & Giannini, C. (2012). *J. Appl. Cryst.* 45, 1228-1235.

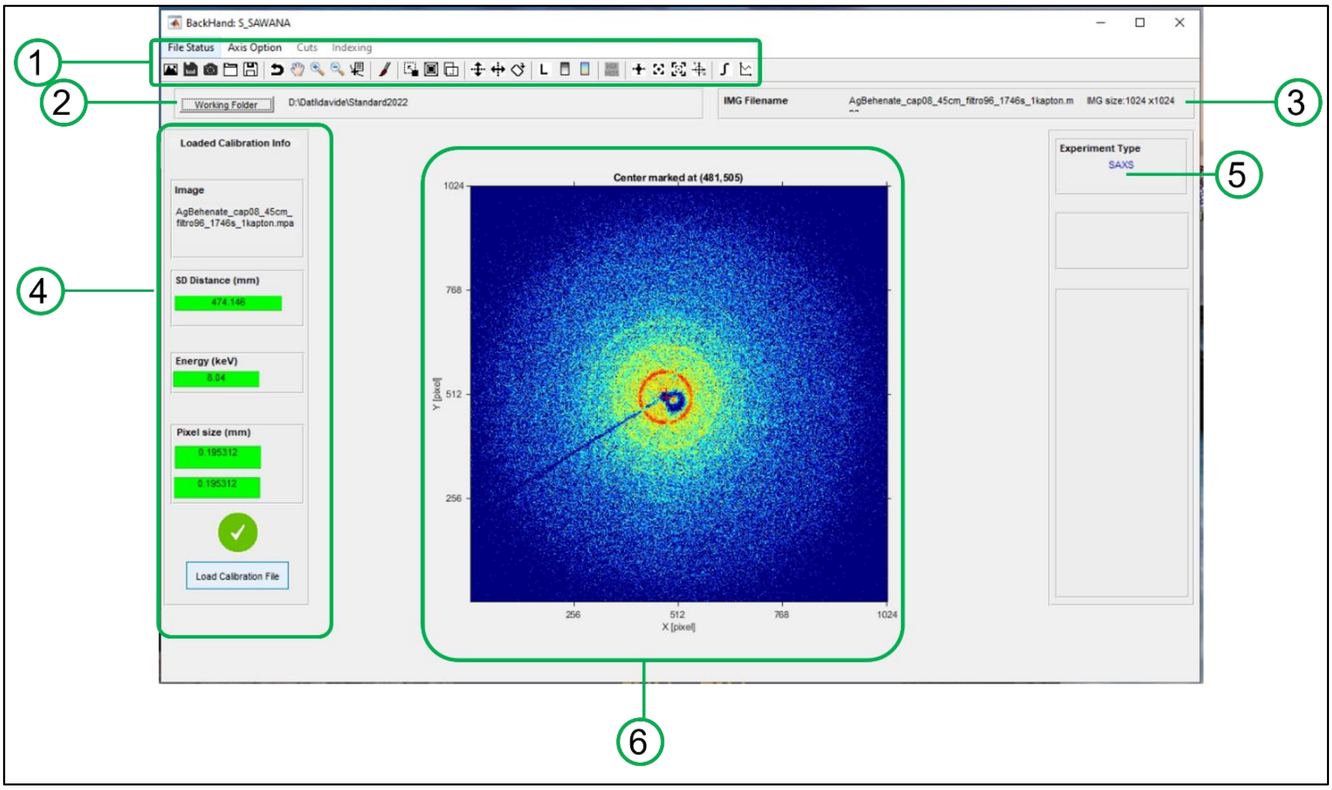
[2] De Caro, L., Altamura, D., Sibillano, T., Siliqi, D., Filograsso, G., Bunk, O. & Giannini, C. (2013). *J. Appl. Cryst.* 46, 672-678.

[3] Sibillano, T, De Caro, L., Altamura, D., Siliqi, D., Ramella, M., Boccafoschi, F., Ciasca, G., Campi, G., Tirinato, L., di Fabrizio E. and Giannini C. (2014) *Sci. Rep.* **4**, 6985.

3.4 S-SAWANA (Single scan SWAXS and Data Analysis window)

To open S-SAWANA window click on "S-saw" icon or select "S-SAWANA (Single scan SWAXS and Data Analysis window)" from the "Programs" menu of the main SUNBIM window. The window allows to select the experiment type (SAXS or GISAXS or WAXS or GIWAXS).





a. Menu and toolbar
b. Working Folder selection
c. File Name
d. General information about the:
    i. File name of calibration image
    ii. Sample-distance in mm
    iii. Energy beam in keV
    iv. Pixel size of the detector in mm

e. Experimental Information:

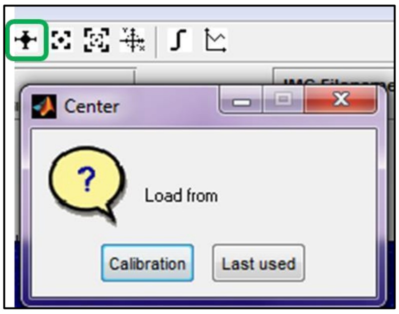
  i. Experiment type (SAXS/GISAXS or WAXS/GIWAXS)

f. The loaded image

3.4.1 Menu and toolbar

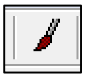
The commands contained in the main toolbar are mostly identical to those described in section 3.2.1, with the addition of some basic commands (such as window screenshot  and figure pan ), except for the "Load Center" and "Hide Draws" commands.

Load center

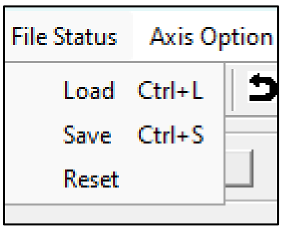


If the command is selected a window will open where user can click "Calibration" for loading the same center of the calibration file, or can click "Last used" for loading the center position used in the last analysis.

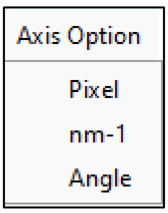
Hide draws



"Hide draws" command allows to hide all the lines and/or points drawn on the image. This command is useful for hiding selected "Cuts", which will be described in the following section about GISAXS measurements (sec. 3.4.1.1).



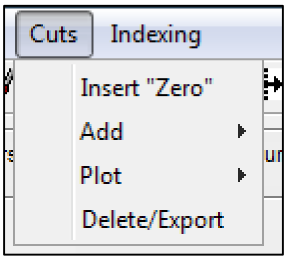
The "File Status" menu contains the options for reading and writing files. User can load an image file and then save a calibrated image after loading a calibration file. The "Reset" command resets all the fields of the Calibration Window and of the opened image to restart the entire procedure.



The "Axis" menu contains three options to change the axis unit in pixel, nm^{-1} or angle.

3.4.2 Cuts Menu

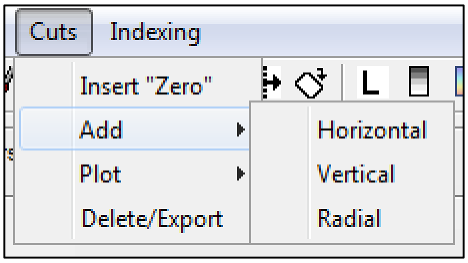
When working on a single 2D GISAXS frame it is possible to access a SUNBIM program section dedicated to Cuts.



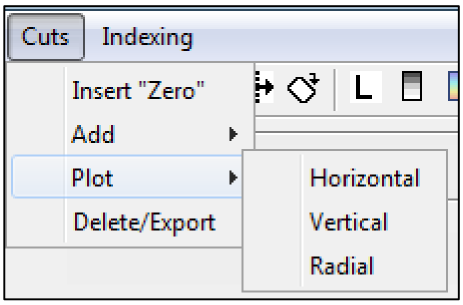
From the "Cuts" menu, choose "Insert Zero": the Zero position can be directly guessed through the mouse, or the x,y coordinates can be set, if previously determined. If the last option is chosen, the Crosshair will be enabled. Press "ENTER" to confirm.

Hint: if the"Zero"angle position (corresponding to the sample horizon) is also defined, the 2D pattern can be plotted against the scattering vector components (qy, qz) or the corresponding scattering angle components (2θ, α_f).

