
gisansexplorer

Release 1.0.0

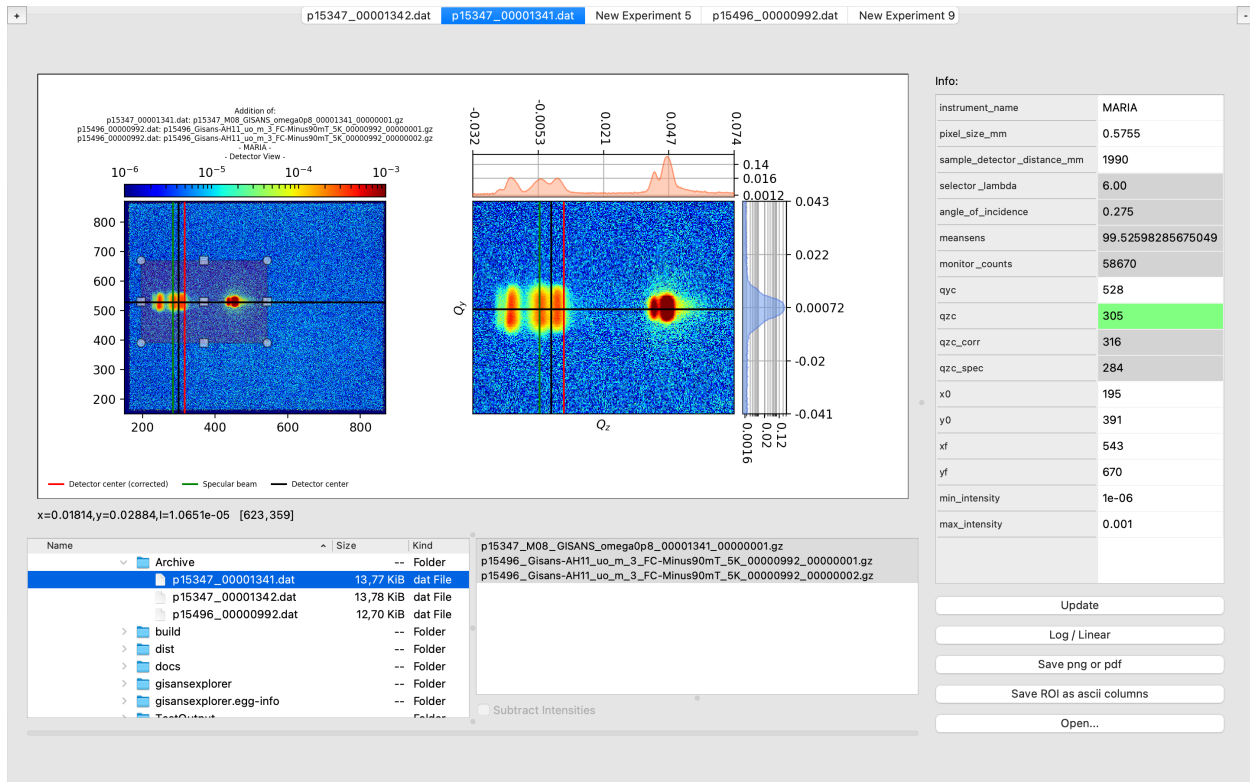
Juan M. Carmona-Loaiza

Jan 05, 2021

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Simple App that interactively helps in the reduction of **NICOS** files for **GISA(NIX)S** data.



INSTALL - WINDOWS, MAC, LINUX; PYTHON 3.6

Open a terminal and use pip:

```
$ pip install gisansexplorer
```

CHAPTER TWO

RUN:

Once installed, open a terminal and simply call `gisansexplorer`:

```
$ gisansexplorer
```

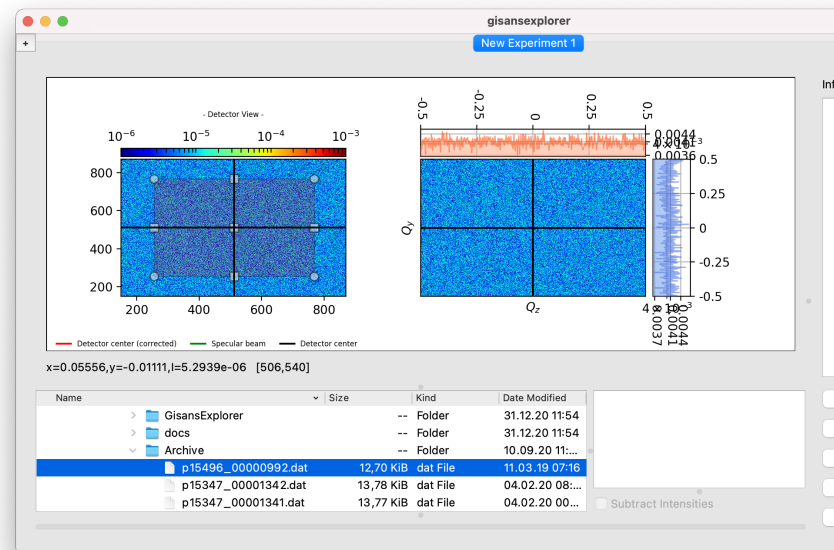
CHAPTER THREE

HOW TO...

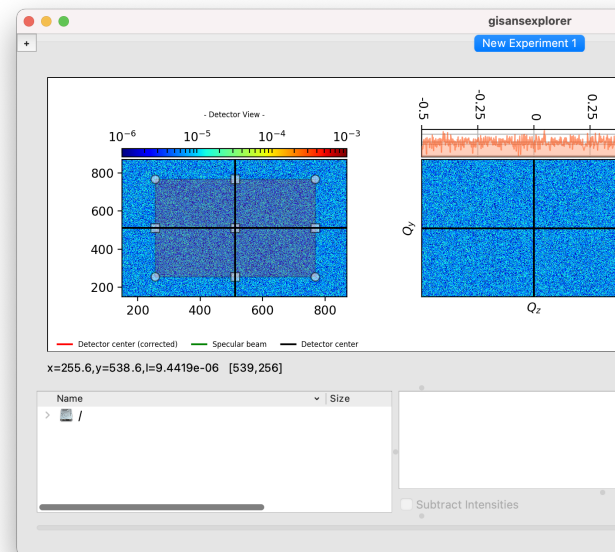
Developed by Juan M. Carmona Loaiza - MLZ Scientific Computing Group, in collaboration with Alexandros Koutsoumpas.

