JUPYLABBOOK: USER MANUAL

Date de diffusion	Rédacteur	Vérificateur	Approbateur	Modifications
2020/07/13	A. Hemmerle (Beamline Scientist)			Creation for release of v1.0
2020/10/02	A.. Hemmerle			Deal with problems in saving the nb
Destinataires	SIRIUS Users. https://github.com/ArnaudHemmerle/JupyLabBook			

PUBLIC

La version électronique fait foi.

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1. INTRODUCTION

1.1. WHAT IS JUPYLABBOOK?

JupyLabBook is an interactive lab book to be used on SIRIUS. It is meant to be as close as possible as the paper-like lab book that you would use on the beamline (except for the ruler and the tape).

The user can easily plot raw data, do data reduction, and write sample description without typing a single line of code. A PDF with a linear presentation of the notebook can be generated at any time of the experiment.

Expert users can define their own functions to perform more involved data analysis or presentation of the data, if needed.

The development of JupyLabBook is tracked on GitHub:
https://github.com/ArnaudHemmerle/JupyLabBook

1.2. WHAT IS NOT JUPYLABBOOK?

JupyLabBook was not designed to be a notebook for **analysis,** but for **data reduction** only. Think of it as the traditional lab book, that should remain untouched after the end of the experiment. Notebooks for specific analysis (GIXS, GIXD, XRF ...) can be provided as well on demand.

JupyLabBook is not made of paper: it can crash, it can be corrupted, it can be deleted by mistake ... In the present state of development, we advise users to keep a written paper-like lab book in parallel with any type of digital notebook. Especially for all the info concerning the samples used, that cannot be retrieved afterwards.

2. INSTALLATION & START UP

2.1. INSTALL JUPYTER

JupyLabBook works within the framework of the Project Jupyter (https://jupyter.org/). It only requires a proper install of Jupyter, and can therefore work on Windows, Linux, or MacOS. For installing Jupyter on your work station, refer directly to Jupyter website.

Few recommendations:
- Use anaconda Python >= 3.7 (conda -version >= 4.8.3)
- If used on Windows, it requires the installation of MikTex >= 2.9.7 for rendering the notebook as a PDF.
- The packages *lmfit* and *ipysheet* are required and not necessarily provided within the anaconda distribution.

2.2. SET UP CRONTAB

An automatic copy of the logs and scripts should be set up from srv4 to the Ruche. First create a folder `logs/` and a folder `scripts/` in the user's folder on the Ruche.

Then edit the crontab file in a terminal on srv4:
- Type `crontab -e` (works like vi)
- Add two lines (or modify if already there):
  - `*/1 * * * * cp -u /home/experiences/sirius/com-sirius/log/spyc/_*.log /nfs/pathToUser/logs/`
  - `*/1 * * * * cp -u /home/pathToUser/*py /nfs/pathToUser/scripts/`

This will copy the files every minute (only if the files are modified).

2.3. DOWNLOAD THE LATEST VERSION OF JUPYLABBOOK

To download the latest version of JupyLabBook:
- Go to https://github.com/ArnaudHemmerle/JupyLabBook
- Click on the button "Code"
- Download and extract the zip file
- Rename the JupyLabBook-master with the experiment name: User_PropNumber (for ex.: Doe_20200712
- Rename the file JupyLabBook.ipynb with experiment name: User_PropNumber.ipynb (for ex.: Doe_20200712.ipynb)

2.4. RUN JUPYLABBOOK

Start Jupyter Notebook in a folder from where you can access your working folder.

Contrary to its name, JupyLabBook cannot be used with Jupyter Lab. It has to be used with Jupyter Notebook. If you want to use Jupyter Lab, use the option "Launch Classic Notebook" in the Help menu.

Find and open the .ipynb file, which should now have the name User_PropNumber.ipynb

2.5. SET UP AND RUN THE FIRST CELL

A few thing must be modified in the first code cell:
- Change the value of `expt.notebook_name = 'JupyLabBook.ipynb'` with your notebook name.
  For ex.: `expt.notebook_name = 'Doe_20200712.ipynb'`
- Change the value of `expt.working_dir` with the full path to your working directory (where the data reduction will be saved).
  For ex.: `expt.working_dir = "C:\\Users\\SIRIUS\\Documents\\SIRIUS_Users\\Doe_20200712\\working\\"`
- Change the value of `expt.recording_dir` with the full path to your recording directory (where the nexus files are saved).
  For ex.: `expt.working_dir = "Z:\\com-sirius\\users\\2020\\doe\\"`

- Change the value of `expt.logs_dir` with the full path to the directory containing the logs.

