Quantum Metrology with Photoelectrons Vol. 3

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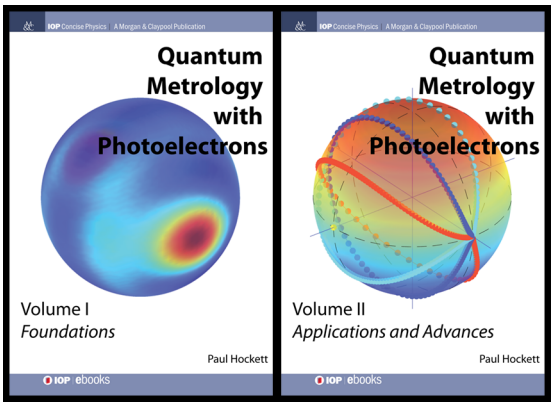
CONTENTS

Quantum metrology with photoelectrons volume 3, open source executable book. This repository contains the source documents (mainly Jupyter Notebooks in Python) and notes for the book, as of Jan 2022 writing is in progress, and the current HTML build can be found online. The book is due to be finished in 2023, and will be published by IOP Press - see below for more details.

Series abstract

Photoionization is an interferometric process, in which multiple paths can contribute to the final continuum photoelectron wavefunction. At the simplest level, interferences between different final angular momentum states are manifest in the energy and angle resolved photoelectron spectra: metrology schemes making use of these interferograms are thus phase-sensitive, and provide a powerful route to detailed understanding of photoionization. In these cases, the continuum wavefunction (and underlying scattering dynamics) can be characterised. At a more complex level, such measurements can also provide a powerful probe for other processes of interest, leading to a more general class of quantum metrology built on phase-sensitive photoelectron imaging. Since the turn of the century, the increasing availability of photoelectron imaging experiments, along with the increasing sophistication of experimental techniques, and the availability of computational resources for analysis and numerics, has allowed for significant developments in such photoelectron metrology.

About the books



- Volume I covers the core physics of photoionization, including a range of computational examples. The material is presented as both reference and tutorial, and should appeal to readers of all levels. ISBN 978-1-6817-4684-5, http://iopscience.iop.org/book/978-1-6817-4684-5 (IOP Press, 2018)
- Volume II explores applications, and the development of quantum metrology schemes based on photoelectron measurements. The material is more technical, and will appeal more to the specialist reader. ISBN 978-1-6817-4688-3, http://iopscience.iop.org/book/978-1-6817-4688-3 (IOP Press, 2018)

Additional online resources for Vols. I & II can be found on OSF and Github.

- Volume III in the series will continue this exploration, with a focus on numerical analysis techniques, forging a closer link between experimental and theoretical results, and making the methodologies discussed directly accessible via new software. The book is due for publication by IOP due in 2023; this volume is also open-source, with a live HTML version at https://phockett.github.io/Quantum-Metrology-with-Photoelectrons-Vol3/ and source available at https://github.com/phockett/Quantum-Metrology-with-Photoelectrons-Vol3.

For some additional details and motivations (including topical video), see the ePSdata project.