3.1 How to...

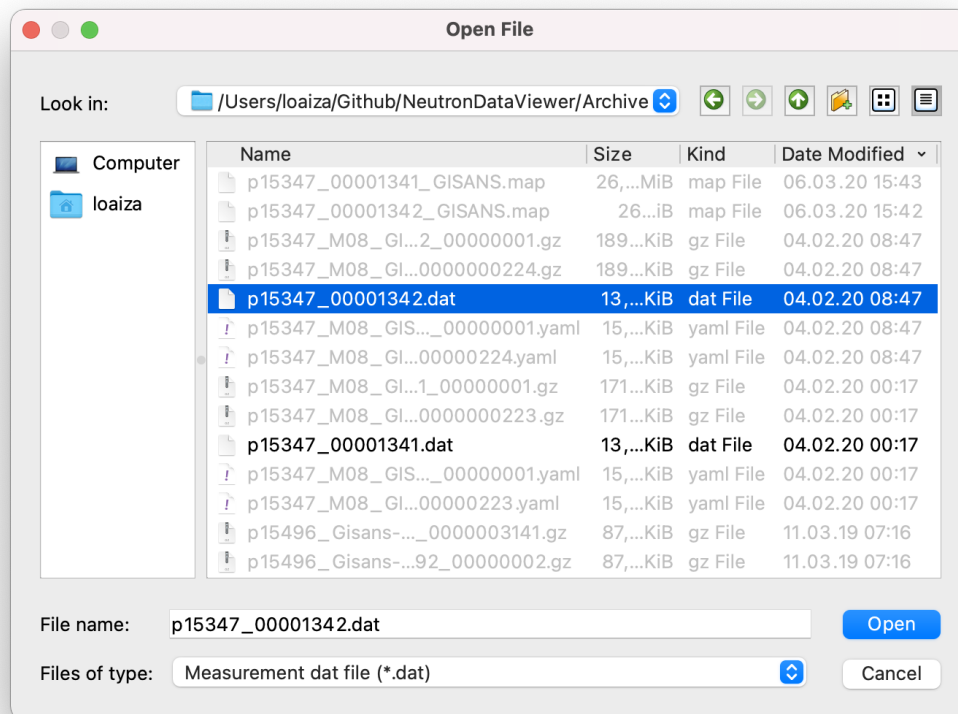
3.1.1 Open a NICOS .dat file



- By navigating to it on the bottom left panel:

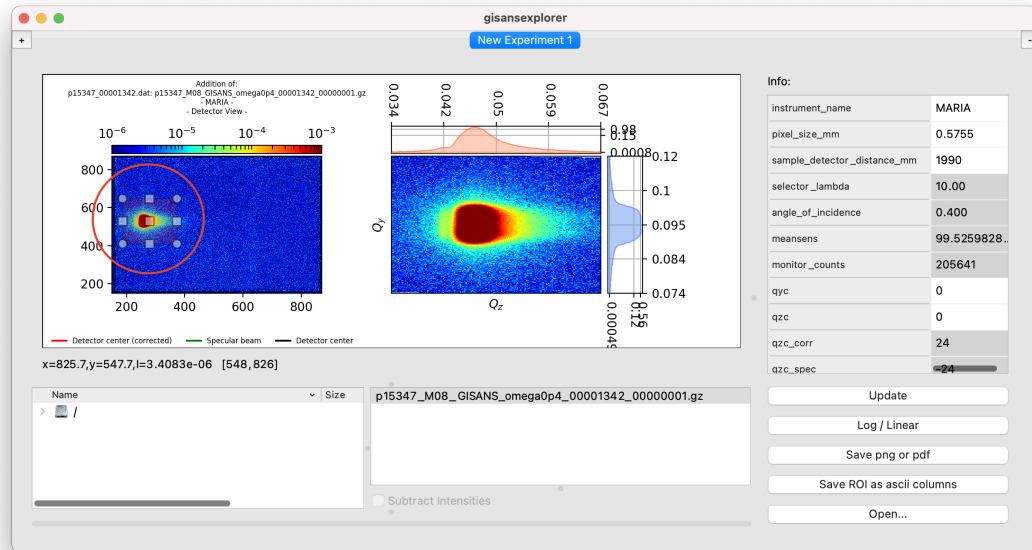


- By browsing to it using the *open...* button on the bottom right:

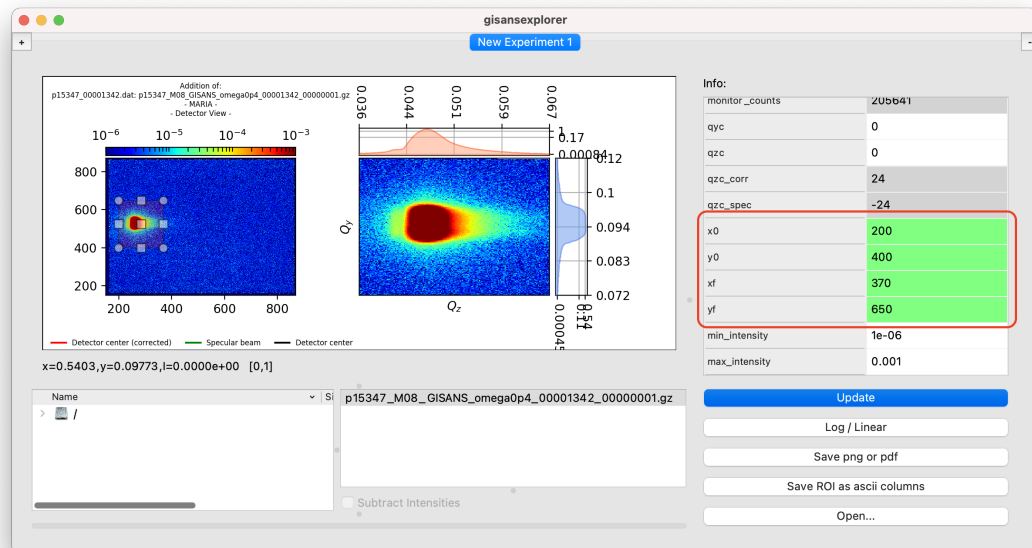


3.1.2 Select the region of interest (ROI)

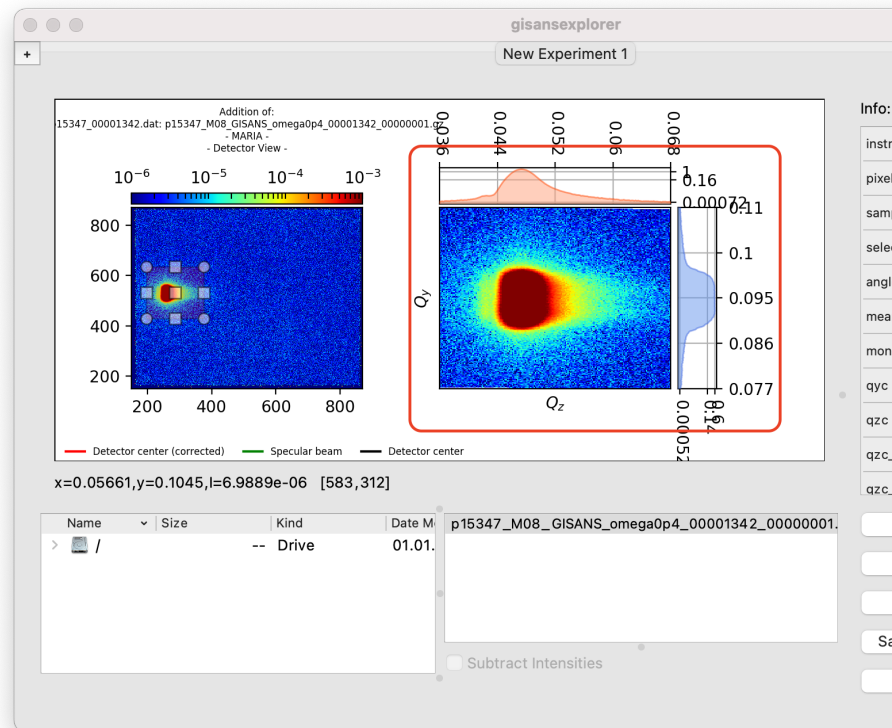
- By using the ROI selector on the left plot:
 - Click a corner and drag **to resize**.
 - Click the center and drag **to move**.