  For ex.: `expt.logs_dir = "Z:\\com-sirius\\users\\2020\\doe\\logs\\"`

Run the first cell. Check that there is no error message.

If everything worked well, a "Choose action" panel with the nexus files should appear at the bottom of the notebook.

```
# Necessary for saving in pdf
expt.notebook_name = 'JupyLabBook.ipynb'

# Directory where the data will be saved
expt.working_dir = "/Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/"

# Directory where the nexus files are
expt.recording_dir = "/Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/recording/"

# Directory where the logs are
expt.logs_dir = "/Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/logs/"
```

Parameters to be changed in the first cell

3. PANEL "CHOOSE ACTION"

Panel "Choose action"

3.1. FILL FORM

Load an empty form to be filled at the beginning of the experiment.

When the form is filled, click on "Print form".
The different text cells can be modified afterwards by double-clicking on them.

3.2. CALIBRATION THETA Z

Do the qz calibration for GIXD.

A code cell is generated with default values.
Change the corresponding values and re-run the cell.

The value of the calibration in radian per channel is stored, and will be automatically used in GIXD.

3.3. CONVERT LOGS

Convert all the logs from your logs directory into a human-readable format.

Results are saved in a folder `readable_logs/` in your working directory.
The original logs are kept intact.

3.4. EXPORT TO PDF

Export the notebook into a PDF stored in the same folder as your notebook.

Check first that the value of `expt.notebook_name` in the first cell is the correct one (especially if you have renamed the notebook during the experiment).

In the present state: Export to PDF does not work on the Windows PC on the beamline, ask for the beamline staff to do the conversion.

3.5. INSERT COMMENT

Create an empty text cell above the panel.

Click on it to enter text. When you are done, click on "Execute" in the top bar.

To enter a title add a symbol # and a space at the beginning of the text.

To insert a line break, put an empty line between the lines.

Example of a text cell before execution.

The same example after cell execution.

3.6. INSERT SCRIPT

Insert a script in the notebook.

Check that the path to the scripts directory is the right one. Click to validate the path.

Choose the script you want to print. If you want an automatic numbering of the scans, put the index of the first scan in the text cell. If not, leave it empty. Click to insert the script.

The script can be modified after import by double clicking on the text cell.

NB: Save the scripts with a different file name each time you modify them.

3.7. INSERT POSITIONS

Get the positions in the logs and insert them in a text cell.

This function searches in the logs all the *wm* commands. First select the log file, then the *wm* you want to print.

The text cell can be edited by double-clicking on it.

3.8. INSERT COMMANDS

Print a series of commands extracted from the logs.

The index of each scan is added after the command. In case of a script, the index of each scan ran by the script is added.

First select the log file, then select one or multiple commands and click on *Insert commands* below the selection window.

To select multiple commands: keep shift pressed while clicking to select a range of commands, keep ctrl pressed while clicking to select the commands individually (cmd on MacOS).

| Fill form | Calib. theta z | Convert logs | Export to PDF |
| Insert comment | Insert script | Insert positions | Insert commands |

_all_171204T111541.log ▾   Select log

Mon, 11 Dec 2017 06:53:05 shclose
SCAN ABORTED: Mon, 11 Dec 2017 06:05:19 run xsw7.ipy #8041 #8042 #8043
Mon, 11 Dec 2017 06:05:19 run xsw7.ipy #8041 #8042 #8043
Mon, 11 Dec 2017 06:05:09 setposition alphax 2.07
Mon, 11 Dec 2017 06:05:01 wm alphax gamma
Mon, 11 Dec 2017 06:04:53 amove alphax CEN
Mon, 11 Dec 2017 06:03:51 dscan alphax -.2 .2 50 .1 #8040
Mon, 11 Dec 2017 06:03:42 shopen
SCAN ABORTED: Mon, 11 Dec 2017 06:03:24 dscan alphax -.2 .2 50 .1 #8039
Mon, 11 Dec 2017 06:03:24 dscan alphax -.2 .2 50 .1 #8039
Mon, 11 Dec 2017 06:03:15 amove xs 2
Mon, 11 Dec 2017 06:03:22 amove alphax 2.07 gamma 4.14

Insert commands with multiple scans selected by keeping shift pressed while clicking.

