

Installation

To run Batch_PDF.py several packages are needed and most do not come with the installation of Anaconda. Before installing any packages python 2.7 must be installed, this can either be done through Python's own homepage:

<https://www.python.org/downloads/>

or with Anaconda:

<https://www.anaconda.com/download/>

Remember to add Python to your path when installing. It is important that your current version of Python is 2.7 since PDFgetX3 is not supported by any other Python version. Should another version of Python already be installed, another environment can be made with the correct Python version. The easiest way to do this is through Anaconda:

<https://conda.io/docs/user-guide/tasks/manage-environments.html>

The following links are guides on how to install and verify the installation of required packages:

h5py <http://docs.h5py.org/en/stable/build.html>

matplotlib <https://matplotlib.org/users/installing.html>

prompter <https://pypi.org/project/prompter/>

tqdm <https://pypi.org/project/tqdm/>

PDFgetX3 <https://www.diffpy.org/doc/pdfgetx/2.0.0/install.html>

After the installations three different files are needed before the script can be used, Batch_PDF.py, Batch_PDF_config.ini and pdfgetx3.cfg. Batch_PDF.py and Batch_PDF_config.ini can be found on:

https://github.com/EmilSkaaning/Batch_PDF

Batch_PDF.py and Batch_PDF_config.ini must be located within the same directory for the script to work. The script can be used without the config file, if this is chosen the script will use the settings put predefined within Batch_PDF.py. This is not recommended.

A simple version of pdfgetx3.cfg can be generated with Batch_PDF.py by setting the variable 'make_cfg = True' under [PDFgetX3] in Batch_PDF_config.ini. For a complete version of the pdfgetx3.cfg see documentation page:

<https://www.diffpy.org/doc/pdfgetx3/quick-start.html>

Now that all three files are downloaded open your command prompt or IDE and navigate to the directory where Batch_PDF.py is located and run the script.