spec2nexus Documentation

Release 1.g74a6e53.dirty

Pete R. Jemian

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Converts SPEC data files and scans into NeXus HDF5 files:

```
$ spec2nexus  path/to/file/specfile.dat
```

Writes `path/to/file/specfile.hdf5`

CHAPTER 1

Provides

- **spec2nexus** : command-line tool: Convert SPEC data files to NeXus HDF5
- **h5toText** : command-line tool: Print the structure of an HDF5 file
- **extractSpecScan** : command-line tool: Save columns from SPEC data file scan(s) to TSV files
- **spec** : library: python binding to read SPEC data files
- **eznx** : library: (Easy NeXus) supports writing NeXus HDF5 files using h5py
- **specplot** : command-line tool: plot a SPEC scan to an image file
- **specplot_gallery** : command-line tool: call **specplot** for all scans in a list of files, makes a web gallery

CHAPTER 2

Package Information

- **author**: Pete R. Jemian
- **email**: prjemian@gmail.com
- **copyright**: 2014-2017, Pete R. Jemian
- **license**: Creative Commons Attribution 4.0 International Public License (see LICENSE.txt file)
- **URL**: documentation: http://spec2nexus.readthedocs.io
- **git**: source: https://github.com/prjemian/spec2nexus
- **PyPI**: Distribution: https://pypi.python.org/pypi/spec2nexus/
- **OpenHub**: Compare open source software: https://www.openhub.net/p/spec2nexus
- **version**: 2017.711.0
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- **published**: Jul 11, 2017

Contents

spec2nexus

Converts SPEC data files and scans into NeXus HDF5 files.

How to use spec2nexus

Convert all scans in a SPEC data file:

```
$ spec2nexus  path/to/file/specfile.dat
```

Writes `path/to/file/specfile.hdf5` (Will not overwrite if the HDF5 exists, use the *-f* option to force overwrite).

show installed version

Verify the version of the installed spec2nexus:

```
$ spec2nexus  -v
2014.03.02
```

command-line options

```
user@host ~$ spec2nexus.py -h
usage: spec2nexus [-h] [-e HDF5_EXTENSION] [-f] [-v] [-s SCAN_LIST] [-t]
                  [--quiet | --verbose]
                  infile [infile ...]

spec2nexus: Convert SPEC data file into a NeXus HDF5 file.

positional arguments:
  infile                SPEC data file name(s)

optional arguments:
  -h, --help            show this help message and exit
  -e HDF5_EXTENSION, --hdf5-extension HDF5_EXTENSION
                        NeXus HDF5 output file extension, default = .hdf5
  -f, --force-overwrite
                        overwrite output file if it exists
  -v, --version         show program's version number and exit
  -s SCAN_LIST, --scan SCAN_LIST
                        specify which scans to save, such as: -s all or -s 1
                        or -s 1,2,3-5 (no spaces!), default = all
  --quiet                     suppress all program output (except errors), do not
                        use with --verbose option
  --verbose                   print more program output, do not use with --quiet
                        option
```

Note: Where's the source code to spec2nexus?

In the source code, the *spec2nexus* program is started from file **nexus.py** (in the *spec2nexus.nexus.main()* method, for those who look at the source code):

```
$ python nexus.py specfile.dat
```

You're not really going to call that from the source directory, are you? It will work, *if* you have put that source directory on your PYTHONPATH.

source code documentation

Converts SPEC data files and scans into NeXus HDF5 files

spec2nexus.nexus.**get_user_parameters**()
configure user's command line parameters from sys.argv

spec2nexus.nexus.**main**()
entry point for command-line interface

spec2nexus.nexus.**parse_scan_list_spec**(*scan_list_spec*)
parses the argument of the -s option, returns a scan number list

spec2nexus.nexus.**pick_scans**(*all_scans*, *opt_scan_list*)
edit opt_scan_list for the scans to be converted

To be converted, a scan number must be first specified in opt_scan_list and then all_scans is checked to make sure that scan exists. The final list is returned.

h5toText

Command line tool to print the structure of an HDF5 file

Caution: h5toText is deprecated

The same capability as *h5toText* is being built into the *punx*[1] project. When that project has its initial release, the *h5toText* code will be removed from *spec2nexus*.

How to use h5toText

Print the HDF5 tree of a file:

```
$ h5toText  path/to/file/hdf5/file.hdf5
```

the usage message:

```
[linux,511]$ h5toText
usage: h5toText [-h] [-n NUM_DISPLAYED] [-V] infile [infile ...]
h5toText: error: too few arguments
```

the version number:

```
[linux,511]$ h5toText -v
2014.03.07
```

the help message:

```
[linux,512]$ h5toText -h
usage: h5toText [-h] [-n NUM_DISPLAYED] [-V] infile [infile ...]

Print the structure of an HDF5 file

positional arguments:
  infile            HDF5 data file name(s)

optional arguments:
  -h, --help        show this help message and exit
```

[1] *punx*: http://punx.readthedocs.io

```
  -n NUM_DISPLAYED  limit number of displayed array items to NUM_DISPLAYED
                    (must be 3 or more or 'None'), default = None
  -a                Do not print attributes
  -v, --version     show program's version number and exit
```

Example

Here's an example from a test data file (**writer_1_3.h5** from the NeXus documentation[2]):

```
  [linux,512]$ h5toText data/writer_1_3.h5
  data/writer_1_3.h5 : NeXus data file
    @default = Scan
    Scan:NXentry
      @NX_class = NXentry
      @default = data
      data:NXdata
        @NX_class = NXdata
        @signal = counts
        @axes = two_theta
        @two_theta_indices = 0
        counts:NX_INT32[31] = __array
          __array = [1037, 1318, 1704, '...', 1321]
          @units = counts
        two_theta:NX_FLOAT64[31] = __array
          __array = [17.926079999999999, 17.925909999999998, 17.925750000000001, '...
↪', 17.92108]
          @units = degrees
```

---

source code documentation

Command line tool to print the structure of an HDF5 file (deprecated, planned for deletion, see docs)

DEPRECATION NOTICE:

The *h5toText* code in *spec2nexus* is being replaced by the same capability in the *punx* project.[3] Once the *punx* project is ready for initial release, the *h5toText* code will be removed from *sxpec2nexus*.

class spec2nexus.h5toText.**H5toText**(*filename*)

Example usage showing default display:

```
mc = H5toText(filename)
mc.array_items_shown = 5
show_attributes = False
txt = mc.report(show_attributes)
```

report(*show_attributes=True*)

return the structure of the HDF5 file in a list of strings

The work of parsing the datafile is done in this method.

spec2nexus.h5toText.**do_filelist**(*filelist*, *limit=5*, *show_attributes=True*)

interpret and print the structure of a list of HDF5 files

[2] writer_1_3 from NeXus: http://download.nexusformat.org/doc/html/examples/h5py/writer_1_3.html

[3] *punx structure*: http://punx.readthedocs.io/en/latest/structure.html#structure

Parameters

- **filelist** (*[str]*) – one or more file names to be interpreted
- **limit** (*int*) – maximum number of array items to be shown (default = 5)

spec2nexus.h5toText.**isHdf5Dataset**(*obj*)
is *obj* an HDF5 Dataset?

spec2nexus.h5toText.**isHdf5ExternalLink**(*obj*)
is *obj* an HDF5 ExternalLink?

spec2nexus.h5toText.**isHdf5File**(*obj*)
is *obj* an HDF5 File?

spec2nexus.h5toText.**isHdf5Group**(*obj*)
is *obj* an HDF5 Group?

spec2nexus.h5toText.**isHdf5Link**(*obj*)
is *obj* an HDF5 Link?

spec2nexus.h5toText.**isNeXusDataset**(*obj*)
is *obj* a NeXus dataset?

spec2nexus.h5toText.**isNeXusFile**(*filename*)
is *filename* is a NeXus HDF5 file?

Tests if `filename` adheres to either "Associating plottable data using attributes applied to the **NXdata** group" (needs URL - NeXus manual is not yet ready to provide it) or "Associating plottable data by name using the `axes` attribute" (needs URL - again, from NeXus manual) or "Associating plottable data by dimension number using the `axis` attribute" (needs URL - again, from NeXus manual)

spec2nexus.h5toText.**isNeXusFile_ByAxes**(*filename*)
is *filename* is a NeXus HDF5 file?

This has been, to date, the most common method in NeXus to define the default plot.

In short, verify this NeXus classpath exists:

```
/NXentry/NXdata/dataset/@signal=1
```

Tests for the existence of any NXentry group containing any NXdata group containing a single dataset with signal=1 attribute (allows either integer or text representation). This is the minimum requirement for a NeXus data file.

This method ignores any exceptions incurred.

spec2nexus.h5toText.**isNeXusFile_ByAxisAttr**(*filename*)
is *filename* is a NeXus HDF5 file?

This is the oldest method in NeXus to define the default plot.

NOTE: **Not implemented yet!**

spec2nexus.h5toText.**isNeXusFile_ByNXdataAttrs**(*filename*)
is *filename* is a NeXus HDF5 file?

This is the "NIAC2014" method. In short, verify these NeXus classpaths exist:

```
/@default={entry_group}
/{entry_group}:NXentry/@default={data_group}
/{entry_group}:NXentry/{data_group}:NXdata
/{entry_group}:NXentry/{data_group}:NXdata/@signal={signal_dataset}
/{entry_group}:NXentry/{data_group}:NXdata/{signal_dataset}
```

```
/{entry_group}:NXentry/{data_group}:NXdata/@axes=["{axes_dataset1}", ...]
/{entry_group}:NXentry/{data_group}:NXdata/@{axes_dataset1}_indices=int[]
...
```

where curly braces ({ and }) denote that the enclosed name is defined in the data file.

spec2nexus.h5toText.**isNeXusGroup**(*obj*, *NXtype*)
is *obj* a NeXus group?

spec2nexus.h5toText.**isNeXusLink**(*obj*)
is *obj* linked to another NeXus item?

spec2nexus.h5toText.**main**()
standard command-line interface

extractSpecScan

Command line tool to extract scan data from a SPEC data file.

How to use extractSpecScan

Extract one scan from a SPEC data file:

```
user@host ~$ extractSpecScan data/APS_spec_data.dat -s 1 -c mr USAXS_PD I0 seconds
```

the usage message:

```
user@host ~$ extractSpecScan
usage: extractSpecScan [-h] [-v] [--nolabels] -s SCAN [SCAN ...] -c COLUMN
                       [COLUMN ...] [-G] [-P] [-Q] [-V] [--quiet | --verbose]
                       spec_file
```

the version number:

```
user@host ~$ extractSpecScan -v
2017.0201.0
```

the help message:

```
user@host ~$ extractSpecScan -h
usage: extractSpecScan [-h] [-v] [--nolabels] -s SCAN [SCAN ...] -c COLUMN
                       [COLUMN ...] [-G] [-P] [-Q] [-V] [--quiet | --verbose]
                       spec_file

Save columns from SPEC data file scan(s) to TSV files URL:
http://spec2nexus.readthedocs.org/en/latest/extractSpecScan.html v2016.1025.0

positional arguments:
  spec_file             SPEC data file name(s)

optional arguments:
  -h, --help            show this help message and exit
  -v, --version         print version number and exit
  --nolabels            do not write column labels to output file (default:
                        write labels)
  -s SCAN [SCAN ...], --scan SCAN [SCAN ...]
```

```
                        scan number(s) to be extracted (must specify at least
                        one)
  -c COLUMN [COLUMN ...], --column COLUMN [COLUMN ...]
                        column label(s) to be extracted (must specify at least
                        one)
  -G                    report scan Geometry (#G) header information
  -P                    report scan Positioners (#O & #P) header information
  -Q                    report scan Q (#Q) header information
  -V                    report scan (UNICAT-style #H & #V) header information
  --quiet               suppress all program output (except errors), do not
                        use with --verbose option
  --verbose             print more program output, do not use with --quiet
                        option
```

Example

Extract four columns (mr, USAXS_PD, I0, seconds) from two scans (1, 6) in a SPEC data file:

```
$ extractSpecScan data/APS_spec_data.dat -s 1 6 -c mr USAXS_PD I0 seconds

program: /path/to/extractSpecScan.py
read: data/APS_spec_data.dat
wrote: data/APS_spec_data_1.dat
wrote: data/APS_spec_data_6.dat
```

Here's the contents of *data/APS_spec_data_6.dat*:

```
# mr  USAXS_PD I0 seconds
15.61017 9.0   243.0 0.3
15.61 13.0  325.0 0.3
15.60984 19.0  460.0 0.3
15.60967 30.0  609.0 0.3
15.6095  54.0  883.0 0.3
15.60934 161.0 1780.0   0.3
15.60917 499.0 3649.0   0.3
15.609   1257.0   6588.0   0.3
15.60884 2832.0   10245.0  0.3
15.60867 7294.0   13118.0  0.3
15.6085  139191.0 16527.0  0.3
15.60834 299989.0 17893.0  0.3
15.60817 299989.0 18276.0  0.3
15.608   299989.0 18240.0  0.3
15.60784 299989.0 18266.0  0.3
15.60767 299989.0 18616.0  0.3
15.6075  299989.0 19033.0  0.3
15.60734 299989.0 19036.0  0.3
15.60717 299988.0 18587.0  0.3
15.607   299989.0 17471.0  0.3
15.60684 123003.0 14814.0  0.3
15.60667 11060.0  11861.0  0.3
15.6065  2217.0   8131.0   0.3
15.60634 637.0 4269.0   0.3
15.60617 254.0 2632.0   0.3
15.606   132.0 1927.0   0.3
15.60584 79.0  1406.0   0.3
15.60567 58.0  1075.0   0.3
```

```
15.6055  32.0  695.0 0.3
15.60534 17.0  374.0 0.3
15.60517 10.0  245.0 0.3
```

source code documentation

Save columns from SPEC data file scan(s) to TSV files

Note: TSV: tab-separated values

Usage:

```
extractSpecScan.py /tmp/CeCoIn5 -s 5 -c HerixE Ana5 ICO-C
extractSpecScan.py ./testdata/11_03_Vinod.dat   -s 2 12   -c USAXS.m2rp Monitor  I0
```

Note: sdpecified column names **MUST** appear in all chosen scans

Compatible with Python 2.7+

spec2nexus.extractSpecScan.**get_user_parameters**()
configure user's command line parameters from sys.argv

spec2nexus.extractSpecScan.**main**()
read the data file, find each scan, find the columns, save the data

Parameters **cmdArgs** (*[str]*) – Namespace from argparse, returned from get_user_parameters()

Note: Each column label must match *exactly* the name of a label in each chosen SPEC scan number or the program will skip that particular scan

If more than one column matches, the first match will be selected.

example output:

```
# mr     I0     USAXS_PD
1.9475     65024     276
1.9725     64845     352
1.9975     65449     478
```

spec2nexus.extractSpecScan.**makeOutputFileName**(*specFile*, *scanNum*)
return an output file name based on specFile and scanNum

Parameters

- **specFile** (*str*) – name of existing SPEC data file to be read
- **scanNum** (*str*) – number of chosen SPEC scan

append scanNum to specFile to get output file name (before file extension if present)

Always add a file extension to the output file. If none is present, use ".dat".

Examples:

specFile	scanNum	outFile
CeCoIn5	scan 5	CeCoIn5_5.dat
CeCoIn5.dat	scan 77	CeCoIn5_77.dat
CeCoIn5.dat	scan 5.1	CeCoIn5_5_1.dat

specplot

Read a SPEC data file and plot a thumbnail image.

This code can be called as a standalone program or it can be imported into another program and called as a subroutine, as shown in the *specplot_gallery* program.

The standard representation of a SPEC scan is a line plot of the last data column *versus* the first data column. Any SPEC macro which name ends with *scan* ([1]) will be plotted as a line plot.

A special case SPEC scan macro is the *hklscan* where one of the three reciprocal space axes is scanned while the other two remain constant. A special handler (*SPEC's hklscan macro*) is provided to pick properly the scanned axis (not always the first column) for representation as a line plot.

Some SPEC macros scan two positioners over a grid to collect a 2-D image one pixel at a time. These scans are represented as color-mapped images where the first two columns are the vertical and horizontal axes and the image is color-mapped to intensity. Any SPEC macro which name ends with *mesh* will be plotted as an image plot.

Different handling can be customized for scan macros, as described in *How to write a custom scan handling for specplot*.

How to use *specplot*

Plot a scan from one of the sample data files supplied with *spec2nexus*:

```
user@host ~$ specplot src/spec2nexus/data/APS_spec_data.dat 2 specplot.png
```

Usage

```
user@host ~$ specplot
usage: specplot.py [-h] specFile scan_number plotFile
```

Help

```
user@host ~$ specplot -h
usage: specplot.py [-h] specFile scan_number plotFile

read a SPEC data file and plot scan n

positional arguments:
  specFile     SPEC data file name
  scan_number  scan number in SPEC file
  plotFile     output plot file name

optional arguments:
  -h, --help   show this help message and exit
```

[1] *scan*: any scan where the last four letters converted to lower case match *scan*, such as *ascan*, *a2scan*, *Escan*, *tscan*, *uascan*, *FlyScan*, *unusual_custom_user_scan*, ...