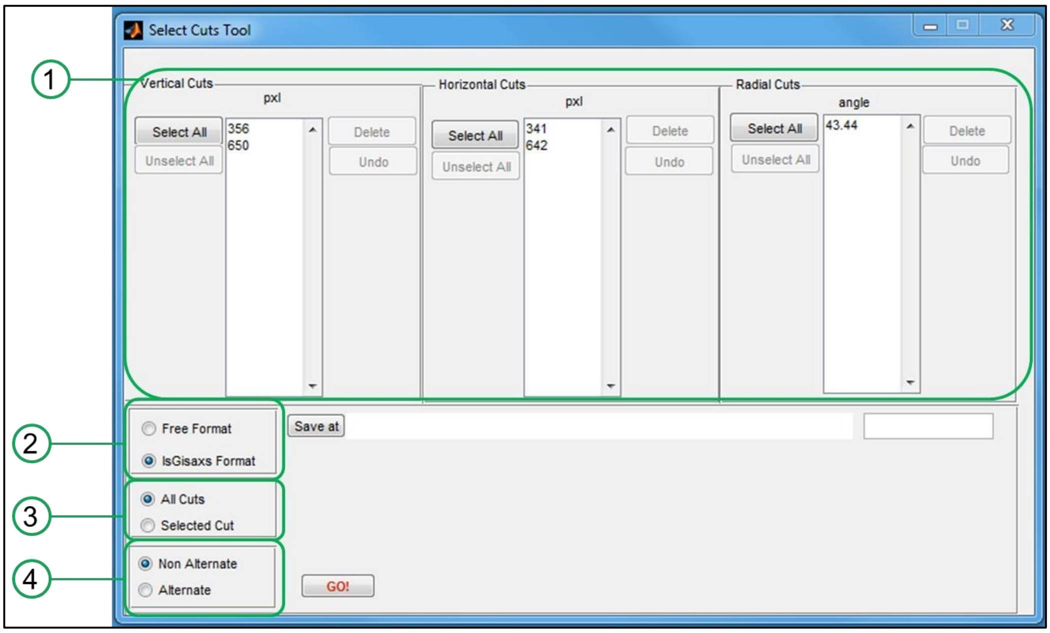
Linear cuts can be extracted along horizontal, vertical or radial directions, as free format or formatted for fitting in the IsGISAXS [1] analysis software. The position of the cuts can be chosen from the "Cuts" menu selecting "Add horizontal/vertical/radial". Then user can define the cut position through the mouse, or insert the (x,y) coordinates, if previously determined. If the last option is chosen, the Crosshair will be enabled. Press "ENTER" to confirm.



Hint: User can hide all cuts drawn on the image using the "Hide Draws" command. To plot the 1D horizontal/vertical/radial profiles, from the "Cuts" menu choose "Plot".



To extract or delete the 1D horizontal/vertical/radial profiles, from the "Cuts" menu, choose "Delete/Export" so the "Select Cuts Tool" window will open.



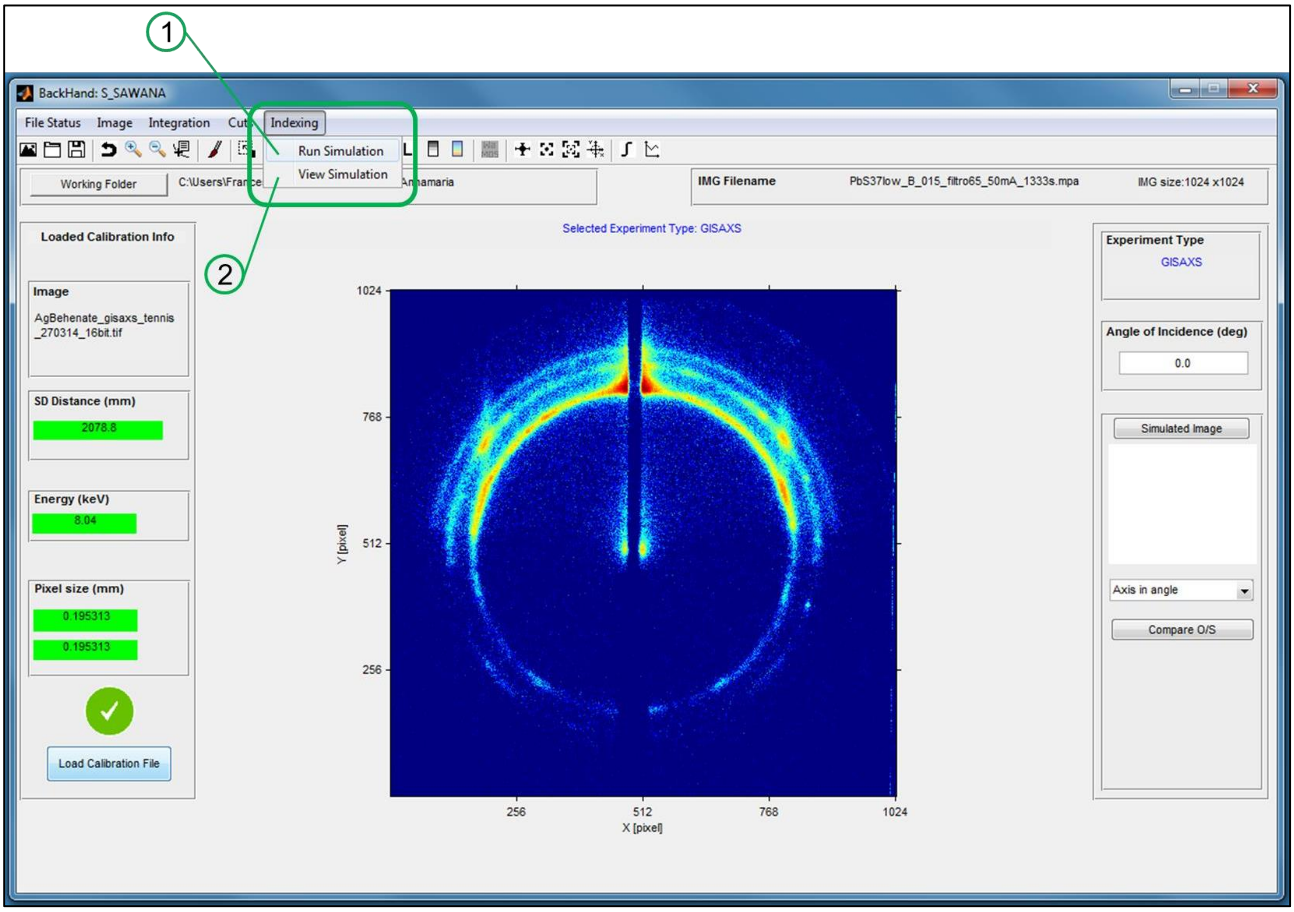
In his window there are the following options:

1. the requested cuts can be selected,
2. saving ".dat" format :"Free" data columns, or formatted for IsGISAXS
3. saving "All Cuts" or "Selected Cut"
4. "Non Alternate/Alternate" allows writing all cuts of the same type consecutively, or alternately, in the ".dat" file.
5. Click on "Go!" button to save the data into the file defined by "Save at".

For more details how to use the "S-SAWANA", please check the video tutorial: **ssawana-gisaxs_4.0.mp4**

3.4.3 Indexing Menu

When working on a single 2D GISAXS frame it is possible to access a SUNBIM program section dedicated to indexing.



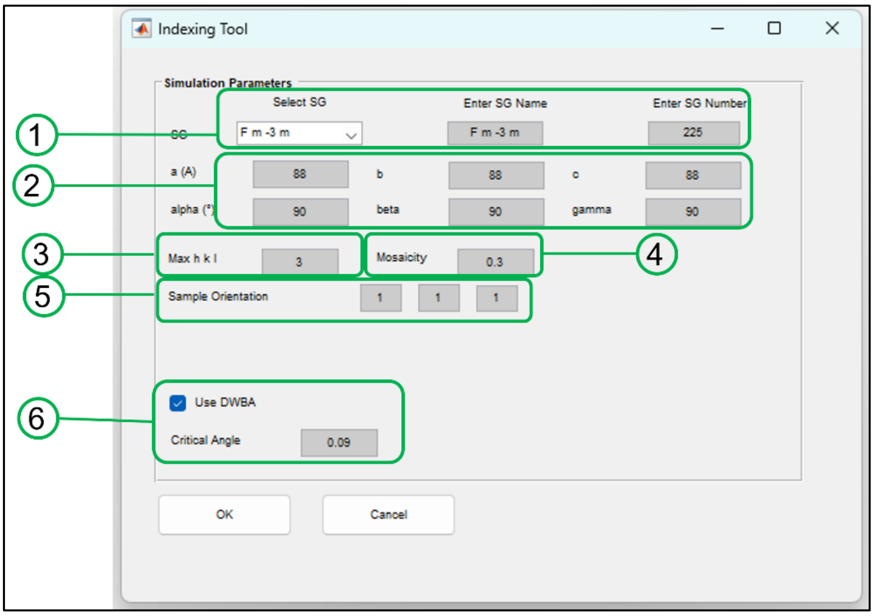
To open the Indexing menu select Indexing from S-SAWANA menu.

The indexing procedure requires the zero and the center for the GISAXS image to be set. The indexing menu allows to:

6. Run a simulation
7. View a simulation

It is possible to visualize the last simulation performed selecting from the indexing menu the “View a simulation” option.

The “Run a simulation” option allows to open the indexing panel and to perform a new indexing operation.