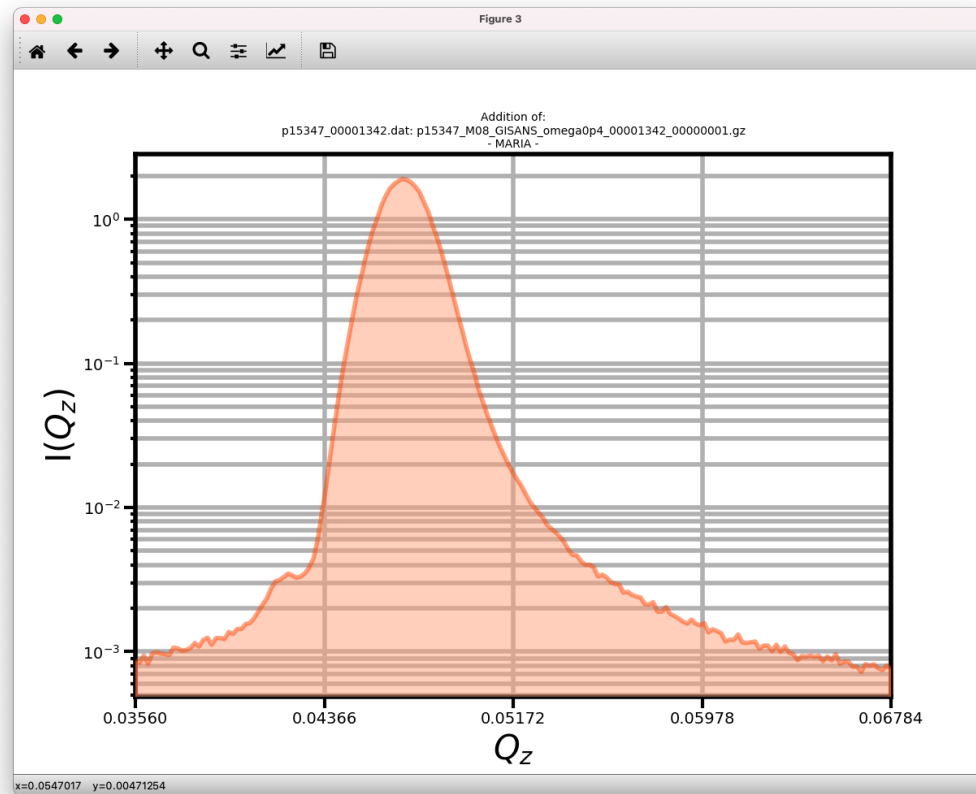
- By setting the limits on the information table on the right:
 - Set the pixel limit values x_0 , y_0 , x_f , y_f (left, bottom, right, top).
 - After they turn green –wrong entries will turn red, click *Update*.



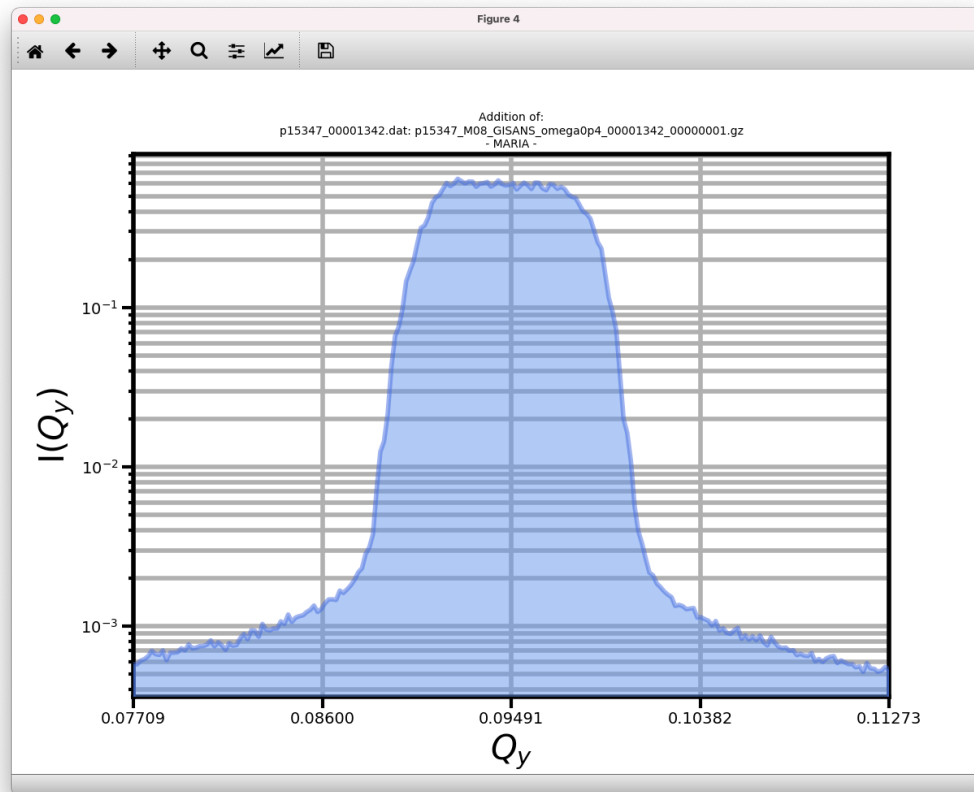
3.1.3 Pop up the ROI plots



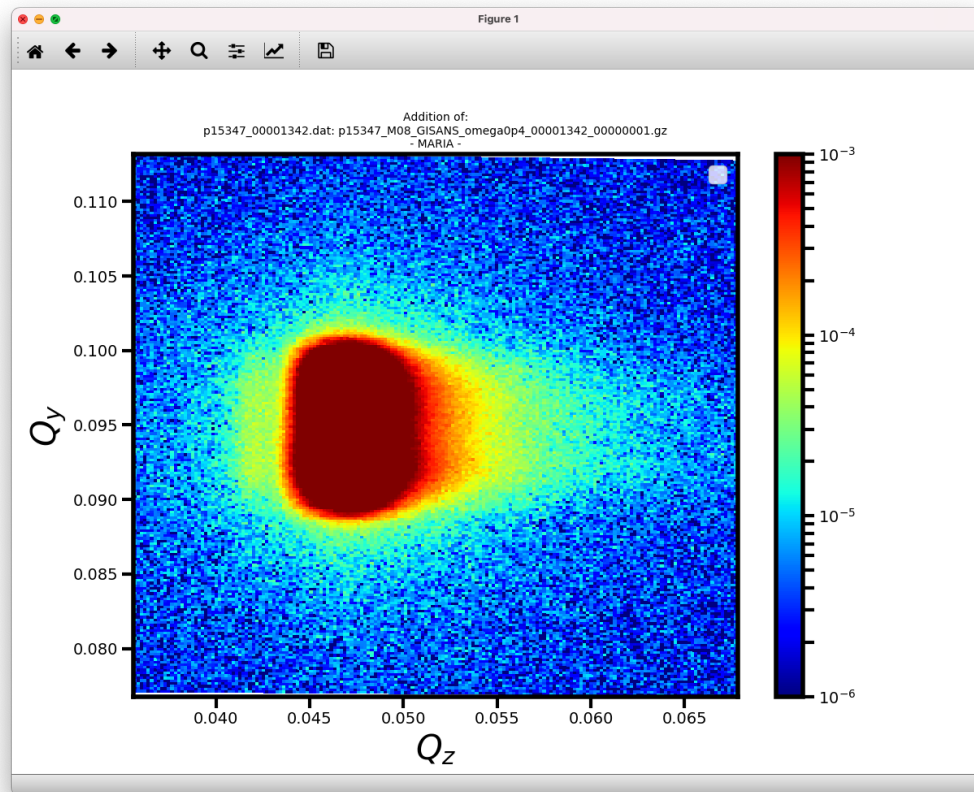
- By double clicking on any of the ROI plots, four pop-up windows will appear:
 - Q_z vs integration along Q_y



