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