PDFgetX3 cheatsheet

Command line options

```
pdfgetx3 [-flag] FILENAME     Launch pdfgetx3
```

Configuration file
A file named "pdfgetx3.cfg" will be read automatically

```
-c CONFIG, --config CONFIG
                Specify a configuration file
                Put NONE to ignore default configuration
-s SECTION, --section SECTION
                Read custom section in the config file
                Standard is "DEFAULT"
--createconfig CREATECONFIG
                Create new template configuration file
                Write to the standard output when "-"
```

Experimental parameters
Will overwrite the ones in the configuration file

```
-w WAVELENGTH, --wavelength WAVELENGTH
        X-ray wavelength in Angstroms
--twothetazero TWOTHETAZERO
        Actual zero angle in diffractometer degrees
--composition COMPOSITION
        Chemical composition of the sample
        Format: "NaCl", "C0.5 Pt 4.5", "CH3 CH2 OH", etc.
```

Calculation options
```
--mode MODE         PDF calculator ('xray', 'neutron', 'sas')
--qmaxinst QMAXINST Maximum Q cutoff for input intensities (1/A)
--qmin QMIN         Lower Q bound for FT (1/A). Default: 0
--qmax QMAX         Upper Q bound for FT (1/A). Default:
qmaxinst
--rmin RMIN         Low limit of the r-grid (A). Default: 0
--rmax RMAX         High limit of the r-grid (A). Default: 30
--rstep RSTEP       r-grid step size (A). Default: 0.01
--rpoly RPOLY       r-limit for the maximum frequency in the
F(Q)

                    correction polynomial. Default: 0.9
```

Background
```
-b BACKGROUNDFILE, --background BACKGROUNDFILE
                    Background datafile
--bgscale BGSCALE   Scaling of the background data. Default: 1
```

Input
```
-d DATAPATH, --datapath DATAPATH
                Extra directory for input files
                When NONE clears previously defined paths
--format {twotheta,QA,Qnm}
                Format of input data files
-ff FORMFACTORFILE, --formfactor FORMFACTORFILE
                Form factor datafile (only in `sas` mode)
```

Output
```
-o OUTPUT, --output OUTPUT
                Customize output files naming
                Write to the standard output when "-".
                @h      the input file head directory or '.'
                @r      the input path with extension removed
                @e      the input file extension without '.'
                @t      the tail component of the input file
                @b      the tail component with extension removed
                @o      the output extension iq, sq, fq or gr
-t OUTPUTTYPES, --outputtypes OUTPUTTYPES
                Results to be saved ("iq", "sq", "fq", "gr", "none")
--force FORCE
                Overwrite output ("yes", "true", "on", "1")
                One-time overwrite when "once"
-p PLOT, --plot PLOT
                Results to be plotted ("iq", "sq", "fq", "gr")
```

See/process files from pattern
```
-f, --find      Process files that matches a pattern
-l, --list      List files that matches a pattern
```

General options & other
```
-h, --help          See the help instructions
-V, --version       Program version
--manual            Online manual
--verbose VERBOSE   Verbosity level (error, warning, info,
                    debug, all) or (0, 1, ..., 5).
```

Interactive mode (ipython)

To activate it
```
-i, --interact          Interactive mode after processing
```
It is also activated using the "-p" or "--plot" flag.

Configuration parameters
```
print(config)  See config parameters on screen
config.
```

Functions for interactive mode
```
tuneconfig()    Launch interactive tuning of parameters (GUI)
processfiles()         Process specified data files
clearsession() Clear variables (inputfiles, iraw, iq, sq, fq, gr)
plotdata()     Plot all or selected columns from a text data file
loaddata()     Load all or selected columns from a text data file
findfiles()    Search for files matching the specified patterns
clf()          Clear the current plot
exit()         Exit from the interactive shell
%pdfgetx3      Reset session
pdfgetter()    Get G(r) - allows step by step process
        pdfgetter.describe()                See options
        var = pdfgetter.getTransformation(N) Save step "N" to var
                                            N in the range 0 - 7
        tuneconfig([var, 'gr'])             Plot var with G(r)
```

Configuration parameters
Can be set directly in interactive mode - e.g.
```
print(config)           See config parameters on screen
print(config.var)       See only the "var" parameter value on screen
config.var = 3.0        Set the value 3.0 to the parameter named
"var"
```
*It is **necessary** to specify the "config." prior to the variable name*

Parameters where to use (real) numbers
```
wavelength    twothetazero  bgscale      rpoly
qmaxinst      qmin          qmax         rmin
rmax          rstep
```

Other parameters
```
configfile     "filename"
configsection  "filename"
dataformat     twotheta/QA/Qnm
inputfiles     ["filename"]
backgroundfile "filename"
datapath       ["path/to/files"]
output         ["basename"]
outputtypes    ["iq", "sq", "fq", "gr", "none"]
force          True/False
mode           xray/neutron/sas
composition    Aa 1.5 Bb 4.5 Cc
plot           ["iq", "sq", "fq", "gr"]
interact       True/False
verbose        None, error, warning, info, debug, all
```

Simple plotting

Use of the plotdata tool bundled with pdfgetx3
Also invocable from the interactive mode with plotdata()

```
plotdata FILENAME1 FILENAME2 ...    Plot data (overlay)
```

Find & select data
```
-f, --find     Plot files that matches a pattern
-l, --list     List files that matches a pattern
```

Plotting options
```
-x X    Select X column name or position (first is 0)
-y Y    Select Y columns name or positions
        First is 0. Ranges can be used as "start,stop,step"

-s STYLE, --style STYLE     Line / markers style (e.s. "--", "o")
                            See matplotlib manual.
-L LOG, --log LOG           Plot in logscale ("x", "y", "xy")
```

Other
```
-h, --help         See the help instructions
-V, --version      Program version
--manual           Online manual
```