User Guide for the Laue-Camera Application

Software-Version: 1.1.2
Datum: 19.01.2022
Author: Julian Kaiser

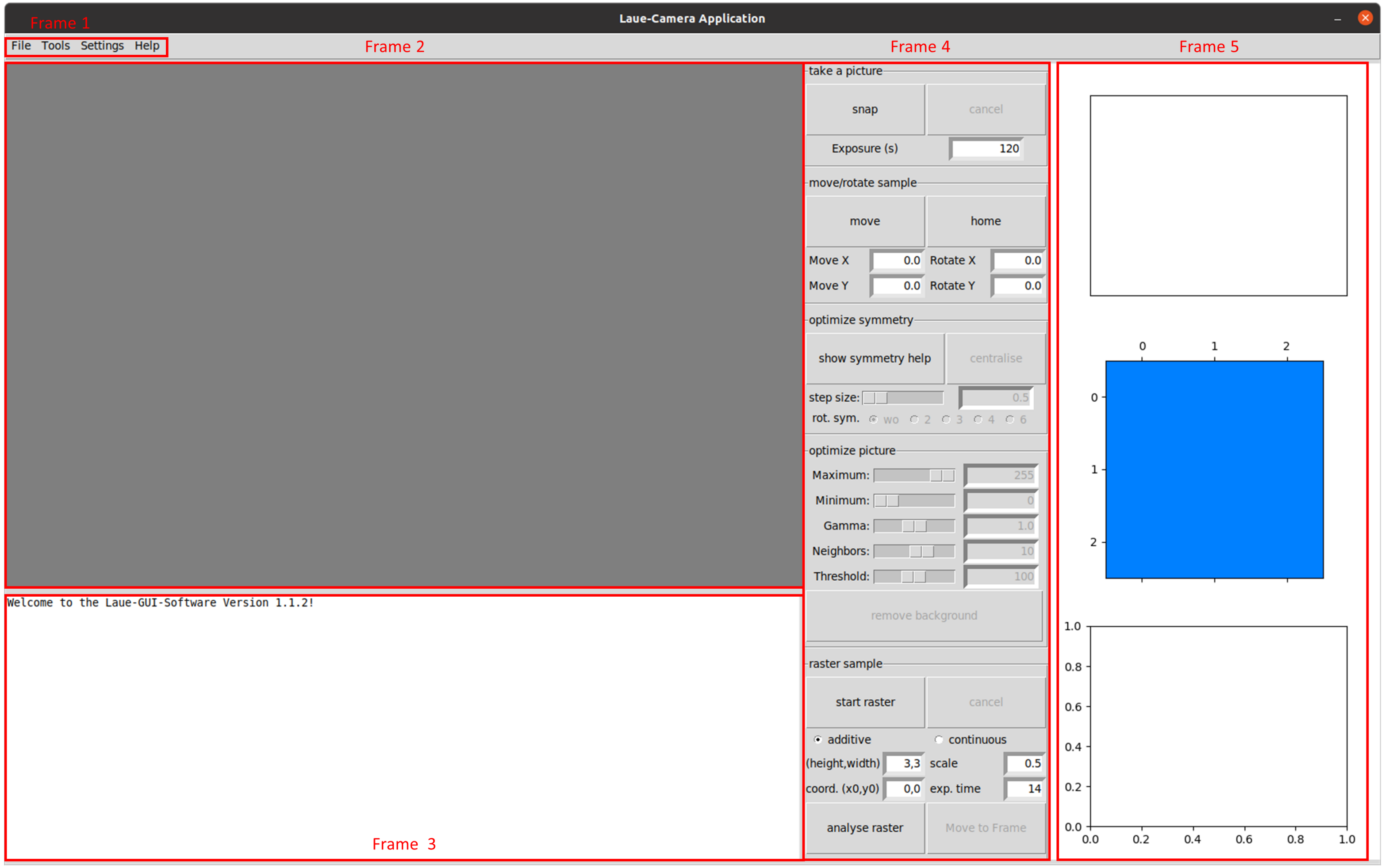


Fig. 0.1: Laue-Camera Application after starting

Contents

System requirement

This application is coded in python version 3.8.10 for PSLViewer version 3I-CFL from Photonic Science. It's purpose is to simplify and optimize the handling of the Laue-Diffraktometer from the chair of applied physics 6, the motorized goniometer and the image processing. Basic functions for the communication with the server and goniometer are adopted from Marvin Klinger and enhanced.
It is recommend to use the Laue-Diffraktometer and this application only with 20 kV and 30 mA, because this application was developed specifically for this values. Furthermore it is optimized for the visualisation of Na_2IrO_3 crystals, which produce rather bad images. For other crystals, all the possible functions for image processing may don't be necessary. Also other settings may be more beneficial, so many default settings can be changed. If any non changeable value should be changeable, please contact the author! Moreover not only the goniometer is accessible, but also the Windowscomputer with the corresponding programm PSLViewer, so that a full remote control is possible. If PSLViewer crashed, two important settings on the Windowscomputer have to be adjusted in advance, that a remote restart is possible:

- The application „cports.exe“ has to be in the folder with the same name at „Local Disk (C:)“. If it was deleted, a download is possible here.
- At „Task Scheduler Library“ the task „restart_PSL_Viewer_2“ has to exist. If not, this tutorial will explain the required steps (without changing the icon). The application that has to be selected is „restart_PSL_Viewer_2.bat“ at the folder „PSLViewer-3I“ and the resulting connection must be callable from „restart_PSL_Viewer.bat“ at the folder „PSLViewer-3I“.

Changelog

1.1.1

- Convert a .tif- to a .bmp-raster
- Detection of areas with complete different alignments through the detection of the center and the orientation of the diffraction pattern
- Different visualization options for rasters with center detection data
- New evaluation of a kontur for long exposure times
- Save a flipped image at the horizontal or vertical image center

1.1.2

- Bug-fixes for the center-detection option in rasters
- Detection of small and big transition in advanced raster analysis

Frame 1 - menu

At the menu bar in the sub menu File, the user can save the displayed picture on Frame 2 and display a recorded image or raster. In the sub menu Tools, several tools can be used and in Settings the user can change the value of important parameters. In the sub menu Help, this PDF file will be displayed.

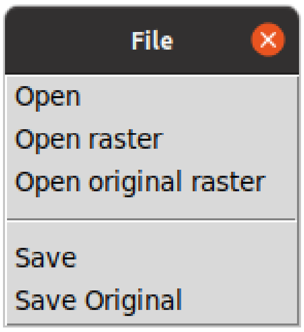


Fig. 1.1: File-menu with all available functions

File

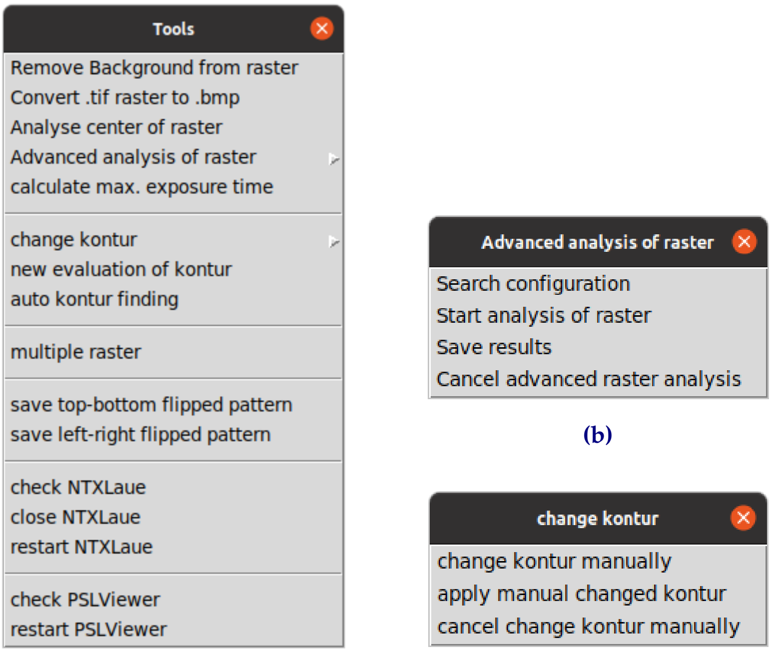
- Open: Opens a dialog to select a recorded grayscale image with the dimensions 975x643 pixel, either a 8-bit („.bmp“) or higher data formatted („.tif“) images. This command is also available with the shortcut „STRG + o“.

- Open raster: Opens a dialog to select a recorded raster, saved as 8-bit and multiplot image. The dialog only displays folders, so the user has to select only the corresponding folder (dialog has to be inside the folder). For correct visualization, the order of the saved rasterframes is very important (name-sorted must be equal to the acquisition order). This command is also available with the shortcut „STRG + r“.

- Open original raster: Opens a dialog similar to „Open raster“ with the same requirements on the file-order, but in this command only „.tif“ are opend. This command is also available with the shortcut „STRG + SHIFT + R“.