3.9. REFRESH

Refresh the list of nexus files.

Click on *Refresh* if your scan is finished but does not appear in the list.

It does not refresh the list of scripts/logs. These files are automatically updated every minute.

3.10. TREAT SCAN(S)

Open the panel Choose Treatment.

First select a scan in the scan selection window. The command which led to this scan is extracted from the logs and printed below the window for your information. Use it to confirm that the selected scan is the right one, and click on *Treat scan(s).*

This will delete the panel "Choose Action", print the command which led to the scan as a subtitle, and open a panel "Choose Treatment".

It is possible to select multiple scans and apply the same treatment on each of them.

To select multiple scans: keep shift pressed while clicking to select a range of commands, keep ctrl pressed while clicking to select the commands individually (cmd on MacOS).

Scan selection window. When the scan is selected, click on Treat scan(s).

4. PANEL "CHOOSE TREATMENT"

This panel allows you to choose which type of data reduction you want to apply on the selected scan.

You can have a look on the 1D data contained in the scan by selecting sensors for x and y.

NB: If you want to have this plot in the final PDF, you need to click on *Add plot to report*.
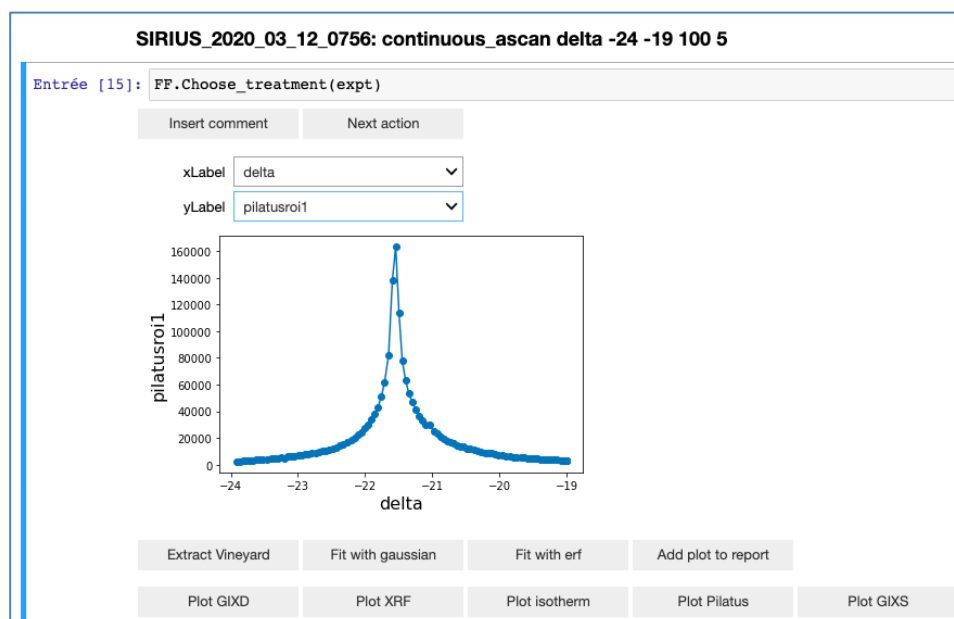
Example of a panel "Choose Treatment". The plot will appear in the PDF only if you click on Add plot to report.

4.1. NEXT ACTION

Bring back the panel "Choose Action".

Click on Next action if there is something wrong or if you do not want to extract the current scan.

Careful, the subtitle with the scan number and its command will stay and needs to be manually erased.

4.2. EXTRACT VINEYARD

Extract the position of the Vineyard from a GIXD scan.

The value of the Vineyard is automatically stored in the variable `expt.channel0` and will appear as the default value in the GIXD panel.

Usually needs to be done once per experiment only.

4.3. FIT WITH GAUSSIAN/ERF

Fit the 1D plot displayed with a gaussian/erf function.

Used during alignment of the beam only.

4.4. ADD PLOT TO REPORT

Add the 1D plot currently displayed in the PDF report.

4.5. PLOT GIXD

Open a panel to plot a GIXD (Grazing Incidence X-ray Diffraction) scan.