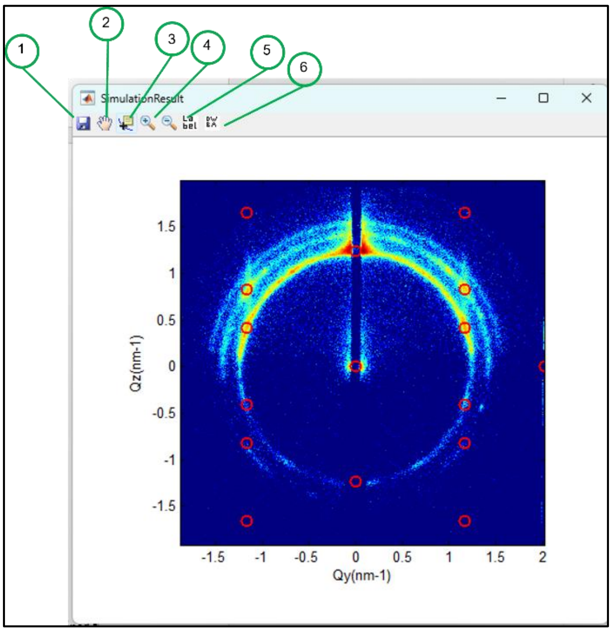
The procedure is able to simulate the pattern produced by a collection of nanoparticles assembled on top of a substrate according to some precise information [2].

The user must insert in the panel:

1. Space group symmetry: choosing it among SG menu possibilities. According to the selected space group the unit cell angle values can be set automatically. The user can also type in the corresponding box either the space group name or its number*
2. Unit cell parameters a, b, c dimensions in Angstrom and alpha beta and gamma angles in degrees*
3. Maximum value of *hkl* to be explored*
4. Mosaicity of the sample (between 0 and 1)*
5. Sample orientation. The h, k, and l values should be inserted into the fields*
6. If the user wants to use the DWBA (Distorted Wave Born Approximation) option, he must check the relative box and specify the critic angle.

(*) Mandatory fields in order to calculate the Bragg peak positions.

Bragg peak positions and corrections by refraction/reflection effects are displayed in the graphical output.



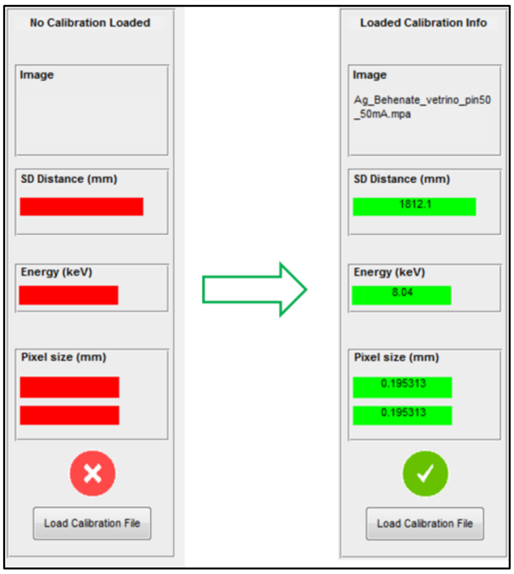
The “Simulation Result” window toolbar contains the commands for saving and visualizing the results obtained.

1. Save a .tif image for the simulation
2. Pan the image
3. Data tips
4. Zoom In and Zoom Out on the image (toggle)
5. Show/hide the indexing labels for each peak
6. Show the refraction (red circle) and reflection (white boxes) correction in DWBA approximation.

Warning: it is not recommended to use the indexing menu on 2D (GI)WAXS data, as the simulation algorithms is not optimized for this type of data.

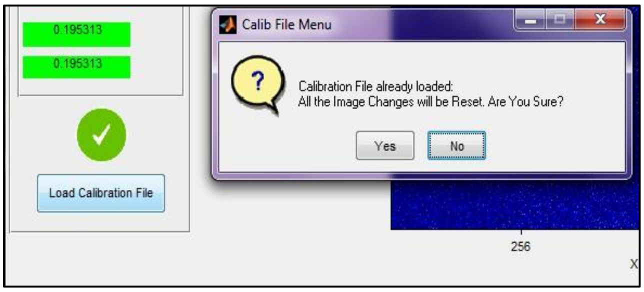
3.4.2 General Information

On the left side of the S-SAWANA window, a panel of general information about the image used for Calibration, the Sample-to-Detector distance, the energy used for the experiment and the detector and pixel sizes (in mm) is displayed. If no calibration file is loaded all the fields are empty and red colored.

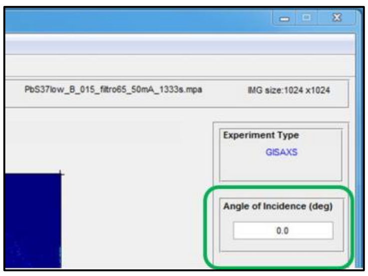


Push “Load calibration file” to load a calibration “.mat” file previously created in the Calibration window. All the fields will filled and green colored.

A new calibration file can be loaded by clicking again on “Load calibration file”: the “Calib File Menu” window allows to reset all the image changes.



3.4.3 Angle of Incidence

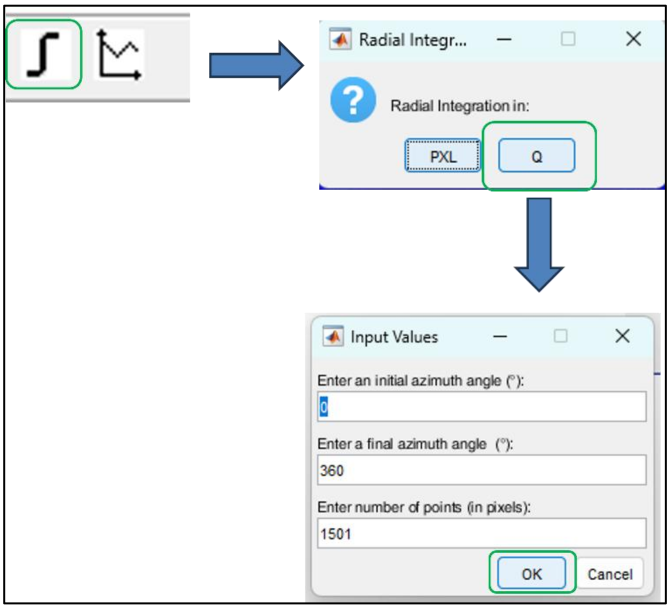


When working on a single 2D GISAXS frame, on the right panel of the S-SAWANA window user can set the angle of incidence in order to provide correct values for the Qz component of the scattering vector [1], when exporting linear cut.

3.4.4 Background correction for (GI)WAXS data

This function performs a semi-automatic background subtraction on the 1D profile obtained from azimuthal integration, which has been corrected for the flat-panel detector geometry. Its main purpose is to enhance the visibility of diffraction peaks, especially at large scattering angles typical of WAXS and GIWAXS data.

When S-SAWANA is opened in WAXS or GIWAXS mode, after completing all preliminary operations — such as importing the calibration file and refining the center — the azimuthal integration can be performed by clicking the corresponding button in the toolbar. The user will then be asked whether to perform the folding in pixels or in Q. To apply background correction, select "Q."



A prompt window will then appear asking for:

a) the azimuthal integration range,

b) the number of pixels to be used for sampling the Q-vector range. (**Hint:** it is recommended to keep the suggested default value.)

The subtraction is based on an adaptive algorithm [3] that estimates and removes the slowly varying background component, improving the signal-to-noise ratio and making weak structural features more discernible. This step is particularly useful when dealing with samples that produce broad or low-intensity peaks, or when the raw data are affected by residual scattering or detector artefacts.

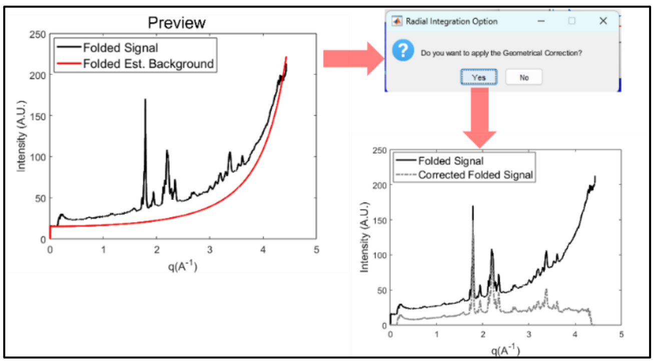
Choose where you would like the background to be evaluated from:

i. Center: near the direct beam position, where the beam stopper is typically located

ii. Corners: where usually the signal can be considered nearly negligible

iii. Manual: select a background area by drawing it manually. A draggable blue circle will appear on the figure, whose size can be adjusted. When the selected area is acceptable, double-click to proceed with the background evaluation.

Subsequently, a constant 2D background image is generated and used to subtract the background signal from the 2D pattern. As the same spherical angle correction is applied to the background image [3], the resulting 1D plot contains, in principle, only the correct scattering signal of the sample projected on a spherical surface.



The program asks whether the evaluated background is satisfactory by showing a preview of both the background and the integrated profile. If accepted, the plot is stored in memory and can be visualized by clicking "Plot," from which it can also be saved as a .dat file.