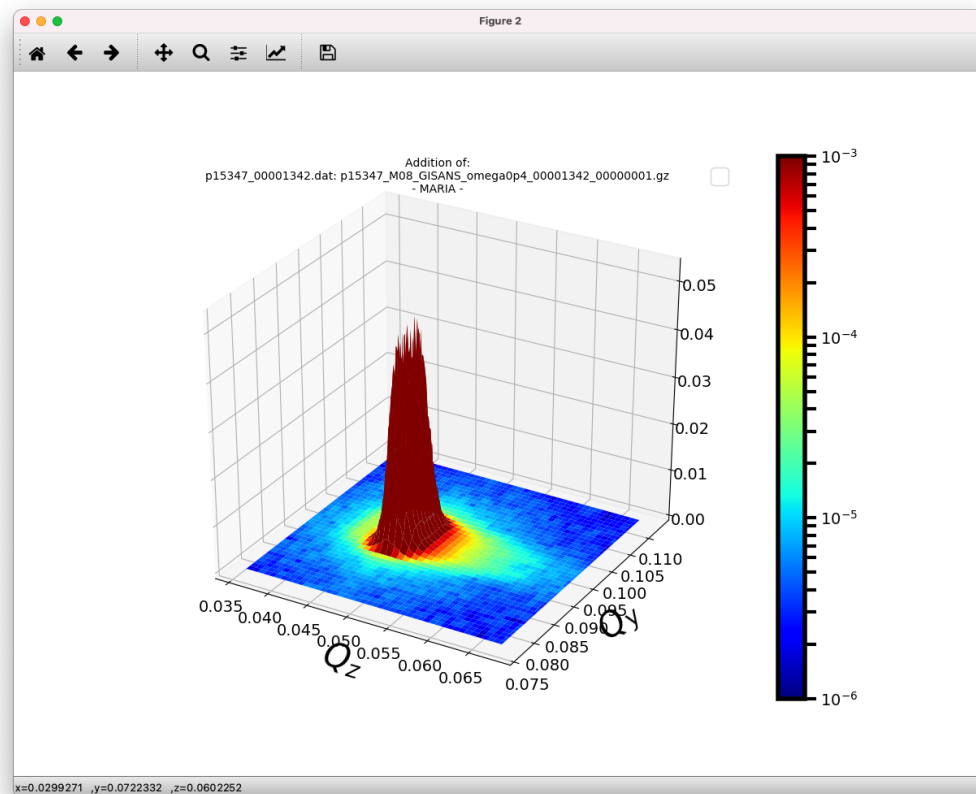
– Q_y vs integration along Q_z



- 2D Intensity map as function of Q_y, Q_z



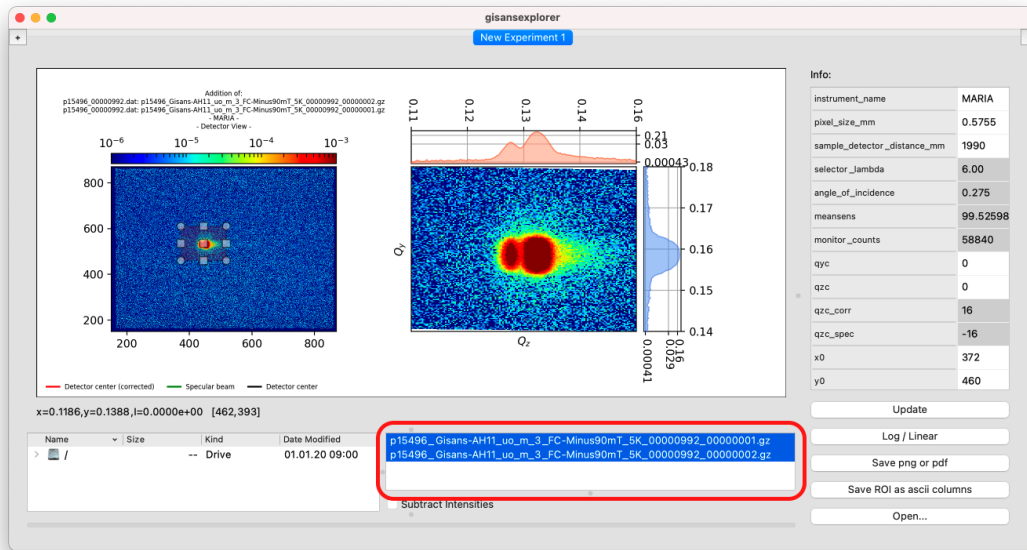
- 3D Intensity surface as function of Q_y, Q_z



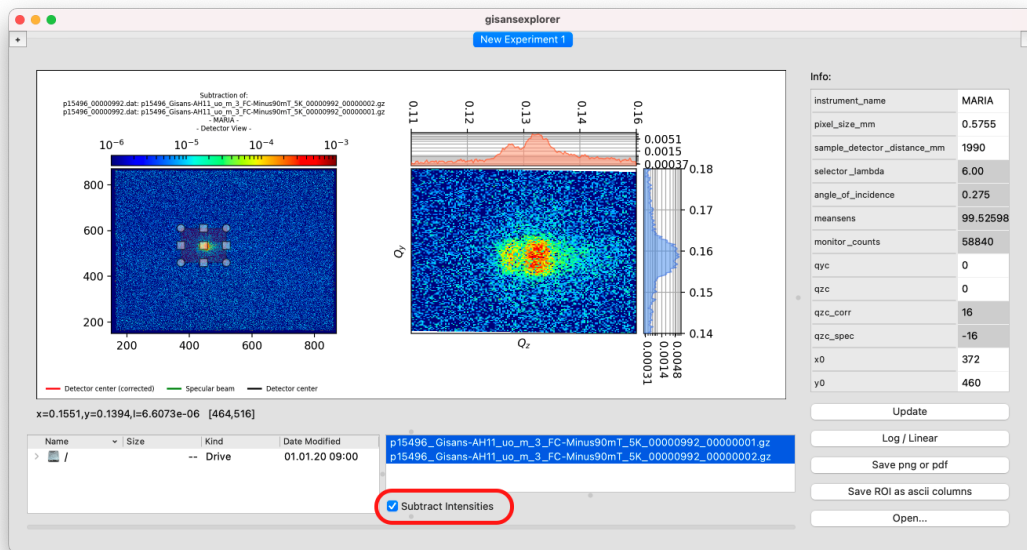
Clicking the floppy disk icon will save individual figures.

3.1.4 Add or subtract intensities from different Gisans maps

- After loading one or more files, click the corresponding maps on the gisans map list. To select several maps, hold the keys `shift` or `ctrl` while clicking on each entry. This will automatically show the **addition** of the intensities of the selected gisans maps. To open several `.dat` files, repeat the procedure to *Open a NICOS .dat file*.