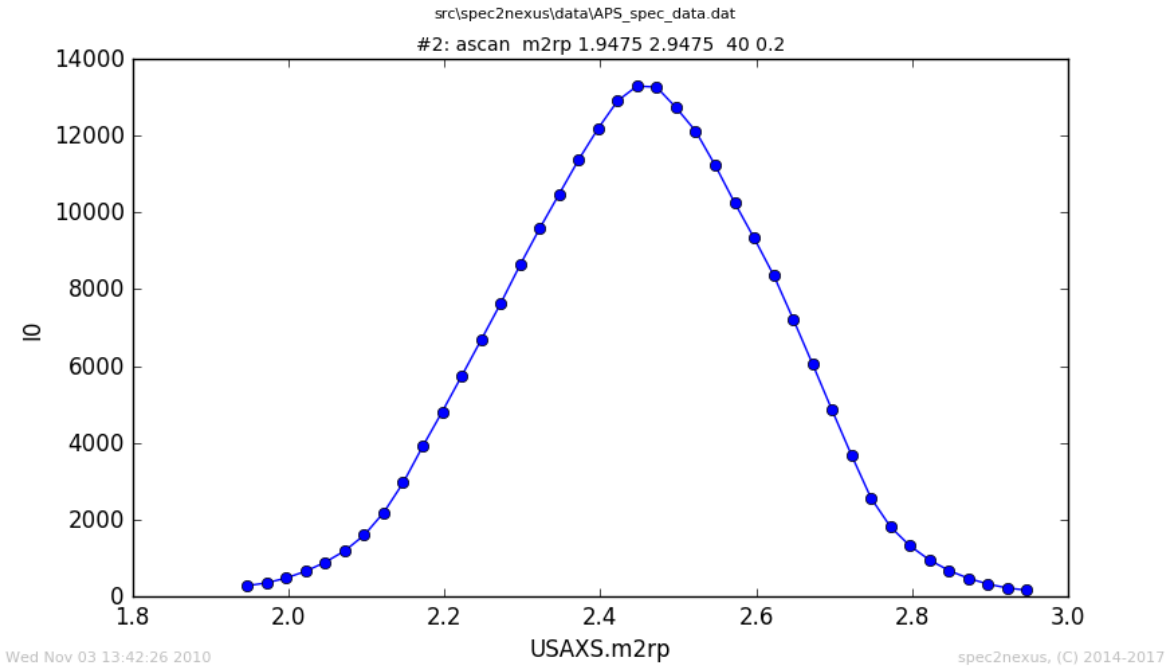

Fig. 2.1: Plot of scan #2 from example data file *APS_spec_data.dat*.

source code documentation

Plot the data from scan N in a SPEC data file

Selector()	associate SPEC scan macro names with image makers
ImageMaker()	superclass to handle plotting of data from a SPEC scan
LinePlotter()	create a line plot
MeshPlotter()	create a mesh plot (2-D image)
openSpecFile(specFile)	convenience routine so that others do not have to *import spec2nexus.spec*

Exceptions:

NoDataToPlot	Exception: scan aborted before any points gathered or data not present in SPEC file
NotPlottable	Exception: No plottable data for this scan
ScanAborted	Exception: Scan aborted before all points acquired
UnexpectedObjectTypeError	Exception: incorrect Python object type: programmer error

class spec2nexus.specplot.**HKLScanPlotter**
create a line plot from hklscan macros

retrieve_plot_data()
retrieve default data from spec data file

class spec2nexus.specplot.**ImageMaker**
superclass to handle plotting of data from a SPEC scan

Internal data model

Signal name of the 'signal' data (default data to be plotted)

Data values of various collected arrays {label: array}

Axes names of the axes of signal data

EXAMPLE

```
class LinePlotter(ImageMaker):
    'create a line plot'

    def make_image(self, plotFile):
        """
        make MatPlotLib chart image from the SPEC scan

        :param obj plotData: object returned from :meth:`retrieve_plot_data`
        :param str plotFile: name of image file to write
        """
        assert(self.signal in self.data)
        assert(len(self.axes) == 1)
        assert(self.axes[0] in self.data)

        y = self.data[self.signal]
        x = self.data[self.axes[0]]
        xy_plot(x, y,  plotFile,
               title = self.plot_title(),
               plot_subtitle = self.plot_subtitle(),
               xtitle = self.x_title(),
               ytitle = self.y_title(),
               xlog = self.x_log(),
               ylog = self.y_log(),
               timestamp_str = self.timestamp())

sfile = specplot.openSpecFile(specFile)
scan = sfile.getScan(scan_number)
plotter = LinePlotter()
plotter.plot_scan(scan, plotFile, y_log=True)
```

data_file_name()
the name of the file with the actual data

Usually, this is the SPEC data file but it *could* be something else

data_is_newer_than_plot(*plotFile*)
only proceed if mtime of SPEC data file is newer than plotFile

make_image(*plotFile*)
make MatPlotLib chart image from the SPEC scan

The data to be plotted are provided in:

- *self.signal*
- *self.axes*
- *self.data*

Parameters **plotFile** (*str*) – name of image file to write

plot_options()
re-define any plot options in a subclass

plot_scan(*scan*, *plotFile*, *maker=None*)
make an image plot of the data in the scan

Parameters

- **scan** (*obj*) – instance of *SpecDataFileScan*
- **plotFile** (*str*) – file name for plot output

plot_subtitle()
return the plot_subtitle

plot_title()
return the plot title

plottable()
can this data be plotted as expected?

retrieve_plot_data()
retrieve default plottable data from spec data file and store locally

This method must retrieve the data to be plotted, either from the SPEC data file scan or from a file which name is provided in the scan detalis.

These attributes must be set by this method:

Data dictionary containing values of the various collected arrays {label: array}

Signal name of the 'signal' data (default data to be plotted)

Axes names of the axes of signal data

Example data

```
self.data = {
    'angle': [1, 2, 3, 4, 5],
    'counts': [0. 2. 55. 3. 0]}
self.signal = 'counts'
self.axes = ['angle']
```

Raise any of these exceptions as appropriate:

NoDataToPlot	Exception: scan aborted before any points gathered or data not present in SPEC file
NotPlottable	Exception: No plottable data for this scan
ScanAborted	Exception: Scan aborted before all points acquired

set_plot_subtitle(*text*)
set the plot_subtitle

set_plot_title(*text*)
set the plot title

set_timestamp(*text*)
set the plot time stamp

set_x_log(*choice*)
set the x axis logarithmic if True

set_x_title(*text*)
set the x axis title

set_y_log(*choice*)
set the y axis logarithmic if True

set_y_title(*text*)
set the y axis title

set_z_log(*choice*)
set the z axis (image) logarithmic if True

timestamp()
return the time of this scan as a string

x_log()
boolean: should the X axis be plotted on a log scale?

x_title()
return the title for the X axis

y_log()
boolean: should the Y axis be plotted on a log scale?

y_title()
return the title for the Y axis

z_log()
boolean: should the Z axis (image) be plotted on a log scale?

class spec2nexus.specplot.**LinePlotter**
create a line plot

make_image(*plotFile*)
make MatPlotLib chart image from the SPEC scan

Parameters **plotFile** (*str*) – name of image file to write

plot_options()
define the settings for this, accepting any non-default values first

plottable()
can this data be plotted as expected?

retrieve_plot_data()
retrieve default data from spec data file

class spec2nexus.specplot.**MeshPlotter**
create a mesh plot (2-D image)

..rubric:: References:

Mesh 2-D parser http://www.certif.com/spec_help/mesh.html

```
mesh motor1 start1 end1 intervals1 motor2 start2 end2 intervals2 time
```

Hklmesh 2-D parser http://www.certif.com/spec_help/hklmesh.html

```
hklmesh Q1 start1 end1 intervals1 Q2 start2 end2 intervals2 time
```

make_image(*plotFile*)
make MatPlotLib chart image from the SPEC scan

Parameters **plotFile** (*str*) – name of image file to write

plot_options()
define the settings for this, accepting any non-default values first

plottable()
can this data be plotted as expected?

retrieve_plot_data()
retrieve default data from spec data file

exception spec2nexus.specplot.**NoDataToPlot**
Exception: scan aborted before any points gathered or data not present in SPEC file

exception spec2nexus.specplot.**NotPlottable**
Exception: No plottable data for this scan

exception spec2nexus.specplot.**ScanAborted**
Exception: Scan aborted before all points acquired

class spec2nexus.specplot.**Selector**
associate SPEC scan macro names with image makers

Image maker subclass of *ImageMaker*

To include a custom image maker from outside this module, create the subclass and then add it to an instance of this class. Such as this plotter that defaults to a logarithmic scale for the X axis for all *logxscan* macros:

from spec2nexus import specplot

class LogX_Plotter(specplot.ImageMaker):

def x_log(self): return True

...

selector = specplot.Selector() selector.add('logxscan', LogX_Plotter)

...

image_maker = specplot.Selector().auto(scan) plotter = image_maker() plotter.plot_scan(scan, fullPlotFile)

This class is a singleton which means you will always get the same instance when you call this class many times in your program.

auto(scan)	automatically choose a scan image maker based on the SPEC scan macro
add(key, value[, default])	register a new value by key
update(key, value[, default])	replace an existing key with a new value
get(key)	return a value by key
exists(key)	is the key known?
default()	retrieve the value of the default key

add(*key*, *value*, *default=False*)
register a new value by key

Parameters **key** (*str*) – name of key, typically the macro name

Raises

- **KeyError** – if key exists
- ***UnexpectedObjectTypeError*** – if value is not subclass of *ImageMaker*

auto(*scan*)
automatically choose a scan image maker based on the SPEC scan macro

Selection Rules:

•macro ends with "scan": use *LinePlotter*

•macro ends with "mesh": use *MeshPlotter*

•default: use default image maker (initially *LinePlotter*)

default()
retrieve the value of the default key

exists(*key*)
is the key known?

get(*key*)
return a value by key

Returns subclass of *ImageMaker* or *None* if key not found

update(*key*, *value*, *default=False*)
replace an existing key with a new value

Parameters **key** (*str*) – name of key, typically the macro name

Raises

- **KeyError** – if key does not exist
- ***UnexpectedObjectTypeError*** – if value is not subclass of *ImageMaker*

exception spec2nexus.specplot.**UnexpectedObjectTypeError**
Exception: incorrect Python object type: programmer error

spec2nexus.specplot.**openSpecFile**(*specFile*)
convenience routine so that others do not have to *import spec2nexus.spec*

specplot_gallery

Read a list of SPEC data files (or directory(s) containing SPEC data files) and plot images of all scans. *specplot_gallery* will store these images in subdirectories of the given base directory (default: current directory) based on this structure:

```
{base directory}
   /{year}
      /{month}
         /{spec file name}
             /index.html
              s00001.png
              s00002.png
```

The year and month are taken from the SPEC data file when the data were collected. The plot names include the scan numbers padded with leading zeroes to five places (so the file names sort numerically).

The results will be shown as a WWW page (*index.html*) of thumbnail images *and* a separate list of any scans that could not generate plots. A reason will accompany these scans, as shown in the example.

How to use *specplot_gallery*: command line

Here is an example:

```
user@host ~$ specplot_gallery -d ./__demo__ ../src/spec2nexus/data/33bm_spec.dat
```

Note that one of the scans could not be plotted. Looking at the data file, it shows there is *no data to plot* (this particular scan was aborted before any data was collected):

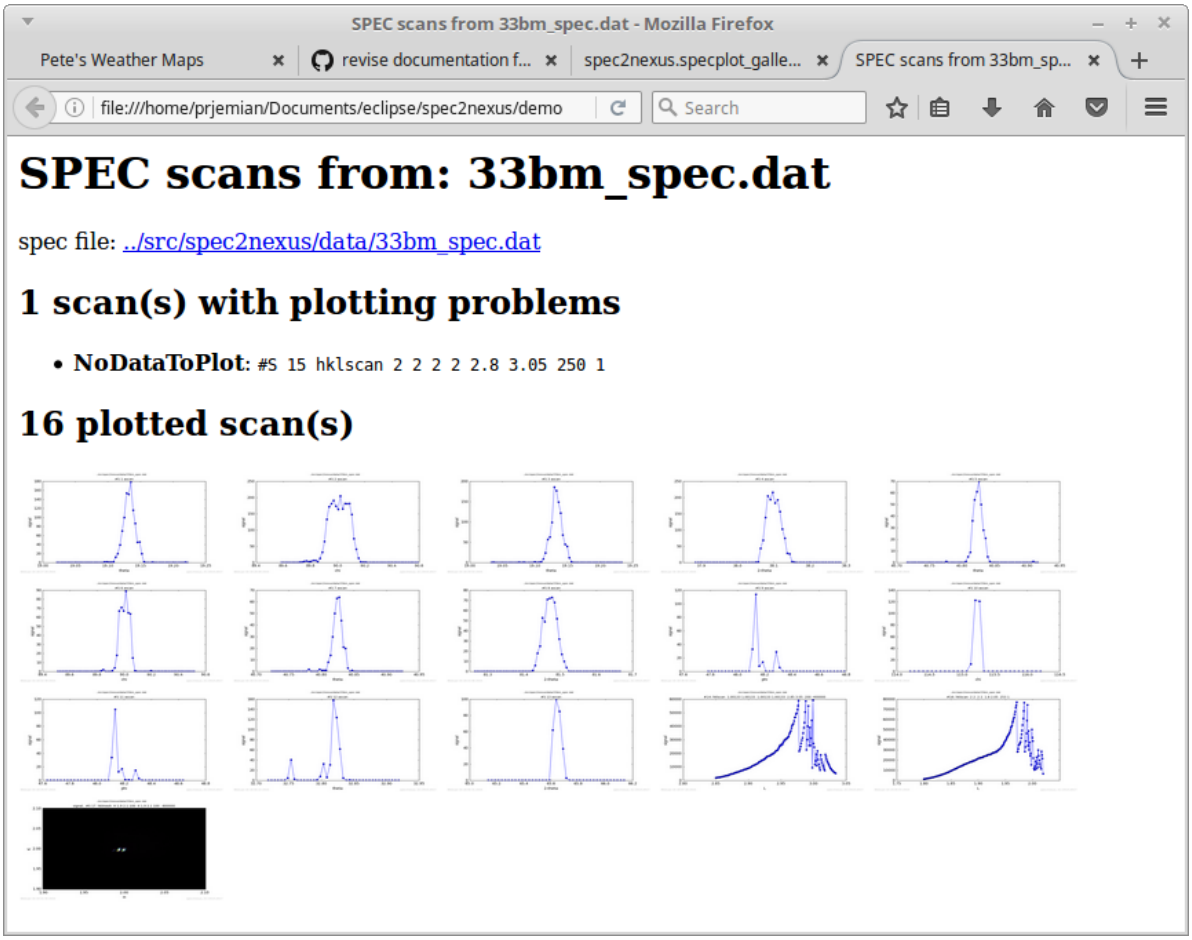

Fig. 2.2: Example of *specplot_gallery* showing scans from test file *33bm_spec.dat*.

```
#C Wed Jun 16 19:00:10 2010.  Scan aborted after 0 points.
```

The last scan shown is from a *hklmesh* (2-D) scan. It is mostly a constant background level, thus the large black area.

Each of the plots in the web page can be enlarged (by clicking on it).

How to use *specplot_gallery*: periodic background task (cron)

This script could be called from a Linux background task scheduler (*cron*) entry. To add the entry, type the *crontab -e* command which opens the task list in a screen editor and add lines such as these to the file:

```
# every five minutes (generates no output from outer script)
0-59/5 * * * *  /path/to/specplot_gallery.py -d /web/page/dir /spec/data/file/dirs
```

If the *specplot_gallery* script is called too frequently and the list of plots to be generated is large enough, it is possible for more than one process to be running. In one extreme case, many processes were found running due to problems with the data files. To identify and stop all processes of this program, use this on the command line:

```
kill -9 `ps -ef | grep python | awk '/specplot_gallery.py/ {print $2}' -`
```

source code documentation

read a list of SPEC data files (or directories) and plot images of all scans

DirectoryNotFoundError	Exception: The requested directory does not exist
PlotSpecFileScans(filelist[, plotDir, ...])	read a SPEC data file and plot thumbnail images of all its scans
Cache_File_Mtime(base_dir)	maintain a list of all known data file modification times
datePath(date)	convert the date into a path: yyyy/mm
get_SpecFileDate(specFile)	return the #D date of the SPEC data file or None
get_file_mtime(filename)	get the file modified time from disk
needToMakePlot(fullPlotFile, mtime_specFile)	Determine if a plot needs to be (re)made.
timestamp()	current time as yyyy-mm-dd hh:mm:ss
build_index_html(specFile, plotted_scans, ...)	build index.html content
logger(message)	log a message or report from this module

RESULT

The images are stored in files within a directory structure that is organized chronologically, such as: `yyyy/mm/spec_file/s1.png`. The root of the directory is either specified by the command line `-d` option or defaults to the current working directory. The `yyyy/mm` (year and month) are taken from the `#D` line of the SPEC data file. The `spec_file` is the file name with file extension and directory name removed. The image file names are derived from the scan numbers.

Linux CRON task

This script could be called from a *cron* entry, such as:

```
# every five minutes (generates no output from outer script)
0-59/5 * * * *  /some/directory/specplot_gallery.py -d /web/page/dir /spec/data/file/
↪dir
```

If this script is called too frequently and the list of plots to be generated is large enough, it is possible for more than one process to be running. In one extreme case, many processes were found running due to problems with the data files. To identify and stop all processes of this program:

```
kill -9 `ps -ef | grep python | awk '/specplot_gallery.py/ {print $2}' -`
```

class spec2nexus.specplot_gallery.**Cache_File_Mtime**(*base_dir*)
maintain a list of all known data file modification times

Parameters **base_dir** (*str*) – name of base directory to store output image thumbnails

This list will allow the code to avoid unnecessary work reparsing and plotting of unchanged SPEC data files.

get(*fname*)
get the file modified time from the cache

Parameters **fname** (*str*) – file name, already known to exist

Returns time (float) cached value of when fname was last modified or None if not known

read()
read the cache from storage

was_file_updated(*fname*)
compare the mtime between disk and cache

Parameters **fname** (*str*) – file name, already known to exist

Return bool True if file is newer than the cache (or new to the cache)

write()
write the cache to storage

exception spec2nexus.specplot_gallery.**DirectoryNotFoundError**
Exception: The requested directory does not exist

exception spec2nexus.specplot_gallery.**PathIsNotDirectoryError**
Exception: The path is not a directory

class spec2nexus.specplot_gallery.**PlotSpecFileScans**(*filelist*, *plotDir=None*, *reverse_chronological=False*)
read a SPEC data file and plot thumbnail images of all its scans

Parameters

- **filelist** (*[str]*) – list of SPEC data files to be checked
- **plotDir** (*str*) – name of base directory to store output image thumbnails

getBaseDir(*basename*, *date*)
find the path based on the date in the spec file

get_PngDir(*specFile*)
return the PNG directory based on the specFile

Parameters **specFile** (*str*) – name of SPEC data file (relative or absolute)

plot_all_scans(*specFile*)
plot all the recognized scans from the file named specFile

spec2nexus.specplot_gallery.**build_index_html**(*specFile*, *plotted_scans*, *problem_scans*)
build index.html content

Parameters

- **specFile** (*str*) – name of SPEC data file (relative or absolute)
- **plotList** (*[str]*) – list of HTML <*a*> elements, one for each plot image

spec2nexus.specplot_gallery.**datePath**(*date*)
convert the date into a path: yyyy/mm

Parameters **date** (*str*) – text date from SPEC file #D line: 'Thu Jun 19 12:21:55 2014'

spec2nexus.specplot_gallery.**developer**()
supply a file and a directory as command-line arguments to "paths"

spec2nexus.specplot_gallery.**get_SpecFileDate**(*specFile*)
return the #D date of the SPEC data file or None

Parameters **specFile** (*str*) – name of SPEC data file (relative or absolute)

spec2nexus.specplot_gallery.**get_file_mtime**(*filename*)
get the file modified time from disk

Parameters **fname** (*str*) – file name, already known to exist

Returns time (float) fname was last modified

spec2nexus.specplot_gallery.**logger**(*message*)
log a message or report from this module

Parameters **message** (*str*) – text to be logged

spec2nexus.specplot_gallery.**needToMakePlot**(*fullPlotFile*, *mtime_specFile*)
Determine if a plot needs to be (re)made. Use mtime as the basis.

Return bool `True` if plot should be made again

spec2nexus.specplot_gallery.**timestamp**()
current time as yyyy-mm-dd hh:mm:ss

Return str

spec2nexus.spec

Library of classes to read the contents of a SPEC data file.