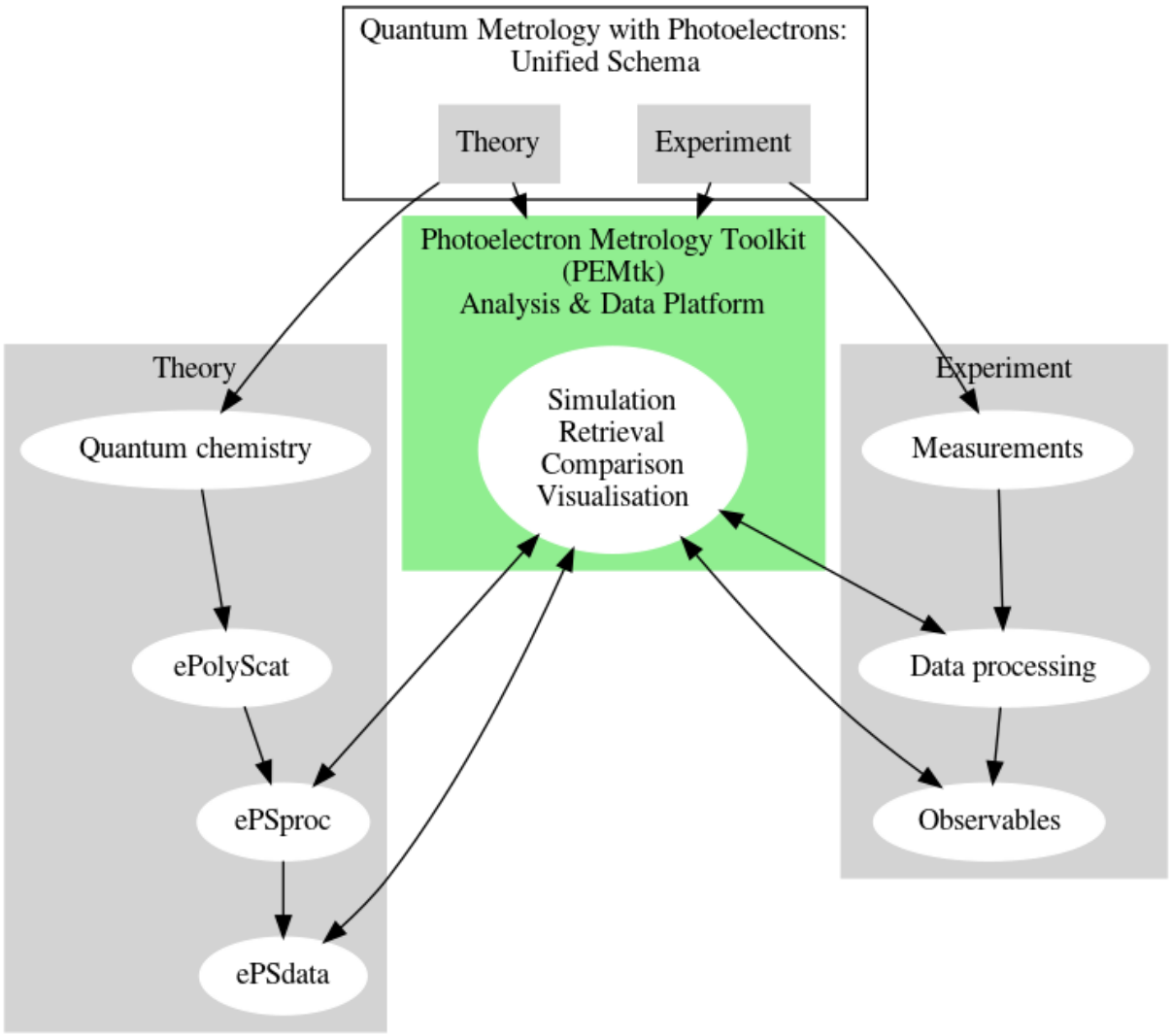
Technical details

This repository contains:

- `doc-source`: the source documents (mainly Jupyter Notebooks in Python)
- `notes`: additional notes for the book,
- the `gh-pages` branch contains the current HTML build, also available at https://phockett.github.io/Quantum-Metrology-with-Photoelectrons-Vol3/

The project has been setup to use the Jupyter Book build-chain (which uses Sphinx on the back-end) to generate HTML and Latex outputs for publication from source Jupyter notebooks & markdown files.

The work *within* the book will make use of the Photoelectron Metrology Toolkit platform for working with experimental & theoretical data.



Running code examples

Each Jupyter notebook (`*.ipynb`) can be treated as a stand-alone computational document. These can be run/used/modified independently with an appropriately setup python environment (details to follow).

Building the book

The full book can also be built from source:

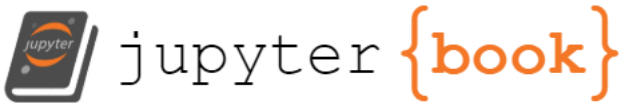
1. Clone this repository
2. Run `pip install -r requirements.txt` (it is recommended you do this within a virtual environment)
3. (Optional) Edit the books source files located in the `doc-source/` directory
4. Run `jupyter-book clean doc-source/` to remove any existing builds
5. For an HTML build:
    - Run `jupyter-book build doc-source/`
    - A fully-rendered HTML version of the book will be built in `doc-source/_build/html/`.
6. For a LaTex & PDF build:
    - Run `jupyter-book build doc-source/ --builder pdflatex`
    - A fully-rendered HTML version of the book will be built in `doc-source/_build/latex/`.

See https://jupyterbook.org/basics/building/index.html for more information.

Credits

This project is created using the open source Jupyter Book project and the executablebooks/cookiecutter-jupyter-book template.