- Save: Opens a dialog to save the displayed 8-bit image at Frame 2 as „.bmp“ file. This command is also available with the shortcut „STRG + ALT + s“. Additionally, the shortcut „STRG + s“ also saves the image, but doesn't open a dialog but saves the image at the selected directory in Settings. The file name contains the name/number of the sample, applied voltage and current, distance to the detector, exposure time, comment and a uprising number starting at „000“, all seperated by „_“ (more information to the parameters is available at save settings).

- Save Original: Opens similar to „Save“ a dialog to save the original image (greater than 8-bit). This command is also available with the shortcut „STRG + ALT + SHIFT + S“. Also the shortcut „STRG + SHIFT + S“ saves similar to „Save“ the original image at the selected directory in Settings with the suffix „original“ in the filename.



(a) (c)

Fig. 1.2: Tools-menu with all available functions

Tools

- Remove Background from raster: Opens a dialog similar to „Open raster“ to select a original raster (no multiplot images!) to remove the background of each frame. After the selection, a new dialog opens to select the save directory, where a new folder is created for the new calculated raster. The command subtracts the background with the selected options at Settings from the whole image.

- convert .tif to .bmp raster: Converts a original raster (.tif files) to a raster with 8-bit (.bmp files). Therefore the user has to set a mean value and then the maximum pixel value is tuned, so that the mean value of the resulting image is near to the defined one. The mean value can be set in a range from 255 (maximum) to the mean value of the original image (minimum).

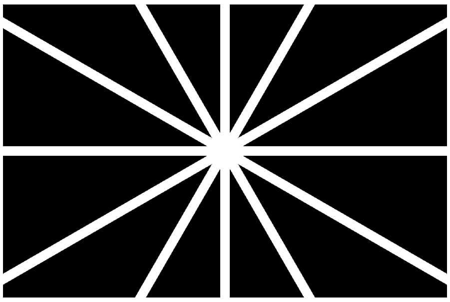


Fig. 1.3: Example of a mask with six lines and a linewidth of 21 pixel

- Analyse center of raster: Opens a dialog to select a raster to analyse and afterwards a dialog to select the save directory for the collected data. The method tries to detect the center and the smallest clockwise degree a „line“ is rotated from the vertical image-center of the centered diffraction image. Therefor, according to the Settings, a mask slightly larger as the image is generated first (see fig. 1.3). The center of this mask is put on each pixel of the search area and then the mean value of all pixel who aren't covered by the mask is calculated. To define the rotated degree, the mask is additionally rotated in steps of 1° until it matches with the original one and for each orientation the mean value of the remaining pixel is caluclated. The idea behind the method is, that for the best orientation of the mask on the image the mean value of the remaining pixel is at a minimum. First for each angle of rotation the mean value of the mean values from the whole search area is calculated and the smallest one is interpreted as the best orientation. Second the center of the diffraction pattern is the center of mass from all minima of the mean values in the search area from the corresponding angle. The results are saved in the logfile from the selected raster additionally, separated by the prefix „$$$beginCenterData$$$“ and the suffix „$$$endCenterData$$$“. Furthermore if a raster with data from the center detection method is loaded, the results can be visualized in Frame 5. With a right-click on the kontur the user can choose between the normal kontur, the diffrent angle of rotations (each color represents one specific angle from minimum (dark blue) to maximum (dark red)), the mean distance from the center to surrounding centers of the diffraction images and the combination of the angle of rotation and distance map (added together).
- Advanced analysis of raster: Offers the possibility of a deeper analysis of a raster than Analyse center of raster, so that minor transitions between two different orientated regions of the sample can be detected and visualized. **Attention!** Only two different areas are supported at the moment to analyse.
  - Search configuration: Switches to the interface for the advanced analysis.

Therefore all buttons in Frame 4 are disabled and the „remove background" button is replaced by the buttons „add rect" and „sub rect". With the „add rect"-button the user can add another rectangle and with the „sub rect"-button the user can delete the selected rectangle. To draw a rectangle, on the one hand side the user can draw a square of 10 pixels by left-clicking inside the image and on the other hand side with the left mouse button holded the user can define an independent rectangle by moving over the screen. To switch between the different rectangles the user has to right click inside the corresponding rectangle, which will be framed blue and all others that are inactive are framed orange. These rectangles represent the data area which is used in the function Start analysis of raster. Also the shape of the current rectangle can be modified by double right-clicking inside the active rectangle, then the user can modify the coordinates of the top left and bottom right corner of the rectangle. Additonally the sliders for „neighborhood" and „threshold" are also active now and can be adjusted for each rectangle separately. In Diagram 1 in Frame 5 the result of the function Start analysis of raster with the data from the actual rectangle plus the defined offset in Settings as the input is displayed, in which all detected spots are visualized but the real maxima in green and the wrong maxima in red (see Fig. 1.4). Moreover the navigation through the raster is also activated to check the result of the analysis function with the adjusted parameters for the whole sample.

- Start analysis of raster: This function try to make a distinction of cases for each defined rectangle between none, one or two maxima inside each area. Therefore the algorithm tries to detect all possible maxima inside one rectangle with a maxima detection function, in which the sliders „neighborhood" and „threshold" are respected. In detail, first a maximum- and a minimum-filter (with the corresponding „neighborhood") is applied and the result is assembled by subtracting the result of the minimum-filter from the result of the maximum-filter and converted into a true-map by setting all values greater than „threshold" to true and the others to false. From every connected area inside the true-map the center is calculated and returned as a potentially maximum. Every maximum is checked with a gaus-function like

$$f(x,y) = A \cdot \exp\left(\frac{(x-x_0)^2}{\sigma_1^2}\frac{(y-y_0)^2}{\sigma_2^2}\right) \tag{1.1}$$

  for separate inspection. The data field is defined as a quadratic area around the corresponding maximum with the defined length in Settings. The constants x_0 and y_0 are the coordinates of the detected maximum in pixel and the variables A,σ_1 and σ_2 are used as fitting parameters in a „least-square"-algorithm. If the algorithm fails to determine the fitting parameters the corresponding maximum is not a „real" maximum but rather a misinterpretation of the noise from the maxima detection function from before. Also it turned out that for false maxima one value of σ_1 and/or σ_2 is huge. For that reason a maximum is only classified as a real maximum when at least one value of σ_1 and σ_2 is lower than the defined maximum value in Settings. For the distinction of cases, another correction of the remaining points is done before. Since only the amount of maxima is important for the separation of cases, the number of the resulting points is given by subtracting the amount of dots that doesn't fulfill the conditions from the whole number of remaining points. In the following the distances between the detected points are investigated. The distance between two points is only allowed to be between the minimum distance (too near points are considered to be one point) and the maximum distance (noise far away from one maximum is misinterpreted as a maximum) in Settings. Remains no point, no reflex can be detected (encoded as 0). Remains only one point, at this point the x-ray beam detected a single crystalline area (encoded as 1) and with two dots remaining, at this point the x-ray beam detected two areas with slightly different orientations due to his dilatation (encoded as 2). Are two rectangles defined, two more cases appear like one point per frame, which represents a greater transition between two areas with different orientations (encoded as 3) and more than one point in one or both of the frames, which represents additionally to the great transition a smaller one in the selected frames (encoded as 4). The result is visualized in the diagram 2 in Frame 5, whereat the color coding describes the encoded values from blue (0) to red (4 or actual position) and also the quality of the detection area at the sample (blue for good and red for bad spots).

  - Save results: Saves the current result (contour in Frame 5) of an advanced analysis in the selected logfile in the opening dialog. The data is saved with the prefix „$$$beginAdvancedData$$$“ and the suffix „$$$endAdvancedData$$$“ to separate it from the other data.
  - Cancel advanced raster analysis: Cancels the actual advanced analysis from one raster and rebuild the normal user interface.

- calculate max. exposure time: Calculates the new maximum exposure time. More information are available at Section 1 in Frame 4
- change kontur: In this sub menu, the user can change an acquired contour, if the algorithm misvalue a frame in a raster. The command „change kontur manually“ makes the current contour at Frame 5 changeable and the user can navigate through the contour with the arrow keys. To change the selected frame, the user has to type in numbers from 0 to 3. With the command „apply manual changed kontur“, a dialog opens to select a logfile.txt, which contour will be overwritten with the displayed contour. With the command „cancel change kontur manually“ the displayed contour isn't changeable any more.