How to use spec2nexus.spec

spec2nexus.spec provides Python support to read the scans in a SPEC data file. (It does not provide a command-line interface.) Here is a quick example how to use *spec*:

```
from spec2nexus.spec import SpecDataFile

specfile = SpecDataFile('data/33id_spec.dat')
print 'SPEC file name:', specfile.specFile
print 'SPEC file time:', specfile.headers[0].date
print 'number of scans:', len(specfile.scans)

for scanNum, scan in specfile.scans.items():
    print scanNum, scan.scanCmd
```

For one example data file provided with *spec2nexus.spec*, the output starts with:

```
SPEC file name: samplecheck_7_17_03
SPEC file time: Thu Jul 17 02:37:32 2003
number of scans: 106
1  ascan  eta 43.6355 44.0355  40 1
2  ascan  chi 73.47 73.87  40 1
3  ascan  del 84.6165 84.8165  20 1
4  ascan  del 84.5199 84.7199  20 1
5  ascan  del 84.3269 84.9269  30 1
...
```

How to read one scan

Here is an example how to read one scan:

```
from spec2nexus.spec import SpecDataFile

specfile = SpecDataFile('data/33id_spec.dat')
specscan = specfile.getScan(5)
print specscan.scanNum
print specscan.scanCmd
```

which has this output:

```
5
ascan  del 84.3269 84.9269  30 1
```

The data columns are provided in a dictionary. Using the example above, the dictionary is `specscan.data` where the keys are the column labels (from the #L line) and the values are from each row. It is possible to make a default plot of the last column vs. the first column. Here's how to find that data:

```
x_label = specscan.L[0]          # first column from #L line
y_label = specscan.L[-1]         # last column from #L line
x_data = specscan.data[x_label]  # data for first column
y_data = specscan.data[y_label]  # data for last column
```

Get a list of the scans

The complete list of scan numbers from the data file is obtained (sorting is necessary since the list of dictionary keys is returned in a scrambled order):

```
all_scans = sorted(specfile.scans.keys())
```

SPEC data files

The SPEC data file format is described in the SPEC manual.[1] This manual is taken as a suggested starting point for most users. Data files with deviations from this standard are produced at some facilities.

[1] SPEC manual: http://www.certif.com/spec_manual/user_1_4_1.html

Assumptions about data file structure

These assumptions are used to parse SPEC data files:

1. SPEC data files are text files organized by lines. The lines can be categorized as: **control lines**, **data lines**, and blank lines.

line type	description
control	contain a # character in the first column followed by a command word[2]
data	generally contain a row of numbers (the scan data)
special data	containing MCA data[3]

2. Lines in a SPEC data file start with a file name control line, then series of blocks. Each block may be either a file header block or a scan block. (Most SPEC files have only one header block. A new header block is created if the list of positioners is changed in SPEC without creating a new file. SPEC users are encouraged to *always* start a new data file after changing the list of positioners.) A block consists of a series of control, data, and blank lines.

   SPEC data files are composed of a sequence of a single file header block and zero or more scan blocks.[4]

3. A SPEC data file always begins with this control lines: #F, such as:

```
#F samplecheck_7_17_03
```

4. A file header block begins with these control lines in order: #E #D #C, such as:

```
#E 1058427452
#D Thu Jul 17 02:37:32 2003
#C psic  User = epix
```

5. A scan block begins with these command lines in order: #S #D, such as:

```
#S 78  ascan  del 84.6484 84.8484  20 1
#D Thu Jul 17 08:03:54 2003
```

Control lines (keys) defined by SPEC

Here is a list[5] of keys (command words) from the comments in the *file.mac* (SPEC v6) macro source file:

[2] See *Example of Control Lines*
[3] See *Example of MCA data lines*
[4] It is very unusual to have more than one file header block in a SPEC data file.
[5] Compare with *Supplied spec plugin modules*

command word	description
#C	comment line
#D date	current date and time in UNIX format
#E num	the UNIX epoch (seconds from 00:00 GMT 1/1/70)
#F name	name by which file was created
#G1 ...	geometry parameters from G[] array (geo mode, sector, etc)
#G2 ...	geometry parameters from U[] array (lattice constants, orientation reflections)
#G3 ...	geometry parameters from UB[] array (orientation matrix)
#G4 ...	geometry parameters from Q[] array (lambda, frozen angles, cut points, etc)
#I num	a normalizing factor to apply to the data
#j% ...	mnemonics of counter (% = 0,1,2,... with eight counters per row)
#J% ...	names of counters (each separated by two spaces)
#L s1 ...	labels for the data columns
#M num	data was counted to this many monitor counts
#N num [num2]	number of columns of data [num2 sets per row]
#o% ...	mnemonics of motors (% = 0,1,2,... with eight motors per row)
#O% ...	names of motors (each separated by two spaces)
#P% ...	positions of motors corresponding to above #O/#o
#Q	a reciprocal space position (H K L)
#R	user-defined results from a scan
#S num	scan number
#T num	data was counted for this many seconds
#U	user defined
#X	a temperature
#@MCA fmt	this scan contains MCA data (array_dump() format, as in `"%16C"`)
#@CALIB a b c	coefficients for `x[i] = a + b * i + c * i * i` for MCA data
#@CHANN n f l r	MCA channel information (number_saved, first_saved, last_saved, reduction coef)
#@CTIME p l r	MCA count times (preset_time, elapsed_live_time, elapsed_real_time)
#@ROI n f l	MCA ROI channel information (ROI_name, first_chan, last_chan)

Example of Control Lines

The command word of a control line may have a number at the end, indicating it is part of a sequence, such as these control lines (see *Control lines (keys) defined by SPEC* for how to interpret):

```
#D Wed Nov 03 13:42:03 2010
#T 0.3  (seconds)
#G0 0
#G1 0
#G3 0
#G4 0
#Q
#P0 -0.5396381 -0.5675 0.395862 0.7425 40.489861 0 5.894899e-07 11
#P1 24 0 -1.19 9.0028278 25.000378 -22.29064 1.5 5
#P2 -43 -0.01 98 11.8 0 -6.3275 111.52875 -8.67896
#P3 -0.11352 1e-05 0.199978 0.4001875 1.2998435 15.6077 0 0
#P4 3.03 0 3.21 6.805 2.835 2.4475 0.9355 -0.072
#P5 1.31 0.0875 2442.673 -0.391 12 -14.4125 15.498553
```

Example of MCA data lines

Lines with MCA array data begin with the **@A** command word. (If such a data line ends with a continuation character \, the next line is read as part of this line.)

This is an example of a 91-channel MCA data array with trivial (zero) values:

```
@A 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\
 0 0 0 0 0 0 0 0 0 0 0
```

Several MCA spectra may be written to a scan. In this case, a number follows **@A** indicating which spectrum, such as in this example with four spectra:

```
    @A1 0 0 0 0 0 0 35 0 0 35
    @A2 0 0 0 0 0 0 0 35 0 35
    @A3 0 0 35 35 0 0 0 0 0 0
    @A4 0 0 0 0 0 35 35 0 35 0
```

Supported header keys (command words)

The SPEC data file keys recognized by *spec* are listed in *Supplied spec plugin modules*.

---

source code summary

classes

SpecDataFile	contents of a spec data file
SpecDataFileHeader	contents of a spec data file header (#F) section
SpecDataFileScan	contents of a spec data file scan (#S) section

methods

strip_first_word	return everything after the first space on the line from the spec data file
is_spec_file	test if a given file name is a SPEC data file

exceptions

SpecDataFileNotFound	data file was not found
SpecDataFileCouldNotOpen	data file could not be opened
SpecDataFileNotFound	data file was not found
DuplicateSpecScanNumber	multiple use of scan number in a single SPEC data file

Continued on next page

Table 2.9 – continued from previous page

UnknownSpecFilePart	unknown part in a single SPEC data file

dependencies

os	OS routines for NT or Posix depending on what system we're on.
re	Support for regular expressions (RE).
sys	This module provides access to some objects used or maintained by the interpreter and to functions that interact strongly with the interpreter.

internal structure of spec2nexus.spec.SpecDataFileScan

The internal variables of a Python class are called *attributes*. It may be convenient, for some, to think of them as *variables*.

scan attributes

parent *obj* - instance of *spec2nexus.spec.SpecDataFile*

scanNum *int* - SPEC scan number

scanCmd *str* - SPEC command line

raw *str* - text of scan, as reported in SPEC data file

scan attributes (variables) set after call to plugins

These attributes are only set *after* the scan's `interpret()` method is called. This method is called automatically when trying to read any of the following scan attributes:

comments *[str]* - list of all comments reported in this scan

data *{label,[number]}* - written by *spec2nexus.plugins.spec_common_spec2nexus.data_lines_postprocessing()*

data_lines *[str]* - raw data (and possibly MCA) lines with comment lines removed

date *str* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_Date*

G *{key,[number]}* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_Geometry*

I *float* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_NormalizingFactor*

header *obj* - instance of *spec2nexus.spec.SpecDataFileHeader*

L *[str]* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_Labels*

M *str* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_Monitor*

positioner *{key,number}* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_Positioners.postprocess*

N *[int]* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_NumColumns*

P *[str]* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_Positioners*

Q *[number]* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_HKL*

S *str* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_Scan*

T *str* - written by *spec2nexus.plugins.spec_common_spec2nexus.SPEC_CountTime*

V *{key,number|str}* - written by *spec2nexus.plugins.unicat_spec2nexus.UNICAT_MetadataValues*

column_first *str* - label of first (ordinate) data column

column_last *str* - label of last (abscissa) data column

internal use only - do not modify

These scan attributes are for internal use only and are not part of the public interface. Do not modify them or write code that depends on them.

postprocessors *{key,obj}* - dictionary of postprocessing methods

h5writers *{key,obj}* - dictionary of methods that write HDF5 structure

__lazy_interpret__ *bool* - Is *lazy* (on-demand) call to `interpret()` needed?

__interpreted__ *bool* - Has `interpret()` been called?

source code documentation

Provides a set of classes to read the contents of a SPEC data file.

author Pete Jemian

email jemian@anl.gov

SpecDataFile() is the only class users will need to call. All other *spec* classes are called from this class. The *read()* method is called automatically.

The user should create a class instance for each spec data file, specifying the file reference (by path reference as needed) and the internal routines will take care of all that is necessary to read and interpret the information.

Note that the SPEC geometry control lines (`#G0 #G1 ...`) have meanings that are unique to specific diffractometer geometries including different numbers of values. Consult the geometry macro file for specifics.

Examples

Get the first and last scan numbers from the file:

```
>>> from spec2nexus import spec
>>> spec_data = spec.SpecDataFile('path/to/my/spec_data.dat')
>>> print spec_data.fileName
path/to/my/spec_data.dat
>>> print 'first scan: ', spec_data.getFirstScanNumber()
1
```

```
>>> print 'last scan: ', spec_data.getLastScanNumber()
22
```

Get plottable data from scan number 10:

```
>>> from spec2nexus import spec
>>> spec_data = spec.SpecDataFile('path/to/my/spec_data.dat')
>>> scan10 = spec_data.getScan(10)
>>> x_label = scan10.L[0]
>>> y_label = scan10.L[-1]
>>> x_data = scan10.data[x_label]
>>> y_data = scan10.data[y_label]
```

Try to read a file that does not exist:

```
>>> spec_data = spec.SpecDataFile('missing_file')
Traceback (most recent call last):
  ...
spec.SpecDataFileNotFound: file does not exist: missing_file
```

Classes and Methods

exception spec2nexus.spec.**DuplicateSpecScanNumber**
multiple use of scan number in a single SPEC data file

exception spec2nexus.spec.**NotASpecDataFile**
content of file is not SPEC data (first line must start with #F)

class spec2nexus.spec.**SpecDataFile**(*filename*)
contents of a spec data file

getFirstScanNumber()
return the first scan

getLastScanNumber()
return the last scan

getMaxScanNumber()
return the highest numbered scan

getMinScanNumber()
return the lowest numbered scan

getScan(*scan_number=0*)
return the scan number indicated, None if not found

getScanCommands(*scan_list=None*)
return all the scan commands as a list, with scan number

getScanNumbers()
return a list of all scan numbers sorted by scan number

getScanNumbersChronological()
return a list of all scan numbers sorted by date

read()
Reads and parses a spec data file

exception spec2nexus.spec.**SpecDataFileCouldNotOpen**
data file could not be opened

class spec2nexus.spec.**SpecDataFileHeader**(*buf*, *parent=None*)
contents of a spec data file header (#F) section

addH5writer(*label*, *func*)
add a function to be processed when writing the scan header

Parameters

- **label** (*str*) – unique label by which this writer will be known
- **func** (*obj*) – function reference of writer

The writers will be called when the HDF5 file is to be written.

addPostProcessor(*label*, *func*)
add a function to be processed after interpreting all lines from a header

Parameters

- **label** (*str*) – unique label by which this postprocessor will be known
- **func** (*obj*) – function reference of postprocessor

The postprocessors will be called at the end of header interpretation.

interpret()
interpret the supplied buffer with the spec data file header

exception spec2nexus.spec.**SpecDataFileNotFound**
data file was not found

class spec2nexus.spec.**SpecDataFileScan**(*header*, *buf*, *parent=None*)
contents of a spec data file scan (#S) section

addH5writer(*label*, *func*)
add a function to be processed when writing the scan data

Parameters

- **label** (*str*) – unique label by which this writer will be known
- **func** (*obj*) – function reference of writer

The writers will be called when the HDF5 file is to be written.

addPostProcessor(*label*, *func*)
add a function to be processed after interpreting all lines from a scan

Parameters

- **label** (*str*) – unique label by which this postprocessor will be known
- **func** (*obj*) – function reference of postprocessor

The postprocessors will be called at the end of scan data interpretation.

add_interpreter_comment(*comment*)
allow the interpreter to communicate information to the caller

see issue #66: https://github.com/prjemian/spec2nexus/issues/66

get_interpreter_comments()
return the list of comments

see issue #66: https://github.com/prjemian/spec2nexus/issues/66

get_macro_name()
name of the SPEC macro used for this scan

interpret()
interpret the supplied buffer with the spec scan data

exception spec2nexus.spec.**UnknownSpecFilePart**
unknown part in a single SPEC data file

spec2nexus.spec.**is_spec_file**(*filename*)
test if a given file name is a SPEC data file

Parameters **filename** (*str*) – path/to/possible/spec/data.file

filename is a SPEC file only if the file starts[6] with these control lines in order:

- #F - original filename
- #E - the UNIX epoch (seconds from 00:00 GMT 1/1/70)
- #D - current date and time in UNIX format
- #C - comment line (the first one provides the filename again and the user name)

such as:

```
#F LNO_LAO
#E 1276730676
#D Wed Jun 16 18:24:36 2010
#C LNO_LAO  User = epix33bm
```

spec2nexus.charts

source code documentation

charting for spec2nexus

make_png(image, image_file[, axes, title, ...])	read the image from the named HDF5 file and make a PNG file
xy_plot(x, y, plot_file[, title, subtitle, ...])	with MatPlotLib, generate a plot of a scan (as if data from a scan in a SPEC file)

spec2nexus.charts.**make_png**(*image*, *image_file*, *axes=None*, *title='2-D data'*, *subtitle=''*, *log_image=False*, *hsize=9*, *vsize=5*, *cmap='cubehelix'*, *xtitle=None*, *ytitle=None*, *timestamp_str=None*)
read the image from the named HDF5 file and make a PNG file

Test that the HDF5 file exists and that the path to the data exists in that file. Read the data from the named dataset, mask off some bad values, convert to log(image) and use Matplotlib to make the PNG file.

Parameters

- **image** (*obj*) – array of data to be rendered
- **image_file** (*str*) – name of image file to be written (path is optional)
- **log_image** (*bool*) – plot log(image)
- **hsize** (*int*) – horizontal size of the PNG image (default: 7)

[6] SPEC manual, *Standard Data File Format*, http://www.certif.com/spec_manual/user_1_4_1.html

- **hsize** – vertical size of the PNG image (default: 3)
- **cmap** (*str*) – colormap for the image (default: 'cubehelix'), 'jet' is another good one

Return str *image_file*

The HDF5 file could be a NeXus file, or some other layout.

spec2nexus.charts.**xy_plot**(*x*, *y*, *plot_file*, *title=None*, *subtitle=None*, *xtitle=None*, *ytitle=None*, *xlog=False*, *ylog=False*, *hsize=9*, *vsize=5*, *timestamp_str=None*)

with MatPlotLib, generate a plot of a scan (as if data from a scan in a SPEC file)

Parameters

- **x** (*[float]*) – horizontal axis data
- **y** (*[float]*) – vertical axis data
- **plot_file** (*str*) – file name to write plot image
- **xtitle** (*str*) – horizontal axis label (default: not shown)
- **ytitle** (*str*) – vertical axis label (default: not shown)
- **title** (*str*) – title for plot (default: date time)
- **subtitle** (*str*) – subtitle for plot (default: not shown)
- **xlog** (*bool*) – should X axis be log (default: False=linear)
- **ylog** (*bool*) – should Y axis be log (default: False=linear)
- **timestamp_str** (*str*) – date to use on plot (default: now)

Tip: when using this module as a background task ...

MatPlotLib has several interfaces for plotting. Since this module runs as part of a background job generating lots of plots, MatPlotLib's standard `plt` code is not the right model. It warns after 20 plots and will eventually run out of memory.

Here's the fix used in this module: http://stackoverflow.com/questions/16334588/create-a-figure-that-is-reference-counted/16337909#16337909

How to write a custom scan handling for *specplot*

Sometimes, it will be obvious that a certain scan macro never generates any plot images, or that the default handling creates a plot that is a poor representation of the data, such as the *hklscan* where only one of the the axes *hkl* is scanned. To pick the scanned axis for plotting, it is necessary to prepare custom handling and replace the default handling.

Overview

It is possible to add in additional handling by writing a Python module. This module creates a subclass of the standard handling, such as *LinePlotter*, *MeshPlotter*, or their superclass *ImageMaker*. The support is added to the macro selection class *Selector* with code such as in the brief example described below: *Change the plot title text in ascan macros*:

```
selector = spec2nexus.specplot.Selector()
selector.add('ascan', Custom_Ascan)
spec2nexus.specplot_gallery.main()
```

Data Model

The data to be plotted is kept in an appropriate subclass of `PlotDataStructure` in attributes show in the next table. The data model is an adaptation of the NeXus *NXdata* base class.[1]

attribute	description
self.signal	name of the dependent data (*y* axis or image) to be plotted
self.axes	list of names of the independent axes[2]
self.data	dictionary with the data, indexed by name

Steps

In all cases, custom handling of a specific SPEC macro name is provided by creating a subclass of *ImageMaker* and defining one or more of its methods. In the simplest case, certain settings may be changed by calling `spec2nexus.specplot.ImageMaker.configure()` with the custom values. Examples of further customization are provided below, such as when the data to be plotted is stored outside of the SPEC data file. This is common for images from area detectors.

It may also be necessary to create a subclass of `PlotDataStructure` to gather the data to be plotted or override the default *spec2nexus.specplot.ImageMaker.plottable()* method. An example of this is shown with the *MeshPlotter* and associated `MeshStructure` classes.