To add: build env & main software packages (see automation for this…)



CHAPTER

ONE

EPSPROC BASE AND MULTIJOB CLASS INTRO

16/10/20

As of Oct. 2020, v1.3.0-dev, basic data classes are now implemented, and are now the easiest/preferred method for using ePSproc (as opposed to calling core functions directly, as illustrated in the functions guide).

A brief intro and guide to use is given here.

Aims:

- Provide unified data architecture for ePSproc, ePSdata and PEMtk.
- Wrap plotting and computational functions for ease of use.
- Handle multiple datasets inc. comparitive plots.

1.1 Setup

```
# For module testing, include path to module here, otherwise use global installation
local = True

if local:
    import sys
    if sys.platform == "win32":
        modPath = r'D:\code\github\ePSproc'  # Win test machine
        winFlag = True
    else:
        modPath = r'/home/femtolab/github/ePSproc/'  # Linux test machine
        winFlag = False

    sys.path.append(modPath)

# Base
import epsproc as ep

# Class dev code
from epsproc.classes.multiJob import ePSmultiJob
from epsproc.classes.base import ePSbase
```

```
* pyevtk not found, VTK export not available.
```

1.2 ePSbase class

The ePSbase class wraps most of the core functionality, and will handle all ePolyScat output files in a single data directory. In general, we'll assume:

- an ePS *job* constitutes a single ionization event/channel (ionizing orbital) for a given molecule, stored in one or more output files.
- the data dir contains one or more files, where each file will contain a set of symmetries and energies, with either
  - one file per ionizing event. In this case, each file will equate to one job, and one entry in the class datastructure.
  - a single ionizing event, where each file contains a different set of energies for the given event (*energy chunked* fileset). In this case, the files will be stacked, and the dir will equate to one job and one entry in the class datastructure.

The class datastructure is (currently) a set of dictionaries, with entries per job as above, and various data for each job. In general the data is stored in Xarrays.

The `multiJob` class extends the base class with reading from multple directories.

1.2.1 Load data

Firstly, set the data path, instantiate a class object and load the data.

```
# Set for ePSproc test data, available from https://github.com/phockett/ePSproc/tree/
 ↪master/data
# Here this is assumed to be on the epsproc path
import os
dataPath = os.path.join(sys.path[-1], 'data', 'photoionization', 'n2_multiorb')
```

```
# Instantiate class object.
# Minimally this needs just the dataPath, if verbose = 1 is set then some useful␣
 ↪output will also be printed.
data = ePSbase(dataPath, verbose = 1)
```

```
# ScanFiles() - this will look for data files on the path provided, and read from␣
 ↪them.
data.scanFiles()
```

```
*** Job orb6 details
Key: orb6
Dir D:\code\github\ePSproc\data\photoionization\n2_multiorb, 1 files.
{   'batch': 'ePS n2, batch n2_1pu_0.1-50.1eV, orbital A2',
    'event': ' N2 A-state (1piu-1)',
    'orbE': -17.096913836366,
    'orbLabel': '1piu-1'}

*** Job orb5 details
Key: orb5
Dir D:\code\github\ePSproc\data\photoionization\n2_multiorb, 1 files.
{   'batch': 'ePS n2, batch n2_3sg_0.1-50.1eV, orbital A2',
    'event': ' N2 X-state (3sg-1)',
    'orbE': -17.341816310545997,
    'orbLabel': '3sg-1'}
```

In this case, two files are read, and each file is a different ePS job - here the $3\sigma_g^{-1}$ and $1\pi_u^{-1}$ channels in N2. The keys for the job are also used as the job names.

1.2.2 Basic info & plots

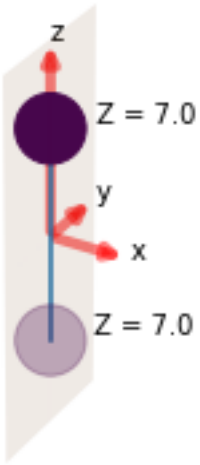
A few basic methods to summarise the data…

```
# Summarise jobs, this will also be output by scanFile() if verbose = 1 is set, as␣
↪illustrated above.
data.jobsSummary()
```

```
*** Job orb6 details
Key: orb6
Dir D:\code\github\ePSproc\data\photoionization\n2_multiorb, 1 files.
{   'batch': 'ePS n2, batch n2_1pu_0.1-50.1eV, orbital A2',
    'event': ' N2 A-state (1piu-1)',
    'orbE': -17.096913836366,
    'orbLabel': '1piu-1'}

*** Job orb5 details
Key: orb5
Dir D:\code\github\ePSproc\data\photoionization\n2_multiorb, 1 files.
{   'batch': 'ePS n2, batch n2_3sg_0.1-50.1eV, orbital A2',
    'event': ' N2 X-state (3sg-1)',
    'orbE': -17.341816310545997,
    'orbLabel': '3sg-1'}
```

```
# Molecular info
# Note that this is currently assumed to be the same for all jobs in the data dir.
data.molSummary()
```

```
*** Molecular structure
```