Panel Plot GIXD

4.5.1. PARAMETERS

- Print sensors: print the list of sensors in the nexus file.
- Print scan info: print several contextual info from the scan.
- Print abs: print the absorber used.
- log x/log y: log on the x and y axis of the integrated profile.
- log z: log on the image.
- cmap: colormap of the image.
- binsize: size in pixels of the vertical binning (along qz), for the image display only.
- nblevels: number of color levels for the image display.
- moy to create: binsize to be saved.
- Vineyard: channel of the Vineyard (automatically filled with *Extract Vineyard*).
- Compute qz: switch from pixels to qz in the vertical direction.
- wavelength: use 12398/E(eV)/10 to have the wavelength in nm.
- thetac: critical angle in rad.
- thetazfactor: factor for conversion from channel to radian in the vertical direction (automatically filled by *Calibration Theta z*).

4.5.2. FORMULA

4.5.2.1. q_{xy}

q_{xy} is extracted from the scan, and is computed with the formula:
$$q_{xy} = 4\pi/\lambda \, \sin(\delta/2)$$
where δ is the in-plane angle of the detector (classical 2θ in diffraction).

4.5.2.2. q_z

q_z is computed using:
$$q_z = 2\pi/\lambda \, \sin(\theta_z)$$
with $\theta_z = \theta_c + \gamma + (channel0 - channel) * \theta_{z,factor}$,where γ is the out-of-plane angle of the detector.

4.5.3. DATA OUTPUT

Files are generated in the working directory.

- XXX_1D.mat: each line corresponds to a position of delta. It is the matrix corresponding to the image displayed.
- XXX_1D.dat: each line corresponds to a position of delta. It contains the value of each sensor, and integration along qz:
    - o QzIntegrated: over the whole detector,
    - o QzIntegratedTop: over its top half,
    - o QzIntegratedBottom: over its bottom half,
    - o QzIntegratedBottomQuarter: over its bottom quarter.

Binned data:
- XXX_1D.matNN: binning of the matrix, with NN the number of points per bin.
- XXX_1D_qz.datNN: to convert bin number to qz in XXX_1D.matNN.
- XXX_1D.moyNN: a more convenient way to represent the binned matrices with a 3 columns (qxy, qz, intensity) display.

4.6. PLOT XRF

Open a panel to plot an XRF (X-Ray Fluorescence) scan.

Panel Plot XRF

4.6.1. PARAMETERS

- Print sensors: print the list of sensors in the nexus file.
- Print scan info: print several contextual info from the scan.
- Print abs: print the absorber used.
- Fast extract: switch off to extract the scan point-by-point (to be used if the memory is saturated).
- Plot spectrogram: plot a spectrogram (spectrums as a function of time).
- Plot first&last spectrums: plot the first and last spectrum of the scan.
- Plot sum of spectrums: plot the sum of the spectrums (i.e. a time integration).

- logz: log on the image and on the plots.
- Elements: the index of the element (i.e. the part of the detector) to be used. For the single-element detector use '4' (by convention). For the four-elements detector use '0,1,2,3' or any combination of these numbers.
- First/Last channel: define the range of channels to be used in the plots.
- Use eV: use eV instead of channels with the formula $Gain * channel + eV0$.

4.6.2. IDENTIFY PEAKS

Click on *Identify peaks* to add positions of peaks on the plots. This will open a spreadsheet with 3 columns:
- Name: the name of the peak.
- Position: the position of the peak (in eVs or channels depending on your choice in the corresponding tick box).
- Use?(y/n): allows you to keep a peak in the list without using it (useful if you alternate between different samples).

Once you are done, click on *Validate peaks.* Your current selection of peaks will be displayed. You can continue to modify the list and click on *Validate peaks* anytime you want to check it on the plot.

Click then on *Plot* to add the series of plots to the report.

	Identify peaks	Plot	
	Validate Peaks		

	Name	Position	Use?(y/n)
1	Cu (Ka1)	8046.3	y
2	Elastic	12000	y
3	Compton	11650	y
4	Mn (Ka1)	5900.3	y
5	Fe (Ka1)	6400.5	y
6	Cu (Kb1)	8903.9	y
7	Ar (Ka1)	2957.5	n
8			

Panel Identify peaks

NB: You have to click on *Validate peaks* to have the peaks on the final plots.

The list of peaks is saved for the next scans as well when you click on *Plot* (i.e. you will not have to enter the list of peaks for every scan, just play with the y/n option).