For more details how to use the "S-SAWANA", please check the video tutorial: **ssawana_giwaxs_4.0.mp4**

References

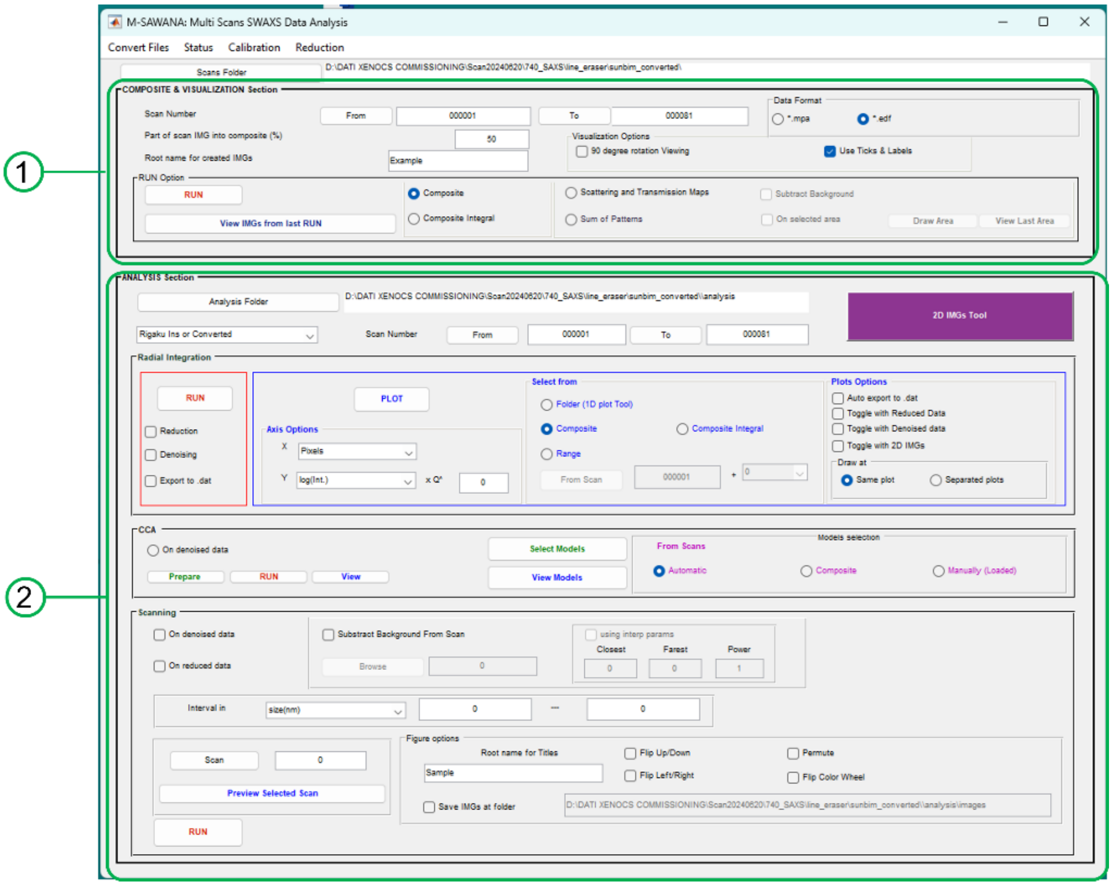
[1] Lazzari, R. (2012). *J. Appl. Cryst*, **35**, 406-421

[2] Tate, M. P., Urade, V. N., Kowalski, J. D., Wei, T., Hamilton, B. D., Eggiman, B. W. & Hillhouse, H.W. (2006). *J. Phys. Chem*. B **110**, 9882–9892

[3] Scattarella, F., Altamura, D., Sibillano, T., De Caro, L., Siliqi, D. & Giannini, C. (2025). *J. Appl. Cryst. 58, 1817-1826*

3.5 M-SAWANA window (Multi scan SWAXS and Data Analysis window)

M-SAWANA is realized to compose the as-acquired raw data into a single map and to analyze them. To open M-SAWANA Panel, click “M-saw” icon from the SUNBIM main window.



The M-SAWANA Panel is divided in 2 main sections:

1. Composite & Visualization Section, to compose the acquired data into a single map
2. Analysis Section, to analyze the composite map

The Composite & Visualization Section and the Analysis Section will be explained in more details.

Hint: Before to start, use “Scan Folder” to select the scan folder where data are stored.

The Menu bar contains the following commands:

- “Convert Files”, option to convert multiple *edf* files into a format readable by SUNBIM
- “Status”, for opening and saving M-SAWANA status previously saved*.
- “Calibration”, for loading calibration files created with SUNBIM Calibration Tool and check “Active Info” of the loaded calibration file
- “Reduction”, for opening the Data Reduction Panel to perform operations such as dark current and background subtraction, calculation of the sample relative thickness map.

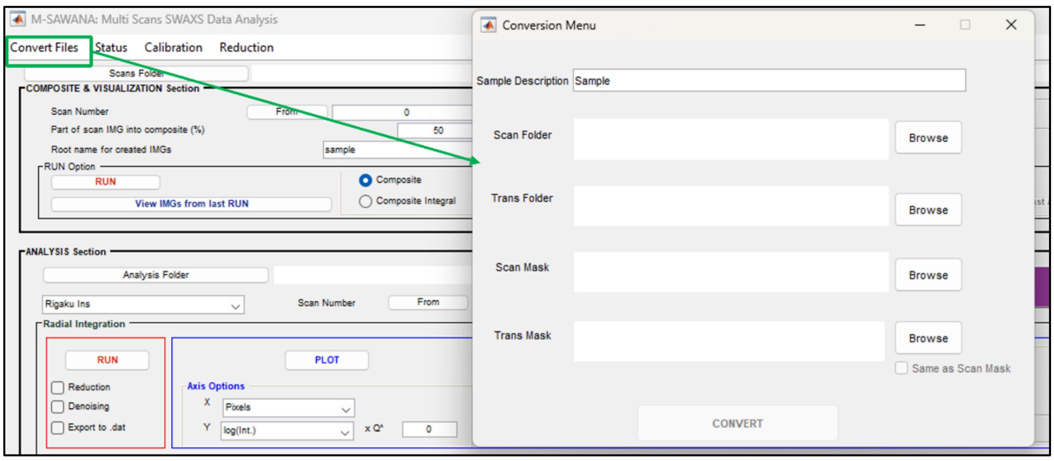
(*) If accidently the M-SAWANA Window has been closed, a temporary “Status” file is automatically created, which can be recalled when the M-SAWANA Window is re-started from the SUNBIM main menu. In fact, when the user opens the M-SAWANA for the second time, software asks him if he wants to recover the last used status or not.

3.5.1 Convert Files

M-SAWANA is designed to read and analyze data in a specific format. Actually, in the previous version of SUNBIM, these features were limited to data collected in a proprietary Rigaku format (.mpa), which associates each acquired frame with a text file (.info) containing information about the collected data, such as scan position, exposure time, and transmitted beam intensity. From SUNBIM 4.0, a new menu has been added that allows for importing of files in .edf format and making them ready for the composite function after an automatic conversion procedure.
Clicking on Convert Files tab from the Menu and selecting ".edf", a window will open.

- Enter the sample name
- Select the SAXS sample folder
- Select the folder where transmission files are stored (**Hint:** If the transmission data are saved in the header of the SAXS data, this will be the same folder as the SAXS sample folder)
- Select the scattering mask (TXT file) (**Hint:** The mask file must be created outside SUNBIM, must contain a binary mask, and must be in TXT format)
- Select the transmission mask (TXT file) (**Hint:** The mask file must be created outside SUNBIM, must contain a binary mask, and must be in TXT format. The "Same as Scan Mask" option should be used if you want to mask transmission data collected independently from the SAXS data, by selecting a mask with the same dimensions as the one used for the SAXS data but in negative (inverted) — meaning that pixels where the scattering mask is *0* become *1*, and vice versa)
- Click the "Convert" button

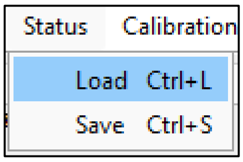
A new folder named "sunbim_converted" will be created inside the sample's SAXS folder.



This folder contains copies of the original EDF files renamed with a six-digit numerical sequence from 000001 to 00000x, together with corresponding .info files where useful metadata (e.g., coordinates, transmission, acquisition time, etc.) are stored to build the composite maps. Additionally, a subfolder named "mat" is created, containing further copies of the EDF files converted into MAT format, which are used by SUNBIM in the background to speed up calculations.
For more details how to use the conversion panel , please check the video tutorial: **Conversion_edf_4.0.mp4**

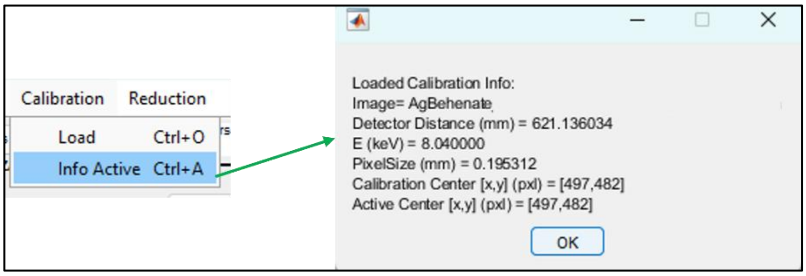
3.5.2 Status

Clicking on Status allows you to load or save an M-SAWANA status.