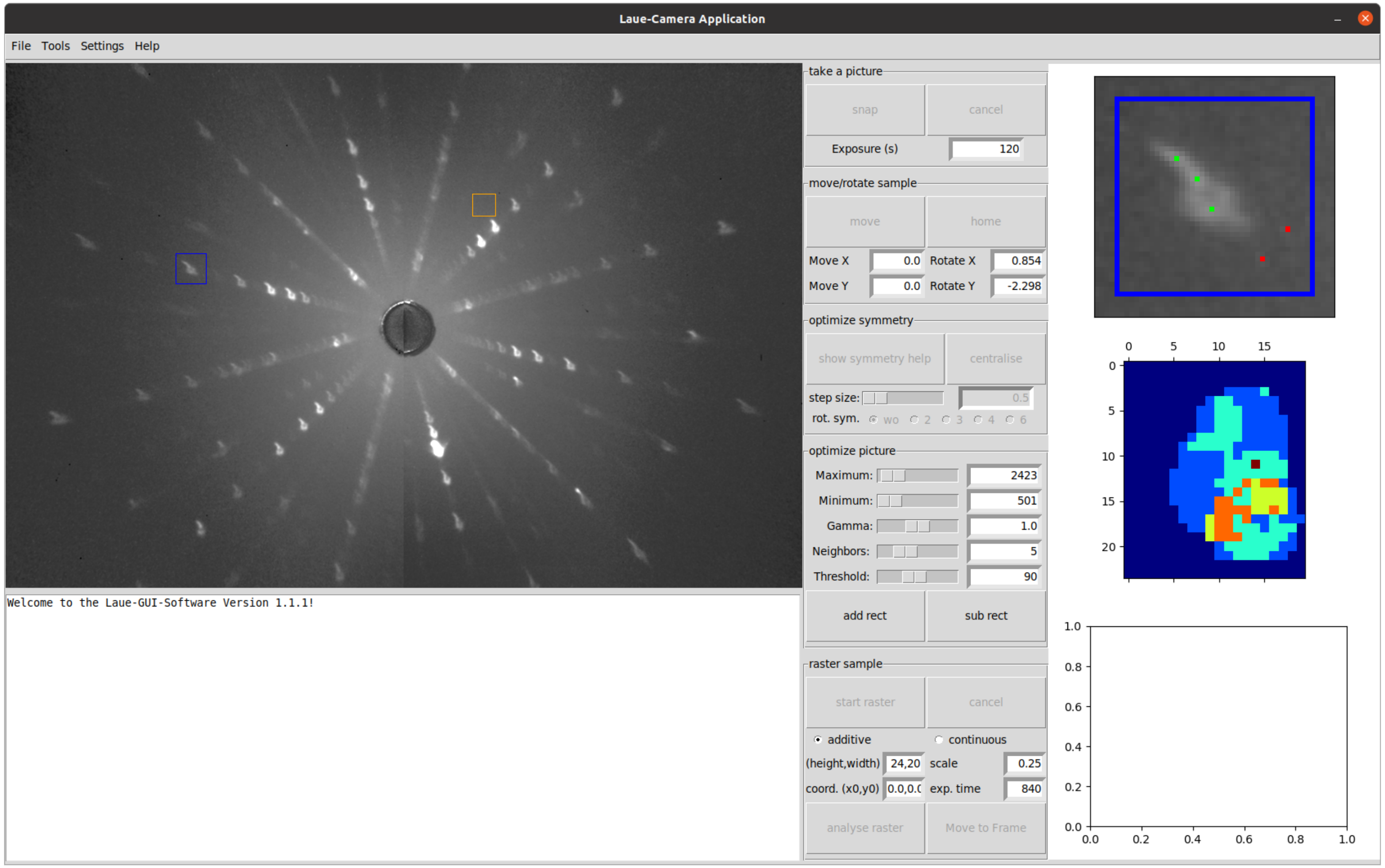


Fig. 1.4: User-interface for the advanced analysis. The different rectangles are visualized inside the image viewer as a blue rectangle for the actual frame and as an orange rectangle for the other frames. In the upper diagram all detected points are shown for the blue rectangle, green dots represent real maxima and red dots false maxima. The diagram in the middle visualized the result of one run of the analyse function and the „remove background"-button is replaced by the two buttons „add rect" and „sub rect".

- new evaluation of kontur: Opens a dialog to select a .tif-raster, from which the kontur will be reevaluate. This method is necessary for long exposure times, because for an appropriate characterization the remove of the background is necessary. The remove of the background is done by the selected method in Settings, rescaled to an 8-bit image and then evaluated by the same algorithm as in a normal kontur acquisition. The new results are saved in the logfile of the selected raster.

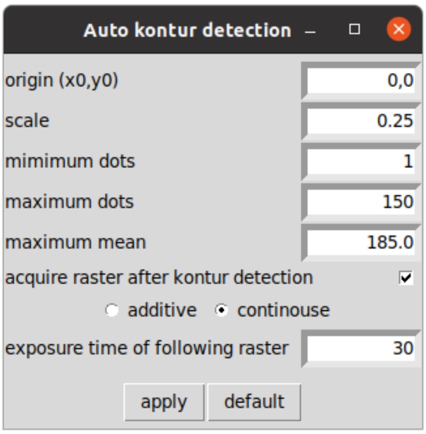


Fig. 1.5: „auto kontur finding" Dialog with all available functions

- auto kontur finding: Opens a dialog to configure the search criteria:
  - origin (x_0,y_0): origin of contour search; $x_0,y_0 \in \mathbb{R}$
  - scale: step size between two frames; scale $\in \mathbb{R}^+$
  - minimum dots: minimum number of detected points, that are necessary to interpret the frame as a hit; $\text{min}_{\text{dots}} \in \mathbb{N}$
  - maximum dots: maximum number of detected points, that are required to interpret the frame as a hit; $\text{max}_{\text{dots}} \in \mathbb{N}$
  - maximum mean: maximum mean value up to a frame is interpreted as a hit; $\text{max}_{\text{mean}} \in \mathbb{R}^+$
  - acquire raster after kontur detection: acquire after the detection of the contour a new raster with the determined parameters;
  - additive/continuous: the user can change between additive (max. 16 s exposure) or continuous (max. exposure) acquisition (for more information see Section 1 in Frame 4)
  - exposure time of following raster: exposure time of a frame in the subsequent raster, exposure $\in \mathbb{N}$

  This method tries to determine the contour of the sample by moving the sample from the origin in steps of step size in every direction until no diffraction pattern can be detected anymore (number of dots isn't in the defined range). Afterwards all edges are analysed to ensure that the whole sample is inside the contour. The exposure time is 31 s.

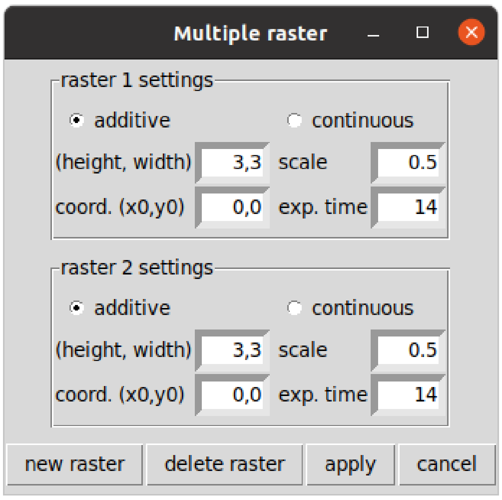


Fig. 1.6: „multiple raster" Dialog with all available functions

- multiple raster: Allow the user to acquire from the same sample various raster. To configure all settings, a dialog will open where more than one raster can be selected with the same settings as a normal raster in Section 5. With the button „apply", all selected rasters are acquired in a row.

- save top-bottom flipped pattern: Saves the image from the diffraction pattern mirrored to the horizontal center of the image because of the same reason in save left-right flipped pattern. Is the sample inserted with left and right match with the left and right from the detector, so top and bottom is inverted due to the 180° rotation. Mirror on the horizontal or vertical image center depends therefor on the insertion of the sample inside the goniometer.

- save left-right flipped pattern: Saves thee diffraction pattern mirrored to the vertical center of the image. This can be helpful for the problem of a correct direction determination on a sample, which results of the different point of views on the image from the microscope and the diffraction pattern. The point of view through the microscope (eye) at the sample is mirrored to the point of view from the computer to the detector (see fig. 1.7). Therefore one image has to be mirrored vertically for this insertion of the sample.

- check NTXLaue: Checks the current status of the camera (if the application is opened at the other computer) and displays the status in Frame 3.

- close NTXLaue: Closes the camera and displays the status in Frame 3

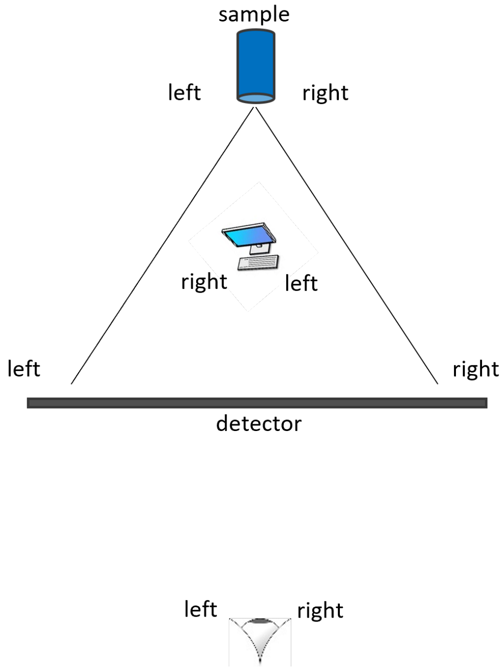


Fig. 1.7: Visualization of the necessity to mirror the diffraction pattern or the image from the microscope for a correct determination of the direction in the sample. Rotating the sample to match right an left lead to swapping top and bottom.