Examples

A few exmaples of custom macro handling are provided, some simple, some complex. In each example, decisions have been made about where to provide the desired features.

Change the plot title text in *ascan* macros

The SPEC *ascan* macro is a workhorse and records the scan of a positioner and the measurement of data in a counter. Since this macro name ends with "scan", the default selection in *specplot* images this data using the *LinePlotter* class. Here is a plot of the default handling of data from the *ascan* macro:

We will show how to change the plot title as a means to illustrate how to customize the handling for a scan macro.

We write `Custom_Ascan` which is a subclass of *LinePlotter*. The `get_plot_data` method is written (overrides the default method) to gain access to the place where we can introduce the change. The change is made by the call to the `configure` method (defined in the superclass). Here's the code:

ascan.py example

```
#!/usr/bin/env python

#-----------------------------------------------------------------------------
# :author:    Pete R. Jemian
# :email:     prjemian@gmail.com
# :copyright: (c) 2014-2017, Pete R. Jemian
#
# Distributed under the terms of the Creative Commons Attribution 4.0 International␣
↪Public License.
```

[1] NeXus *NXdata* base class: http://download.nexusformat.org/doc/html/classes/base_classes/NXdata.html

[2] The number of names provided in *self.axes* is equal to the *rank* of the *signal* data (*self.data[self.signal]*). For 1-D data, *self.axes* has one name and the *signal* data is one-dimensional. For 2-D data, *self.axes* has two names and the *signal* data is two-dimensional.

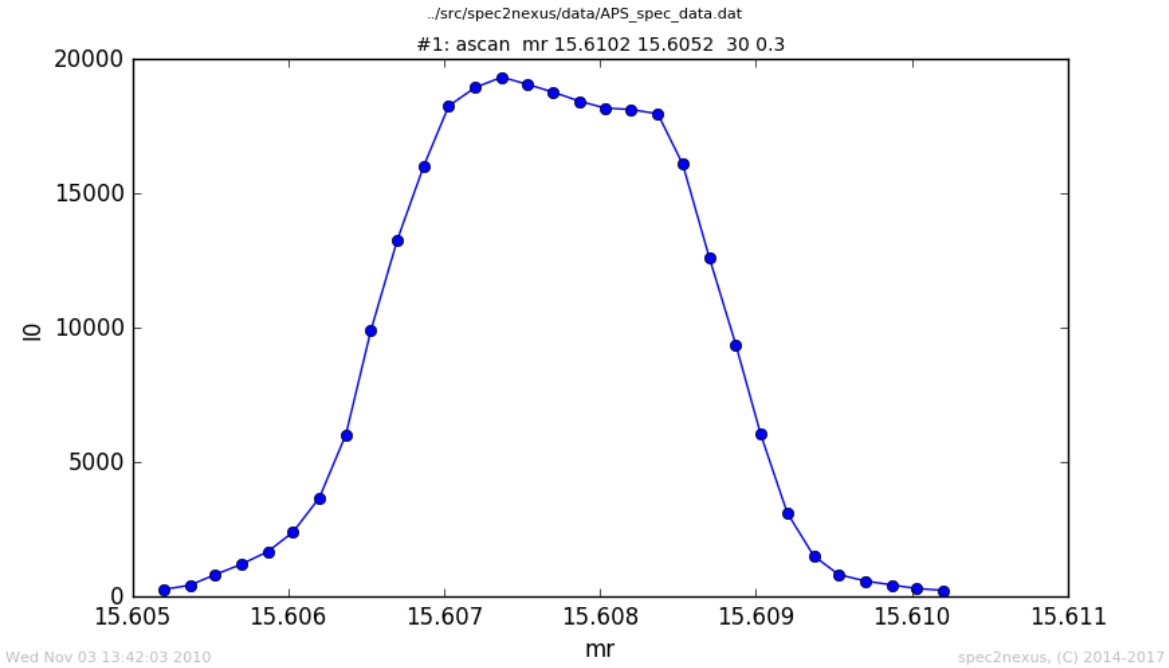

Fig. 2.3: Standard plot of data from *ascan* macro

```
#
# The full license is in the file LICENSE.txt, distributed with this software.
#-----------------------------------------------------------------------------

'''
Plot all scans that used the SPEC `ascan` macro, showing only the scan number (not␣
↪full scan command)

This is a simple example of how to customize the scan macro handling.
There are many more ways to add complexity.
'''

import spec2nexus.specplot
import spec2nexus.specplot_gallery


class Custom_Ascan(spec2nexus.specplot.LinePlotter):
    '''simple customization'''

    def retrieve_plot_data(self):
        '''substitute with the data&time the plot was created'''
        import datetime
        spec2nexus.specplot.LinePlotter.retrieve_plot_data(self)
        self.set_plot_subtitle(str(datetime.datetime.now()))


def main():
    selector = spec2nexus.specplot.Selector()
    selector.add('ascan', Custom_Ascan)
    spec2nexus.specplot_gallery.main()

```

```

if __name__ == '__main__':
    main()
```

See the changed title:

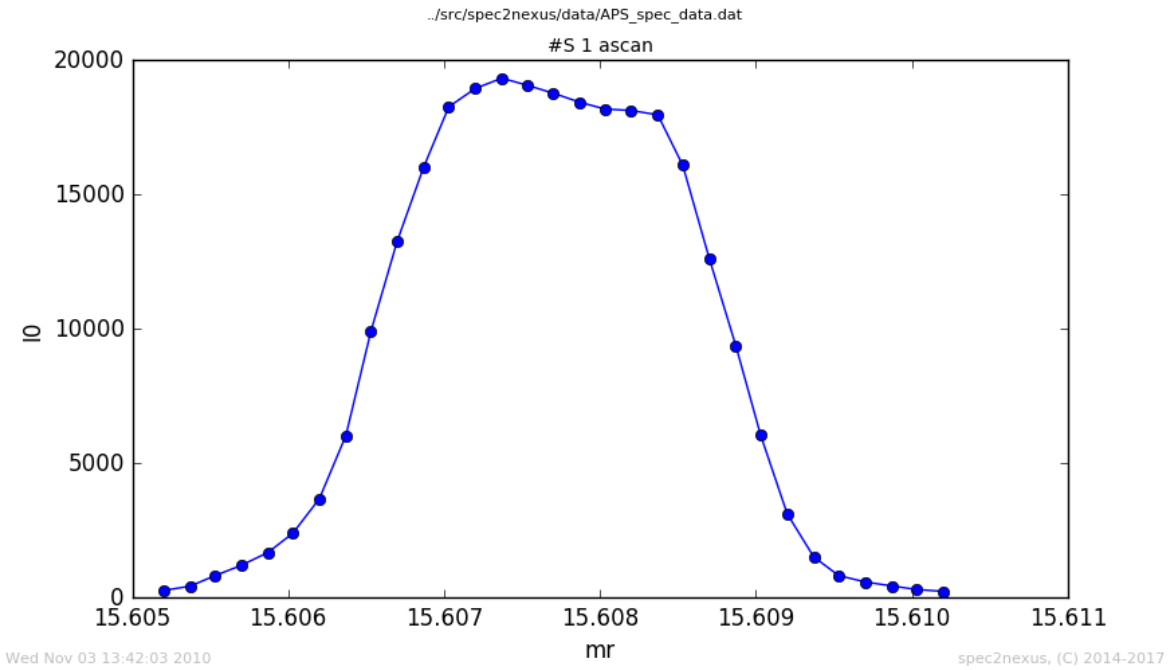

Fig. 2.4: Customized plot of data from *ascan* macro

Make the *y*-axis log scale

A very simple customization can make the Y axis to be logarithmic scale. (This customization is planned for an added feature[3] in a future relase of the *spec2nexus* package.) We present two examples.

modify handling of *a2scan*

One user wants all the *a2scan* images to be plotted with a logarithmic scale on the Y axis. Here's the code:

custom_a2scan_gallery.py example

```
#!/usr/bin/env python

'''
Customization for specplot_gallery: plot a2scan with log(y) axis

This program changes the plotting for all scans that used the *a2scan* SPEC macro.
The Y axis of these plots will be plotted as logarithmic if all the data values are
```

[3] specplot: add option for default log(signal)

```
greater than zero.  Otherwise, the Y axis scale will be linear.
'''

import spec2nexus.specplot
import spec2nexus.specplot_gallery

class Custom_a2scan_Plotter(spec2nexus.specplot.LinePlotter):
    '''plot `a2scan` y axis as log if possible'''

    def retrieve_plot_data(self):
        '''plot the vertical axis on log scale'''
        spec2nexus.specplot.LinePlotter.retrieve_plot_data(self)

        choose_log_scale = False

        if self.signal in self.data:    # log(y) if all data positive
            choose_log_scale = min(self.data[self.signal]) > 0

        self.set_y_log(choose_log_scale)


def main():
    selector = spec2nexus.specplot.Selector()
    selector.add('a2scan', Custom_a2scan_Plotter)
    spec2nexus.specplot_gallery.main()


if __name__ == '__main__':
    # debugging_setup()
    main()

'''
Instructions:

Save this file in a directory you can write and call it from your cron tasks.

Note that in cron entries, you cannot rely on shell environment variables to
be defined.  Best to spell things out completely.  For example, if your $HOME
directory is `/home/user` and you have these directories:

* `/home/user/bin`: various custom executables you use
* `/home/user/www/specplots`: a directory you access with a web browser for your plots
* `/home/user/spec/data`: a directory with your SPEC data files

then save this file to `/home/user/bin/custom_a2scan_gallery.py` and make it␣
↪executable
(using `chmod +x ./home/user/bin/custom_a2scan_gallery.py`).

Edit your list of cron tasks using `crontab -e` and add this (possibly
replacing a call to `specplot_gallery` with this call `custom_a2scan_gallery.py`)::

    # every five minutes (generates no output from outer script)
    0-59/5 * * * *  /home/user/bin/custom_a2scan_gallery.py -d /home/user/www/
↪specplots /home/user/spec/data 2>&1 >> /home/user/www/specplots/log_cron.txt

Any output from this periodic task will be recorded in the file
`/home/user/www/specplots/log_cron.txt`.  This file can be reviewed
for diagnostics or troubleshooting.
```

```
'''
```

custom *uascan*

The APS USAXS instrument uses a custom scan macro called *uascan* for routine step scans. Since this macro name ends with "scan", the default selection in *specplot* images this data using the `LinePlotter` class. Here is a plot of the default handling of data from the *uascan* macro:

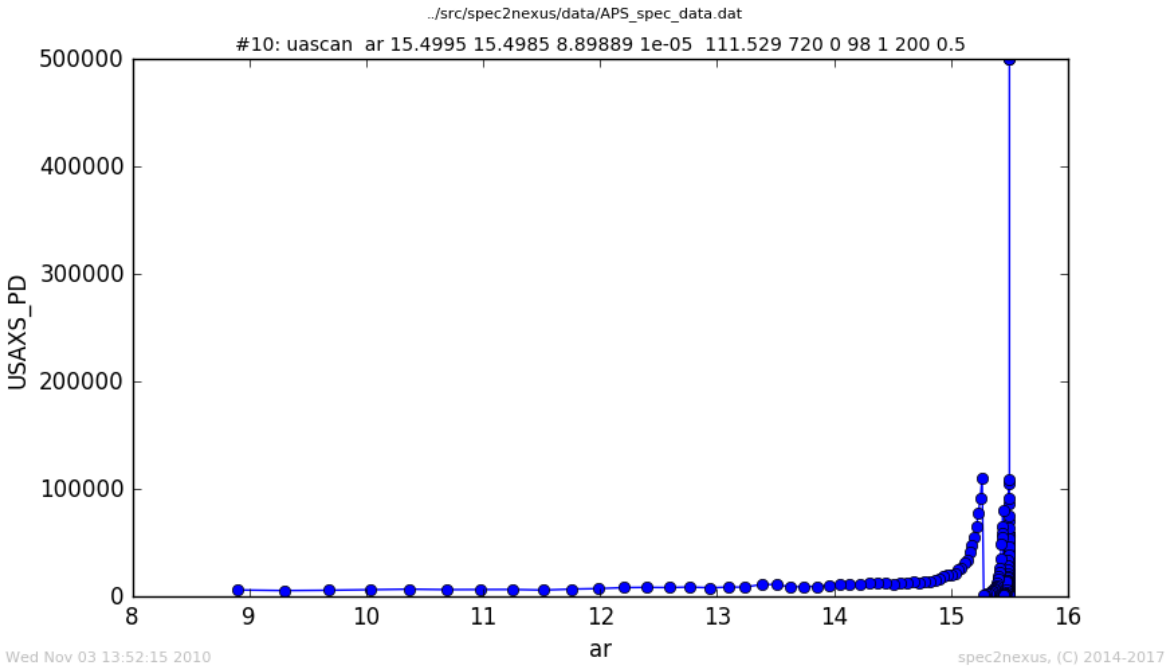

Fig. 2.5: USAXS *uascan*, handled as `LinePlotter`

The can be changed by making the *y* axis log scale. To do this, a custom version of `LinePlotter` is created as `Custom_Ascan`. The `get_plot_data` method is written (overrides the default method) to make the *y* axis log-scale by calling the `configure` method (defined in the superclass). Here's the code:

usaxs_uascan.py example

```
#!/usr/bin/env python

#-----------------------------------------------------------------------------
# :author:    Pete R. Jemian
# :email:     prjemian@gmail.com
# :copyright: (c) 2014-2017, Pete R. Jemian
#
# Distributed under the terms of the Creative Commons Attribution 4.0 International␣
↪Public License.
#
# The full license is in the file LICENSE.txt, distributed with this software.
#-----------------------------------------------------------------------------

```

```
'''
Plot data from the USAXS uascan macro

.. autosummary::

    ~UAscan_Plotter

'''

import spec2nexus.specplot
import spec2nexus.specplot_gallery


class UAscan_Plotter(spec2nexus.specplot.LinePlotter):
    '''simple customize of `uascan` handling'''

    def retrieve_plot_data(self):
        '''plot the vertical axis on log scale'''
        spec2nexus.specplot.LinePlotter.retrieve_plot_data(self)

        if self.signal in self.data:
            if min(self.data[self.signal]) <= 0:
                # TODO: remove any data where Y <= 0 (can't plot on log scale)
                msg = 'cannot plot Y<0: ' + str(self.scan)
                raise spec2nexus.specplot.NotPlottable(msg)

        # in the uascan, a name for the sample is given in `self.scan.comments[0]`
        self.set_y_log(True)
        self.set_plot_subtitle(
            '#%s uascan: %s' % (str(self.scan.scanNum), self.scan.comments[0]))


def debugging_setup():
    import os, sys
    import shutil
    import ascan
    selector = spec2nexus.specplot.Selector()
    selector.add('ascan', ascan.Custom_Ascan)    # just for the demo
    path = '__usaxs__'
    shutil.rmtree(path, ignore_errors=True)
    os.mkdir(path)
    sys.argv.append('-d')
    sys.argv.append(path)
    sys.argv.append(os.path.join('..', 'src', 'spec2nexus', 'data', 'APS_spec_data.dat
↪'))


def main():
    selector = spec2nexus.specplot.Selector()
    selector.add('uascan', UAscan_Plotter)
    spec2nexus.specplot_gallery.main()


if __name__ == '__main__':
    # debugging_setup()
    main()
```

Note that in the *uascan*, a name for the sample provided by the user is given in *self.scan.comments[0]*. The plot title

is changed to include this and the scan number. The customized plot has a logarithmic *y* axis:

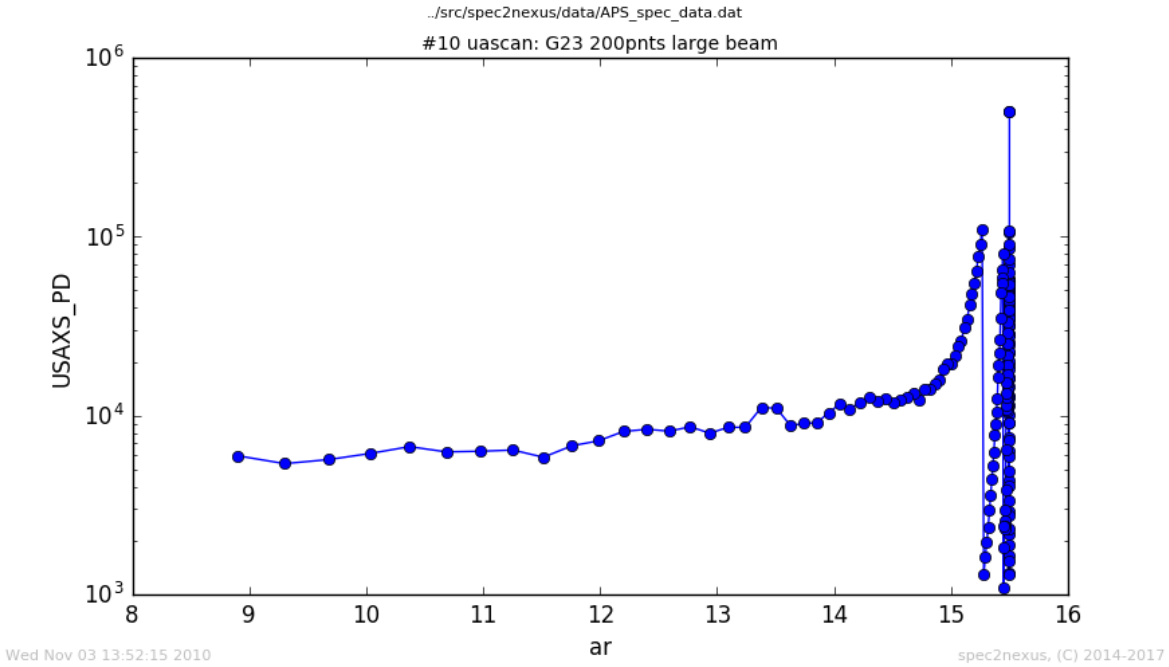

Fig. 2.6: USAXS *uascan*, with logarithmic *y* axis

The most informative view of this data is when the raw data are reduced to $I(Q)$ and viewed on a log-log plot, but that process is beyond this simple example. See the example *Get xy data from HDF5 file* below.

SPEC's *hklscan* macro

The SPEC *hklscan* macro appears in a SPEC data file due to either a *hscan*, *kscan*, or *lscan*. In each of these one of the *hkl* vectors is scanned while the other two remain constant.

The normal handling of the *ascan* macro plots the last data column against the first. This works for data collected with the *hscan*. For *kscan* or *lscan* macros, the *h* axis is still plotted by default since it is in the first column.

To display the scanned axis, it is necessary to examine the data in a custom subclass of `LinePlotter`. The `HKLScanPlotter` subclass, provided with *specplot*, defines the `get_plot_data()` method determines the scanned axis, setting it by name:

```
plot.axes = [axis,]
self.scan.column_first = axis
```

Then, the standard plot handling used by *LinePlotter* uses this information to make the plot.