3.5.3 Calibration

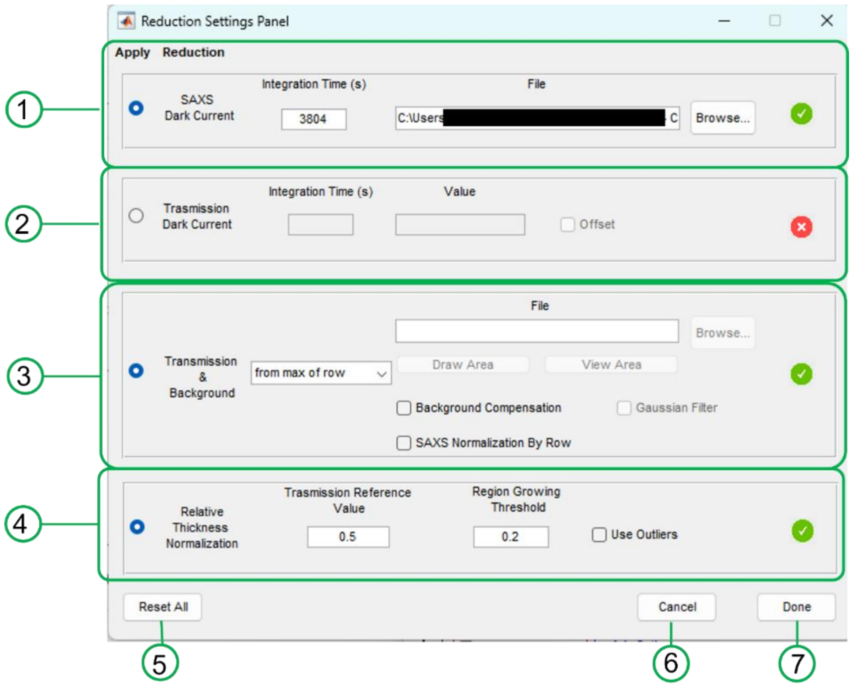
Clicking on Calibration allows you to load calibration files created with the SUNBIM Calibration Tool and to check the "Active Info" of the loaded calibration file.



Warning: "Active Center" info refers to the active center if it differs from the one in the calibration (for example, if it was recalculated with the S-SAWANA tool inside M-SAWANA).

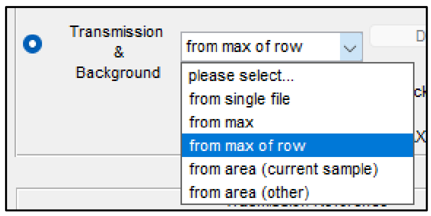
3.5.4 Reduction

Select Reduction, then open the Settings Panel. A new window will appear:



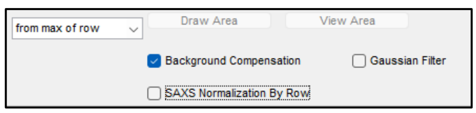
1. Select "SAXS Dark Current" subtraction to correct the main components of the detector artefacts, including bias current, dark current, and readout noise. Click **Browse** to load the file and enter the integration time used to measure the dark current.
2. Select "Transmission Dark Current" subtraction if the transmitted beam intensity is measured by the detector, as in the XMI-Lab setup described by Altamura et al. [7]. Enter the integration time, the recorded value, and select the **Offset** option if you want to shift the minimum transmission to 0 (useful if negative values are recorded).

Hint: Dark-current signals should be obtained for integration times sufficient to achieve a signal statistically comparable to that of the raw data, to avoid noise increase during subtraction. To ensure that the dark-current signal values are compatible with the experimental ones, the program automatically normalizes the loaded values to the actual integration time.



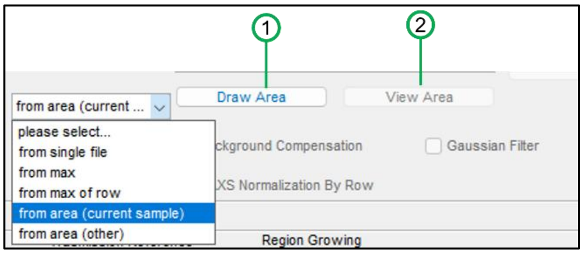
3. Select "Transmission & Background" to evaluate the local transmission coefficient and the background of the scanned area. The Transmission coefficient represents the ratio between the transmitted X-ray intensity measured after the interaction with the sample and the incoming beam intensity [8]. When the scanned area includes a no-sample region, the user can choose one of the following options to estimate the incoming beam intensity:

   - *from single file*: Select a specific file from the scan to be used as reference for the incoming beam intensity (I_0). This option is useful when a particular frame (e.g., a measurement without sample or in a no sample region) is known and should serve as the transmission reference. Click the "Browse" button to load the selected file.
   - *from max:* the incoming intensity I_0 is taken as the maximum transmitted value detected across the entire scan.
   - *from max of row:* The incoming intensity is calculated independently for each scan line, taking the maximum transmitted



value along that line. When this option is selected, additional processing options for the resulting transmission image become available, such as applying an Irregular "Background Compensation" algorithm [9], which is recommended when the background shows irregularities due to beam fluctuations. A "Gaussian Filter" can also be applied, particularly when the sample is weakly absorbing and the transmission signal has low contrast. In addition, "SAXS Normalization By Row" can be enabled when the SAXS map itself shows line irregularities caused by beam fluctuations.

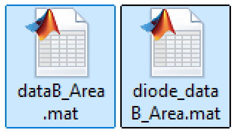
- *from area (current sample):* The incoming intensity is calculated as the average transmitted value within a background area manually defined by the user. Once this option is selected, the "Draw Area" button becomes active, allowing the user to draw a background region directly on the composite or on one of the previously created composites. The user can choose on which composite the background region should be drawn before confirming the selection. Use "View Area" to visualize the drawn area.



Once the area has been drawn, two *.mat* files are saved:

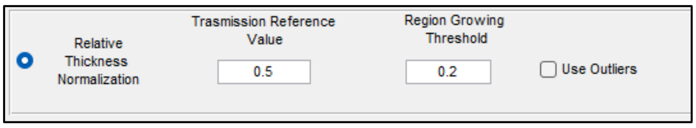
a) "dataB_Area.mat" contains the diffraction pattern image resulting from the sum of all diffraction patterns within the selected background area

b) "diode_dataB_Area.mat" stores the corresponding transmission value.



Hint: If the scanned area does not include any background region, the user can select "*from area (other)*" to load an external file (e.g. from another dataset) containing either a single transmitted intensity value or an averaged value from a specific region. Click "Browse" to import the file.

4. Select "Relative Thickness Normalization" to compute the map of relative thickness [8] by setting a reference value of the transmission coefficient (e.g. "Transmission Reference Value" = 0.5) and, if necessary, use the obtained result to normalize the scattering maps (see section 3.5.5). In the case of scanning areas containing void or non-sample regions, the calculated relative thickness would be approximately zero. Therefore, in order to avoid singularities arising from the normalization to arbitrary low values in those regions, it is possible to use a masking procedure based on the *Region Growing* algorithm, to exclude non-sample areas. Set a value of the "Region Growing" threshold to refine the mask evaluation.



Hint: select the "Use Outliers" option when the sample contains avoid regions within its area.

5. Click "Reset All" button to reset all fields in the panel.

6. Click "Cancel" to close the panel without saving the settings.

7. Click "Done" to validate all settings and close the panel.

Warning: Each field is associated with an icon on the right side of the panel:

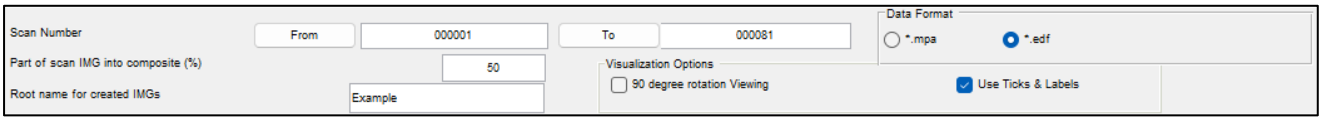
-  indicates that the field has not been completed and will not be applied during data reduction;

- ✓ indicates that the field has been validated clicking “Done”, it will be saved and applied during data reduction.

For more details how to use the reduction panel , please check the video tutorial: **msawana_data_reduction_4.0.mp4**

3.5.5 Composite section

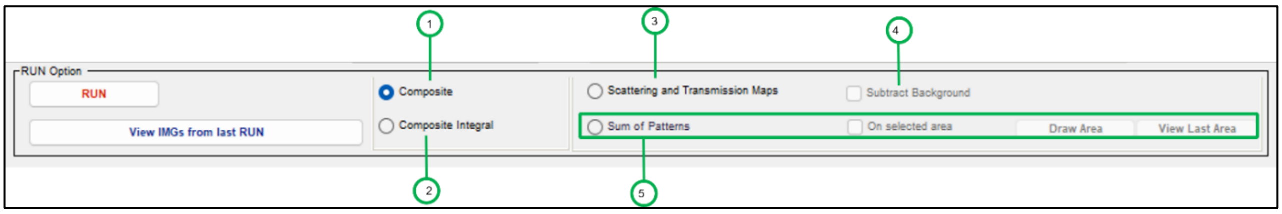
Insert the initial and final scan number clicking the “From” and “To” button respectively. Type the percentage (%) of each data you want to visualize (typically information is contained within 50% of each image from the center). User may decide to display each 2D data as collected or rotated by 90 degrees. The composite image may contain ticks and labels, if flagging the opposite field. Finally, specify in the corresponding box the root name for the images that will be generated and saved in a subfolder named “mesh”.