4.6.3. DATA OUTPUT

Files are generated in the working directory.

- XXX_fluospectrumNN.mat: raw data file converted to a matrix, with NN the index of the detector element. Each line is one data point, each column a channel. For example, if you ran a "*tscan 300 30"* the matrix will contain 301 lines (each being an integration over 30 s), and 2048 columns (corresponding to the 2048 channels of the detector).
- XXX.dat: each line corresponds to a data point and each column the value of a sensor (see the header of the file).

4.7. PLOT ISOTHERM

Open a panel to plot an isotherm.

NB: Try to start/stop the isotherm at the right moment to have a nice plot. In particular, stop the isotherm before emptying the through.

Extract Vineyard	Fit with gaussian	Fit with erf	Add plot to report	
Plot GIXD	Plot XRF	Plot isotherm	Plot Pilatus	Plot GIXS
☐ Print sensors	☐ Print scan info	☑ Fast extract		
Plot				

Panel Plot Isotherm

4.7.1. PARAMETERS

- Print sensors: print the list of sensors in the nexus file.
- Print scan info: print several contextual info from the scan.
- Fast extract: switch off to extract the scan point-by-point (to be used if the memory is saturated).

4.7.2. DATA OUTPUT

Files are generated in the working directory.

- XXX.dat: each line corresponds to a data point and each column the value of a sensor (see the header of the file).

4.8. **PLOT PILATUS**

Open a panel to plot the time-integrated images from the Pilatus.

Panel Plot Pilatus

4.8.1. *PARAMETERS*

- Print sensors: print the list of sensors in the nexus file.
- Print scan info: print several contextual info from the scan.
- Print abs: print the absorber used.
- logz: log on the image and on the plots.
- cmap: choice of the colormap.
- x min/max: x-range in pixels for the plot of the integration along the vertical axis (bottom left plot).
- y min/max: y-range in pixels for the plot of the integration along the horizontal axis (top left profile plot).

4.8.2. *DATA OUTPUT*

Files are generated in the working directory.

- XXX_pilatus_sum.mat: the image saved as a matrix. Each pixel with the value 0 is replaced by the value -2 (easier to filter out the dead zones of the detector in the analysis).
- XXX_pilatus_sum.tiff: the same as the mat file, but saved as a tiff.
- XXX_integrated_x.dat: horizontal integration of **the whole detector** as a function of y (each line is a pixel in the vertical direction).
- XXX_integrated_y.dat: vertical integration of **the whole detector** as a function of x (each line is a pixel in the horizontal direction).

4.9. **PLOT GIXS**

Open a panel to plot a GIXS (Grazing Incidence X-ray Scattering) scan.

Panel Plot GIXS

4.9.1. *PARAMETERS*

- Print sensors: print the list of sensors in the nexus file.
- Print scan info: print several contextual info from the scan.
- Print abs: print the absorber used.
- logz: log on the image and on the plots.
- cmap: choice of the colormap.
- Pixel size: pixel size in microns.
- wavelength: use 12398/E(eV)/10 to have the wavelength in nm.
- distance: distance from the detector to the center of the sample in mm.
- thetai: incident angle on the sample in rad.
- PONIx/PONIy: Coordinates of the Point Of Normal Incidence in pixels. Measured on the direct beam at delta=0 and gamma=0.
- Force gamma&delta: Tick to enforce the value of gamma and delta **if the sensors are in the sensor list but are not correct/relevant** (for example if the detector is on the delta0 platform).
- Forced gamma/delta: Values of gamma and delta in degrees to be used if *Force gamma&delta* is ticked, or if they are absent from the sensor list.
- qxy min/max: qyx-range in nm-1 for the plot of the integration along the vertical axis (bottom left plot).
- qz min/max: qz-range in nm-1 for the plot of the integration along the horizontal axis (top left profile plot).

4.9.2. FORMULA

4.9.2.1. QXY

qxy is computed with the formula:

$$q_{xy} = 4\pi/\lambda \, \sin(2\theta/2),$$

using, for each pixel of horizontal coordinate x:

$$2\theta = \tan^{-1}(pixel\_size * (x - pos\_direct\_x)/D),$$

with pos_direct_x the position of the direct beam on the rotated detector:

$$pos\_direct\_x = PONIx - D/pixel\_size * \tan(\delta),$$

where δ is the in-plane angle of the detector and D the distance detector-sample.