Get *xy* data from HDF5 file

One example of complexity is when SPEC has been used to direct data collection but the data is not stored in the SPEC data file. The SPEC data file scan must provide some indication about where the collected scan data has been stored.

The USAXS instrument at APS has a *FlyScan* macro that commands the instrument to collect data continuously over the desired Q range. The data is written to a NeXus HDF5 data file. Later, a data reduction process converts the arrays

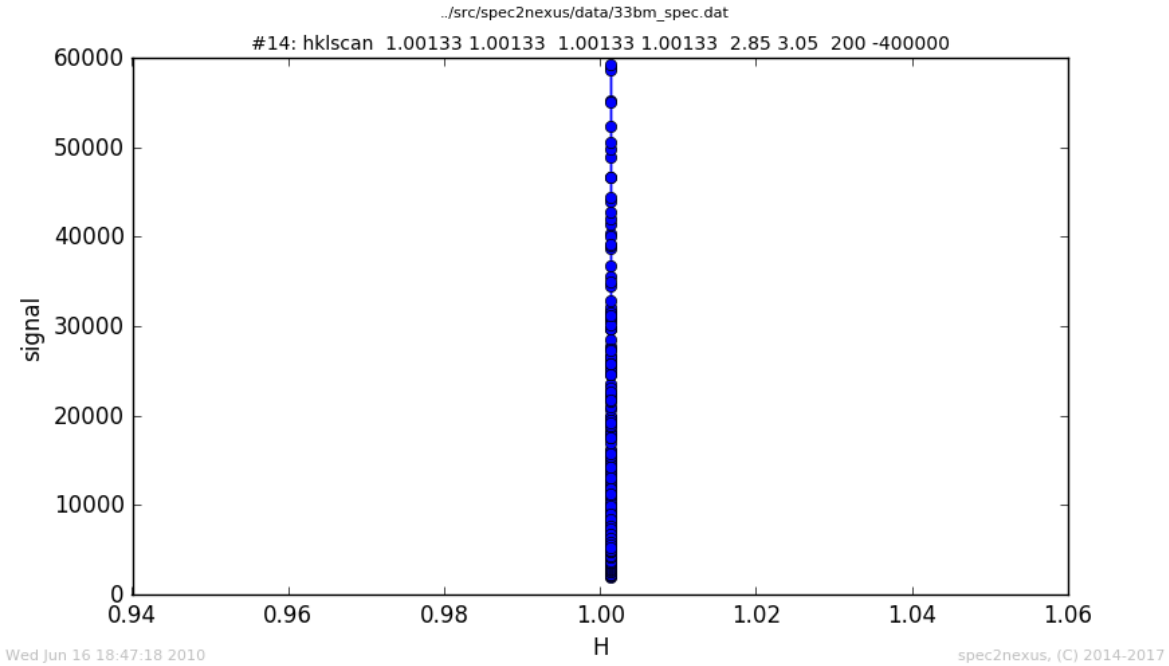

Fig. 2.7: SPEC *hklscan* (*lscan*, in this case), plotted against the (default) first axis *H*

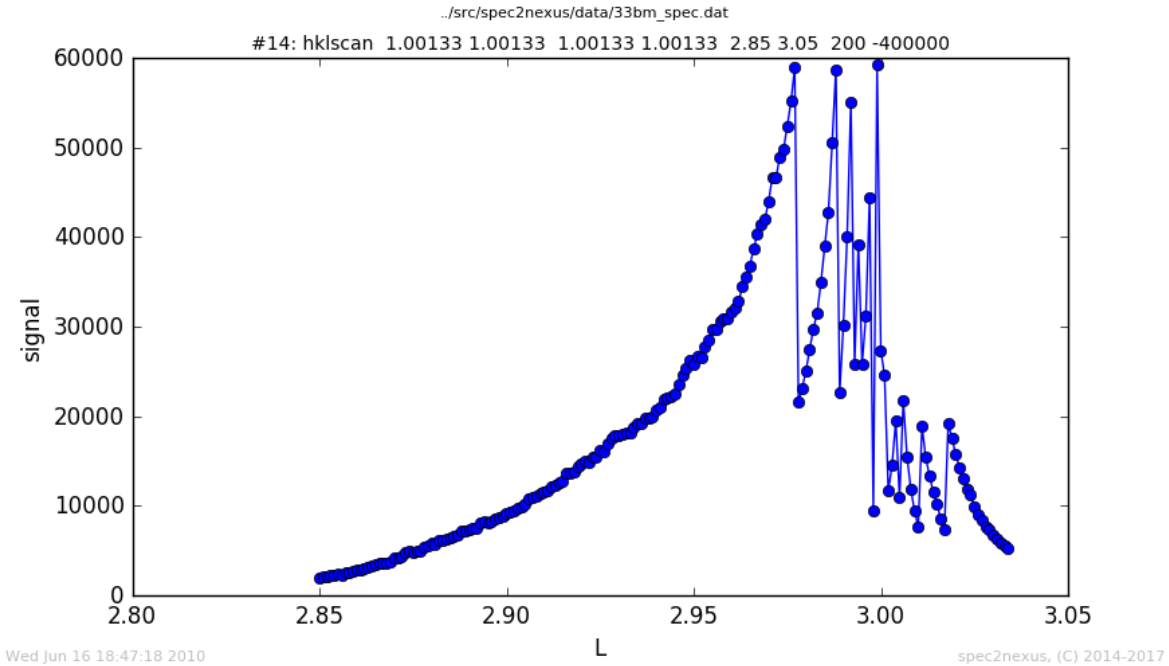

Fig. 2.8: SPEC *hklscan* (*lscan*), plotted against *L*

of raw data to one-dimensional $I(Q)$ profiles. The best representation of this reduced data is on a log-log plot to reveal the many decades of both I and Q covered by the measurement.

With the default handling by `LinePlotter`, no plot can be generated since the dfata is given in a separate HDF5 file. That file is read with the custom handling of the *usaxs_flyscan.py* demo:

usaxs_flyscan.py example

```
#!/usr/bin/env python

#-----------------------------------------------------------------------------
# :author:    Pete R. Jemian
# :email:     prjemian@gmail.com
# :copyright: (c) 2014-2017, Pete R. Jemian
#
# Distributed under the terms of the Creative Commons Attribution 4.0 International␣
↪Public License.
#
# The full license is in the file LICENSE.txt, distributed with this software.
#-----------------------------------------------------------------------------

'''
Plot data from the USAXS FlyScan macro

.. autosummary::

    ~read_reduced_fly_scan_file
    ~retrieve_flyScanData
    ~USAXS_FlyScan_Structure
    ~USAXS_FlyScan_Plotter

'''

import h5py
import numpy
import os

import spec2nexus.specplot
import spec2nexus.specplot_gallery


# methods picked (& modified) from the USAXS livedata project
def read_reduced_fly_scan_file(hdf5_file_name):
    '''
    read any and all reduced data from the HDF5 file, return in a dictionary

    dictionary = {
      'full': dict(Q, R, R_max, ar, fwhm, centroid)
      '250':  dict(Q, R, dR)
      '5000': dict(Q, R, dR)
    }
    '''

    reduced = {}
    hdf = h5py.File(hdf5_file_name, 'r')
    entry = hdf['/entry']
    for key in entry.keys():
```

```
        if key.startswith('flyScan_reduced_'):
            nxdata = entry[key]
            d = {}
            for dsname in ['Q', 'R']:
                if dsname in nxdata:
                    value = nxdata[dsname]
                    if value.size == 1:
                        d[dsname] = float(value[0])
                    else:
                        d[dsname] = numpy.array(value)
            reduced[key[len('flyScan_reduced_'):]] = d
    hdf.close()
    return reduced


# $URL: https://subversion.xray.aps.anl.gov/small_angle/USAXS/livedata/specplot.py $
REDUCED_FLY_SCAN_BINS   = 250       # the default
def retrieve_flyScanData(scan):
    '''retrieve reduced, rebinned data from USAXS Fly Scans'''
    path = os.path.dirname(scan.header.parent.fileName)
    key_string = 'FlyScan file name = '
    comment = scan.comments[2]
    index = comment.find(key_string) + len(key_string)
    hdf_file_name = comment[index:-1]
    abs_file = os.path.abspath(os.path.join(path, hdf_file_name))

    plotData = {}
    if os.path.exists(abs_file):
        reduced = read_reduced_fly_scan_file(abs_file)
        s_num_bins = str(REDUCED_FLY_SCAN_BINS)

        choice = reduced.get(s_num_bins) or reduced.get('full')

        if choice is not None:
            plotData = {axis: choice[axis] for axis in 'Q R'.split()}

    return plotData


class USAXS_FlyScan_Plotter(spec2nexus.specplot.LinePlotter):
    '''
    customize `FlyScan` handling, plot :math:`log(I)` *vs.* :math:`log(Q)`

    The USAXS FlyScan data is stored in a NeXus HDF5 file in a subdirectory
    below the SPEC data file.  This code uses existing code from the
    USAXS instrument to read that file.
    '''

    def retrieve_plot_data(self):
        '''retrieve reduced data from the FlyScan's HDF5 file'''
        # get the data from the HDF5 file
        fly_data = retrieve_flyScanData(self.scan)

        if len(fly_data) != 2:
            raise spec2nexus.specplot.NoDataToPlot(str(self.scan))

        self.signal = 'R'
        self.axes = ['Q',]
```

```
        self.data = fly_data

        # customize the plot just a bit
        # sample name as given by the user?
        subtitle = '#' + str(self.scan.scanNum)
        subtitle += ' FlyScan: ' + self.scan.comments[0]
        self.set_plot_subtitle(subtitle)
        self.set_x_log(True)
        self.set_y_log(True)
        self.set_x_title(r'$|\vec{Q}|, 1/\AA$')
        self.set_y_title(r'USAXS $R(|\vec{Q}|)$, a.u.')

    def plottable(self):
        '''
        can this data be plotted as expected?
        '''
        if self.signal in self.data:
            signal = self.data[self.signal]
            if signal is not None and len(signal) > 0 and len(self.axes) == 1:
                if len(signal) == len(self.data[self.axes[0]]):
                    return True
        return False


def debugging_setup():
    import os, sys
    import shutil
    sys.path.insert(0, os.path.join('..', 'src'))
    path = '__usaxs__'
    shutil.rmtree(path, ignore_errors=True)
    os.mkdir(path)
    sys.argv.append('-d')
    sys.argv.append(path)
    sys.argv.append(os.path.join('..', 'src', 'spec2nexus', 'data', '02_03_setup.dat
↪'))


def main():
    selector = spec2nexus.specplot.Selector()
    selector.add('FlyScan', USAXS_FlyScan_Plotter)
    spec2nexus.specplot_gallery.main()


if __name__ == '__main__':
    # debugging_setup()
    main()
```

The data is then rendered in a customized log-log plot of $I(Q)$:

Usage

When a custom scan macro handler is written and installed using code similar to the *custom ascan* handling above:

```
def main():
    selector = spec2nexus.specplot.Selector()
    selector.add('ascan', Custom_Ascan)
    spec2nexus.specplot_gallery.main()
```

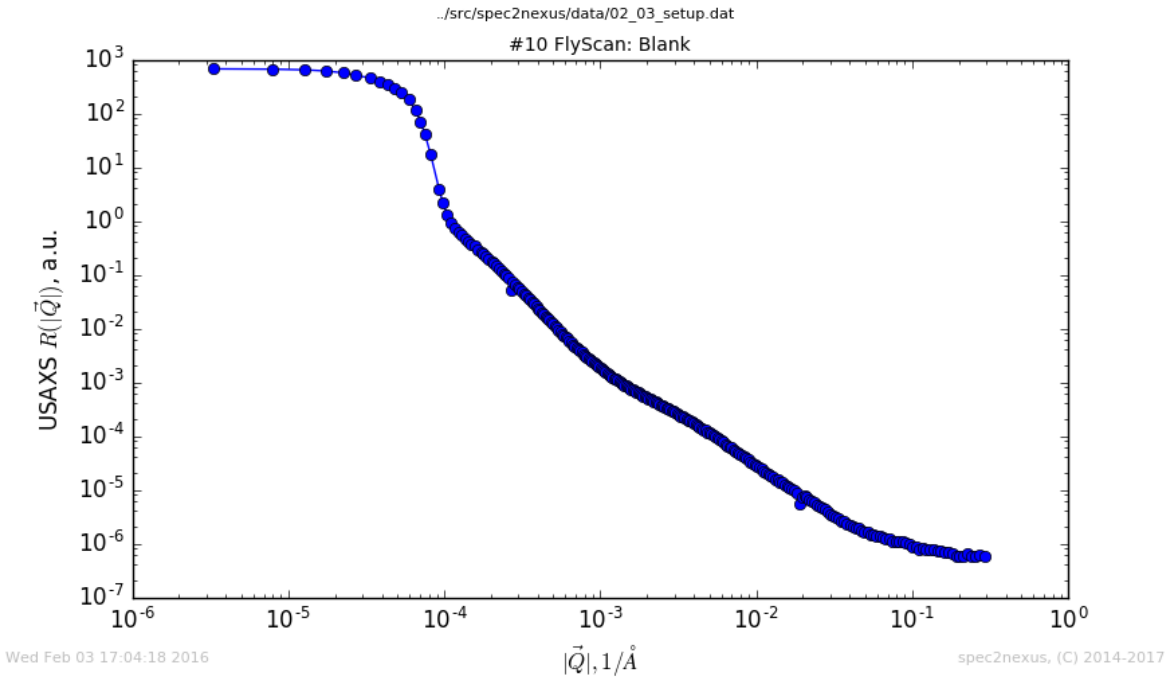

Fig. 2.9: USAXS *FlyScan*, handled by `USAXS_FlyScan_Plotter`

```
if __name__ == '__main__':
    main()
```

then the command line arugment handling from `spec2nexus.specplot_gallery.main()` can be accessed from the command line for help and usage information.

Usage:

```
user@localhost ~/.../spec2nexus/demo $ ./ascan.py
usage: ascan.py [-h] [-r] [-d DIR] paths [paths ...]
ascan.py: error: too few arguments
```

Help:

```
user@localhost ~/.../spec2nexus/demo $ ./ascan.py -h
usage: ascan.py [-h] [-r] [-d DIR] paths [paths ...]

read a list of SPEC data files (or directories) and plot images of all scans

positional arguments:
  paths              SPEC data file name(s) or directory(s) with SPEC data
                     files

optional arguments:
  -h, --help         show this help message and exit
  -r                 sort images from each data file in reverse chronolgical
                     order
  -d DIR, --dir DIR  base directory for output (default:/home/prjemian/Documen
```

```
                    ts/eclipse/spec2nexus/demo)
```

spec2nexus.eznx

(Easy NeXus) support library for reading & writing NeXus HDF5 files using h5py

How to use spec2nexus.eznx

Here is a simple example to write a NeXus data file using eznx:

```
#!/usr/bin/env python
# -*- coding: utf-8 -*-

'''
Writes a simple NeXus HDF5 file using h5py with links.

This example is based on ``writer_2_1`` of the NeXus Manual:
http://download.nexusformat.org/doc/html/examples/h5py/index.html
'''

import eznx


HDF5_FILE = 'eznx_example.hdf5'

I_v_TTH_DATA = '''
17.92608    1037
17.92558    2857
17.92508    23819
17.92458    49087
17.92408    66802
17.92358    66206
17.92308    64129
17.92258    56795
17.92208    29315
17.92158    6622
17.92108    1321
'''
#---------------------------

tthData, countsData = zip(*[map(float,_.split()) for _ in I_v_TTH_DATA.strip().
↪splitlines()])

f = eznx.makeFile(HDF5_FILE)  # create the HDF5 NeXus file
f.attrs['default'] = 'entry'

nxentry = eznx.makeGroup(f, 'entry', 'NXentry', default='data')
nxinstrument = eznx.makeGroup(nxentry, 'instrument', 'NXinstrument')
nxdetector = eznx.makeGroup(nxinstrument, 'detector', 'NXdetector')

tth = eznx.makeDataset(nxdetector, "two_theta", tthData, units='degrees')
counts = eznx.makeDataset(nxdetector, "counts", countsData, units='counts')

nxdata = eznx.makeGroup(nxentry, 'data', 'NXdata',
                        signal=1, axes='two_theta', two_theta_indices=0)
```

```
eznx.makeLink(nxdetector, tth, nxdata.name+'/two_theta')
eznx.makeLink(nxdetector, counts, nxdata.name+'/counts')

f.close()    # be CERTAIN to close the file
```

The output of this code is an HDF5 file (binary). It has this structure:

```
    eznx_example.hdf5:NeXus data file
      @default = entry
      entry:NXentry
        @NX_class = NXentry
        @default = data
        data:NXdata
          @NX_class = NXdata
          @signal = counts
          @axes = two_theta
          @two_theta_indices = 0
          counts --> /entry/instrument/detector/counts
          two_theta --> /entry/instrument/detector/two_theta
        instrument:NXinstrument
          @NX_class = NXinstrument
          detector:NXdetector
            @NX_class = NXdetector
            counts:NX_FLOAT64[11] = __array
              @units = counts
              @target = /entry/instrument/detector/counts
              __array = [1037.0, 2857.0, 23819.0, '...', 1321.0]
            two_theta:NX_FLOAT64[11] = __array
              @units = degrees
              @target = /entry/instrument/detector/two_theta
              __array = [17.926079999999999, 17.92558, 17.925080000000001, '...', 17.
↪92108]
```

NeXus HDF5 File Structure

The output of this code is an HDF5 file (binary). It has this general structure (indentation shows HDF5 groups, @ signs describe attributes of the preceding item):

```
  hdf5_file:NeXus data file
     @default = S1
     S1:NXentry      (one NXentry for each scan)
        @default = data
        title = #S
        T or M: #T or #M
        comments: #C for entire scan
        date: #D
        scan_number: #S
        G:NXcollection
           @description = SPEC geometry arrays, meanings defined by SPEC␣
↪diffractometer support
           G0:NX_FLOAT64[] #G0
           G1:NX_FLOAT64[] #G1
           ...
        data:NXdata
           @description = SPEC scan data (content from #L and data lines)
           @signal = I0
```

```
            @axes = mr
            @mr_indices = 0
            Epoch:NX_FLOAT64[]
            I0:NX_FLOAT64[]          (last data column)
              @spec_name = I0
            mr:NX_FLOAT64[]          (first data column)
            ...
         metadata:NXcollection
            @description = SPEC metadata (UNICAT-style #H & #V lines)
            ARenc_0:NX_FLOAT64 = 0.0
            ...
         positioners:NXcollection
            @description = SPEC positioners (#P & #O lines)
            mr:NX_FLOAT64
            ...
```

APIs provided:

spec2nexus.writer

This is an internal library of the **spec2nexus** software. It is not expected that users of this package will need to call the writer module directly.

source code documentation

(internal library) Parses SPEC data using spec2nexus.eznx API (only requires h5py)

class spec2nexus.writer.**Writer**(*spec_data*)

writes out scans from SPEC data file to NeXus HDF5 file

Parameters **spec_data** (*obj*) – instance of *SpecDataFile*

mca_spectra(*nxdata*, *scan*, *primary_axis_label*)

internal: parse for optional 2-D MCA spectra

mesh(*nxdata*, *scan*)

internal: data parser for 2-D mesh and hklmesh

oneD(*nxdata*, *scan*)

internal: generic data parser for 1-D column data, returns signal and axis

root_attributes()

internal: returns the attributes to be written to the root element as a dict

save(*hdf_file*, *scan_list=[]*)

save the information in this SPEC data file to a NeXus HDF5 file

Each scan in scan_list will be converted to a **NXentry** group. Scan data will be placed in a **NXdata** group where the attribute **signal=1** is the last column and the corresponding attribute **axes=<name of the first column>**. There are variations on this for 2-D and higher dimensionality data, such as mesh scans.