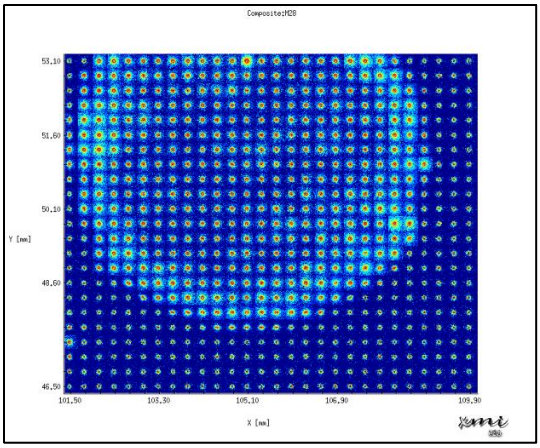
Hint: If you want to analyze a set of EDF data converted in SUNBIM, you must select the "edf" flag in the Data Format section; otherwise, leave "mpa" selected (the other format available for multiple analysis).

RUN Option sub-panel

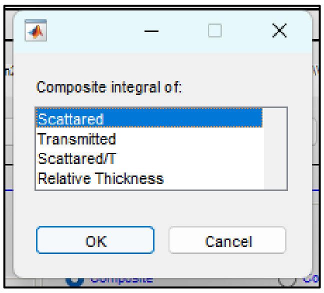
Select the option listed below, then click to the RUN. Clicking the RUN button opens a small window that allows the user to enter the step values in the horizontal (x) and vertical (y) directions to be used for generating the Composites and the Maps. By default, the values applied during the scan are automatically set.



1. Composite: it is the command to display raw data according to a (x,y) array (see figure)

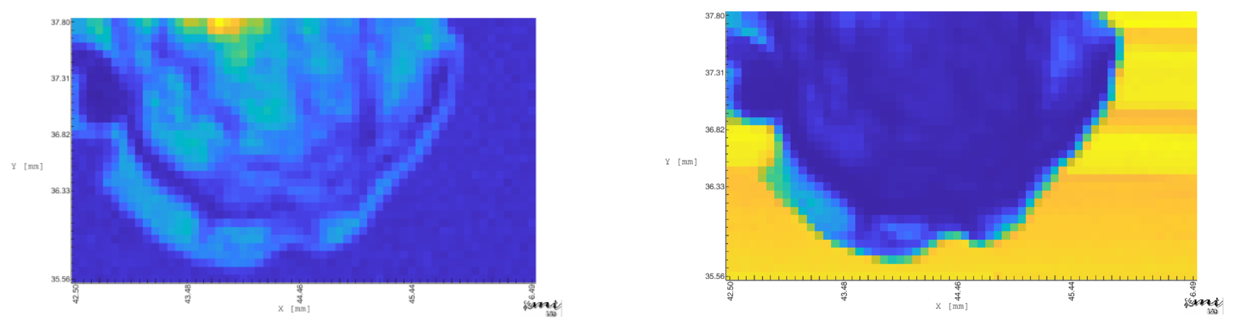


2. Composite Integral: it is the command to display (i) scattering, (ii) transmission, (iii) scattering normalized to the transmission coefficient signal integrated over the entire scattering angle range, (iv) relative thickness according to a (x,y) array



Hint 1: If the Composite Integral of Scattered/T is selected, it is important to note that transmission coefficient T is calculated as I_{trans} / I_0, where I_{trans} is the local transmitted signal I_0 is the maximum transmitted signal recorded during the scan (i.e no sample region).

Hint 2: Relative Thickness Composite will be calculated only if corresponding option in the Data Reduction panel has been set. See "Reduction" section for more details.



Scattered Composite Integral   Transmitted Composite Integral

3. Scattering and Transmission maps: displays scattering and transmission maps where each pixel of the (x,y) array corresponds to the totally scattered intensity (in the entire q range) and the transmitted intensity respectively. Each intensity is converted in different colors. If the options for calculating the transmission coefficient (T) and the relative thickness (n) have been set in the Data Reduction panel, the corresponding maps will also be generated, together with the effective scattering map (see "Reduction" section for more details).
4. Subtract Background: this option allows subtracting the background signal from each diffraction pattern of the scan.

   Warning: This option can only be enabled if the background region has been defined in the Data Reduction panel.
5. Sum of Patterns: this function sums all the diffraction patterns of the scan. It automatically saves three files in the mesh folder: a TIFF image, a raw TIFF, and a MAT file.
   - The TIFF image provides a quick view of the result,
   - the raw TIFF is the summed pattern that can also be imported into S-SAWANA for analysis
   - the MAT file contains the numerical matrix of the summed data, without any filtering effects from the conversion (i.e., it may include negative pixels).

   Hint: the MAT file is recommended if you want to analyze the summed pattern in S-SAWANA.

   The Sum of the Patterns can also be performed on a well-defined area by selecting the corresponding box "On selected area" and drawing a region on the scan composite. The "Draw Area" button allows you to define this region directly on the composite, while the "View Last Area" button lets you display the previously selected area.

For more details how to use the Composite Visualization please check the video tutorial "**2D_composite_4.0.mp4**"

3.5.6 Analysis section

The analysis folder is a subdirectory (Ex: C:\Desktop\data\XMILAB\analysis) automatically created in the same folder (Ex: C:\Desktop\data\XMILAB\) where data are stored.

Insert the initial and final scan number of raw data you want to analyze. A calibration file has to be loaded before proceeding with any further analysis.

The "2D IMGs Tool" allows to visualize one or more data/image in the array for additional checks (for example on the center previously evaluated).

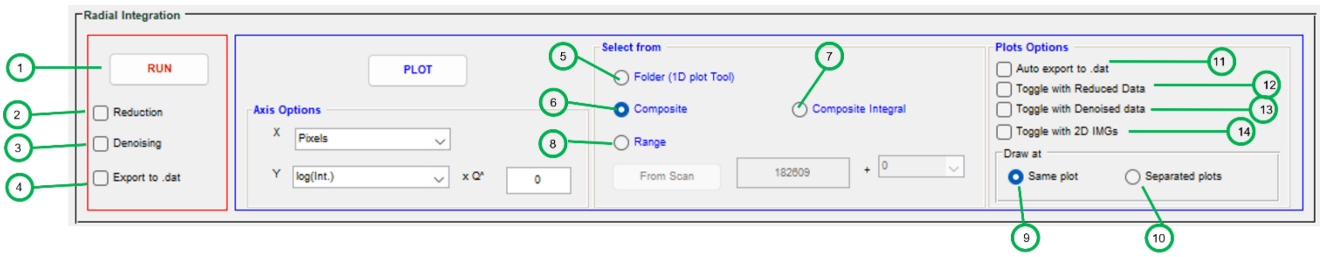
The drop-down menu on the left allows you to select the type of files to be analyzed:

i. Select "Rigaku Ins and Converted" for *.mpa* files or converted *.edf* files.

ii. Select "cSAXS" for data acquired at the cSAXS beamline.

iii. Select "Manual" for setting manual coordinates and step of the scan.

Radial Integration commands



1. Click "RUN" to fold the 2D raw data into 1D raw profiles. This procedure will be automatically repeated for all data. Note that a calibration file must be loaded before running this operation. After clicking "RUN", a prompt will ask within which angular range (0–360°) the folding should be performed. Subsequently, a subfolder named *analysis* is created inside the working folder. Within it, another subfolder called *radial_integration* is generated, where all 1D profiles are exported in *.mat* format. Each file name includes the number of the corresponding 2D pattern followed by the suffix "_integ".
2. The "Reduction" option allows the user to run the folding procedure using the data reduction settings defined in the panel (e.g, transmission, relative thickness, background, etc.). This procedure will be automatically repeated for all data. Subsequently, a subfolder named *reduct* within the folder *radial_integration* is generated, where all 1D profiles are exported in *.mat* format. Each file name includes the number of the corresponding 2D pattern followed by the suffix "_integ".
3. The "Denoising" option allows the user to run the procedure needed to denoise [1,2,3] the 1D raw profiles. This procedure will be automatically repeated for all data. Subsequently, a subfolder named *denoise* within the folder *radial_integration* is generated, where all 1D profiles are exported in *.mat* format. Each file name includes the number of the corresponding 2D pattern followed by the suffix "_integ".
4. The "Export to .dat" option allows the user to run the procedure and save all the profiles in *dat* format in a subfolder named "dat". Actually, by clicking "RUN", if the "Reduction" and "Denoising" options have been enabled, the corresponding profiles will also be saved in the *reduction* and *denoise* subfolders, respectively.

Warning: When performing the folding operation for the first time, it is necessary to run it on the raw data, without selecting the “Reduction” or “Denoising” options. These options can be applied only after the initial folding has been completed.

User may PLOT the integrated, reduced and denoised profiles either selecting them:

5. from the folder where they are stored
6. directly from the composite map
7. directly from the composite integral map
8. from a selected range (scan number using button From/To).

They can be plotted:

9. in the same frame plot
10. as separate plots.