4.9.2.2. QZ

qz is computed with the formula:

$$q_z = 2\pi/\lambda \, (\sin(\alpha_f) + \sin(\alpha_i)),$$

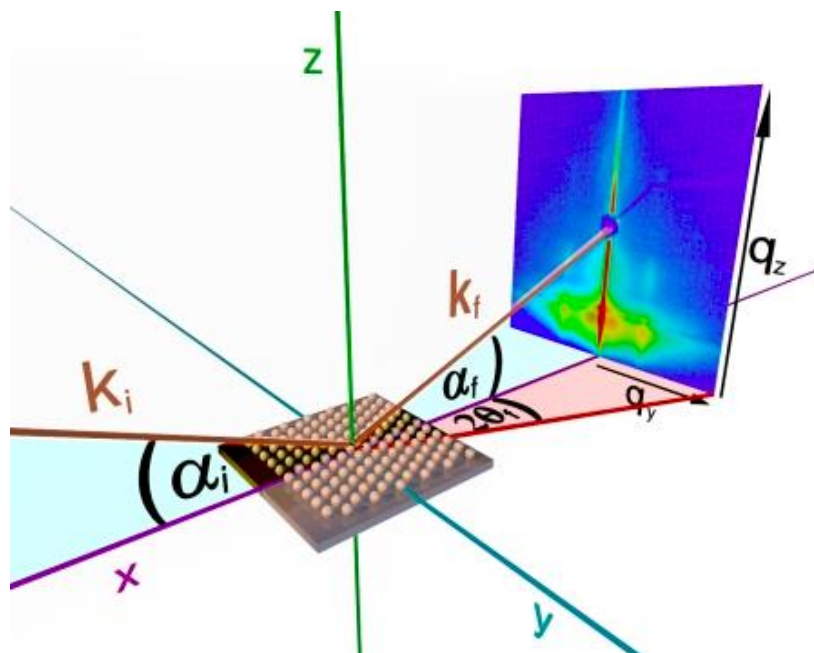using, for each pixel of vertical coordinate y:

$$\alpha_f = \tan^{-1}(\, (pixel\_size * (pos\_direct\_y - y) - \Delta y0)/D),$$

with pos_direct_y the position of the direct beam on the rotated detector:

$$pos\_direct\_y = PONIy - distance/pixel\_size * \tan(\gamma),$$

where γ is the out-of-plane angle of the detector.

$\Delta y0 = distance * \tan(\alpha_i)$ is the distance between the direct beam and the horizon defined by $\alpha_f = 0$, and α_i the incident angle.

Geometry for GIXS. Image from Prof. Andreas Meyer, U.Hamburg. See
http://gisaxs.com/files/Strzalka.pdf as well.

4.9.3. DATA OUTPUT

Files are generated in the working directory.

- XXX_pilatus_sum.mat: the image saved as a matrix. Each pixel with the value 0 is replaced by the value -2 (easier to filter out the dead zones of the detector in the analysis).
- XXX_pilatus_sum.tiff: the same as the mat file, but saved as a tiff.
- XXX_integrated_qxy.dat: horizontal integration of **the whole detector** as a function of qz (in nm-1).
- XXX_integrated_qz.dat: vertical integration of **the whole detector** as a function of qxy (in nm-1).

5. MISCELLANEOUS

5.1. GET BACK THE SCAN SELECTION PANEL

If you have deleted by mistake the scan selection panel, or if you are simply lost and do not know how to continue filling the notebook:
- Select the very first code cell of the notebook (click inside),
- Execute it.

A new panel will be created at the very bottom of the notebook.