- restart NTXLaue: Restarts the camera and displays the status in Frame 3. If the camera is closed, the camera will be opened.

- check PSLViewer: Checks if the application „PSLViewer“ and the data connection to „server control“ is open and connected.

- restart PSLViewer: Restarts the application „PSLViewer“ with „server control“ on the other windows computer with a batch-file. It is useful, if the application crashed or isn't responding. To restart the application, the data connection still has to be open to send the command to the other computer. With this command, a reasonable remote control of the PSLViewer application is possible via, for example, TeamViewer.

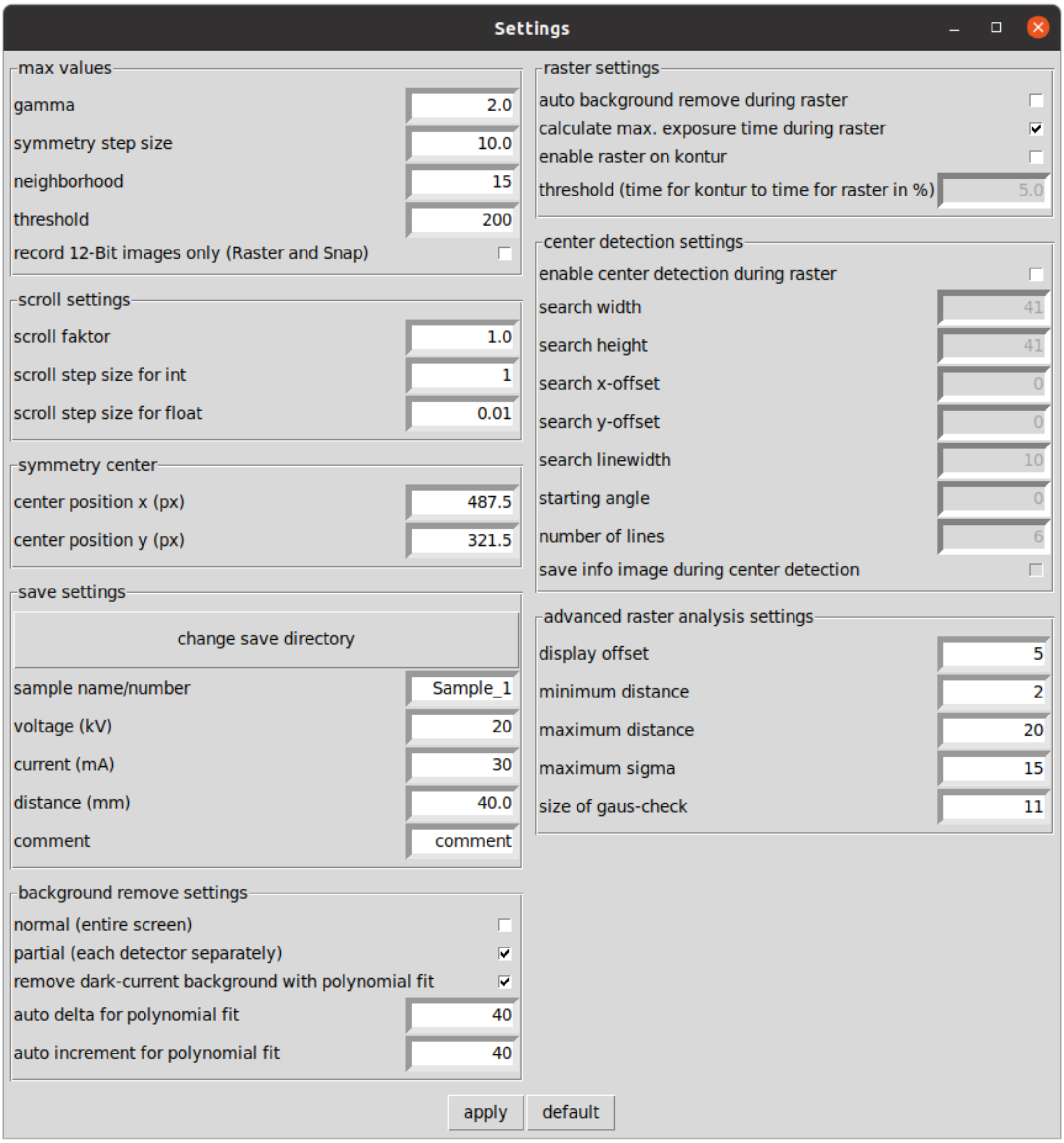


Fig. 1.8: „Settings“ Dialog with all available functions

Settings

max values:

- gamma: maximum value of gamma (Minimum is 0); $max_{gamma} \in \mathbb{R}^+$
- symmetry step size: maximum value of the angle of rotation for the symmetry help (Minimum is 0.5); $max_{sym} \in \mathbb{R}^+$
- neighborhood: maximum value of the selectable neighborhood (Minimum is 1); $max_{neigh} \in \mathbb{N}$
- threshold: maximum value of the threshold in the maximum detection (Minimum is 1); $max_{thres} \in \mathbb{N}$
- record 12-Bit images only (Raster and Snap): defines if only 12-bit gray scale images (values up to 4095 possible) or more detailed images (values greater than 4095 are possible) have to be recorded.

scroll settings:

- scroll faktor: factor which will be multiplied to the stepsize of the sliders in Frame 4; faktor$\in \mathbb{R}^+$
- scroll step size for int: stepsize of the sliders in Frame 4 with integers; $stepsize_{int} \in \mathbb{N}$
- scroll step size for float: stepsize of the sliders in Frame 4 with floats; $stepsize_{float} \in \mathbb{R}^+$

symmetry center:

- center position x (px): X-coordinate of the point, on which the diffraction pattern will be symmetrized in Frame 4 in Section 3. Unfortunately, not all points on the detector are suitable for a center position due to the limitation of the goniometer. Is state in pixels between 0 and 975. $center_x \in \mathbb{R}^+$
- center position y (px): Y-coordinate of the point, on which the diffraction pattern will be symmetrized in Frame 4 in Section 3. Unfortunately, not all points on the detector are suitable for a center position due to the limitation of the goniometer. Is state in pixels between 0 and 643. $center_y \in \mathbb{R}^+$

save settings:

- change save directory: Opens a dialog to select a directory, which is the origin for save and load dialogs and the save directory for the auto save commands.
- sample name/number: Defines the name or number of the current sample, which is used for the filename in the auto save commands. Shouldn't contain the symbol „/", due to possible errors while saving.

- voltage (kV): Defines the applied voltage at the x-ray tube in kV. Attention: other values than the default value may result in bad or false results during background subtraction! $U \in \mathbb{N}$.

- current (mA): Defines the applied cuurent at the x-ray tube in mA. Attention: other values than the default value may result in bad or false results during background subtraction! $I \in \mathbb{N}$.

- distance (mm): Defines the distance between sample and detector. Value is also used in Frame 4 in Section 3 to calculate the rotational angels to symmetrize the diffraction pattern. $d \in \mathbb{R}^+$

- comment: Defines a addition comment which is added to the filename in the auto save commands. Shouldn't contain the symbol „/", due to possible errors while saving.

background remove settings:

- normal (entire screen): Fitfunction for background remove is calculated for the whole area of the detector (see also remove background)

- partial (each detector separately): Fitfunction for background remove is calculated and removed for every half of the detector separately (see also remove background)

- remove dark-current background with polynomial fit: If activated, it removes also the background from the dark-current with a polynomial function (see also remove background)

- auto delta for polynomial fit: Defines the parameter δ for the automatic calculation of the maximum pixel value in the subtraction of the background due to the dark-current. (see also remove background). $\delta \in \mathbb{N}^+$

- auto increment for polynomial fit: Defines the parameter inkrement for the automatic calculation of the maximum pixel value in the subtraction of the background due to the dark-current. (see also remove background). Inkrement $\in \mathbb{N}^+$

raster settings:

- auto background remove during raster: If selected, the background of each frame from every raster with an exposure time greater than 60 s will be subtracted while the raster is acquired. Is saved in an addition folder.

- calculate max. exposure time during raster: If selected, the new maximum exposure will be calculated on every frame.

- enable raster on kontur: If selected, before a raster is acquired, a faster raster with 31 s exposure time will be acquired and according to the resulting contour, only the frames where a hit was detected will be acquired.