In general, the tree structure of the NeXus HDF5 file is:

```
hdf5_file: NXroot
    @default="S1"
    definition="NXspecdata"
    # attributes
```

```
    S1:NXentry
        @default="data"
        # attributes and metadata fields
        data:NXdata
            @signal=<name of signal field>
            @axes=<name(s) of axes of signal>
            @<axis>_indices=<list of indices in "axis1">
            <signal_is_the_last_column>:NX_NUMBER[number of points] = ...␣
↪data ...
                @signal=1
                @axes='<axis_is_name_of_first_column>'
                @<axis>_indices=<list of indices in "axis1" used as dimension␣
↪scales of the "signal">
            <axis_is_name_of_first_column>:NX_NUMBER[number of points] = ...␣
↪data ...
            # other columns from the scan
```

Parameters

- **hdf_file** (*str*) – name of NeXus/HDF5 file to be written
- **scanlist** (*[int]*) – list of scan numbers to be read

save_data (*nxdata*, *scan*)
internal: store the scan data

save_dict (*group*, *data*)
internal: store a dictionary

save_scan (*nxentry*, *scan*)
internal: save the data from each SPEC scan to its own NXentry group

write_ds (*group*, *label*, *data*, ***attr*)
internal: writes a dataset to the HDF5 file, records the SPEC name as an attribute

---

source code methods

addAttributes	add attributes to an h5py data item
makeFile	create and open an empty NeXus HDF5 file using h5py
makeDataset	create and write data to a dataset in the HDF5 file hierarchy
makeExternalLink	create an external link from sourceFile, sourcePath to targetPath in hdf5FileObject
makeGroup	create a NeXus group
openGroup	open or create the NeXus/HDF5 group, return the object
makeLink	create an internal NeXus (hard) link in an HDF5 file
read_nexus_field	get a dataset from the HDF5 parent group
read_nexus_group_fields	return the fields in the NeXus group as a dict(name=dataset)
write_dataset	write to the NeXus/HDF5 dataset, create it if necessary, return the object

source code documentation

(Easy NeXus) support reading & writing NeXus HDF5 files using h5py

predecessor NeXus h5py example code: `my_lib.py`[1]

Dependencies

- h5py: interface to HDF5 file format

Exceptions raised

- None

Example (using ipython)

```
In [1]: from spec2nexus import eznx
In [2]: root = eznx.makeFile('test.h5', creator='eznx', default='entry')
In [3]: nxentry = eznx.makeGroup(root, 'entry', 'NXentry')
In [4]: eznx.write_dataset(nxentry, 'title', 'simple test data', default='data')
Out[4]: <HDF5 dataset "title": shape (), type "|O8">
In [5]: nxdata = eznx.makeGroup(nxentry, 'data', 'NXdata', signal='counts', axes='tth
↪', tth_indices=0)
In [6]: eznx.write_dataset(nxdata, 'tth', [10.0, 10.1, 10.2, 10.3], units='degrees')
Out[6]: <HDF5 dataset "tth": shape (4,), type "<f8">
In [7]: eznx.write_dataset(nxdata, 'counts', [1, 50, 1000, 5], units='counts')
Out[7]: <HDF5 dataset "counts": shape (4,), type "<i8">
In [8]: root.close()
```

The resulting (binary) data file has this structure:

```
test.h5:NeXus data file
  @creator = eznx
  @default = 'entry'
  entry:NXentry
    @NX_class = NXentry
    @default = 'data'
    title:NX_data = simple test data
    data:NXdata
      @NX_class = NXdata
      @signal = 'counts'
      @axes = 'tth'
      @axes_indices = 0
      counts:NX_INT64[4] = [1, 50, 1000, 5]
        @units = counts
        @axes = tth
      tth:NX_FLOAT64[4] = [10.0, 10.1, 10.199999999999999, 10.300000000000001]
        @units = degrees
```

[1] http://download.nexusformat.org/doc/html/examples/h5py/index.html#mylib-support-module

Classes and Methods

spec2nexus.eznx.**addAttributes**(*parent*, ***attr*)
add attributes to an h5py data item

Parameters

- **parent** (*obj*) – h5py parent object
- **attr** (*dict*) – optional dictionary of attributes

spec2nexus.eznx.**makeDataset**(*parent*, *name*, *data=None*, ***attr*)
create and write data to a dataset in the HDF5 file hierarchy

Any named parameters in the call to this method will be saved as attributes of the dataset.

Parameters

- **parent** (*obj*) – parent group
- **name** (*str*) – valid NeXus dataset name
- **data** (*obj*) – the information to be written
- **attr** (*dict*) – optional dictionary of attributes

Returns h5py dataset object

spec2nexus.eznx.**makeExternalLink**(*hdf5FileObject*, *sourceFile*, *sourcePath*, *targetPath*)
create an external link from sourceFile, sourcePath to targetPath in hdf5FileObject

Parameters

- **hdf5FileObject** (*obj*) – open HDF5 file object
- **sourceFile** (*str*) – file containing existing HDF5 object at sourcePath
- **sourcePath** (*str*) – path to existing HDF5 object in sourceFile
- **targetPath** (*str*) – full node path to be created in current open HDF5 file, such as `/entry/data/data`

Note: Since the object retrieved is in a different file, its ".file" and ".parent" properties will refer to objects in that file, not the file in which the link resides.

See http://www.h5py.org/docs-1.3/guide/group.html#external-links

This routine is provided as a reminder how to do this simple operation.

spec2nexus.eznx.**makeFile**(*filename*, ***attr*)
create and open an empty NeXus HDF5 file using h5py

Any named parameters in the call to this method will be saved as attributes of the root of the file. Note that `**attr` is a dictionary of named parameters.

Parameters

- **filename** (*str*) – valid file name
- **attr** (*dict*) – optional dictionary of attributes

Returns h5py file object

spec2nexus.eznx.**makeGroup**(*parent*, *name*, *nxclass*, ***attr*)
create a NeXus group

Any named parameters in the call to this method will be saved as attributes of the group. Note that `**attr` is a dictionary of named parameters.

Parameters

- **parent** (*obj*) – parent group
- **name** (*str*) – valid NeXus group name
- **nxclass** (*str*) – valid NeXus class name
- **attr** (*dict*) – optional dictionary of attributes

Returns h5py group object

spec2nexus.eznx.**makeLink**(*parent*, *sourceObject*, *targetName*)
create an internal NeXus (hard) link in an HDF5 file

Parameters

- **parent** (*obj*) – parent group of source
- **sourceObject** (*obj*) – existing HDF5 object
- **targetName** (*str*) – HDF5 node path to be created, such as `/entry/data/data`

spec2nexus.eznx.**openGroup**(*parent*, *name*, *nx_class*, ***attr*)
open or create the NeXus/HDF5 group, return the object

Parameters

- **parent** (*obj*) – h5py parent object
- **name** (*str*) – valid NeXus group name to open or create
- **nxclass** (*str*) – valid NeXus class name (base class or application definition)
- **attr** (*dict*) – optional dictionary of attributes

spec2nexus.eznx.**read_nexus_field**(*parent*, *dataset_name*, *astype=None*)
get a dataset from the HDF5 parent group

Parameters

- **parent** (*obj*) – h5py parent object
- **dataset_name** (*str*) – name of the dataset (NeXus field) to be read
- **astype** (*obj*) – option to return as different data type

spec2nexus.eznx.**read_nexus_group_fields**(*parent*, *name*, *fields*)
return the fields in the NeXus group as a dict(name=dataset)

This routine provides a mass way to read a directed list of datasets (NeXus fields) in an HDF5 group.

Parameters

- **parent** (*obj*) – h5py parent object
- **name** (*str*) – name of the group containing the fields
- **fields** (*[name]*) – list of field names to be read

Returns dictionary of {name:dataset}

Raises **KeyError** – if a field is not found

spec2nexus.eznx.**write_dataset**(*parent*, *name*, *data*, ***attr*)
write to the NeXus/HDF5 dataset, create it if necessary, return the object

Parameters

- **parent** (*obj*) – h5py parent object
- **name** (*str*) – valid NeXus dataset name to write
- **data** (*obj*) – the information to be written
- **attr** (*dict*) – optional dictionary of attributes

spec2nexus.plugin

An extensible plug-in architecture is used to handle the different possible control lines (such as **#F**, **#E**, **#S**, ...) in a SPEC data file.

Plugins can be used to parse or ignore certain control lines in SPEC data files. Through this architecture, it is possible to support custom control lines, such as **#U** (SPEC standard control line for any user data). One example is support for the *UNICAT-style* of metadata provided in the scan header.

Plugins are now used to handle all control lines in *spec2nexus.spec*. Any control line encountered but not recognized will be placed as text in a NeXus **NXnote** group named `unrecognized`.

Supplied spec plugin modules

These plugin modules are supplied:

spec_common_spec2nexus	SPEC data file standard control lines
fallback_spec2nexus	Fallback handling for any SPEC data file control lines not recognized by other handlers
unicat_spec2nexus	**#H** & **#V** - Metadata in SPEC data files as defined by APS UNICAT
uim_spec2nexus	**#UIM** : Image header information from EPICS areaDetector
XPCS_spec2nexus	SPEC data file control lines unique to the APS XPCS instrument

XPCS plugin

SPEC data file control lines unique to the APS XPCS instrument

class spec2nexus.plugins.XPCS_spec2nexus.**XPCS_CCD**
#CCD

class spec2nexus.plugins.XPCS_spec2nexus.**XPCS_VA**
#VA

writer(*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to write VA data

class spec2nexus.plugins.XPCS_spec2nexus.**XPCS_VD**
#VD

writer(*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to write VD data

class spec2nexus.plugins.XPCS_spec2nexus.**XPCS_VE**
#VE

writer (*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to write VE data

class spec2nexus.plugins.XPCS_spec2nexus.**XPCS_XPCS**
#XPCS

Fallback plugin

Fallback handling for any SPEC data file control lines not recognized by other handlers

class spec2nexus.plugins.fallback_spec2nexus.**UnrecognizedControlLine**
unrecognized control line

process (*text*, *spec_obj*, **args*, ***kws*)

writer (*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
write the data in a NeXus group named `unrecognized`

SPEC standard plugin

SPEC data file standard control lines

see SPEC manual, *Standard Data File Format*, http://www.certif.com/spec_manual/user_1_4_1.html

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_Comment**
#C – any comment either in the scan header or somewhere in the scan

IN-MEMORY REPRESENTATION

- (SpecDataFileHeader): **comments**
- (SpecDataFileScan): **comments**

HDF5/NeXus REPRESENTATION

- file root-level attribute: **SPEC_comments** : string array of all comments from first header block
- dataset named **comments** under */NXentry* group, such as */S1/comments* : string array of all comments from this scan block

writer (*h5parent*, *writer*, *scan*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_CountTime**
#T – counting against this constant number of seconds (see #M)

IN-MEMORY REPRESENTATION

- (SpecDataFileScan): **T**

HDF5/NeXus REPRESENTATION

- Dataset named **T** in the *NXentry* group, such as */S1/T*
- Dataset named **counting_basis** in the *NXentry* group with value *SPEC scan with constant counting time*, such as */S1/counting_basis*

writer (*h5parent*, *writer*, *scan*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_CounterMnemonics**
#j – mnemonics of counter (new with SPEC v6)

IN-MEMORY REPRESENTATION

•(SpecDataFileHeader): **j** : mnemonics

HDF5/NeXus REPRESENTATION

•*NXnote* group named **counter_cross_reference** in the *NXentry* group, such as */S1/counter_cross_reference*

–datasets with names supplied as SPEC counter mnemonics, string values supplied as SPEC counter names

writer (*h5parent*, *writer*, *header*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_CounterNames**
#J – names of counters (each separated by two spaces) (new with SPEC v6)

IN-MEMORY REPRESENTATION

•(SpecDataFileHeader): **J** : mnemonics

HDF5/NeXus REPRESENTATION

•*NXnote* group named **counter_cross_reference** in the *NXentry* group, such as */S1/counter_cross_reference*

–datasets with names supplied as SPEC counter mnemonics, string values supplied as SPEC counter names

writer (*h5parent*, *writer*, *header*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_DataLine**
(scan data) – scan data line

Scan data could include interspersed MCA data or even describe 2-D or 3-D data. T his method reads the data lines and buffers them for post-processing in *spec2nexus.plugins.spec_common_spec2nexus.data_lines_postprocessing()*.

IN-MEMORY REPRESENTATION

•(SpecDataFileScan): **data_lines** : values

•(SpecDataFileScan): **data** : {labels: values}

HDF5/NeXus REPRESENTATION

•*NXdata* group named **data** in the *NXentry* group, such as */S1/data*

–datasets with names supplied in **L**, array values collected in **data_lines**

match_key (*text*)
Easier to try conversion to number than construct complicated regexp

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_Date**
#D – date/time stamp

IN-MEMORY REPRESENTATION

•(SpecDataFileHeader): **date** *str*, ISO8601 format

HDF5/NeXus REPRESENTATION

•file root-level attribute: **SPEC_date** *str* (value for 1st header block is used)

writer (*h5parent*, *writer*, *scan*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_Epoch**
#E – the UNIX epoch (seconds from 00:00 GMT 1/1/70)

In SPEC data files, the `#E` control line indicates the start of a *header* block.

IN-MEMORY REPRESENTATION

•(SpecDataFileHeader): **epoch** *int*

HDF5/NeXus REPRESENTATION

•file root-level attribute: **SPEC_epoch** *int*

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_File**
#F – original data file name (starts a file header block)

Module *spec2nexus.spec* is responsible for handling this control line.

IN-MEMORY REPRESENTATION

•(SpecDataFile): **fileName**

•(SpecDataFileHeader) : **file**

HDF5/NeXus REPRESENTATION

•file root-level attribute: **SPEC_file**

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_Geometry**
#G – diffractometer geometry (numbered rows: #G0, #G1, ...)

IN-MEMORY REPRESENTATION

•(SpecDataFileScan): **G**

HDF5/NeXus REPRESENTATION

•*NXnote* group named **G** in the *NXentry* group, such as */S1/G*

–Datasets created from dictionary <scan>.G (indexed by number from the scan block, such as `G0`, `G1`, ...). Meaning of contents for each index are defined by geometry-specific SPEC diffractometer support.

writer (*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_HKL**
#Q – *Q* (*hkl*) at start of scan

IN-MEMORY REPRESENTATION

•(SpecDataFileScan): **Q**

HDF5/NeXus REPRESENTATION

•Dataset named **Q** in the *NXentry* group, such as */S1/M*

writer (*h5parent*, *writer*, *scan*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_Labels**
#L – data column labels

IN-MEMORY REPRESENTATION

•(SpecDataFileScan): **L** : labels

•(SpecDataFileScan): **data** : {labels: values}

HDF5/NeXus REPRESENTATION

•*NXdata* group named **data** in the *NXentry* group, such as */S1/data*

–datasets with names supplied in **L**, array values collected in **data_lines**

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_MCA**
#@MCA – MCA data formatting declaration (ignored for now)

declares this scan contains MCA data (SPEC's array_dump() format, such as `"#@MCA 16C"`)

From documentation provided by the ESRF BLISS group: (http://www.esrf.eu/blissdb/macros/getsource.py?macname=mca.mac)

#@MCA 16C Format string passed to data_dump() function. This format string is held by the global variable "MCA_FMT" and can then been adapted to particular needs. "%%16C" is the default. It dumps data on 1 line, cut every 16 points:

```
@A 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\
 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\
 0 0 0 0 0 0 0 0 0 0 0 0 ...
```

"%%16" would do the same without any backslash "1" would dump 1 point per line, ...

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_MCA_Array**
@A – MCA Array data

MCA data. Each value is the content of one channel, or an integrated value over several channels if a reduction was applied.

Since the MCA Array data is interspersed with scan data, this method reads the data lines and buffers them for post-processing in *spec2nexus.plugins.spec_common_spec2nexus.data_lines_postprocessing()*.

IN-MEMORY REPRESENTATION

•(SpecDataFileScan): **data_lines** : values

•(SpecDataFileScan): **data** : {labels: values}

HDF5/NeXus REPRESENTATION

•*NXdata* group named **data** in the *NXentry* group, such as */S1/data*

–Dataset **_mca_** : *float* MCA data reported on *@A* lines

–Dataset _mca_channel_: provided as HDF5 dimension scale for _mca_ dataset

* if CALIB data specified: *float* scaled MCA channels – $x_k = a + bk + ck^2$
* if CALIB data not specified: *int* MCA channel numbers

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_MCA_Calibration**
#@CALIB – coefficients to compute a scale based on the MCA channel number

$x_k = a + bk + ck^2$ for MCA data, k is channel number

IN-MEMORY REPRESENTATION

•(SpecDataFileScan): **MCA['CALIB']** = `dict(a, b, c)`

HDF5/NeXus REPRESENTATION

- defines a dimension scale for MCA data
- *NXnote* group named **MCA** in the *NXentry* group, such as */S1/MCA*
  - Dataset **calib_a** : *float*
  - Dataset **calib_b** : *float*
  - Dataset **calib_c** : *float*

writer (*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_MCA_ChannelInformation**
#@CHANN – MCA channel information

number_saved, first_saved, last_saved, reduction_coef

IN-MEMORY REPRESENTATION

- (SpecDataFileScan): **MCA['CALIB']** = `dict(number_saved, first_saved, last_saved, reduction_coef)`

HDF5/NeXus REPRESENTATION

- *NXnote* group named **MCA** in the *NXentry* group, such as */S1/MCA*
  - Dataset **number_saved** : *int* number of channels saved
  - Dataset **first_saved** : *int* first channel saved
  - Dataset **first_saved** : *int* last channel saved
  - Dataset **reduction_coef** : *float* reduction coefficient

writer (*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_MCA_CountTime**
#@CTIME – MCA count times

preset_time, elapsed_live_time, elapsed_real_time

IN-MEMORY REPRESENTATION

- (SpecDataFileScan): **MCA['CALIB']** = `dict(preset_time, elapsed_live_time, elapsed_real_time)`

HDF5/NeXus REPRESENTATION

- *NXnote* group named **MCA** in the *NXentry* group, such as */S1/MCA*
  - Dataset **preset_time** : *float*
  - Dataset **elapsed_live_time** : *float*
  - Dataset **elapsed_real_time** : *float*

writer (*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_MCA_RegionOfInterest**
#@ROI – MCA ROI (Region Of Interest) channel information

ROI_name, first_chan, last_chan

IN-MEMORY REPRESENTATION

- (SpecDataFileScan): **MCA['ROI']** = {ROI_name:dict(first_chan, last_chan)}

HDF5/NeXus REPRESENTATION

- *NXnote* group **ROI** in in *NXnote* group named **MCA** in the *NXentry* group, such as */S1/MCA/ROI*
  - Dataset **{ROI_name}** : *int* [first_chan, last_chan]

writer (*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_Monitor**
#M – counting against this constant monitor count (see #T)

IN-MEMORY REPRESENTATION

- (SpecDataFileScan): **M**

HDF5/NeXus REPRESENTATION

- Dataset named **M** in the *NXentry* group, such as */S1/M*
- Dataset named **counting_basis** in the *NXentry* group with value *SPEC scan with constant monitor count*, such as */S1/counting_basis*

writer (*h5parent*, *writer*, *scan*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_NormalizingFactor**
#I – intensity normalizing factor

IN-MEMORY REPRESENTATION

- (SpecDataFileScan): **I**

HDF5/NeXus REPRESENTATION

- Dataset named **intensity_factor** in the *NXentry* group, such as */S1/intensity_factor*

writer (*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_NumColumns**
#N – number of columns of data [num2 sets per row]

IN-MEMORY REPRESENTATION

- (SpecDataFileScan): **N** : [int]

HDF5/NeXus REPRESENTATION

- not written to file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_PositionerMnemonics**
#o – positioner mnemonics (new with SPEC v6)

IN-MEMORY REPRESENTATION

- (SpecDataFileHeader): **o** : mnemonics

HDF5/NeXus REPRESENTATION

- *NXnote* group named **positioner_cross_reference** in the *NXentry* group, such as */S1/positioner_cross_reference*
  - datasets with names supplied as SPEC positioner mnemonics, string values supplied as SPEC positioner names

writer (*h5parent*, *writer*, *header*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_PositionerNames**
#O – positioner names (numbered rows: #O0, #O1, ...)

