

Software installation for data processing at LiX

Data collection for solution scattering at LiX involves 3 detectors, 2 of which are positioned 184756 an angle from the beam. This geometry is necessary to provide a continuous q-range of $\sim 0.005\text{--}3.2 \text{ \AA}^{-1}$ for all measurements. However, this also requires specialized software to stitch together the data from the 3 detectors with all necessary corrections. These functionalities are provided in the python package *py4xs*. Users will also need the package *lixtools* in orders and to take advantage of data processing GUIs and access functions needed for mail-in measurements.

In order for *py4xs*, *lixtools*, and Jupyter notebooks to run on your computer, you will need a working python environment. The easiest way to get this is to install Anaconda (see <https://docs.anaconda.com/anaconda/install/>), which includes most modules already. If you are worried about disk space, install Miniconda (<http://conda.pydata.org/miniconda.html>) instead. Be sure to use python version ≥ 3.6 .

You might want to set up a conda environment just for data processing and activate that environment. For instance, in a terminal window, type:

```
conda create -n py36 python=3.6  
conda activate py36
```

If you use Anaconda Navigator, you can do this using the “create” button, then run a terminal window from the environment you’ve just created.

py4xs is now deposited in PyPI. In order to process data on your computer using *ipython/jupyter* notebook, you simply need to run this:

```
pip install py4xs lixtools jupyter notebook
```

This should take care of everything. If you run into problems, you will find it useful to read about how to install software using *pip* and *conda*.

You could also install *py4xs* or *lixtools* from the notebook if you use Anaconda Navigator. Open a notebook from the Navigator. In the first cell, run the following to install *py4xs* into the default conda environment.

```
!pip install py4xs
```

You will find on our Google drive some demo ipython notebooks and the data files used by these notebooks. You will receive an up-to-date template data processing notebook and supporting files during your beam time at LiX.

Note that the notebooks saved on Google drive can be opened using Google Colaboratory. This can be used as a minimal data processing environment, or used for communication with beamline staff for troubleshooting. However, the notebook may need to be revised slightly.

We use HDF5 files for all raw and processed data. You will find it handy to have a HDF file viewer to inspect the contents of the data files. You could install h5pyViewer using pip. However, you will need to create a new conda environment based on python 2.7. It also requires wxPython, which you can also install using pip. Alternatively, you can get java-based [HDFView](#).

Update regarding matplotlib in the data processing GUI (July 2020)

We have observed issues displaying plots from newer versions of matplotlib in the data processing GUI in Jupyter notebook. The workaround is to use jupyter-lab instead. This will require installation of a few other packages:

```
pip install jupyterlab  
conda install nodejs  
pip install ipywidgets npm ipympl  
jupyter labextension install @jupyter-widgets/jupyterlab-manager  
jupyter labextension install jupyter-matplotlib  
jupyter nbextension enable --py widgetsnbextension
```

The latter steps could be performed within the extension manager of jupyter-lab. And be sure to use “%matplotlib widget” at the beginning of the notebook.