Different choices can be made in “Axis Options” section for the X (pixels, Q(Å-1), Q(nm-1) …) and Y (Int, Log(Int), 1/Int) axes using the corresponding drop-down menu. It is also possible to multiply the Y axis for Q, Q^2, Q^3 etc.

As “Plots Options” user may decide to:

11. auto export (during plotting) the profiles as dat (e.g. saved in the subdirectory “\analysis\radial_integration\plots”),
12. to visualized the raw profile along with the corresponding reduced one
13. to visualized the raw profile along with the corresponding denoised one
14. to visualize the profile along with the corresponding 2D image

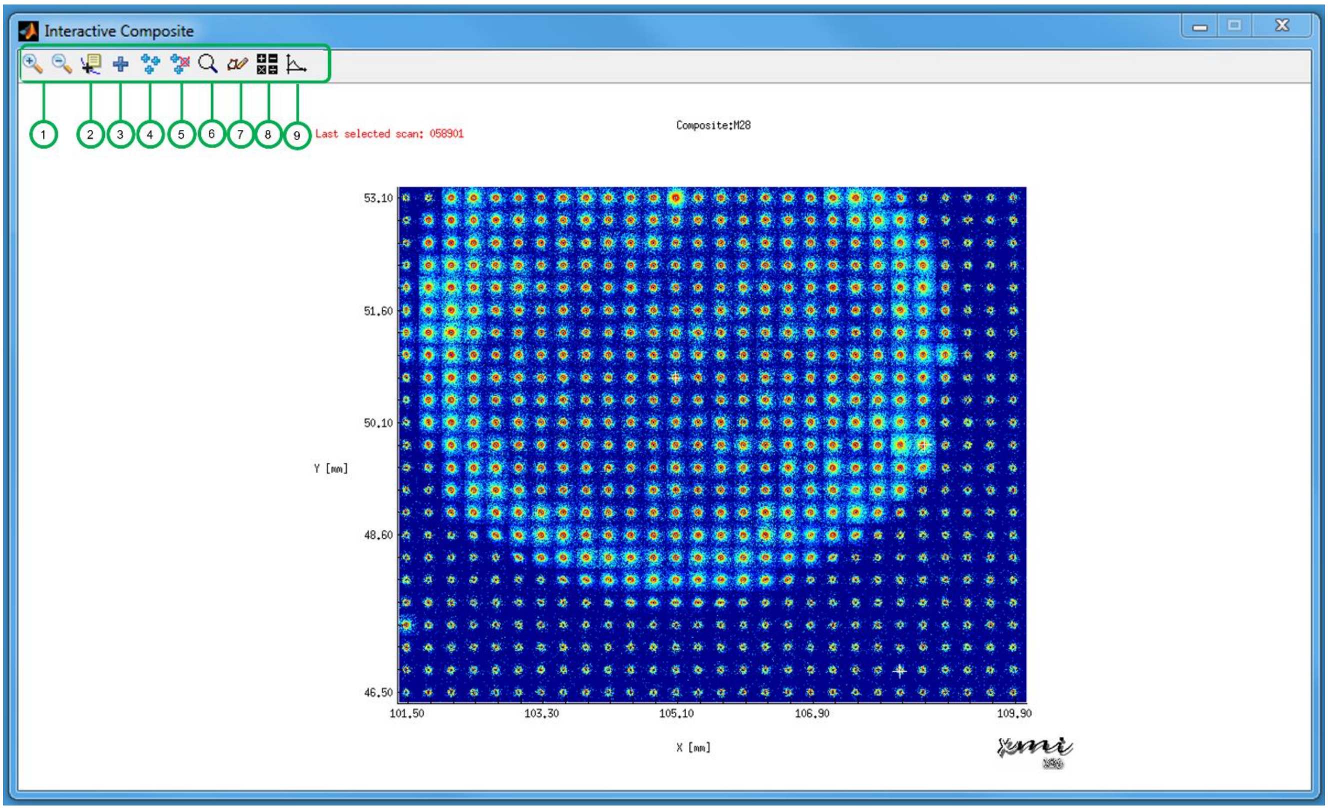
Click PLOT to launch the procedure.

Hint: If the “Toggle with Reduced Data” and/or “Toggle with Denoised Data” options are selected, *plots* subfolders will also be created in the corresponding *Reduction* and *Denoise* folders where corresponding profiles are saved.

Plotting from Composite

Use this option to select or plot data directly from the composite. The user can also choose to pick data from the composite integral. After clicking "PLOT", the program will ask which composite integral should be used for selecting the profile.

A windows opens and a tool bar allows the user to:



1. zoom in/out,
2. place a data cursor onto a specific pixel to know the corresponding scan number and (x,y) position in the array;
3. click inside the composite on a precise position to select a scan;
4. toggle a multi scans selection;

   Hint: Activate the multi scans selection button and, for each point, click button 3 to select the frame. <u>Warning:</u> keep the multi scans selection button enabled if you want to plot all frames simultaneously. If the button is deactivated, only the last selected frame will remain in memory.

5. delete a previously selected scan in the composite;
6. find the corresponding scan number on the composite;
7. draw an area in the composite (rectangle, circle, polygon);

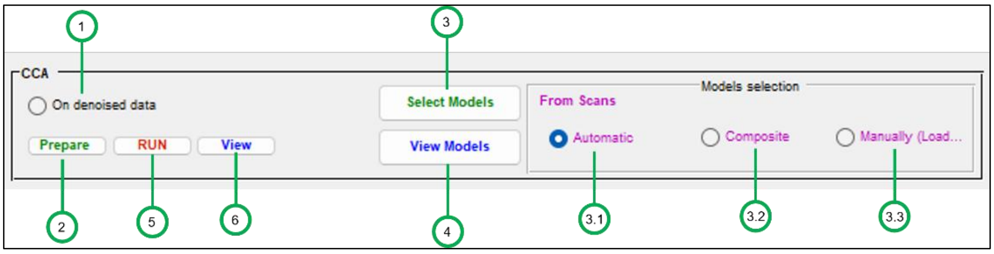
   Hint: Once the area is drawn, double-click to validate it (it will change from red to green)
8. compute the average scattered intensity/number of the scans/q-range inside the drawn area (as in 7). The drawn area in can be dragged using the mouse, inside the composite area;

9. plot selected scans from composite.

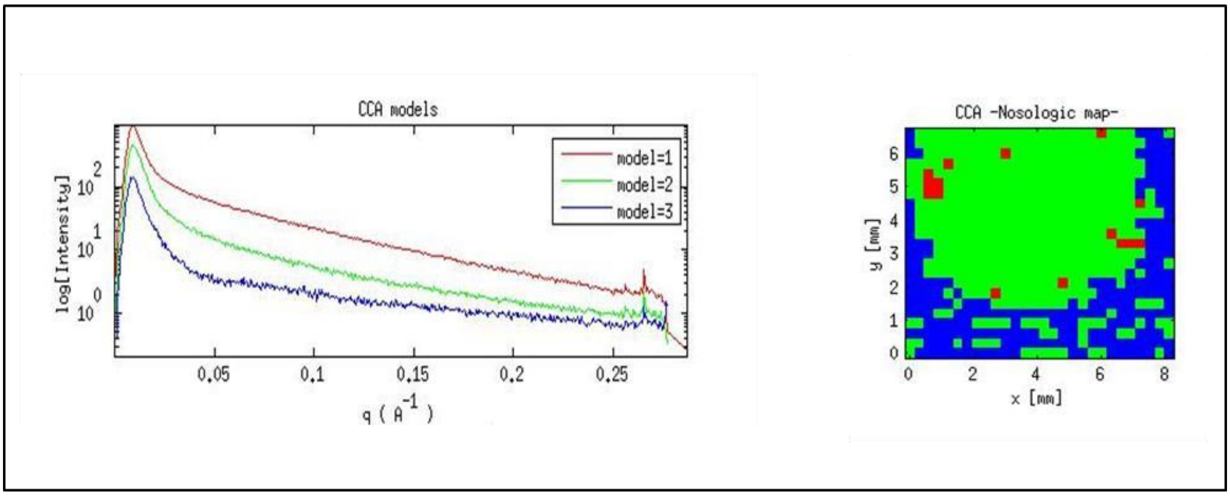
For more details how to use the "Plotting from Composite", please check the video tutorial "**msawana-composite2plot_4.0.mp4**"