IN-MEMORY REPRESENTATION

- (SpecDataFileHeader) : **O** : label
- (SpecDataFileScan): **positioner** : {label: value}

HDF5/NeXus REPRESENTATION

- *NXnote* group named **positioners** in the *NXentry* group, such as */S1/positioners*
  - datasets created from dictionary <scan>.positioner
- *NXnote* group named **positioner_cross_reference** in the *NXentry* group, such as */S1/positioner_cross_reference*
  - datasets with names supplied as SPEC positioner mnemonics, string values supplied as SPEC positioner names

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_Positioners**
#P – positioner values at start of scan (numbered rows: #P0, #P1, ...)

IN-MEMORY REPRESENTATION

- (SpecDataFileHeader) : **O** : label
- (SpecDataFileScan): **positioner** : {label: value}

HDF5/NeXus REPRESENTATION

- *NXnote* group named **positioners** in the *NXentry* group, such as */S1/positioners*
  - datasets created from dictionary <scan>.positioner

postprocess(*scan*, **args*, ***kws*)
interpret the motor positions from the scan header

Parameters **scan** (SpecDataFileScan) – data from a single SPEC scan

writer(*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_Scan**
#S – SPEC scan

In SPEC data files, the `#S` control line indicates the start of a *scan* block. Each scan will be written to a separate **NXentry** group in the HDF5 file.

NXentry: "The top-level NeXus group which contains all the data and associated information that comprise a single measurement."

– http://download.nexusformat.org/doc/html/classes/base_classes/NXentry.html

IN-MEMORY REPRESENTATION

- (SpecDataFile):
- (SpecDataFileHeader):

HDF5/NeXus REPRESENTATION

- */NXentry* group named 'S%d' scan_number at root level, such as */S1*

class spec2nexus.plugins.spec_common_spec2nexus.**SPEC_TemperatureSetPoint**
#X – Temperature Set Point (desired temperature)

The default declaration of the #X control line is written:

```
def Fheader '_cols++;printf("#X %gKohm (%gC)\n",TEMP_SP,DEGC_SP)'
```

The supplied macro alters this slightly (replacing %g with %f) and uses the *spec2nexus.scanf.scanf()* implementation with this format:

```
fmt = "#X %fKohm (%fC)"
```

Depending on the circumstances, this might be a good candidate to override with a custom *ControlLineHandler* that parses the data as written. If the conversion process fails for any reason in this implementation, the *#X* line is ignored.

IN-MEMORY REPRESENTATION

- (SpecDataFileScan): **TEMP_SP**
- (SpecDataFileScan): **DEGC_SP**

HDF5/NeXus REPRESENTATION

- Dataset named **TEMP_SP** in the *NXentry* group, such as */S1/TEMP_SP*
- Dataset named **DEGC_SP** in the *NXentry* group, such as */S1/DEGC_SP*

writer(*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)
Describe how to store this data in an HDF5 NeXus file

spec2nexus.plugins.spec_common_spec2nexus.**data_lines_postprocessing**(*scan*)
interpret the data lines from the body of the scan

Parameters **scan** (SpecDataFileScan) – data from a single SPEC scan

spec2nexus.plugins.spec_common_spec2nexus.**data_lines_writer**(*h5parent*, *writer*, *scan*, **args*, ***kws*)
Describe how to store scan data in an HDF5 NeXus file

UIM plugin

#UIM : Image header information from EPICS areaDetector

deprecated in favor of UXML

class spec2nexus.plugins.uim_spec2nexus.**UIM_generic**
#UIM – various image header information

UNICAT metadata plugin

#H & **#V** - Metadata in SPEC data files as defined by APS UNICAT

Handles the UNICAT control lines which write additional metadata in the scans using #H/#V pairs of labels/values.

class spec2nexus.plugins.unicat_spec2nexus.**UNICAT_MetadataMnemonics**
#H – UNICAT metadata names (numbered rows: #H0, #H1, ...)

IN-MEMORY REPRESENTATION

- (SpecDataFileHeader) : **H** : labels
- (SpecDataFileScan): **metadata** : {labels: values}

HDF5/NeXus REPRESENTATION

•*NXnote* group named **metadata** below the *NXentry* group, such as **/entry/metadata**

–datasets created from dictionary <scan>.metadata

class spec2nexus.plugins.unicat_spec2nexus.**UNICAT_MetadataValues**

#V – UNICAT metadata values (numbered rows: #V0, #V1, ...)

IN-MEMORY REPRESENTATION

•(SpecDataFileScan): **V** : values

•(SpecDataFileScan): **metadata** : {labels: values}

HDF5/NeXus REPRESENTATION

•*NXnote* group named **metadata** below the *NXentry* group, such as **/entry/metadata**

–datasets created from dictionary <scan>.metadata

postprocess(*scan*, **args*, ***kws*)

interpret the UNICAT metadata (mostly floating point) from the scan header

Parameters **scan** (SpecDataFileScan) – data from a single SPEC scan (instance of SpecDataFileScan)

writer(*h5parent*, *writer*, *scan*, *nxclass=None*, **args*, ***kws*)

Describe how to store this data in an HDF5 NeXus file

Writing a custom plugin

While **spec2nexus** provides a comprehensive set of plugins to handle the common SPEC control lines, custom control lines are used at many facilities to write additional scan data and scan metadata into the SPEC data file. Custom plugins are written to process these additions.

How to write a custom plugin module

A custom plugin module for *spec2nexus.spec* is provided in a python module (Python source code file). In this custom plugin module are subclasses for each *new* control line to be supported. An exception will be raised if a custom plugin module tries to provide support for an existing control line.

Give the custom plugin module a name ending with `_spec2nexus.py`. Ensure this name is different than any other plugin module you will use (currently, avoid `spec_common_spec2nexus.py`, `uim_spec2nexus.py`, and `unicat_spec2nexus.py`) to avoid possible duplication.

The custom plugin module can be stored in any directory that is convenient. Define the environment variable `SPEC2NEXUS_PLUGIN_PATH` with the directory (directories, comma delimited) where your plugin file(s) reside. On linux, with the bash shell, this might be:

```
export SPEC2NEXUS_PLUGIN_PATH="/home/jemian/.spec2nexus_plugins, /tmp"
```

The custom plugin module should contain, at minimum one subclass of *spec2nexus.plugin.ControlLineHandler*. A custom plugin module can contain many such handlers, as needs dictate.

Note: It is also useful to import the utility method `spec2nexus.plugin.strip_first_word()`

To get *spec2nexus.plugin.ControlLineHandler*, it will be necessary to import in some form, such as:

```
from spec2nexus.plugin import ControlLineHandler, strip_first_word
```

regular expressions

There are several regular expression testers available on the web. Try this one, for example: http://regexpal.com/

Each subclass must define `key` as a regular expression match for the control line key. It is possible to override any of the supplied plugins for scan control lines. Caution is advised to avoid introducing instability.

Each subclass must also define a `process()` method to process the control line. A `NotImplementedError` exception is raised if `key` is not defined.

For difficult regular expressions (or other situations), it is possible to replace the function that matches for a particular control line key. Override the handler's `match_key()` method. For more details, see the section *Custom key match function*.

Example for #U control line

Consider the **#U** user data control line that allows the user to put any data in the scan file header. The content is to be decided by the user.

Suppose we take this content to be three floating point numbers, this subclass could be written:

```
from spec2nexus.plugin import ControlLineHandler, strip_first_word

class User_ControlLine(ControlLineHandler):
    '''**#U** -- User data (#U user1 user2 user3)'''

    key = '#U'

    def process(self, text, spec_obj, *args, **kws):
        args = strip_first_word(text).split()
        user1 = float(args[0])
        user2 = float(args[1])
        user3 = float(args[2])
        spec_obj.U = [user1, user2, user3]
```

When the scan parser encounters a **#U** line in a SPEC data file, it will call this `process()` code with the full text of the line and the object where this data should be stored. We will choose to store this (following the pattern of other data names in *spec2nexus.spec.SpecDataFileScan*) as `scan_obj.U` using a list.

It is up to the user what to do with the `scan_obj.U` data.

Example to ignore a #Y control line

Suppose it is necessary to ignore a control line found in a SPEC file. Consider that one SPEC file contains the control line: `#Y 1 2 3 4 5`. Since there is no standard handler for this control line, we create one that ignores processing by doing nothing:

```
from spec2nexus.plugin import ControlLineHandler

class Ignore_Y_ControlLine(ControlLineHandler):
    '''**#Y** -- as in ``#Y 1 2 3 4 5``'''
```

```
    key = '#Y'

    def process(self, text, spec_obj, *args, **kws):
        pass
```

Postprocessing

Sometimes, it is necessary to defer a step of processing until after the complete scan data has been read. One example is for 2-D or 3-D data that has been acquired as a vector rather than matrix. The matrix must be constructed only after all the scan data has been read. Such postprocessing is handled in a method in a plugin file. The postprocessing method is registered from the control line handler by calling the `addPostProcessor()` method of the `spec_obj` argument received by the handler's `process()` method. A key name[1] is supplied when registering to avoid registering this same code more than once. The postprocessing function will be called with the instance of *spec2nexus.spec.SpecDataFileScan* as its only argument.

An important role of the postprocessing is to store the result in the scan object. It is important not to modify other data in the scan object. Pick an attribute named similarly to the plugin (e.g., MCA configuration uses the **MCA** attribute, UNICAT metadata uses the **metadata** attribute, ...) This attribute will define where and how the data from the plugin is available. The `writer()` method (see *below*) is one example of a user of this attribute.

Example postprocessing

Consider the **#U** control line example above. For some contrived reason, we wish to store the sum of the numbers as a separate number, but only after all the scan data has been read. This can be done with the simple expression:

```
spec_obj.U_sum = sum(spec_obj.U)
```

To build a postprocessing method, we write:

```
def contrived_summation(scan):
    '''
    add up all the numbers in the #U line

    :param SpecDataFileScan scan: data from a single SPEC scan
    '''
    scan.U_sum = sum(scan.U)
```

To register this postprocessing method, place this line in the `process()` of the handler:

```
spec_obj.addPostProcessor('contrived_summation', contrived_summation)
```

Summary Example Custom Plugin with postprocessing

Gathering all parts of the examples above, the custom plugin module is:

```
from spec2nexus.plugin import ControlLineHandler, strip_first_word

class User_ControlLine(ControlLineHandler):
    '''**#U** -- User data (#U user1 user2 user3)'''
```

[1] The key name must be unique amongst all postprocessing functions. A good choice is the name of the postprocessing function itself.

```
    key = '#U'

    def process(self, text, spec_obj, *args, **kws):
        args = strip_first_word(text).split()
        user1 = float(args[0])
        user2 = float(args[1])
        user3 = float(args[2])
        spec_obj.U = [user1, user2, user3]
        spec_obj.addPostProcessor('contrived_summation', contrived_summation)


def contrived_summation(scan):
    '''
    add up all the numbers in the #U line

    :param SpecDataFileScan scan: data from a single SPEC scan
    '''
    scan.U_sum = sum(scan.U)


class Ignore_Y_ControlLine(ControlLineHandler):
    '''**#Y** -- as in ``#Y 1 2 3 4 5``'''

    key = '#Y'

    def process(self, text, spec_obj, *args, **kws):
        pass
```

Custom HDF5 writer

A custom HDF5 writer method defines how the data from the *plugin* will be written to the HDF5+NeXus data file. The writer will be called with several arguments:

h5parent: *obj* : the HDF5 group that will hold this plugin's data

writer: *obj* : instance of *spec2nexus.writer.Writer* that manages the content of the HDF5 file

scan: *obj* : instance of *spec2nexus.spec.SpecDataFileScan* containing this scan's data

nxclass: *str* : (optional) name of NeXus base class to be created

Since the file is being written according to the NeXus data standard[2], use the NeXus base classes[3] as references for how to structure the data written by the custom HDF5 writer.

One responsibility of a custom HDF5 writer method is to create *unique* names for every object written in the *h5parent* group. Usually, this will be a *NXentry*[4] group. You can determine the NeXus base class of this group using code such as this:

```
>>> print h5parent.attrs['NX_class']
<<< NXentry
```

If your custom HDF5 writer must create group and you are uncertain which base class to select, it is recommended to use a **NXcollection**[5] (an unvalidated catch-all base class) which can store any content. But, you are encouraged to

[2] http://nexusformat.org
[3] http://download.nexusformat.org/doc/html/classes/base_classes/
[4] http://download.nexusformat.org/doc/html/classes/base_classes/NXentry.html
[5] http://download.nexusformat.org/doc/html/classes/base_classes/NXcollection.html

find one of the other NeXus base classes that best fits your data. Look at the source code of the supplied plugins for examples.

The writer uses the *spec2nexus.eznx* module to create and write the various parts of the HDF5 file.

Here is an example `writer()` method from the *spec2nexus.plugins.unicat_spec2nexus* module:

```
def writer(self, h5parent, writer, scan, nxclass=None, *args, **kws):
    '''Describe how to store this data in an HDF5 NeXus file'''
    if hasattr(scan, 'metadata') and len(scan.metadata) > 0:
        desc='SPEC metadata (UNICAT-style #H & #V lines)'
        group = eznx.makeGroup(h5parent, 'metadata', nxclass, description=desc)
        writer.save_dict(group, scan.metadata)
```

Custom key match function

The default test that a given line matches a specific *spec2nexus.plugin.ControlLineHandler* subclass is to use a regular expression match.

```
def match_key(self, text):
    '''default regular expression match, based on self.key'''
    t = re.match(self.key, text)
    if t is not None:
        if t.regs[0][1] != 0:
            return True
    return False
```

In some cases, that may prove tedious or difficult, such as when testing for a floating point number with optional preceding white space at the start of a line. This is typical for data lines in a scan or continued lines from an MCA spectrum. in such cases, the handler can override the `match_key()` method. Here is an example:

```
def match_key(self, text):
    '''
    Easier to try conversion to number than construct complicated regexp
    '''
    try:
        float( text.strip().split()[0] )
        return True
    except ValueError:
        return False
```

Summary Requirements for custom plugin

- file name must end in `_spec2nexus.py`
- file can go in any directory
- add directory to `SPEC2NEXUS_PLUGIN_PATH` environment variable (comma-delimited for multiple directories)
- multiple control line handlers can go in a single file
- for each control line:
  - subclass *spec2nexus.plugin.ControlLineHandler*
  - identify the control line pattern

  - define `key` with a regular expression to match[6]
    * `key` is used to identify control line handlers
    * redefine existing supported control lines to replace supplied behavior (use caution!)
    * Note: `key="scan data"` is used to process the scan data: *spec2nexus.plugins.spec_common_spec2nexus.SPEC_DataLine()*
  - (optional) define `match_key()` to override the default regular expression to match the key
  - define `process()` to handle the supplied text
  - define `writer()` to write the in-memory data structure from this plugin to HDF5+NeXus data file
- for each postprocessing function:
  - write the function
  - register the function with spec_obj.addPostProcessor(key_name, the_function) in the handler's `process()`

Overview of the supplied spec plugins

Plugins for these control lines[1] are provided in **spec2nexus**:

SPEC_File	**#F** – original data file name (starts a file header block)
SPEC_Epoch	**#E** – the UNIX epoch (seconds from 00:00 GMT 1/1/70)
SPEC_Date	**#D** – date/time stamp
SPEC_Comment	**#C** – any comment either in the scan header or somewhere in the scan
SPEC_Geometry	**#G** – diffractometer geometry (numbered rows: #G0, #G1, ...)
SPEC_NormalizingFactor	**#I** – intensity normalizing factor
SPEC_CounterNames	**#J** – names of counters (each separated by two spaces) (new with SPEC v6)
SPEC_CounterMnemonics	**#j** – mnemonics of counter (new with SPEC v6)
SPEC_Labels	**#L** – data column labels
SPEC_Monitor	**#M** – counting against this constant monitor count (see #T)
SPEC_NumColumns	**#N** – number of columns of data [num2 sets per row]
SPEC_PositionerNames	**#O** – positioner names (numbered rows: #O0, #O1, ...)
SPEC_PositionerMnemonics	**#o** – positioner mnemonics (new with SPEC v6)
SPEC_Positioners	**#P** – positioner values at start of scan (numbered rows: #P0, #P1, ...)
SPEC_HKL	**#Q** – Q (hkl) at start of scan
SPEC_Scan	**#S** – SPEC scan
SPEC_CountTime	**#T** – counting against this constant number of seconds (see #M)
SPEC_TemperatureSetPoint	**#X** – Temperature Set Point (desired temperature)
SPEC_DataLine	**(scan data)** – scan data line
SPEC_MCA	**#@MCA** – MCA data formatting declaration (ignored for now)
SPEC_MCA_Array	**@A** – MCA Array data

Continued on next page

[6] It is possible to override the default regular expression match in the subclass with a custom match function. See the *spec2nexus.plugins.spec_common_spec2nexus.SPEC_DataLine.match_key()* method for an example.