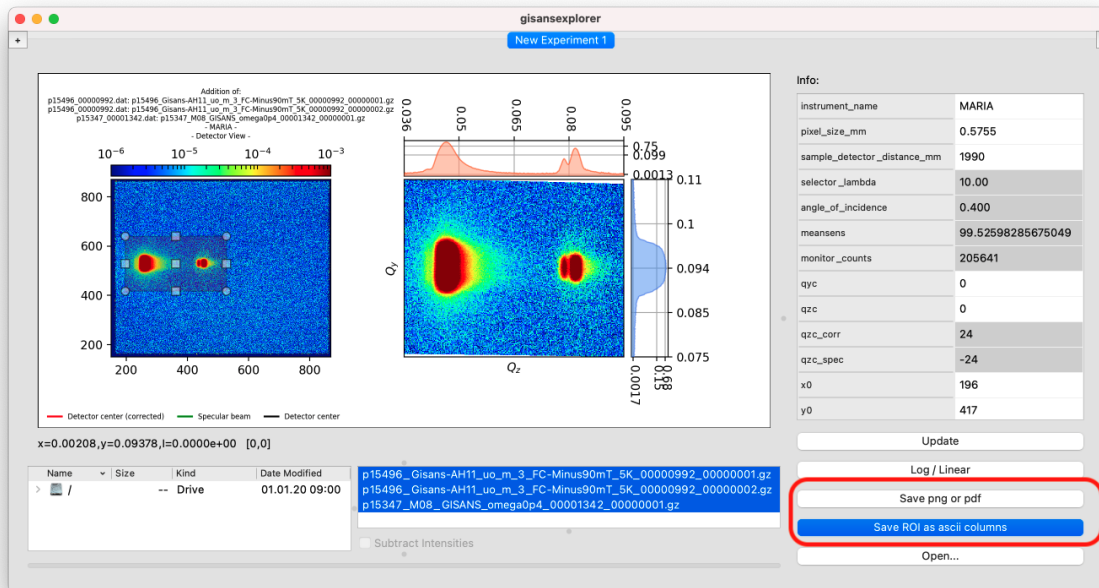


- To show the **subtraction** of the intensities, select any two entries on the list and tick the checkbox *Subtract intensities*



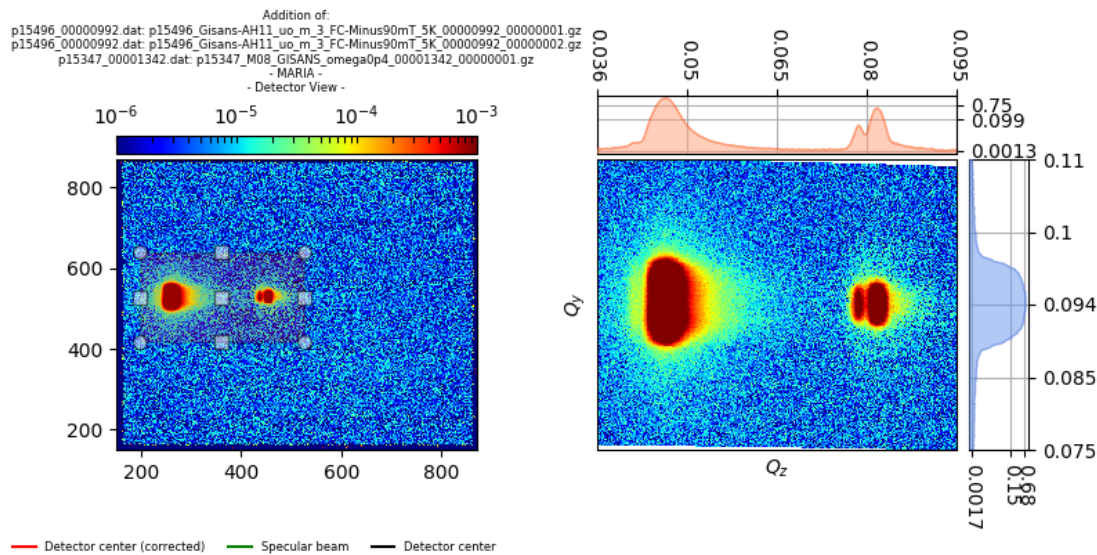
N.B. While addition is calculated in the obvious way, $I = I_A + I_B$, subtraction is calculated as $I = |I_A - I_B|$.

3.1.5 Save the ROI



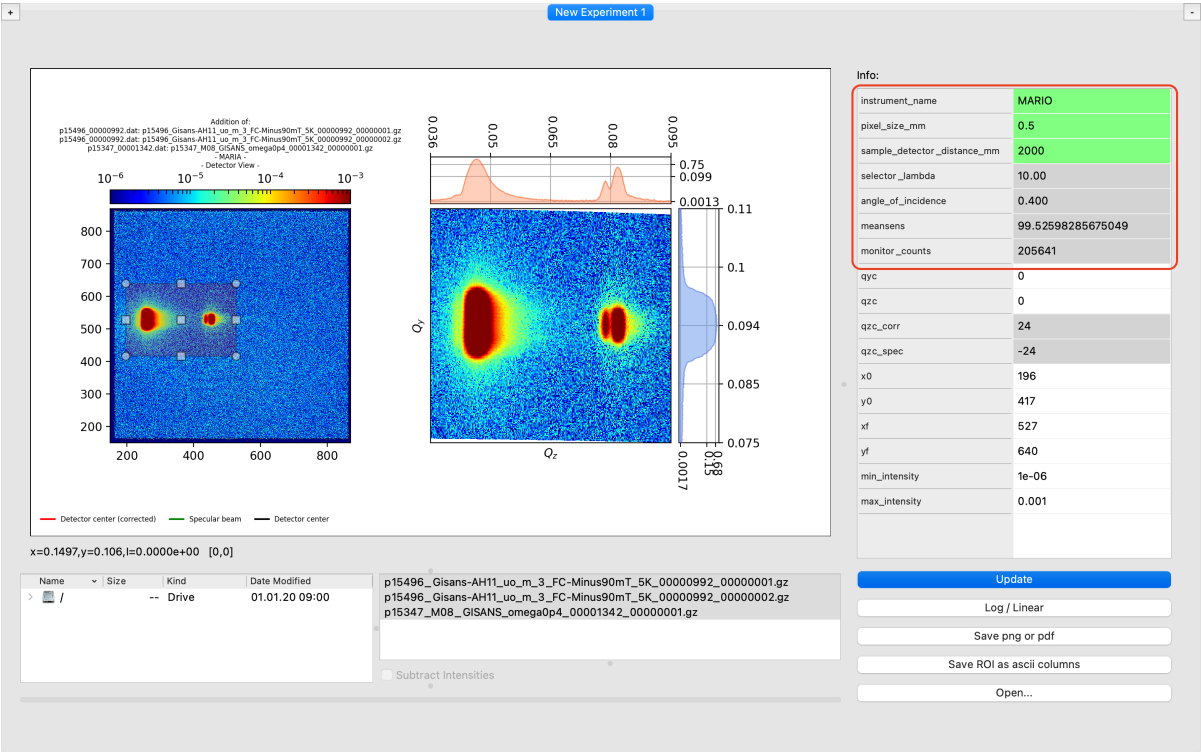
- The button *Save ROI as ascii columns* opens a dialog asking for a location and a filename. After the filename is given (e.g. MyGivenFilename), three files are saved:
 - MyGivenFilename_xI_.txt - two columns: the first one, the x coordinate of the detector in Q -space (i.e. Q_z); the second one, $I(Q_z)$, i.e. the intensity integrated along Q_y .
 - MyGivenFilename_yI_.txt - two columns: the first one, the y coordinate of the detector in Q -space (i.e. Q_y); the second one, $I(Q_y)$, i.e. the intensity integrated along Q_z .
 - MyGivenFilename_xyI_.txt - three columns: analogously to the two previous files, each column represents Q_z , Q_y , $I(Q_z, Q_y)$.
- The button *Save png or pdf* also opens a dialog asking for a location and a filename. After the filename is given (e.g. MyGivenFilename), five files are saved:
 - MyGivenFilename.png (or .pdf)
 - MyGivenFilename-integration_qy.png (or .pdf)
 - MyGivenFilename-integration_qz.png (or .pdf)
 - MyGivenFilename-gisans_surface.png (or .pdf)
 - MyGivenFilename-gisans_map.png (or .pdf)

The first file is practically a screenshot of the plotting area,



, and the other four files correspond to the figures described in Section *Pop up the ROI plots*.

