Introduction

Welcome to a short introduction on how to fully convert your scattering data the Pair Distribution Function (PDF). In this section we will discuss how to setup and run the program. The program is written in Python 3.7 but requires no programming experience to operate. However, to execute the program a Python environment is needed. If you are familiar with Python you can head down to Calibration and Integration or Data Reduction GUI where the program is explained in more detail.

If you have little to no experience with programming and setting up a Python environment I suggest that you go to google or YouTube and search 'Anaconda install'. Anaconda is a helpful tool for managing your Python library and is strongly recommended. How to install Anaconda will depend on your operating system so remember to choose the right one. When installing Anaconda remember to add Path to environmental variables, this will allow you to call Python from your terminal. To check if you have successfully installed Python open you terminal/command prompt and write 'python'. If everything went well your current version of python should be printed.

Now that python is recognized by your computer you are able to proceed with installing the packages needed to run the program. The two most important packages are PyFAI (used for calibrating and integrating your data) and PDFgetX3 (used for calculating the PDFs). How to install can be found on the following links:

link 1

link 2 XXX this might be diffpy

Depending on whether you chose to install Anaconda, Anaconda mini or Python will affect which packages you need. I will not go through all the packages needed but merely describe how you can solve the problem. All of the packages needed can be installed with either conda (how to call Anaconda in the prompt) or pip. When the code is executed it will start with importing all packages needed, hence it will tell us what we are missing. Lets say that we are missing the package 'tqdm'. (XXX screenshot of could not import tqdm). We fix this by opening the terminal and typing 'conda install tqdm' or 'pip install tqdm'. Proceed like this until the everything is working and you will be good to go.

Run Program

Here I will explain the function of file located within the program (e.g. how to run the program) and how to load desired files. Some files can easily be customized to enhance user preference while customizing other files could corrupt the program.

Integration

In this section we will discuss how to make the program integrate your data. So far it is not possible to calibrate in this program since several programs provide that feature (PyFAI, Dioptas and Fit2D). If you have already integrated your data go on to the last section where the Data Reduction GUI will be explain.

Data Reduction GUI

This section is dedicated to explaining how to fully operate the Data Reduction GUI, the GUI is shown on Figure 1.

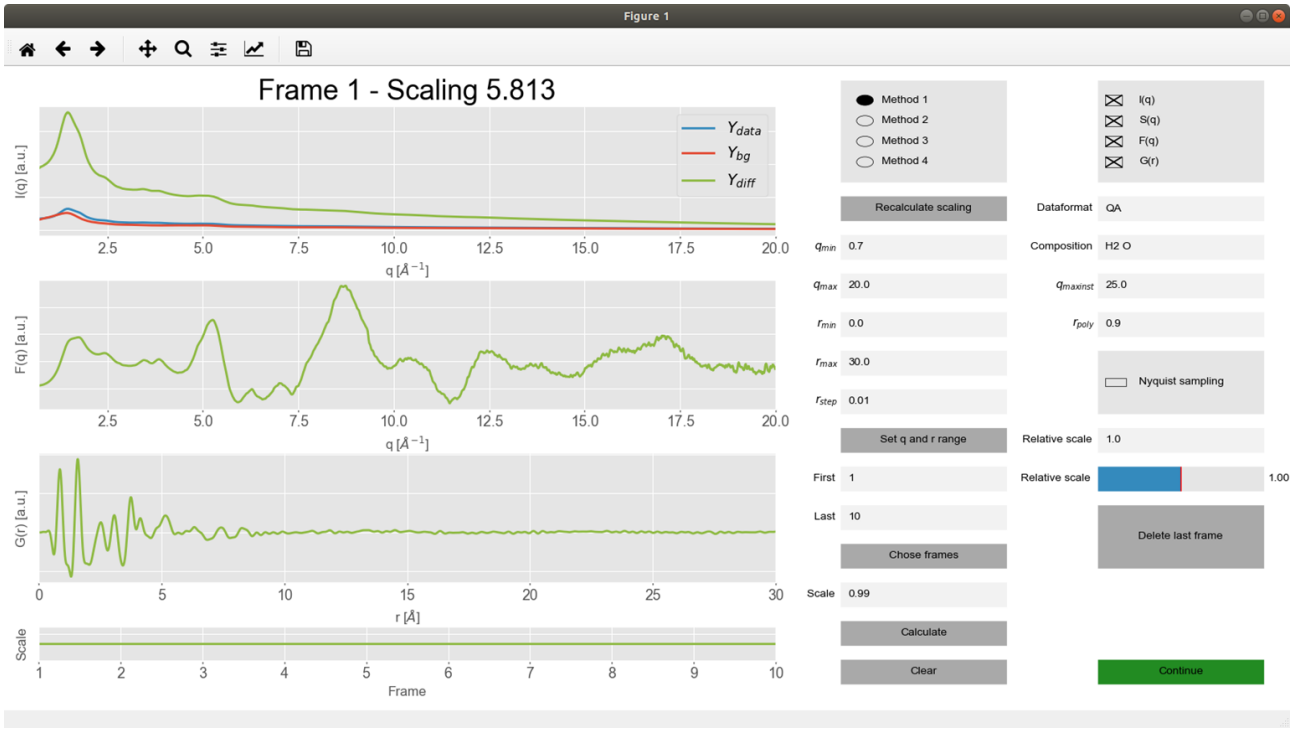

Figure 1: Data Reduction GUI.

Author and License

Should there be any question, desired improvement or bugs they can be reported to me through me email: etsk@chem.ku.dk or GitHub: EmilSkaaning.

This program is under the MIT license and is fully open source. This code was written as part of my M.Sc. and hopefully it can save people for more hours than I spend on writing it.