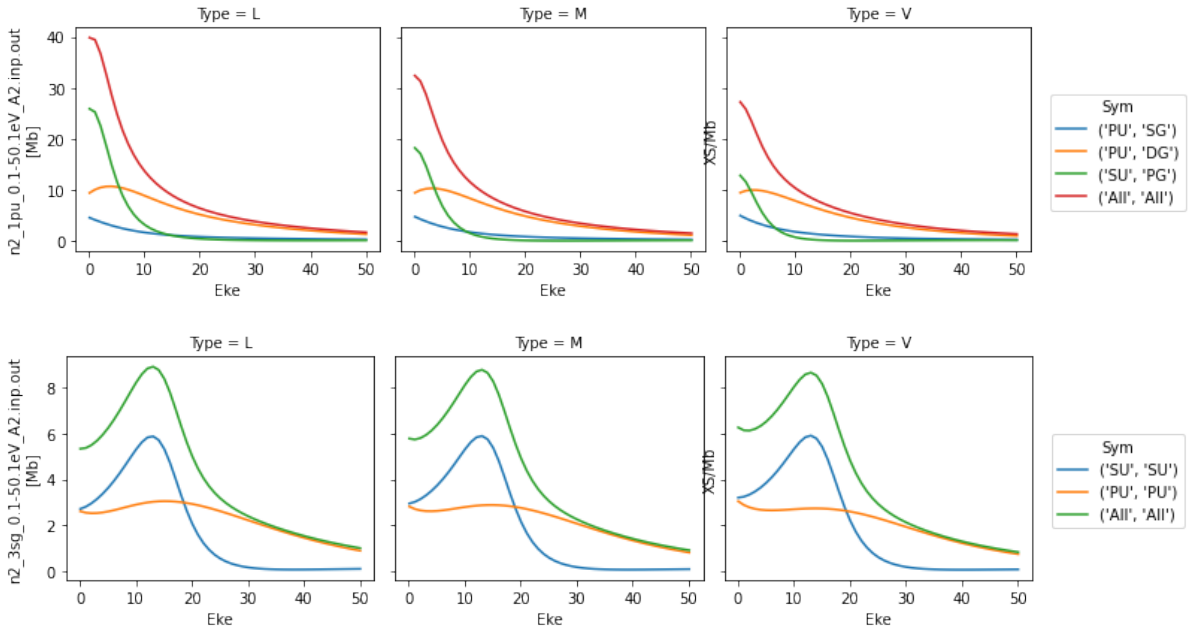
```
*** Molecular orbital list (from ePS output file)
EH = Energy (Hartrees), E = Energy (eV), NOrbGrp, OrbGrp, GrpDegen = degeneracies␣
↪and corresponding orbital numbering by group in ePS, NormInt = single centre␣
↪expansion convergence (should be ~1.0).
```

props	Sym	EH	Occ	E	NOrbGrp	OrbGrp	GrpDegen	NormInt
orb								
1	SG	-15.6719	2.0	-426.454121	1.0	1.0	1.0	0.999532
2	SU	-15.6676	2.0	-426.337112	1.0	2.0	1.0	0.999458
3	SG	-1.4948	2.0	-40.675580	1.0	3.0	1.0	0.999979
4	SU	-0.7687	2.0	-20.917392	1.0	4.0	1.0	0.999979
5	SG	-0.6373	2.0	-17.341816	1.0	5.0	1.0	1.000000
6	PU	-0.6283	2.0	-17.096914	1.0	6.0	2.0	1.000000
7	PU	-0.6283	2.0	-17.096914	2.0	6.0	2.0	1.000000