3.1.6 Change instrument and detector parameters



The **name of the instrument**, the **pixel size** (in mm) and the **sample-detector distance** (in mm) can be modified by double-clicking the corresponding entries in the *Info* table. Once the new entries turn green, the *Update* button must be clicked for the changes to take effect. the **wavelength selector**, the **angle of incidence**, the **mean sensitivity**, and the **monitor counts** are read from the NICOS *.dat* file and thus are not adjustable.

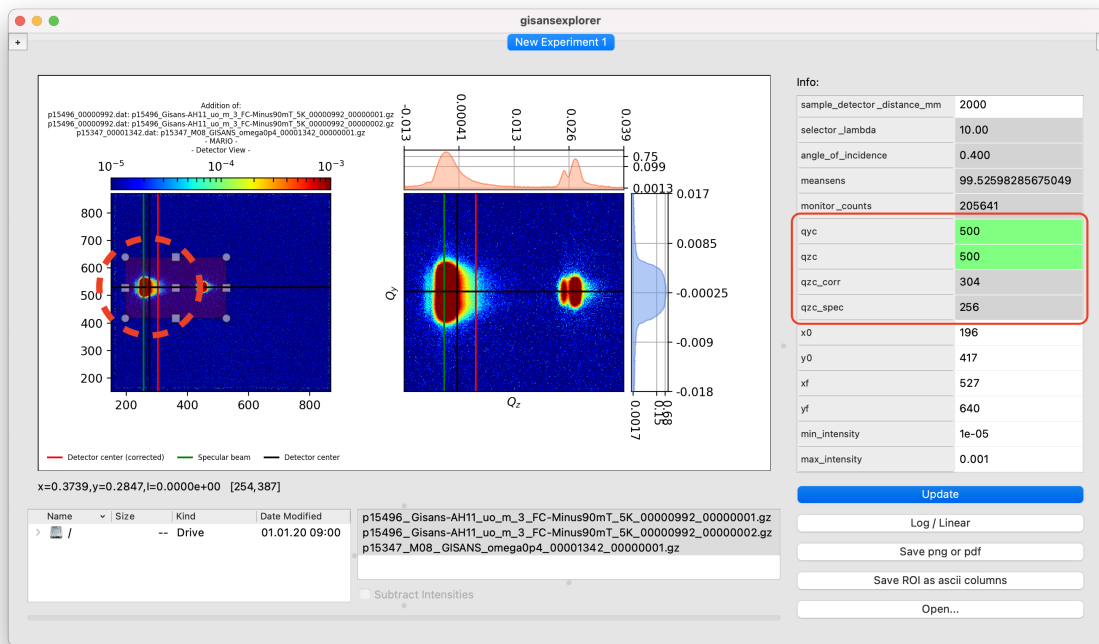
The `instrument_name` parameter only affects the title of the figures and the header of the ascii file when saving;

instead, `sample_detector_distance_mm` and `pixel_size_mm` affect also the way in which the $[Q_y, Q_z]$ map is computed for the ROI plot.

Default values for the `sdd` and the pixel size are 1990 and 0.5755 respectively.

3.1.7 Adjust the beam center position

The detector pixel corresponding to the beam center can be adjusted via the parameters `qyc` and `qzc`. By modifying this parameters on the info table, black crosshairs appear on the detector view (left plot) and, if they are inside the ROI, they appear also on the q-space view (right plot). Two additional lines are calculated: a red one, corresponding to the corrected beam center and a green one, corresponding to the specular reflection. For the changes to take effect, the *Update* button must be clicked after the parameters turn green after being edited.

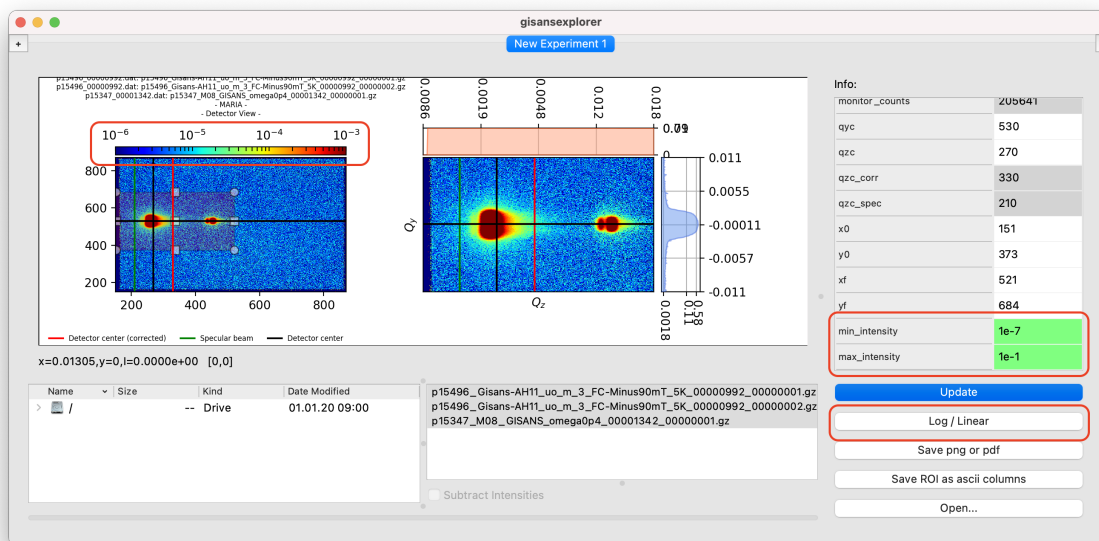


The location of the green and red lines are properties of the class `Experiment` and are calculated inside the class `MyFrame` according to:

```
experiment.qzc_corr = experiment.qzc + int( ( experiment.sample_detector_distance_mm_
↳ * np.tan( np.pi * float(experiment.angle_of_incidence) / 180.0 ) ) / experiment.
↳ pixel_size_mm )
experiment.qzc_spec = experiment.qzc - int( ( experiment.sample_detector_distance_mm_
↳ * np.tan( np.pi * float(experiment.angle_of_incidence) / 180.0 ) ) / experiment.
↳ pixel_size_mm )
```

3.1.8 Modify the intensity gradient range

The intensity gradient can be shown either in linear scale or in logarithmic scale (default). To switch between these two scales, press the *Log/Linear* button.