- threshold (time for kontur to time for raster): If „enable raster on kontur“ is selcted, this entry is editable. If the ratio of total time for the fast raster to total time for the normal raster is lower than the defined threshold in this entry, the fast raster will be acquired. If not, then only the normal raster will be acquired. Is state in percent and from 0 to 100.

center detection settings:

- enable center detection during raster: Enables the analysis of the center detection method from Tools during the acquisition of a raster, whereby the collected data is available direct after the finish of the acquisition. To guarantee that, the exposure time of one image should be greater than the process time of the method for one picture.
- search width: Defines the width of the search area in pixel. Has to be even to guarantee a symmetric dispersion relative to the center of the search area. width $\in \{1{,}975\} \subset \mathbb{N}$
- search height:Defines the height of the search area in pixel. Has to be even to guarantee a symmetric dispersion relative to the center of the search area. height $\in \{1{,}643\} \subset \mathbb{N}$
- search x-offset: Defines the offset in x-direction (cartesian coordinate system) in pixel from the center of the image to the center of the search area. x-offset $\in \{1{,}487\} \subset \mathbb{N}$
- search y-offset: Defines the offset in y-direction (cartesian coordinate system) in pixel from the center of the image to the center of the search area. y-offset $\in \{1{,}321\} \subset \mathbb{N}$
- search linewidth: Defines the half of the linewidth of each line in a mask in pixel. Values greater than 100 should be avoided, because otherwise a too small area is left to calculate the results and the results aren't significant. linewidth $\in \mathbb{N}$
- starting angle: Defines by which angle the first mask is rotated before the other masks are generated. It's important for the case that one „line“ of the diffraction pattern is nearly vertical, so a good boundary isn't visible any more in the visualisation of the rotated angle. angle $\in \{0{,}360\} \subset \mathbb{N}$
- number of lines: Defines the number of lines in one mask, which are all rotated by equally spaced angles. Therefor only numbers up to 10 are supported. $\in \{1{,}10\} \subset \mathbb{N}$
- save info image during center detection: Defines if an info-image is saved additional to the other acquired data. The info-image contains a visualisation of the search field and the detected center on the image and the information of the rotated angle and coordinates from the center.

advanced raster analysis settings:

- display offset: Defines the additional number of pixel which are also displayed in the first diagram of Frame 5 on each side additional to the selected area. offset $\in \{1{,}300\} \subset \mathbb{N}$
- minimum distance: Defines the minimum distance between to detected maxima to classify them as tow different maxima. $\mathrm{min}_{\mathrm{dist}} \in \{2,\mathrm{max}_{\mathrm{dist}}\} \subset \mathbb{N}$
- maximum distance: Defines the maximum distance between to detected maxima. All greater distances are classified as two different orientations. $\mathrm{max}_{\mathrm{dist}} \in \{\mathrm{min}_{\mathrm{dist}},300\} \subset \mathbb{N}$
- maximum sigma: Defines the maximum value for one sigma in the fitting function for the gaus-check, to classify a maximum as a true maximum. $\mathrm{max}_{\mathrm{sigma}} \in \{2,\infty\} \subset \mathbb{N}$
- size of gaus-check: Defines the length of a square for checking a detected maximum, from which the data is used to fit the gaus function. Has to be even for a symmetric devision relative to the center. size $\in \mathbb{N}$

apply:

Saves the changes and inspect all values for format errors. If a format or value error is arised, the settings dialog will not be closed and the corresponding error is print at Frame 3

default:

All entries are set to their default values. To change the default values, the user can modify the corresponding textfile (see also fig. 1.9) in the application folder where all default values are saved. The textfile is formated in lines according to the order in the settings frame. Name and value of the parameter have to be separated by „:“ (without space!) and the value has to be in the same format like in the settings. The values of the checkboxes are 0 for not ticked and 1 for ticked.

```
gamma max:2.0
step size max:10.0
neighborhood max:15
threshold max:200
record  12-Bit images:0
scroll faktor:1.0
scroll step size int:1
scroll step size float:0.01
symmetry center x:487.5
symmetry center y:321.5
sample name:Sample_1
voltage:20
current:30
distance:40.0
comment:comment
normal bg-remove:0
remove dark-current:1
auto delta for polyfit:40
auto increment for polyfit:40
auto bg-remove during raster:0
calculate max exposure during raster:1
enable raster on kontur:0
threshold for kontur-raster:5.0
center detection during raster:0
search width for center detection:41
search height for center detection:41
search x offset for center detection:0
search y offset for center detection:0
linewidth for center detection:10
starting angle for center detection:0
number of lines:6
save info images during center detection:0
display offset:5
minimum distance:2
maximum distance:20
maximum sigma:15
size gaus-check:11
```

Fig. 1.9: default settings of the default settings in the textfile.

Frame 2 - image viewer

Frame 2 is a 8-bit grayscale image viewer, who can display images with 975x643 pixel. All modification made in Section 4 will be immediately visible in this frame.

Frame 3 - console

In frame 3, important messages for the user will be displayed, so no editing is possible. If the console doesn't show any text, a simple mouseclick onto the frame or scroll the mousewheel is normally enough to update the console, if the mouse is in the frame.

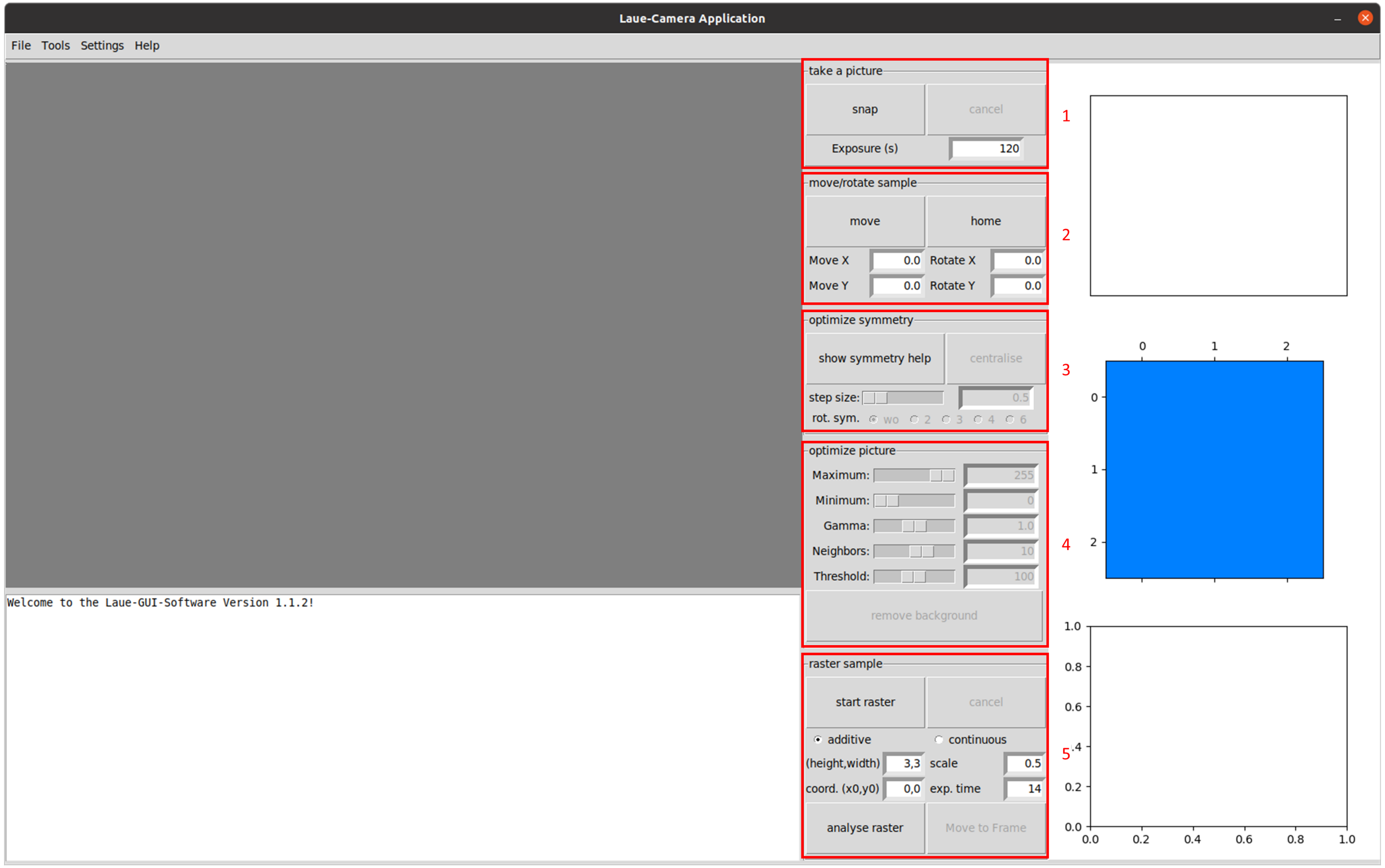


Fig. 4.1: Frame 4 divided into sections

Frame 4 - area of operations

Section 1 - image acquisition

snap:
An image with the defined exposure time will be acquired and afterwards displayed at Frame 2, also the values of Section 4 will be updated. Unfortunately the detector contains only a built-in 12-bit grayscale converter, so the resulting image is limited to 12-bit (0-4095). Therefore for all images with exposure times greater than 90 s (empirical value), the specific maximum exposure time has to be calculated. To achieve this, a separate image with 30 s exposure time will be acquired. With the maximum pixel value g_{30s} of this image and due to a linear correlation of maximum pixel value g_{max} and exposure time, the maximum exposure time t_{max} can be approximated with:

$$t_{max} = \frac{g_{max} - 100}{g_{30s} - 100} \cdot 30\,\text{s}. \tag{4.1}$$

The necessary offset of 100 results from the mean background noise. The maximum pixel value is set to 3900, so that the approximation doesn't reach by accident the limit value. If the calculation is completed, the defined exposure time will be divided into frames with the maximum exposure time plus one frame with the remaining exposure time. Afterwards all frames will be added to form the actual image.

cancel:
Cancels the actual image acquisition and reset the displayed image at Frame 2.