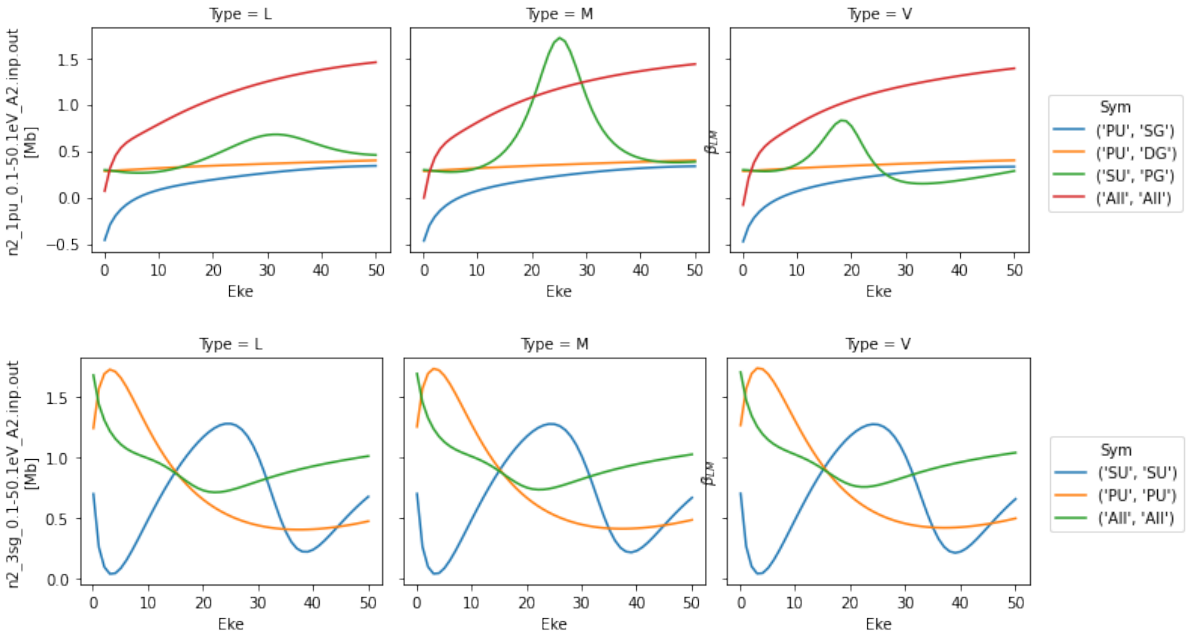
1.2.3 Plot cross-sections and betas

These are taken from the `GetCro` segments in the ePS output files, and correspond to results for an isotropic ensemble of molecules, i.e. observables in the lab frame (LF) for 1-photon ionization (see the ePS tutorial for more details).

```
# Minimal method call will plot cross-sections for all ePS jobs found in the data␣
↪directory.
data.plotGetCro()
```




```
# Plot beta parameters with the 'BETA' flag
data.plotGetCro(pType = 'BETA')
```



TODO: fix labelling here.

1.2.4 Compute MFPADs

The class currently wraps just the basic numerical routine for MFPADs. This defaults to computing MFPADs for all energies and (z, x, y) polarization geometries (where the z-axis is the molecular symmetry axis, and corresponds to the molecular structure plot shown above).

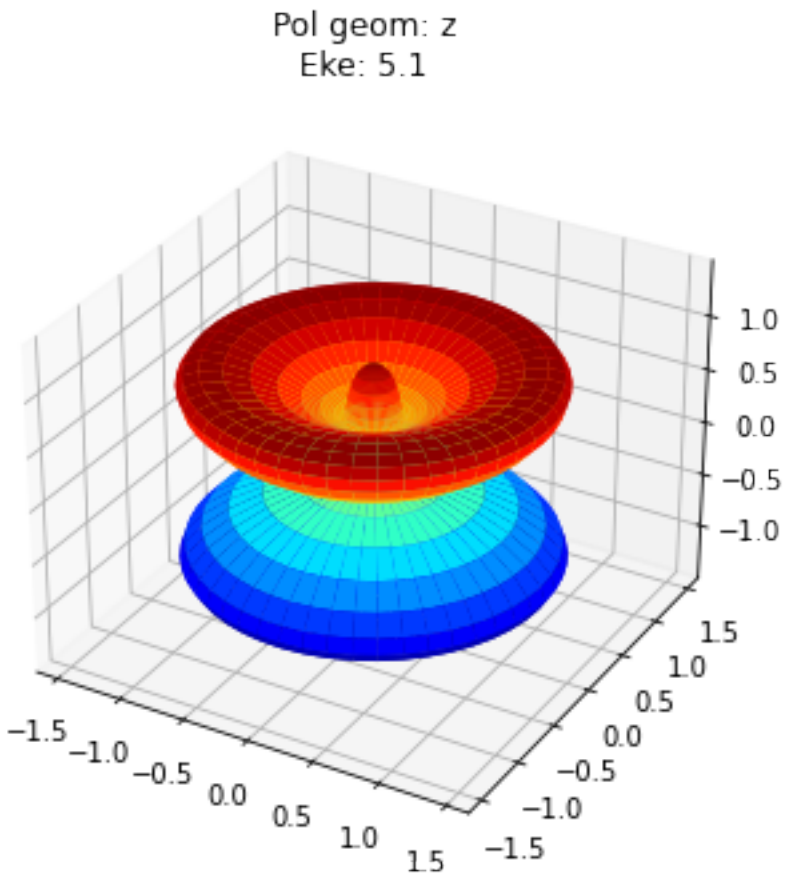
```
# Compute MFPADs...
data.mfpadNumeric()
```