Changing the range of the colormap can be achieved in two ways:

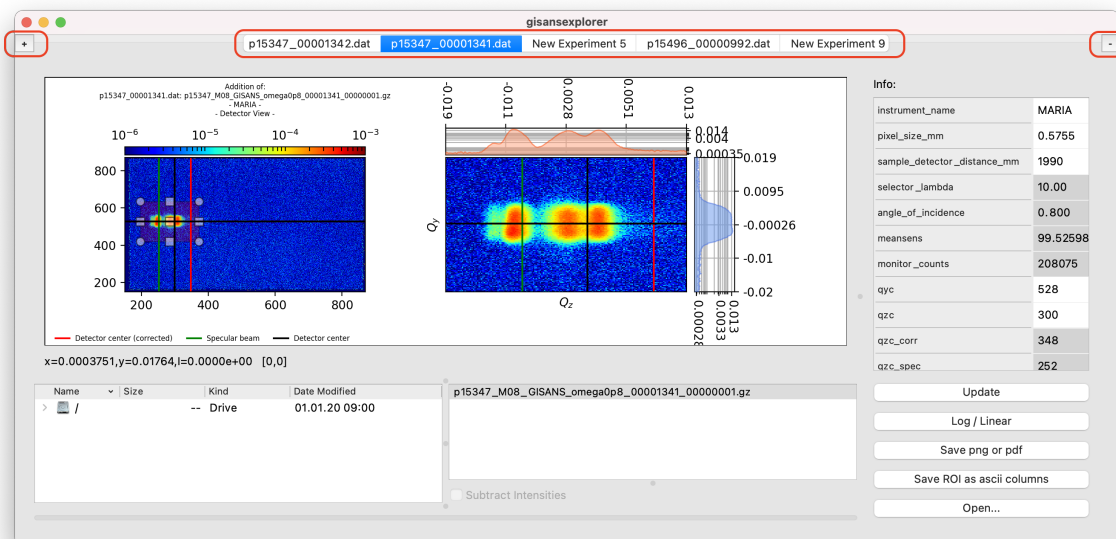
- By specifying the minimum and maximum intensity values of the colormap in the Info Table.
- By using the mouse wheel while hovering over the detector view (left plot) color bar.

The default min- and max- intensity values are $1e-06$ and $1e-03$ respectively.

3.1.9 Open and close experiment tabs

Creating new experiments allows to analyse data using different instruments and different sets of parameters in general.

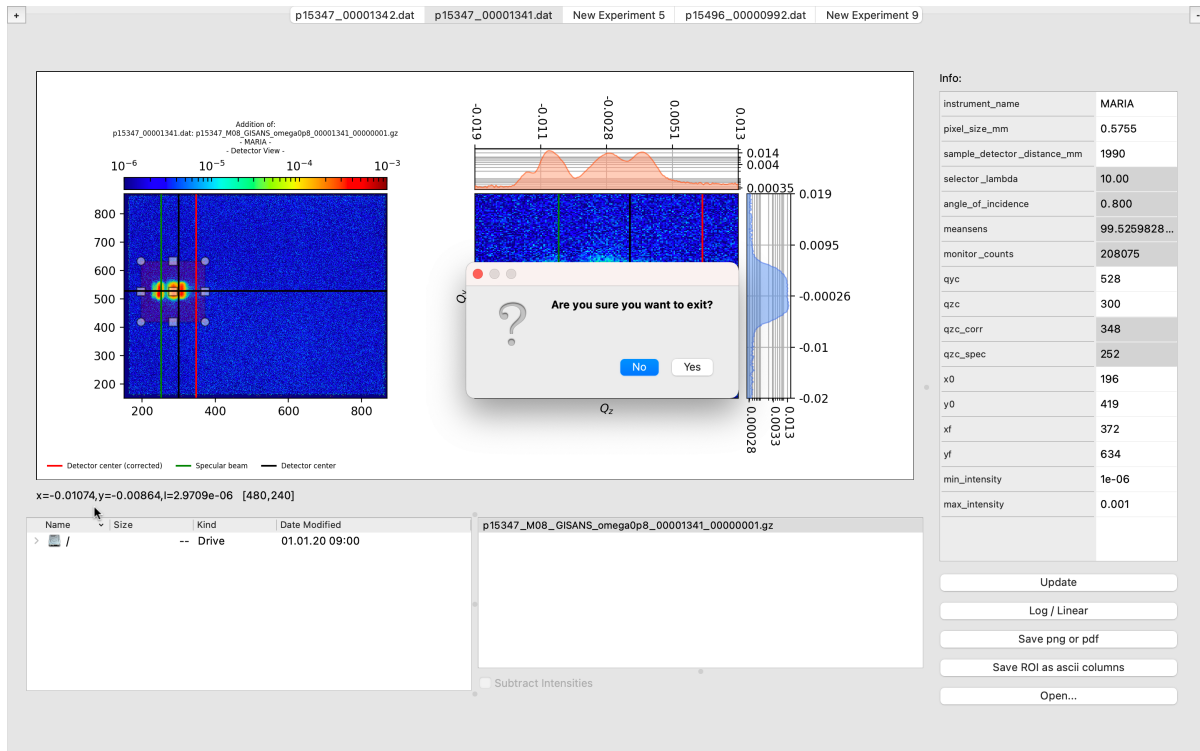
- Clicking the left + button will open a new experiment tab.
- Clicking the right - button will delete the current experiment tab.



After a new experiment tab is opened, the previous tabs are renamed according to the experimental `.dat` file opened in them. The new tab will have the default name “New Experiment N ”, with N increasing by 1 every time the + button is pressed. **The names of experiment tabs are non-editable.**

3.1.10 Save progress

Saving the partial progress is not possible. When the *close* button is pressed (Usually an *X* in a top corner of the window, depending on the Operating System), a pop-up dialog asks whether to quit the application. After clicking *Yes*, the application will close and all progress will be lost. **Make sure that all the reduced ascii data and the figures required are correctly saved before closing the application** –refer to sections [Pop up the ROI plots](#) and [Save the ROI](#).



3.2 gisansexplorer package

3.2.1 Submodules

3.2.2 gisansexplorer.GUI module

class gisansexplorer.GUI.**MyFrame**

Bases: `PyQt5.QtWidgets.QFrame`, `gisansexplorer.utils.Frozen`

[summary]

Parameters

- **qtw** (*[type]*) – [description]
- **Frozen** (*[type]*) – [description]

addExperimentInfo ()

[summary]

addFileTreeAndList (*botSplitter*)

[summary]

Parameters **botSplitter** (*[type]*) – [description]

addFunctionalityButtons ()

[summary]

addPanels ()

[summary]

build_ascii_header()

[summary]

Returns [description]

Return type [type]

color_outdated()

[summary]

Returns [description]

Return type [type]

static color_validate (*table_item*, *value_a*, *value_b*)

[summary]

Parameters

- **table_item** ([*type*]) – [description]
- **value_a** ([*type*]) – [description]
- **value_b** ([*type*]) – [description]

Returns [description]

Return type [type]

compute_Q()

[summary]

Returns [description]

Return type [type]

doStuff (*datFilePath*)

[summary]

Parameters **datFilePath** ([*type*]) – [description]

initFrame()

[summary]

on_cell_changed()

[summary]

on_click_loglinear()

[summary]

on_click_open_file()

on_click_save_ascii()

[summary]

on_click_save_png()

[summary]

Returns [description]

Return type [type]

on_click_update()

[summary]

on_file_double_clicked()

[summary]

on_file_selection_changed()
[summary]

on_graph_updated()
[summary]

on_progress_emited(*value*)
[summary]

Parameters **value** ([*type*]) – [description]

on_subtract_checkbox_changed()
[summary]

openFileNameDialog()
[summary]

Returns [description]

Return type [type]

parse_dat(*file*)
[summary]

Parameters **file** ([*type*]) – [description]

Returns [description]

Return type [type]

parse_intensity_map(*inputd*)
[summary]