CCA commands

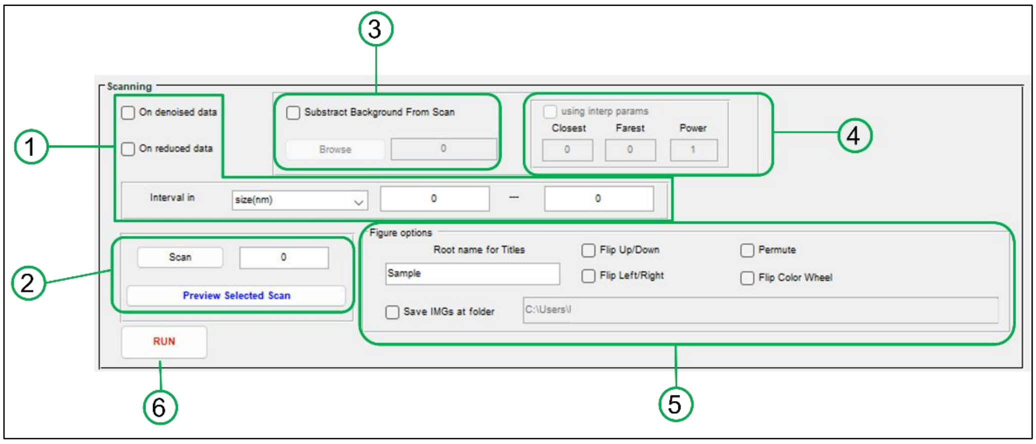
The items in this frame enable the user to perform the Canonical Correlation Analysis (CCA) on the selected data. CCA is a multichannel generalization of ordinary correlation analysis (a statistical technique that quantifies the relationship between two sets of variables); it aims at evincing the relationship between two random variables x and y by means of the so-called correlation coefficient: the algorithm is described, for instance, in.[4]. Application of CCA to X-ray diffraction data is detailed at [5]



1. Tick the box to perform the analysis on denoised data (radial integration outcome, see Analysis section).
2. One dimensional profiles are meshed within a matrix.
3. Current models are selected and will be used throughout the CCA algorithm. Model profiles are selected by:
    3.1 (unsupervised, default) adaptive binning method as described in [6]
    3.2 models are chosen according to the actual patterns mesh (user supervised);
    3.3 models are retrieved from external files.
4. Select the button to open a new window and to plot the chosen model profiles therein.
5. Perform Canonical Correlation Analysis (CCA).
6. Show the nosologic map (see figure below).



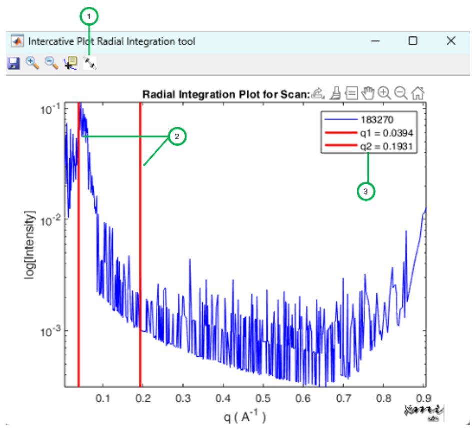
For more details how to use the “CCA”, please check the video tutorial: “**msawana-cca_4.0.mp4**”



1. Select which data you want to use for microscopy (Multi-modal imaging approach [10]). If no option is selected, the original integrated data will be used.

   It is possible to manually set a q-range (in A^{-1} or in nm^{-1}) or a size range of interest, to be used for the Scanning section analysis, from the drop-down menu.

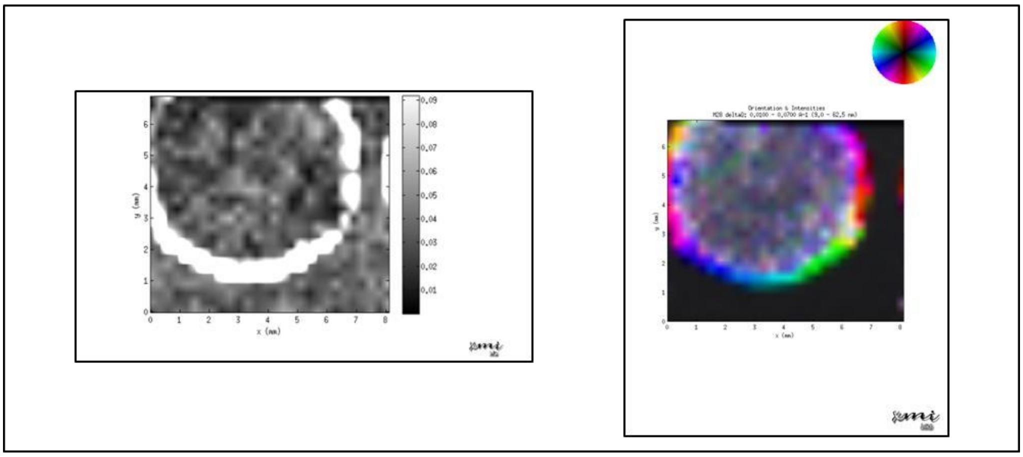
2. The "Preview Selected Scan" button allows you to view a chosen profile and to graphically select the range. The scan is selected from the data folder or from one of the available composite maps. On an interactive plot two vertical red bars will appear to highlight the selected range. User can visualize one single scan, alone, or the scan together with another profile considered as background.



1) The button Allows you to position the two vertical lines using the mouse.
2) The two red vertical lines mark the boundaries of the q range.
3) The legend displays the file name corresponding to the profile and the two numerical values of the q-range. The two values are automatically entered into the boxes in the panel.

3. Activate "Subtract Background From Scan" if user wants to select a background profile entering the scan number or picking it up from the data folder or from one of the available composite maps (clicking "Browse" button). A window opens to visualize the profiles (scan and background) and their difference. **Warning:** this option is not available when already reduced data is selected.
4. If "Subtract Background From Scan" is active, user can use background interpolation: picking the "using interpolation" option , the user can insert values of "Closest" point, "Farthest" point and the "Background Intensity Power" and used them for interpolation.
5. *Figure Options sub-panel:* a root name has to be inserted which will be used by the program when saving the images produced by the Scanning section. These images are labelled as Orientation & Intensities and Orientation Degree. These images are saved in the folder \analysis\images with the root name plus the identification of the selected Δq range, and corresponding size.
6. Click RUN to perform scanning and view the results (see figure below). Along with the orientation figures,

the scattering image for the selected q-range is also displayed.



Orientation degree Orientation Intensity

For more details how to use the "Scanning", please check the video tutorial: "**msawana_scanning_4.0.mp4**"

References

[1] De Caro, L., Altamura, D., Vittoria, F.M., Carbone, G., Qiao, F., Manna L. & Giannini, C. (2012). *J. Appl. Cryst*. 45, 1228-1235.

[2] De Caro, L., Altamura, D., Sibillano, T., Siliqi, D., Filograsso, G., Bunk, O. & Giannini, C. (2013). *J. Appl. Cryst*. 46, 672-678.

[3] Sibillano, T, De Caro, L., Altamura, D., Siliqi, D., Ramella, M., Boccafoschi, F., Ciasca, G., Campi, G., Tirinato, L., di Fabrizio E. and Giannini C. (2014) *Sci. Rep.* **4**, 6985.

[4] Laudadio, T. *et al (2005). Magn. Reson. Med. 54, 1519–1529*

[5] Ladisa, M. *et al. , EURASIP, Journal on Advances in Signal Processing, Volume 2007, Article ID 19260.*

[6] Guagliardi A. *et al*, *J. Appl. Cryst*. (2007). **40**, 865–873;

[7] Altamura, D., Lassandro, R., De Caro, L., Siliqi, D., Ladisa M. & Giannini, C. (2012). *J. Appl. Cryst. 45, 869–873.*

[8] Scattarella, F., Altamura, D., Sibillano, T., De Caro, L., Siliqi, D. & Giannini, C. (2025). *J. Appl. Cryst. 58, 1817-1826*

[9] Scattarella, F., De Caro, L., Siliqi, D. & Carlino, E. (2017).*Crystals* **7**, 186.

[10] O Bunk *et al* 2009 *New J. Phys.* **11** 123016

4 Tutorials

All the video tutorials can be found at the following website

https://www.ba.ic.cnr.it/softwareic/sunbim/tutorials/

The list of the video tutorials.

1. BatchScript_4.0.mp4
2. Calibration_4.0.mp4
3. one_plot_4.0.mp4
4. ssawana-gisax_4.0.mp4
5. ssawana-giwax_4.0.mp4
6. Conversion_edf_4.0.mp4
7. msawana_data_reduction_4.0.mp4
8. 2D_Composite_4.0.mp4
9. msawana_composite2plot_4.0.mp4
10. msawana-cca_4.0.mp4
11. msawana_scanning_4.0.mp4

5 Examples

From the website http://wwwba.ic.cnr.it/content/sunbim-examples is possible to download (examples.zip) some useful examples to test the package

- Calibration:
  - saxs_gisaxs_calibrant
    - AgBehenate_saxs_gisaxs.xxx → calibration image for SAXS/GIWAXS examples
  - waxs_giwaxs_calibrant
    - Si_NIST_waxs.tif → calibration image file for WAXS example
    - AgBehenate_giwaxs.tif → calibration image file for GIWAXS example
- M-SAWANA:
  - Composite:
    - multiscans_2: Several scan images for Composite and M-SAWANA procedure
    - DC: DarkCurrent_1m_3804s.mpa
  - Conversion:
    - Masks: several MASK_XXXXXXX.txt files for different detector configurations
    - multi_scan_edf: Several scan images in edf format

- S-SAWANA:
  - gisaxs.mpa → scan image for GISAXS test
  - saxs.mpa → scan image for SAXS test (indexing)
  - giwaxs.mpa → scan image for GIWAXS test
  - waxs.tif → scan image for WAXS test
  - isgisaxs: folder containing files from IsGISAXS analysis software

- Plot Deconvolution:
    - Two text data files to test the denoising and deconvolution procedure