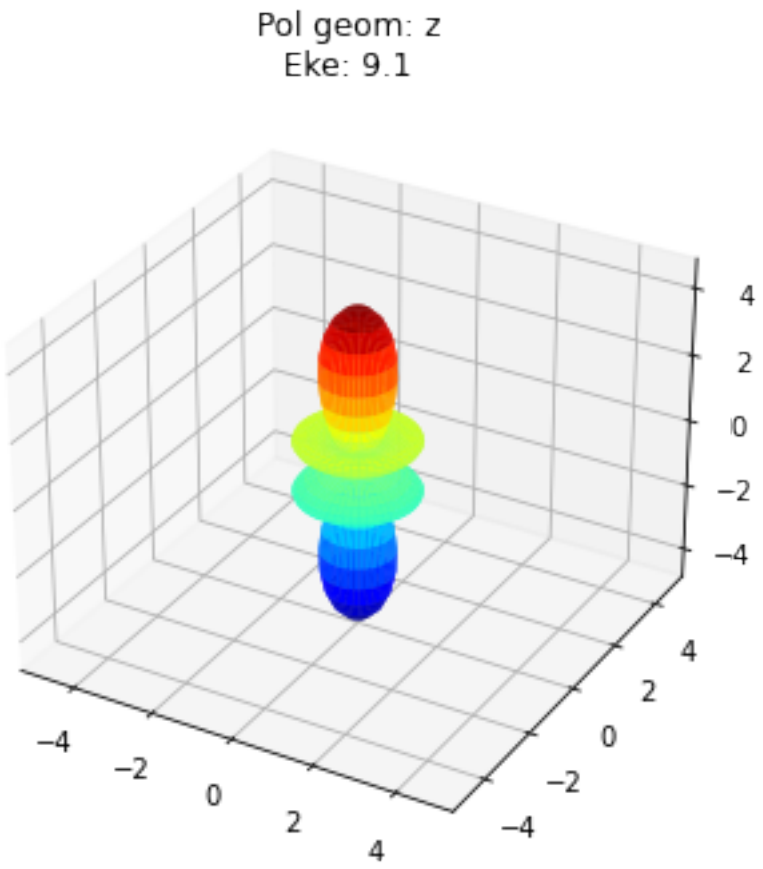
To plot it's advisable to set an enery slice, `Erange = [start, stop, step]`, since MFPADs are currently shown as individual plots in the default case, and there may be a lot of them.

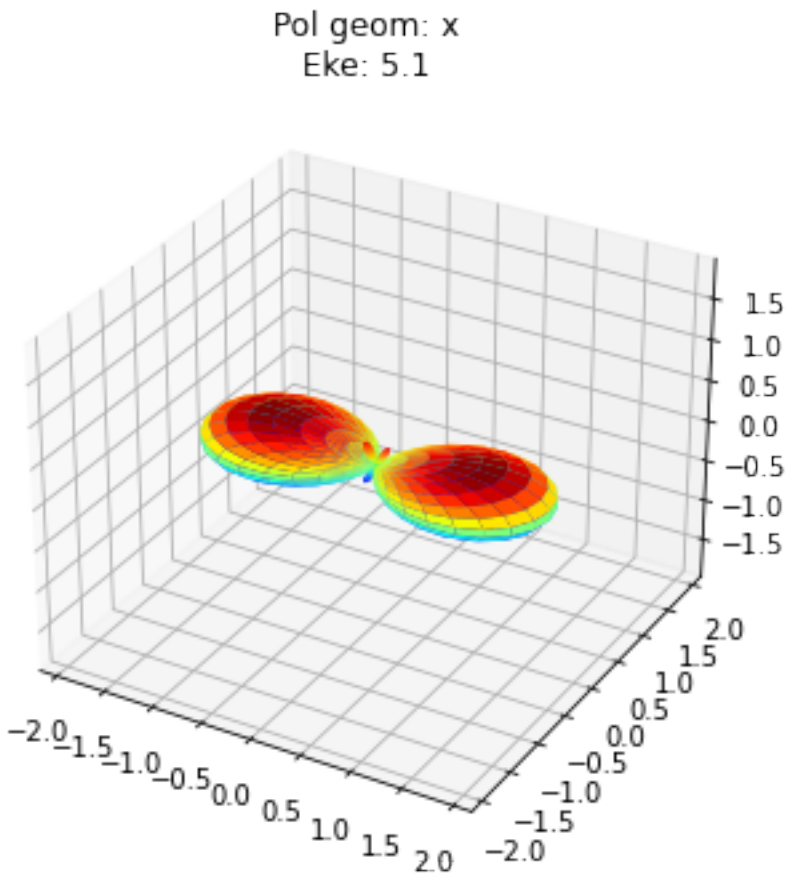
We'll also just set for a single key here, otherwise all jobs will be plotted.