Exposure (s):
Defines the exposure time. $\exp \in \mathbb{N}$

Section 2 - translation and rotation of the sample

move:
The goniometer will be moved and rotated to the defined absolute values. To avoid the critical areas of the goniometer, only translations to ± 15 mm and rotations to $\pm 19°$ are possible. To ensure this, it is recommend to manually reorientate the goniometer every time at the beginning of a measurement with a

new sample. Specifically the user has to push the home-Button, then manually adjust the rotators into their null positions and adjust the sample, so that the x-ray beam hits the center of the sample. Also it is importend, that the coordinate system of the goniometer isn't a normal Cartesian coordinate system (see fig. 4.1).

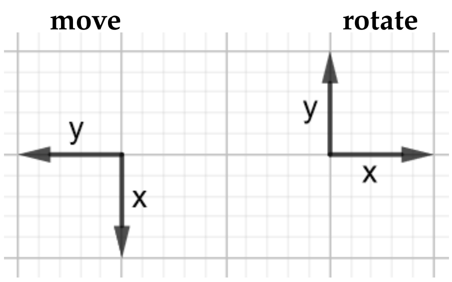


Fig. 4.1: coordinate systems of the goniometer.

home:
Reset all values to 0 and moves/rotates the goniometer in null position.

Move X:
Moves to the absolute value in x direction of the goniometer coordinate system, is state in mm. $\text{move}_x \in (-15.0, 15.0)$

Move Y:
Moves to the absolute value in y direction of the goniometer coordinate system, is state in mm. $\text{move}_y \in (-15.0, 15.0)$

Rotate X:
Rotates to the absolute value in x direction of the goniometer coordinate system, is state in °. $\text{rotate}_x \in (-19.0, 19.0)$

Rotate Y:
Rotates to the absolute value in y direction of the goniometer coordinate system, is state in °. $\text{rotate}_y \in (-19.0, 19.0)$

Section 3 - symmetrization

show symmetry help:
A red dot appears in Frame 2 at the defined symmetry position in Settings. If in „rot. sym." a symmetry is additionally selected, a vertical line from the dot to the upper edge is drawn plus the corresponding lines of the selected symmetry. The dot is movable with the arrow keys in „step size"-pixel steps and if the user clicks with the left mouse button in Frame 2, the dot appears at this position. If the symmetry help lines are displayed, the user can rotate each

of these lines by „step size“-degree by scrolling with the mousewheel.
This method offers the user on the one hand the opportunity to measure the angle between two points respectively to another point and on the other hand to centralize a reflex in the dead zone of the detector (see also „centralise“).
If symmetry help is active, the user can disable this method by pushing the button again.

centralise:
This method offers the user to centralize the selected point via „show symmetry help“ on the symmetry coordinates. The main reason for this is to hide a bright reflex at the dead area of the detector, so minor reflexes are easier to detect. If the certain reflex is already inside the dead area, the lines from symmetry help allows a simpler way of detection.

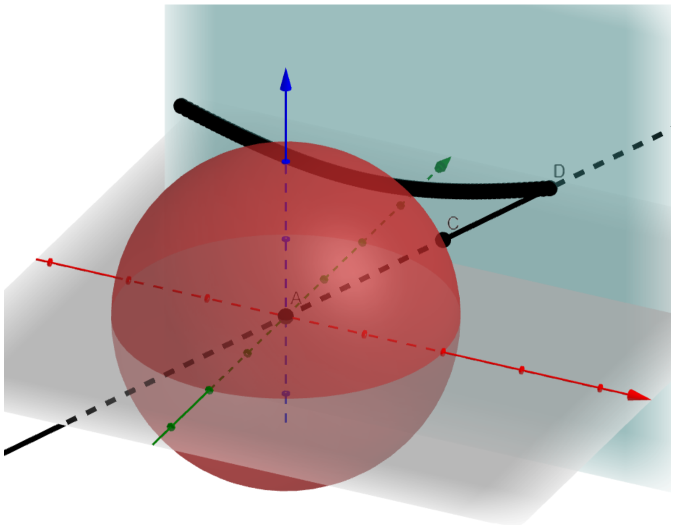


Fig. 4.2: Model to calculate the necessary rotational angles to centralize a reflex at a certain point at the detector. Moreover the variation of ϕ is displayed, to visualize the ϕ-dependency of θ.

The model for the necessary calculation is shown in fig. 4.2 with the target in the origin of the coordinate system and the detector at a distance d in xz-plane. With the help of a spherical coordinate system, the point of intersection D of line AC with the detector can be expressed and thus also the angles θ und ϕ by:

$$\phi = \arctan\left(\frac{d}{x}\right) \tag{4.2}$$

$$\theta = \arctan\left(\frac{d}{y \cdot \sin(\phi)}\right) \tag{4.3}$$

With both angles, the goniometer has to be rotated by these negated values to centralize the defined point to the center. Adapted to the coordinate system of the goniometer and respectively to the current rotational values r_x and r_y, the new values can be determined with:

$$\text{rotate}_x = r_x - \frac{(90° - \phi)}{2} \tag{4.4}$$

$$\text{rotate}_y = r_y - \frac{\theta - (90°)}{2} \tag{4.5}$$

step size:
Defines the step size for the translation of the red dot of „show symmetry help" in pixel and the rotation of the symmetry help lines in degree by scrolling the mousewheel. Is always rounded to the next number divisible by 0.5. stepsize $\in \mathbb{R}^+$

rot. sym.:
Defines the number of symmetry help lines. Selectable are values between 2 and 6 or none (wo).

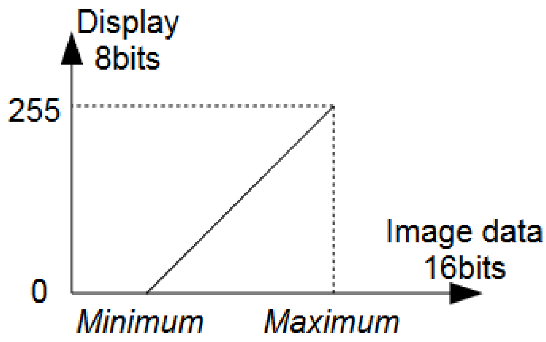


Fig. 4.3: Transformation between the selected range of minimum and maximum using the example of a transformation from 16-bit to 8-bit.

Section 4 - optimize picture

Maximum:
Defines the maximal value of the grayscale image, which is displayed in Frame 2. All greater values are set to this maximum value. The selected interval between minimum and maximum is linear converted to 8-bit to display the resulting image at Frame 2 (see fig. 4.3). Selectable range is between minimum and maximum pixel value. max $\in \mathbb{N}$

Minimum:
Defines the minimal value of the grayscale image, which is displayed in Frame 2. All smaller values are set to this minimum value. The selected interval between minimum and maximum is linear converted to 8-bit to display the resulting image at Frame 2 (see fig. 4.3). Selectable range is between minimum pixel value and maximum. min $\in \mathbb{N}$

gamma:
Defines the gamma exponent, if a non linear contrast optimization is desired. Is applied on the image A after the definition of minimum and maximum, but before the transformation to an 8-bit image B, which is displayed at Frame 2. The mathematical expression is:

$$B = A^{\gamma} \cdot 255^{1-\gamma} \tag{4.6}$$

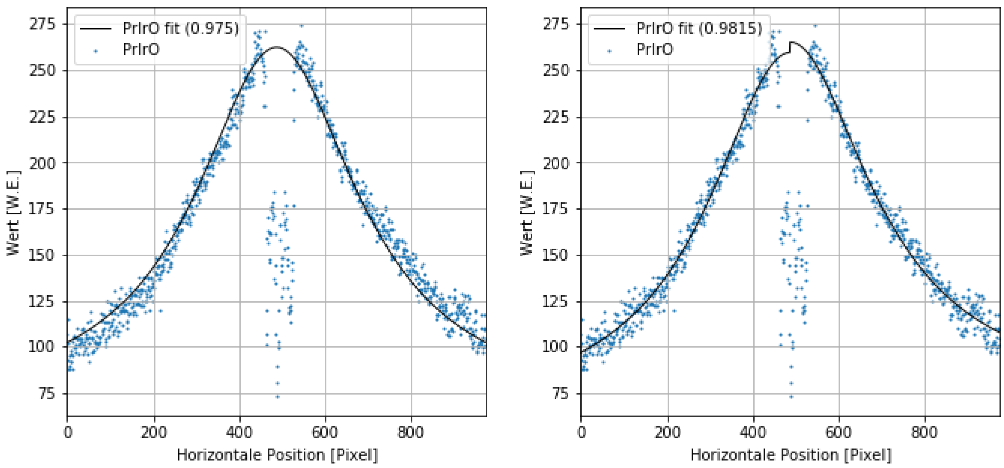
Neighbors:
Defines the size of the data area around each pixel for the maxima detection, which is used as the input for the filter functions. Both filters (maximum- and minimum-filter) redefines the value of each pixel by the maximum or the minimum value of the input data.