[1] Compare this list with *Control lines (keys) defined by SPEC*

Table 2.14 – continued from previous page

SPEC_MCA_Calibration	**#@CALIB** – coefficients to compute a scale based on the MCA channel number
SPEC_MCA_ChannelInformation	**#@CHANN** – MCA channel information
SPEC_MCA_CountTime	**#@CTIME** – MCA count times
SPEC_MCA_RegionOfInterest	**#@ROI** – MCA ROI (Region Of Interest) channel information
UnrecognizedControlLine	unrecognized control line
UNICAT_MetadataMnemonics	**#H** – UNICAT metadata names (numbered rows: #H0, #H1, ...)
UNICAT_MetadataValues	**#V** – UNICAT metadata values (numbered rows: #V0, #V1, ...)
UIM_generic	**#UIM** – various image header information
XPCS_VA	**#VA**
XPCS_VD	**#VD**
XPCS_VE	**#VE**

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define the plug-in architecture

Create a subclass of *spec2nexus.plugin.ControlLineHandler* for each SPEC control line. In each subclass, it is necessary to:

- define a string value for the `key` (class attribute)
- override the definition of `process()`

It is optional to:

- override the definition of `match_key()`
- override the definition of `postprocess()`
- override the definition of `writer()`

Classes

ControlLineHandler	Plugin to handle a single control line in a SPEC data file
PluginManager()	Manage the set of SPEC data file control line plugins

Exceptions

DuplicateControlLineKey	This control line key regular expression has been used more than once.
DuplicateControlLinePlugin	This control line handler has been used more than once.
DuplicatePlugin	This plugin file name has been used more than once.

class spec2nexus.plugin.**ControlLineHandler**
Plugin to handle a single control line in a SPEC data file

Parameters **key** (*str*) – regular expression to match a control line key, up to the first space

Returns None

Class Methods

getKey()	return this handler's unique identifying key
match_key(text)	test if this plugin's key matches the supplied text
process(*args, **kw)	Parse this text from the SPEC data file according to the control line key.
postprocess(*args, **kw)	apply additional interpretation after all control lines have been read
writer(*args, **kw)	write in-memory structure to HDF5+NeXus data file

getKey()
return this handler's unique identifying key

match_key(*text*)
test if this plugin's key matches the supplied text

Parameters **text** (*str*) – first word on the line, up to but not including the first whitespace

The default test is to apply a regular expression match using `self.key` as the regular expression to match.

If this method is to be used, then override this method in the plugin or a `NotImplementedError` exception will be raised.

postprocess(**args*, ***kw*)
apply additional interpretation after all control lines have been read

queue this method by calling:

```
scan.addPostProcessor('unique label', self.postprocess)
```

in the *process()* method. It will be called called after all control lines in a scan have been read.

If this method is to be used, then override this method in the plugin or a `NotImplementedError` exception will be raised.

process(**args*, ***kw*)
Parse this text from the SPEC data file according to the control line key.

A plugin will receive *text* and one of these objects: * *SpecDataFile* * *SpecDataFileHeader* * *SpecDataFileScan*

The plugin will parse the text and store the content into the object.

All plugins **must** override this method or a `NotImplementedError` exception will be raised.

writer(**args*, ***kw*)
write in-memory structure to HDF5+NeXus data file

queue this by calling:

```
scan.addWriter('unique_label', self.writer)
```

in the process() method. It will be called called as the HDF5 file is being constructed.

If this method is to be used, then override this method in the plugin or a `NotImplementedError` exception will be raised.

exception spec2nexus.plugin.**DuplicateControlLineKey**
This control line key regular expression has been used more than once.

exception spec2nexus.plugin.**DuplicateControlLinePlugin**
This control line handler has been used more than once.

exception spec2nexus.plugin.**DuplicatePlugin**
This plugin file name has been used more than once.

class spec2nexus.plugin.**PluginManager**
Manage the set of SPEC data file control line plugins

Class Methods

register(handler)	add this handler to the list of known handlers
hasKey(key)	Is this key known?
getKey(spec_data_file_line)	Find the key that matches this line in a SPEC data file.
get(key)	return the handler identified by key or None
load_plugins()	Call this once to load all plugins that handle SPEC control lines
process(key, *args, **kw)	pick the control line handler by key and call its process() method

get(*key*)
return the handler identified by key or None

getKey(*spec_data_file_line*)
Find the key that matches this line in a SPEC data file. Return None if not found.

Parameters **spec_data_file_line** (*str*) – one line from a SPEC data file

hasKey(*key*)
Is this key known?

load_plugins()
Call this once to load all plugins that handle SPEC control lines

process(*key*, **args*, ***kw*)
pick the control line handler by key and call its process() method

register(*handler*)
add this handler to the list of known handlers

Common Methods: spec2nexus.utils

source code documentation

(internal library) common methods used in **spec2nexus** modules

clean_name(key)	create a name that is allowed by both HDF5 and NeXus rules
get_all_plugins()	load all spec2nexus plugin modules
iso8601(date)	convert SPEC time (example: Wed Nov 03 13:39:34 2010) into ISO8601 string

Continued on next page

Table 2.19 – continued from previous page

strip_first_word(line)	return everything after the first space on the line from the spec data file
sanitize_name(group, key)	make name that is allowed by HDF5 and NeXus rules
reshape_data(scan_data, scan_shape)	Shape scan data from raw to different dimensionality

spec2nexus.utils.**clean_name**(*key*)
create a name that is allowed by both HDF5 and NeXus rules

Parameters **key** (*str*) – identifying string from SPEC data file

See http://download.nexusformat.org/doc/html/datarules.html

The "sanitized" name fits this regexp:

```
[A-Za-z_][\w_]*
```

An easier expression might be: `[\w_]*` but this will not pass the rule that valid NeXus group or field names cannot start with a digit.

spec2nexus.utils.**get_all_plugins**()
load all spec2nexus plugin modules

spec2nexus.utils.**iso8601**(*date*)
convert SPEC time (example: Wed Nov 03 13:39:34 2010) into ISO8601 string

Parameters **date** (*str*) – time string from SPEC data file

Example

SPEC Wed Nov 03 13:39:34 2010

ISO8601 2010-11-03T13:39:34

spec2nexus.utils.**reshape_data**(*scan_data*, *scan_shape*)
Shape scan data from raw to different dimensionality

Some SPEC macros collect data in a mesh or grid yet report the data as a 1-D sequence of observations. For further processing (such as plotting), the scan data needs to be reshaped according to its intended dimensionality.

modified from nexpy.readers.readspec.reshape_data

spec2nexus.utils.**sanitize_name**(*group*, *key*)
make name that is allowed by HDF5 and NeXus rules

Note **deprecated** use *clean_name()* instead (`group` is never used)

Parameters

- **group** (*str*) – unused
- **key** (*str*) – identifying string from SPEC data file

See http://download.nexusformat.org/doc/html/datarules.html

sanitized name fits this regexp:

```
[A-Za-z_][\w_]*
```

An easier expression might be: `[\w_]*` but this will not pass the rule that valid names cannot start with a digit.

spec2nexus.utils.**strip_first_word**(*line*)
return everything after the first space on the line from the spec data file

spec2nexus.scanf

Simple scanf-implementation. This module provides an easy way to parse simple formatted strings. It works similar to the version C programmers are used to.

source code documentation

Small scanf-implementation.

- Created by Henning Schroeder on Mon, 12 Feb 2007
- PSF license

Python has powerful regular expressions but sometimes they are totally overkill when you just want to parse a simple-formatted string. C programmers use the scanf-function for these tasks (see link below).

This implementation of scanf translates the simple scanf-format into regular expressions. Unlike C you can be sure that there are no buffer overflows possible.

source: http://code.activestate.com/recipes/502213-simple-scanf-implementation/

For more information see:

- http://www.python.org/doc/current/lib/node49.html
- http://en.wikipedia.org/wiki/Scanf

spec2nexus.scanf.**scanf**(*fmt*, *s=None*)

scanf supports the following formats:

format	description
%c	One character
%5c	5 characters
%d	int value
%7d	int value with length 7
%f	float value
%o	octal value
%X, %x	hex value
%s	string terminated by whitespace

Examples: >>> scanf("%s - %d errors, %d warnings", "/usr/sbin/sendmail - 0 errors, 4 warnings") ('/usr/sbin/sendmail', 0, 4) >>> scanf("%o %x %d", "0123 0x123 123") (66, 291, 123)

If the parameter s is a file-like object, s.readline is called. If s is not specified, stdin is assumed.

The function returns a tuple of found values or None if the format does not match.

spec2nexus.singletons

This is an internal library of the **spec2nexus** software. It is not expected that users of this package will need to call the *singletons* module directly.

source code documentation

singletons: Python 2 and 3 Compatible Version

see http://stackoverflow.com/questions/6760685/creating-a-singleton-in-python

USAGE:

```
class Logger(Singleton):
    pass
```

Installation

Released versions of spec2nexus are available on PyPI.

If you have `pip` installed, then you can install:

```
$ pip install spec2nexus
```

If you are using Anaconda Python and have `conda` installed, then you can install:

```
$ conda install -c http://conda.anaconda.org/prjemian spec2nexus
```

The latest development versions of spec2nexus can be downloaded from the GitHub repository listed above:

```
$ git clone http://github.com/prjemian/spec2nexus.git
```

To install in the standard Python location:

```
$ cd spec2nexus
$ python setup.py install
```

To install in user's home directory:

```
$ python setup.py install --user
```

To install in an alternate location:

```
$ python setup.py install --prefix=/path/to/installation/dir
```

Required Libraries

These libraries are required to write NeXus data files. They are not required to read SPEC data files.

Library	URL
h5py	http://www.h5py.org
numpy	http://numpy.scipy.org/

Optional Libraries

These libraries are used by the *specplot* and *specplot_gallery* modules of the *spec2nexus* package but are not required just to read SPEC data files or write NeXus data files.

Library	URL
MatPlotLib	http://matplotlib.org/

Unit Testing

Since release 2017.0201.0, this project relies on the Python *unittest*[1] package to apply unit testing[2] to the source code. The test code is in the *tests* directory. Various tests have been developed starting with the *2017.0201.0* release to provide features or resolve problems reported. The tests are not yet exhaustive yet the reported code coverage[3] is well over 80%.

The unit tests are implemented in a standard manner such that independent review[4] can run the tests on this code based on the instructions provided in a *.travis.yml* configuration file in the project directory.

This command will run the unit tests locally:

```
python tests
```

Additional information may be learned with a Python package to run the tests:

```
coverage run -a tests && coverage report -m
```

The *coverage* command ([5]), will run the tests and then prepare a report of the percentage of the Python source code that has been executed during the unit tests.

Note: The number of lines reported by *coverage* may differ from that reported by *travis-ci*. The primary reason is that certain tests involving access to information from GitHub may succeed or not depending on the "Github API rate limit".[6]

Example data

About these example data files

These files are examples of various data files that may be read by **spec2nexus**. They are used to test various components of the interface.

[1] Python *unittest* package: https://docs.python.org/2/library/unittest.html
[2] unit testing: https://en.wikipedia.org/wiki/Unit_testing
[3] *coveralls* code coverage: https://coveralls.io/github/prjemian/spec2nexus
[4] *travis-ci* continuous intregration: https://travis-ci.org/prjemian/spec2nexus
[5] *coverage*: https://coverage.readthedocs.io
[6] Github API rate limit: https://developer.github.com/v3/rate_limit/

file		type description
02_03_setup.dat	SPEC scans	1-D scans, some have no data lines (data are stored in HDF5 file)
33bm_spec.dat	SPEC scans	1-D & 2-D scans (includes hklscan & hklmesh)
33id_spec.dat	SPEC scans	1-D & 2-D scans (includes mesh & Escan scans & MCA data)
APS_spec_data.dat	SPEC scans	1-D scans (ascan & uascan), includes lots of metadata and comments
CdOsO	SPEC scans	1-D scans (ascan), four #E (2, 3659, 3692, 3800) and two #S 1 (35, 3725)
CdSe	SPEC scans	1-D scans (ascan), problem with scan abort on lines 5918-9, in scan 92
compression.h5	NeXus HDF5	2-D compressed image, also demonstrates problem to be resolved in code
Data_Q.h5	NeXus HDF5	2-D image at /entry/data/{I,Q}, test file and variable-length strings
lmn40.spe	SPEC scans	1-D & 2-D scans (hklmesh), two #E lines, has two header sections
mca_spectra_example.dat	SPEC scans	1-D scans (cscan) with 4 MCA spectra in each scan (issue #55)
writer_1_3.h5	NeXus HDF5	1-D NeXus User Manual example
YSZ011_ALDITO_Fe2O3_planar_fired_1.spc	SPEC scans	1-D scans, text in #V metadata, also has #UIM control lines
03_06_JanTest.dat	SPEC scans	1-D scans, USAXS scans, Fly scans, #O+#o and #J+#j control lines
user6idd.dat	SPEC scans	1-D scans, aborted scan, control lines: #R #UB #UE #UX #UX1 #UX2 #X, non-default format in #X lines

Downloads

These downloads are also available online: https://github.com/prjemian/spec2nexus/tree/master/src/spec2nexus/data

- `33bm_spec.dat`
- `33id_spec.dat`
- `APS_spec_data.dat`
- `CdSe`
- `compression.h5`
- `Data_Q.h5`
- `lmn40.spe`
- `mca_spectra_example.dat`
- `user6idd.dat`
- `writer_1_3.h5`
- `YSZ011_ALDITO_Fe2O3_planar_fired_1.spc`

Change History

Production

2017.711.0

- **#110** Ownership of info between #L/data & #S n
- #109 Spaces in data labels on *#L* and other lines

2017.522.1

- #105 ignore extra content in *#@CALIB* control lines
- #104 use versioneer (again)
- **#101** documentation URL & date/time added to every gallery page
- #100 conda package installs properly on Windows now
- #99 BUG: specplot_gallery: plots of hklscan from file *lmn40.spe*
- #98 BUG: specplot_gallery: identify as directory not found
- #52 remove deprecated *prjPySpec* code

2017.317.0

- minor update of the *2017.3.0* release

2017.3.0

- #103 changed *converters* back to *utils*
- #97 PyPI project description now formatted properly
- #90 use *versioneer* (again)

2017-0202.0

- #99 fix list index error in *hklscan* when hkl are all constant
- #96 combine steps when publishing to PyPI

2017-0201.0

- milestone punch list
- #73 refactor mesh and MCA data parsing code
- #67 apply continuous integration via travis-ci
- #66 add verbosity option
- #65 apply unit testing
- #64 *extractSpecScan*: fixed list index out of range
- #63 *extractSpecScan*: command line option to select range of scans
- #56 *specplot* and *specplot_gallery*: add from USAXS instrument and generalize

2016.1025.0 standardize the versioning kit with pyRestTable and pvWebMonitor

2016.1004.0

- #61 release info from git (dropped versioneer package)

2016.0829.0

- #60 Add new plugin test for XPCS plugin (thanks to John Hammonds)

2016.0615.1

- #57 keep information from unrecognized control lines,
- #56 add *specplot* support,
- #55 accept arbitrary number of MCA spectra

2016.0601.0 match complete keys, use unix EOL internally, do not fail if no metadata

2016.0216.0

- #36 identify NIAC2014-compliant NeXus files

2016.0210.0 bugfix: eznx.makeGroup() now correctly sets attributes on new group + documentation for NIAC2014 attributes

2016.0204.0

- #45 handle case when no data points in scan ,
- #46 spec.getScan() ensures argument is used as `str`

2016.0201.0 added spec.getScanNumbersChronological(), spec.getFirstScanNumber(), and spec.getLastScanNumber()

2016.0131.0

- #43 support new NeXus method for default/signal/axes/_indices,

2016.0130.0 fixed #44

2015.1221.1

- #40 added versioneer support

2015.1221.0

- #39 read scans with repeated scan numbers

2015.0822.0 extractSpecScan: add option to report scan heading data, such as positioners and Q

2015.0214.0 h5toText: handle HDF5 'O' data type (variable length strings)

2015.0127.0 spec: ignore bad data lines

2015.0125.0 spec: change handling of #L & #X, refactor detection of scanNum and scanCmd

2015.0113.0 dropped requirement of *lxml* package

2014.1228.1 spec: build mne:name cross-references for counters and positioners

2014.1228.0 show version in documentation

2014.1028.0 spec: quietly ignore unrecognized scan content *for now*

2014.1027.1 spec: major changes in SPEC file support: **custom plugins**

- **spec** based on plugins for each control line, users can add plugins
- declared **prjPySpec** module as legacy, code is frozen at *2014.0623.0* release
- added **spec** module to replace **prjPySpec**

2014.0623.0 updated argparse settings

2014.0622.2 added extractSpecScan.py to the suite from the USAXS project

2014.0410.0 restore scan.fileName variable to keep interface the same for some legacy clients

2014.0404.1 fix sdist utf8 problem, see: http://bugs.python.org/issue11638

2014.0404.0 tree_api_parser moved back into NeXpy project

2014.0320.6 handle multiple header sections in SPEC data file

2014.0320.5 fix the new project URL

2014.0320.4 Sphinx cannot build PDF with code-block in a footnote

2014.0320.3 note the new home URL in the packaging, too, drop nexpy requirement, default docs theme

2014.0320.2 tree_api_parse will go back into nexpy project, remove docs of it here

2014.0320.1 allow readthedocs to build Sphinx without extra package requirements

2014.0320.0

- new home page at http://spec2nexus.readthedocs.org, easier to publish there
- move common methods from __init__.py so docs will build at readthedocs.org
- new test case fails existing SPEC reader, ignore blank lines

2014.03.11 documentation

2014.03.09 h5toText: option to suppress printing of attributes, put URLs in command-line usage documentation, better test of is_spec_file()

2014.03.08 fixed string writer and content display bug in eznx, added h5toText.py, prjPySpec docs improved again

2014.03.051 prjPySpec now handles SPEC v6 data file header additions, add new getScanCommands() method

2014.03.04 (2014_Mardi_Gras release) removed nexpy project requirement from setup, prjPySpec raises exceptions now

2014.03.02 drops nexus tree API (and its dependencies) in favor of native h5py writer

Development: GitHub repository

2014.02.20 version number fits PEP440, LICENSE file included in sdist, more documentation and examples

2014-02-19 reference published documentation (re-posted)

2014-02-19 add documentation framework

2014-02-18 fork to GitHub to make generally available

Development: NeXpy branch

2014-01 briefly, a branch in https://github.com/nexpy/nexpy

- spec2nexus added during this phase
- relies on nexpy.api.nexus for NeXus support

Production: USAXS livedata

2010-2014 production use

- support livedata WWW page of APS USAXS instrument
  - (http://usaxs.xray.aps.anl.gov/livedata/),
- https://subversion.xray.aps.anl.gov/trac/small_angle/browser/USAXS/livedata/prjPySpec.py
- converted from Tcl

2000-2010 Tcl code (*readSpecData.tcl*) in production use at APS sectors 32, 33, & 34

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