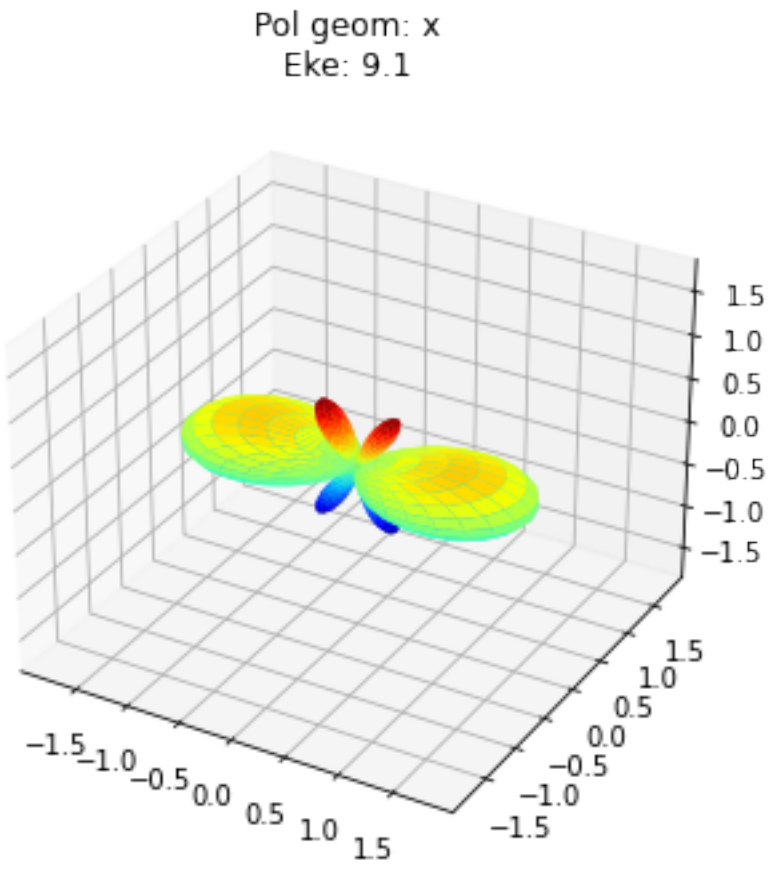
```
data.padPlot(keys = 'orb5', Erange = [5, 10, 4])

#TODO: fix plot layout!
```