Threshold:
Defines the threshold for detecting a maximum at the maxima-detection. For the visualization of the results from the maxima-detection in diagram 2 in Frame 5 the input data is not the displayed 8-bit data from the current image but the raw data from the original image. Therefore a change from the sliders for contrast optimization won't have an effect on the detected points.

remove background:
Removes the background of the image. Therefore a central pixel line is selected from the original image, to which data the function

$$I = I_0 \cdot \left[\arctan\left(\frac{d - a \cdot (x - 487.5)}{g}\right) - \arctan\left(\frac{-d - a \cdot (x - 487.5)}{g}\right) \right] + c \tag{4.7}$$

for the pixel values (I) depending on the distance in pixels from the left edge of the image (x) is fitted. This fitfunction is from a model, where an emitter with a $2d$ spread (depending on the aperture) is at the distance g to the detector. The parameter a represent the ratio between distance and pixel density, thus the horizontal spread of one pixel. The parameter d is set so $d = 40.2$, otherwise the fitfunction converges not every time and if it converges, no noteworthy differences are visible. Therefore it is recommend to choose approximately 40 mm as the distance between sample and detector. Other models, for examples the detector is angled relative to the x-ray beam or a round surface-emitter, are taken into account, but the resulting fitfunctions only converge very infrequently and if it converges, again no noteworthy differences are visible. On the other hand the asymmetry of both detector halves can be corrected easily. Therefore again a centered pixel line is selected, but this time the line is divided in the middle and both sectors are fitted separately with the fitfunction. Also both resulting fitfunction are subtracted separately from the image. The differences of both fitmodi can be seen in fig. 4.4.



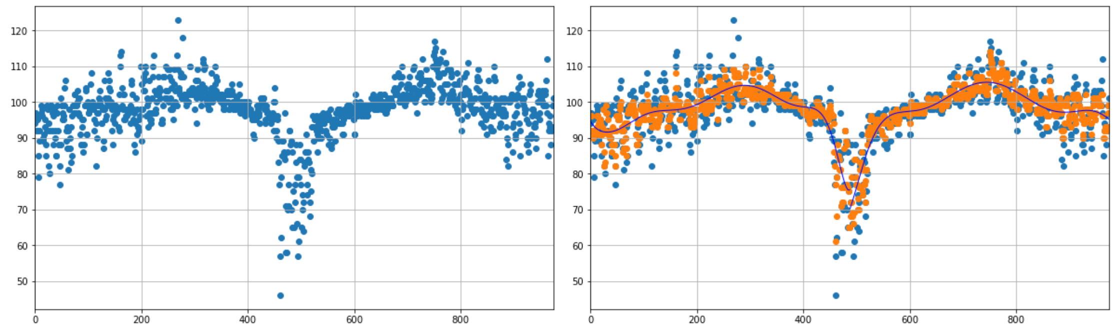
(a)

(b)

Fig. 4.4: Different reusults of both fitmodi. In (a) a normal fit with the data of the whole line is displayed and in (b) a partial fit for every detector half separately is displayed.

The passed image to the function is the original picture after the evaluation of minimum, maximum and gamma exponent, but before the transformation to an 8-bit grayscale image. Therefore the return image is also a grayscale image with greater values than 8-bit. The original image with removed background can also be saved by Save Original.
Despite the background remove another background remains (see fig. 4.6c), which can be lead back to a dark-current inside the detector. To minimize this background, another method must be used, in which also the whole image is passed to the correspondig method if it is in Settings ticked. First, all pixel values greater than a maximum value are sorted out, so that the profile only contains the background and no great maxima. This maximum value is either calculated or determined manually with the bg fine-tuning-button. For the automatic calculation, the image is divided into the two detector halves and the mean value of every line of both sections is calculated, but at both sides of every line δ-pixel are excluded to avoid bad results due to the borders and the dead area in the center. The maximum value is set to the greates mean value plus

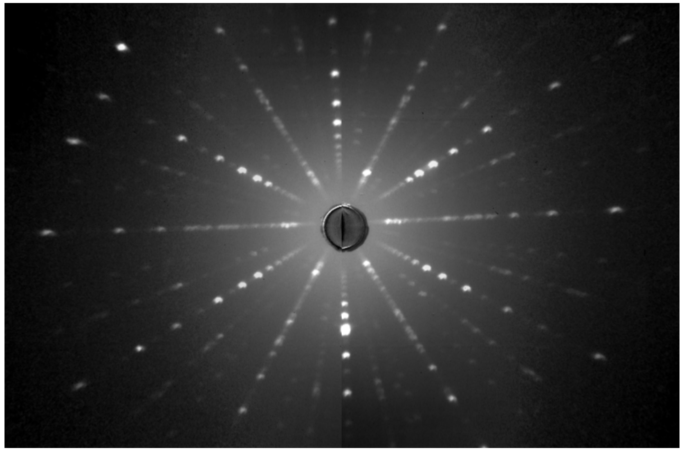
an increment, which can be defined in Settings with δ. In fig. 4.5a a resulting line profile is shown exemplary. Because the profile is fluctuating very much, a 3x3-median filter is applied, so that the orange dots result in fig. 4.5b. Finally for each line in each detector half a polynomial function of 10th degree (blue line) is fitted and subtracted from the corresponding line. At the end in fig. 4.6d the result of this correction can be seen.



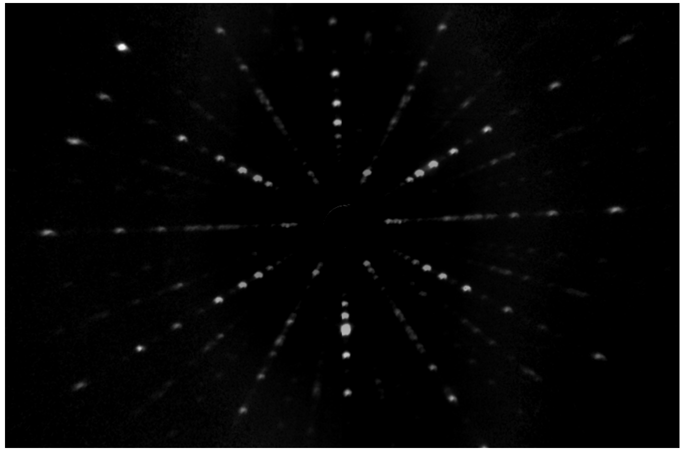
(a) **(b)**

Fig. 4.5: In (a) a resulting line profile from the dark-current background is shown exemplary. In (b) a 3x3-median filter is applied onto the whole image and for each half a polynomial of 10th degree is fitted. This fitfunction describes the profile relatively good and is below the weak maxima, so that these maxima won't be immediately subtracted with the noise.

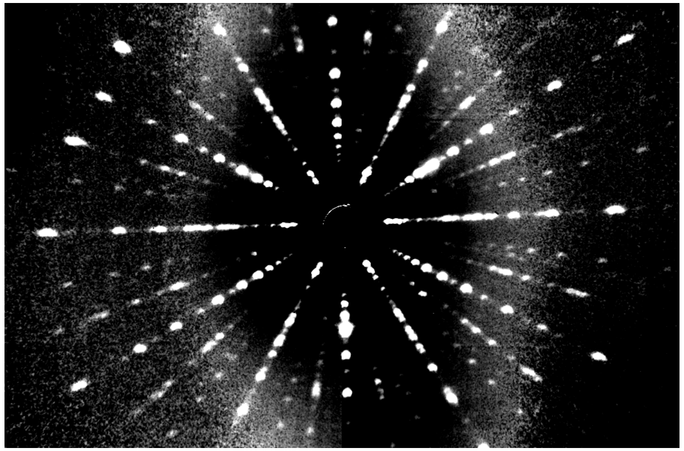
bg fine-tuning:
Because the automatic calculation of the maximum pixel value is good but not perfect all the time, this method gives the user a opportunity to adjust the value manually. In the opening window the actual image without background is displayed, but all pixel values greater than the defined maximum value at the slider aren't displayed. With the slider, the user can vary the maximum value and see the resulting image immediately. In general only the reflexes should be excluded and the background from the dark-current should remain. With the apply-button, the new maximum value is set to the selected value and the displayed image in the main window is updated. With the default-button the slider is set back to the calculated value.