If you are lost, select the first code cell and click on execute.
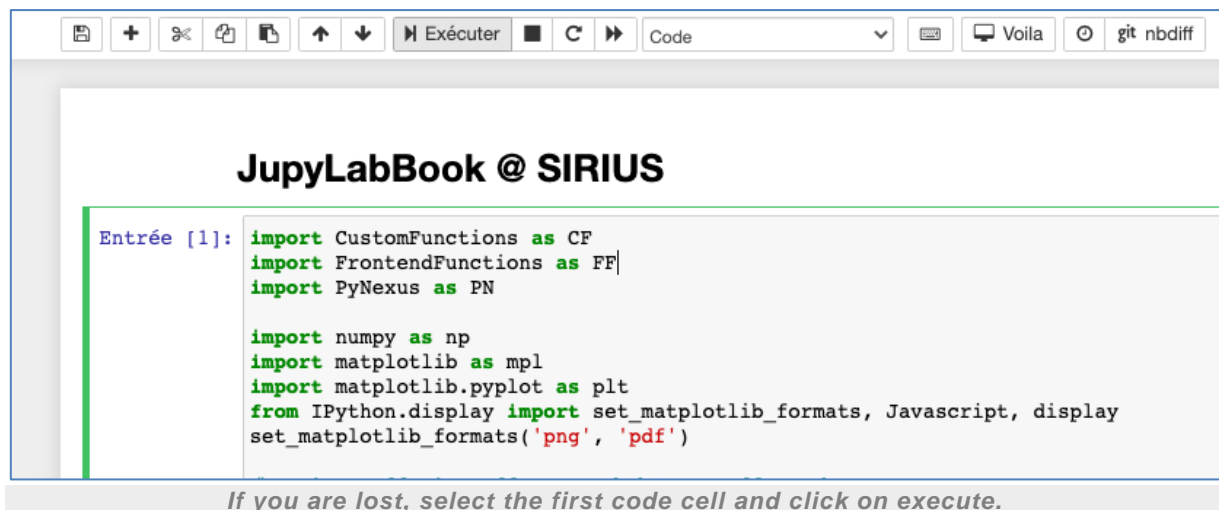
5.2. THE NOTEBOOK HAS CRASHED

If the notebook has crashed (weird code output when executing a cell), or if the notebook was closed by mistake, you need to restart the kernel. Click on the refresh button in the tool bar, or in the menu *Kernel* choose *Restart*.

*Click on the Restart Kernel button in the tool bar if the notebook has crashed (the refresh-like button)*

Unfortunately all the info put into the panel boxes will be reset to default values. You will have to fill each of them back again.

5.3. MODIFY A TEXT CELL

To modify a text cell double-click on it. Re-execute it when done.
See the section "Insert comment" for more details.

5.4. THE LAST SCAN IS MISSING IN THE SCAN LIST

Wait for the scan to be finished. Click on *Refresh* in the panel *Choose action.*
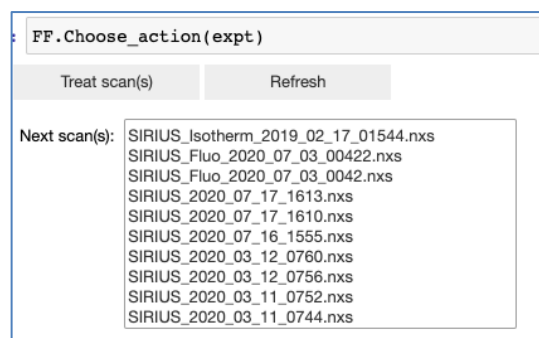
Click on Refesh if the last scan is finished and does not appear in the list.

5.5. DELETE A CELL

The easiest way to delete a cell is to select it and click on the scissors in the tool bar. **Be sure that you have selected the right cell!**

It happens frequently that the user deletes the wrong cell by mistake. If doing so, try to paste back the cell by clicking on Paste in the toolbar.
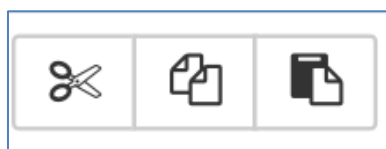
Delete a cell by selecting it and clicking on the scissors. If you want to put it back, click on Paste (extreme right button).

5.6. SAVE/COPY THE NOTEBOOK

Save regularly the notebook by clicking on *Save* in the toolbar.

It is also good to make a hard copy of the notebook every day, in case a mistake happens.
To do so, copy/paste directly the .ipynb file in the file explorer.

5.7. IT IS IMPOSSIBLE TO SAVE THE NOTEBOOK

If it is impossible to save the notebook (check the time since the last save in the top bar), and if there is an error in red "'_xsrf' argument missing from post":
- open a new notebook (File/new notebook), and the issue is magically gone; you can again save the notebook.
- if it still does not work, try to restart the Kernel (Kernel/Restart)
- do not close the notebook if you cannot save it!

See as well: https://stackoverflow.com/questions/55014094/jupyter-notebook-not-saving-xsrf-argument-missing-from-post

5.8. EXAMPLE

An example of what the final PDF can look like is available is the folder *example*.