Parameters **inputd** ([*type*]) – [description]

Returns [description]

Return type [type]

parse_sensitivity_map(*sens*)
[summary]

Parameters **sens** ([*type*]) – [description]

Returns [description]

Return type [type]

parse_yaml(*fp*)
[summary]

Parameters **fp** ([*type*]) – [description]

Returns [description]

Return type [type]

read_dat_file(*datFilePath=None*)
[summary]

Parameters **datFilePath** ([*type*], *optional*) – [description], by default None

Returns [description]

Return type [type]

read_intensity_file()
[summary]

Returns [description]

Return type [type]

read_sensitivity_file()
[summary]

Returns [description]

Return type [type]

read_yaml_file()
[summary]

Returns [description]

Return type [type]

safe_parse(*parse_func, file_path*)
[summary]

Parameters

- **parse_func** ([*type*]) – [description]
- **file_path** ([*type*]) – [description]

Returns [description]

Return type [type]

safe_parse_numpy(*parse_func, file_path, dtype='i', delimiter=' '*)
[summary]

Parameters

- **parse_func** ([*type*]) – [description]
- **file_path** ([*type*]) – [description]
- **dtype** (*str, optional*) – [description], by default 'i'
- **delimiter** (*str, optional*) – [description], by default ' '

Returns [description]

Return type [type]

saveFileNameDialog()
[summary]

Returns [description]

Return type [type]

save_gisans_map_filepath(*inputd*)
[summary]

Parameters **inputd** ([*type*]) – [description]

Raises **NotImplementedError** – [description]

subtract_intensities_from_selected_files()
[summary]

Returns [description]

Return type [type]

Raises ValueError – [description]

sum_intensities_from_selected_files()
[summary]

Returns [description]

Return type [type]

update_from_info_table()
[summary]

Returns [description]

Return type [type]

update_from_selection_list()
[summary]

update_gui()
[summary]

Returns [description]

Return type [type]

Raises Exception – [description]

update_multi_experiment_values()
[summary]

Returns [description]

Return type [type]

update_single_experiment_values(experiment)
[summary]

Parameters experiment ([type]) – [description]

Returns [description]

Return type [type]

update_table()
[summary]

Returns [description]

Return type [type]

class gisansexplorer.GUI.MyTabs
Bases: PyQt5.QtWidgets.QTabWidget, *gisansexplorer.utils.Frozen*
Collection of tabs hosting gisans data frames

tabButton_add
Adds a new tab

Type QToolButton

tabButton_rmv
Removes the current tab

Type QToolButton

frameList
List of gisans frames

Type List

last_num

index of last tab created

Type int

addTab()

Adds a new tab

initCornerButton()

Adds and creates connections for the add/rmv tab buttons

removeTab()

Removes the current tab

3.2.3 gisansexplorer.experiment_data_handling module

```
class gisansexplorer.experiment_data_handling.Experiment (instrument=<gisansexplorer.experiment_data_handling.Experiment object>)
```

Bases: *gisansexplorer.utils.Frozen*

cos_alpha_f(pixel_j)

property cos_alpha_i

sin_2theta_f(pixel_i)

sin_alpha_f(pixel_j)

property sin_alpha_i

property two_pi_over_lambda

```
class gisansexplorer.experiment_data_handling.FileReadingThread (myframe)
```

Bases: PyQt5.QtCore.QThread

progress_signal

run(self)

```
class gisansexplorer.experiment_data_handling.Instrument (name,  
                                                         pixel_size_mm=None,  
                                                         sam-  
                                                         ple_detector_distance_mm=None,  
                                                         data_root_dir='/')
```

Bases: *gisansexplorer.utils.Frozen*

```
class gisansexplorer.experiment_data_handling.Settings
```

Bases: *gisansexplorer.utils.Frozen*

basename()

datFilePath()

gisans_cut_filepath(y_or_z='z')

gisans_map_filepath()

gzFilePaths()

sensFilePath()

yamlFilePaths()

3.2.4 gisansexplorer.main_app module

```
class gisansexplorer.main_app.App
    Bases: PyQt5.QtWidgets.QMainWindow, gisansexplorer.utils.Frozen

    addTab()

    closeEvent(self, QCloseEvent)

gisansexplorer.main_app.icon_file()
```

3.2.5 gisansexplorer.plotting module

```
class gisansexplorer.plotting.AreaSelector(ax, line_select_callback)
    Bases: gisansexplorer.utils.Frozen

class gisansexplorer.plotting.MyGraphView(graph_title, parent=None)
    Bases: PyQt5.QtWidgets.QWidget

    build_cbar()

    build_norm(**kwargs)

    define_axes()

    define_layout()

    finishedUpdating

    init_canvas_connections()

    init_data_and_parameters()

    init_xyzLabel()

    line_select_callback(eclick, erelease)

    on_mouse_click(event)

    on_mouse_move(event)

    on_mouse_wheel(event)

    save(**kwargs)

    save_figures(filePath)

    save_gisans_map(filePath=None)

    save_gisans_surface(filePath=None)

    save_qy_integration(filePath=None)

    save_qz_integration(filePath=None)

    show_figures()

    take_care_of_negative_values()

    test_show()

    update_area_selector(**kwargs)

    update_ax(**kwargs)

    update_axes(**kwargs)
```

```
    update_cax()
    update_data(**kwargs)
    update_graph(**kwargs)
    update_xax()
    update_yax()
    update_zoom_ax()

class gisansexplorer.plotting.PlotData
    Bases: gisansexplorer.utils.Frozen

class gisansexplorer.plotting.PlotStyle
    Bases: object

    classmethod apply_style(ax)

    axisLabelFontSize = 30.0

    borderWidth = 3

    figSize = (12, 9)

    fontSize = 20

    lineWidth = 4.0

    majorTickLength = 20

    minorTickLength = 6.0

    titleFontSize = 10.0

gisansexplorer.plotting.create_gisans_figure(data, cnorm, draw_surface_plot=False)
gisansexplorer.plotting.create_qy_integration_figure(data)
gisansexplorer.plotting.create_qz_integration_figure(data)
```

3.2.6 gisansexplorer.utils module

```
class gisansexplorer.utils.FloatValidator(*args, **kwargs)
    Bases: PyQt5.QtGui.QValidator

    fixup(self, str) → str

    validate(self, str, int) → Tuple[QValidator.State, str, int]

class gisansexplorer.utils.Frozen
    Bases: object

gisansexplorer.utils.enable_high_dpi_scaling()

gisansexplorer.utils.format_float(value)
    Modified form of the 'g' format specifier.

gisansexplorer.utils.handle_exception(e)

gisansexplorer.utils.is_file(path)

class gisansexplorer.utils.mySciSpinBox(*args, **kwargs)
    Bases: PyQt5.QtWidgets.QDoubleSpinBox

    fixup(self, str) → str
```

```
stepBy (self, int)  
textFromValue (self, float) → str  
validate (self, str, int) → Tuple[QValidator.State, str, int]  
valueFromText (self, str) → float  
gisansexplorer.utils.profile_dec (fnc)  
    A decorator that uses cProfile to profile a function  
gisansexplorer.utils.profile_function_with_arguments (*args, **kwargs)  
gisansexplorer.utils.valid_float_string (string)
```

3.2.7 Module contents

```
gisansexplorer.entry_point ()
```

3.3 gisansexplorer

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Developed by Juan M. Carmona Loaiza - MLZ Scientific Computing Group, in collaboration with Alexandros Koutsoumpas.

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