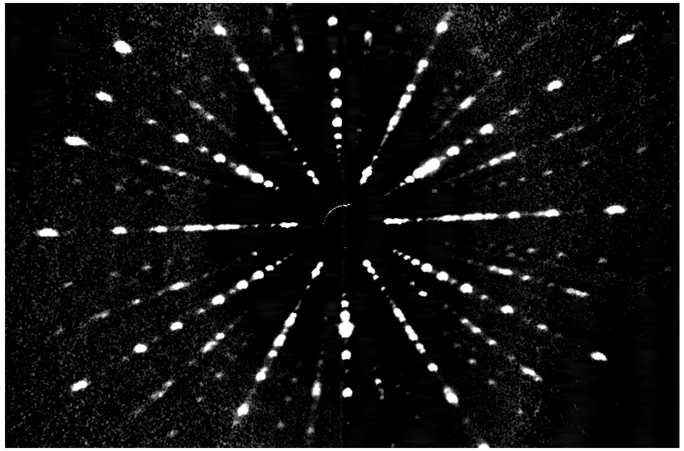
(a) original image



(b) image without background



(c) image without background and with contrast optimization



(d) image without background, with contrast optimization plus polynomial fitting and so without dark-current background

Fig. 4.6: Demonstration of a possible image processing of a original laue-image

Section 5 - raster sample

start raster:
Starts a new raster with the defined values and the selected settings in Settings. Furthermore for each acquired frame a classification is made on how good the diffraction pattern is (from 0 (not visible) to 2 (good)). In the contour diagram in Frame 5 the actual progress is displayed and in Frame 2 the last acquired image is visible. At this image also the methods from Section 4 are applicable. In the beginning of the acquisition of a raster, a new folder is created at the selected directory with the filename „name/number of sample" _ „voltage" „current" _ „distance to detector in mm" _ „RASTER" _ „exposure time" _ „height x width" _ „stepsize im mm" _ „additive or continuous"
Additionally at the end of a raster a „logfile.txt" is created which contains all information of the raster settings and the acquired contour (for the format see a corresponding logfile.txt). With this logfile also raster which were acquired before this application was written can be displayed by creating a logfile.txt by hand and use „change kontur manually" to change the contour.

cancel:
Cancels the actual raster.

additive, continuous:
Defines if a frame is acquired with a maximum exposure time of 16 s (additive) or with the calculated maximum exposure time (continuous). The advantage of additive over continuous is a better contour detection of the algorithm, but the advantage of the continuous method is a longer uninterrupted exposure time, thus weak reflexes can be seen better.

height, width:
Defines the height and width of the raster, thus how many single frames are acquired by each row and column. h,w $\in \mathbb{N}^+,\mathbb{N}^+$

scale:
Defines the step size in mm between two frames in a raster. scale $\in \mathbb{R}^+$

coord. (x_0, y_0):
Defines the center of the raster, from which the corresponding raster will start. $x_0, y_0 \in \mathbb{R}^+,\mathbb{R}^+$

exp. time:
Defines the exposure time in seconds of each frame. exposure $\in \mathbb{R}^+$

analyse raster:
If a raster is acquired or loaded, with this button the particular contour can be analysed. It gives the user the opportunity to navigate with the arrow keys

through the raster. Furthermore the current frame is visualized through a brown frame and the corresponding diffraction image is shown in Frame 2, ready to be modified by the optimization methods from Section 4. Immediately after a raster acquisition, the contour is deposit in Frame 5.
The contour navigation can be canceled by clicking the button again.

move to frame:
If the current raster and the current coordinate system of the goniometer are the same, the position of the sample can be set to the selected frame of the contour.

Frame 5 - diagram viewer

Diagram 1 - maximum finder

In this diagram all positions of the detected maxima of the current frame in an acquired raster is displayed. With this additional information the user can confirm or falsify the classification done by the algorithm. If a mulitplot raster is loaded, only the corresponding part of the image is displayed.
If an original raster is loaded, the maxima will be detected by the same function as in the multiplot but this method will first be applied if the current position of the contour changes.

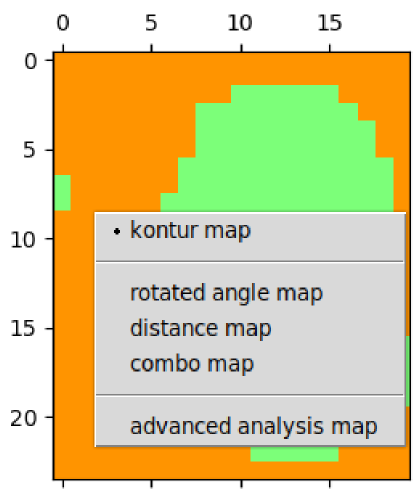
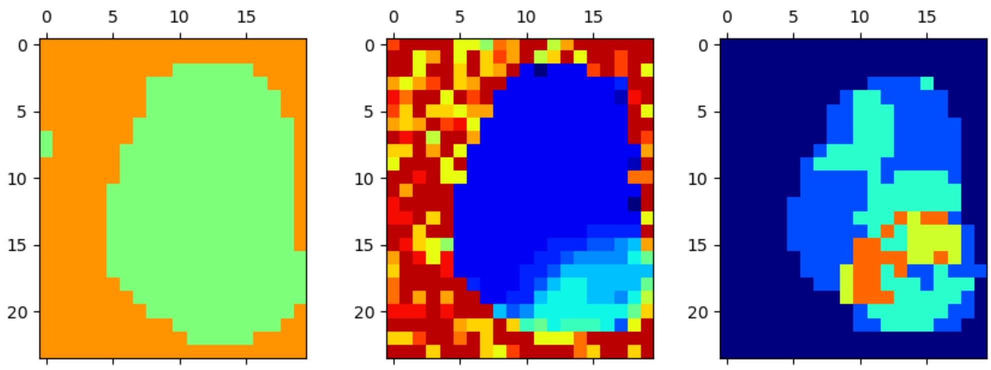


Fig. 5.1: All types of the visualization of the kontur from a raster with center detection data and advanced analysis data.

Diagram 2 - contour diagram

In this diagram the current contour is displayed, which will show the current progress of a raster acquisition or the whole contour of an already measured raster. If the navigation on the raster is active, the current position is marked by a brown frame. If a raster with center detection data or/and advanced analysis data is loaded, these data can be visualized in this diagram with different types,

selectable through a right-click on the diagram(see Fig. 5.2).
In the method „auto find kontur“, the contour will build up time after time, so the user can visually comprehend the contour detection.



(a) normal contour **(b)** rotated angle map **(c)** advanced analysis map

Fig. 5.2: Different types of the visualization of the kontur from a raster with center detection data and advanced analysis data.

Diagram 3 - backgroundfit

If the background is removed from an image, this diagram will visualize the fit with the data from the image (blue dots) and the fitfunction (black line). The left axis shows the pixel value of the corresponding pixel and the lower axis shows the horizontal pixel number from the left image border.

Outsorced Code

The following methods are deprecated and not longer necessary, but are not deleted if another purpose will show up.

angle corr.:
This optimization is only available after the background subtraction to reduce the remaining background noise. This function is only a experimentally method, which changes the data, so the usage must be marked and restricted to visual optimization, it is not useful for intensity comparison.
The remaining background noise is only located in the border area of the picture, so it will be concentrated on this area. The main idea is, that all reflexes will appear at the same point, but the background noise will be randomly spread. If the diffraction image is rotated around the center by small angles and subtracted from the original image, the noise will average out partially but the subtraction of the noise from the reflex will not affect it very much. Also several negative values will appear, which can be set to 0. Furthermore the image has to be rotated in both directions and weight half to avoid artefacts. This method will be applied to the image after minimum, maximum and gamma parameters are evaluated and the image is an 8-bit image. For a better visualization, the mean value of the picture will be subtracted and all negative values are set to 0 plus a transformation to the complete range of an 8-bit image. Selectable are rotation angles between 0 and the defined maximum value in Settings.

radius corr.:
Because the method angle corr. is only suitable for border areas and arise false maxima in the center, this method enables to define the radius of a circle around the center in pixel, which displays the original image. The resulting image is way better than the former one, although the transition between the original image and the calculated image is visible. Selectable are radii between 0 and 321 (half height of the image). radius corr. $\in \mathbb{N}^+$

Outlook

Upcoming improvements:

- Another visualization of the contours, which takes into account that the detected area of the sample is circular and not quadratic and frames are overlapping with a small stepsize.
- Drop out of a raster before it is completely acquired, if the sample is fully detected but several frames are in the line. The remaining frames will be filled up with standard images, so that an analysis with the application still will be possible.
- Automatising of the centralise-method for good diffraction images.
- Introduce another nonlinear optimization function for the contrast besides the gamma factor, to make weak reflexes better visible.

If unknown errors or other questions raise or more extensions are reasonable, please contact the author!