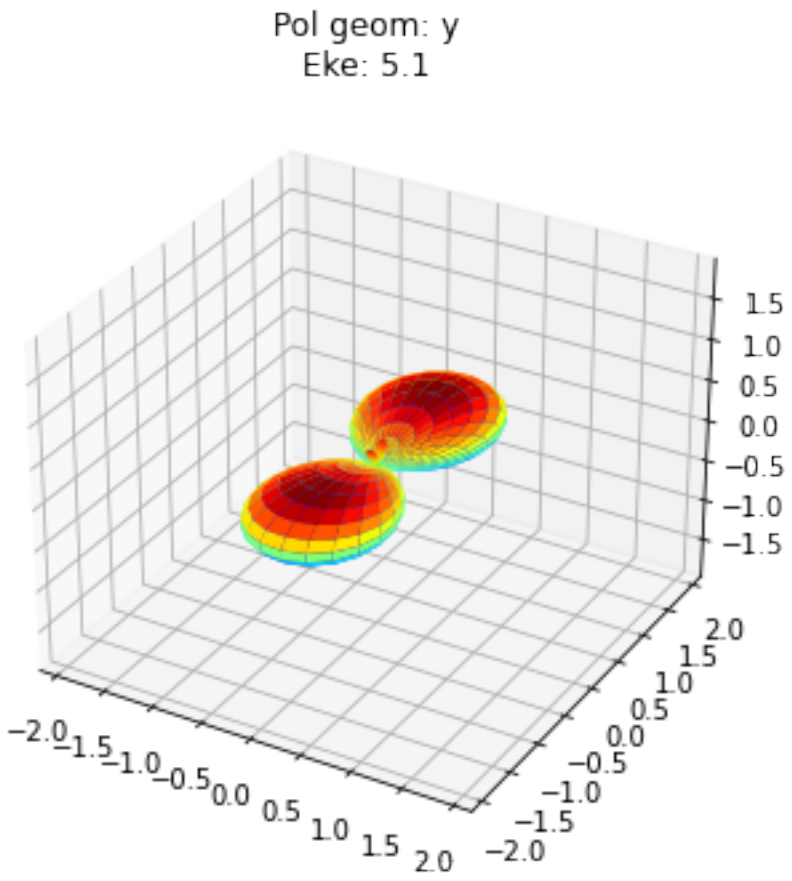
```
Found dims ('Labels', 'Phi', 'Theta', 'Eke', 'Sym'), summing to reduce for plot.␣
↪Pass selDims to avoid.
Sph plots: Pol geom: z
Plotting with mpl
Data dims: ('Phi', 'Theta', 'Eke'), subplots on Eke
Sph plots: Pol geom: x
Plotting with mpl
Data dims: ('Phi', 'Theta', 'Eke'), subplots on Eke
Sph plots: Pol geom: y
Plotting with mpl
Data dims: ('Phi', 'Theta', 'Eke'), subplots on Eke
```

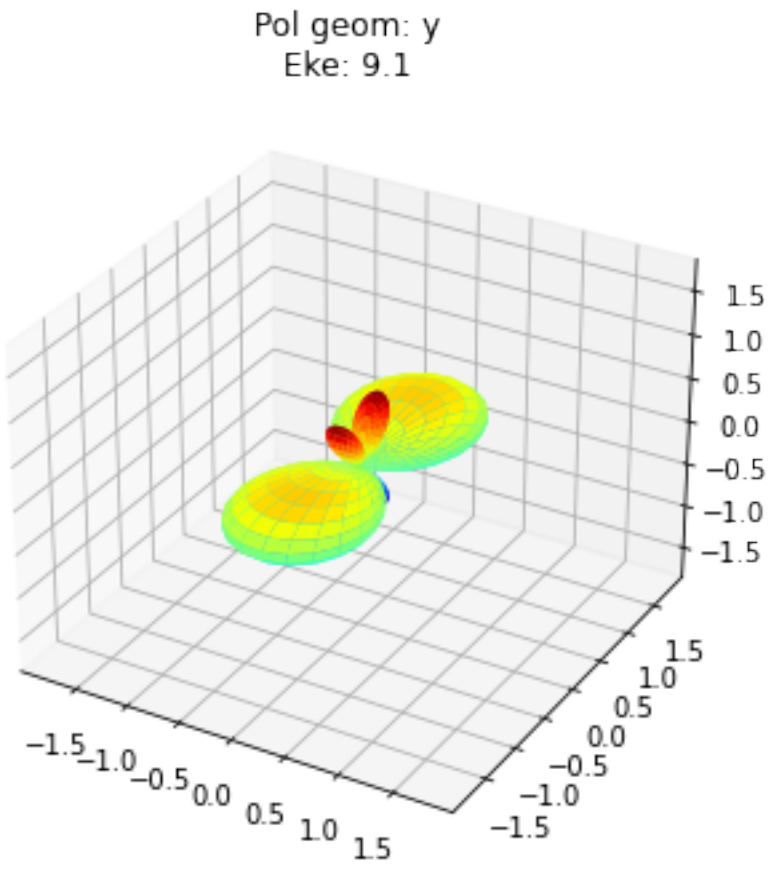

Pol geom: z
Eke: 5.1
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5


Pol geom: z
Eke: 9.1
4
2
0
−2
−4
−4
−2
0
2
4
4
2
0
−2
−4


Pol geom: x
Eke: 5.1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0


Pol geom: x
Eke: 9.1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5

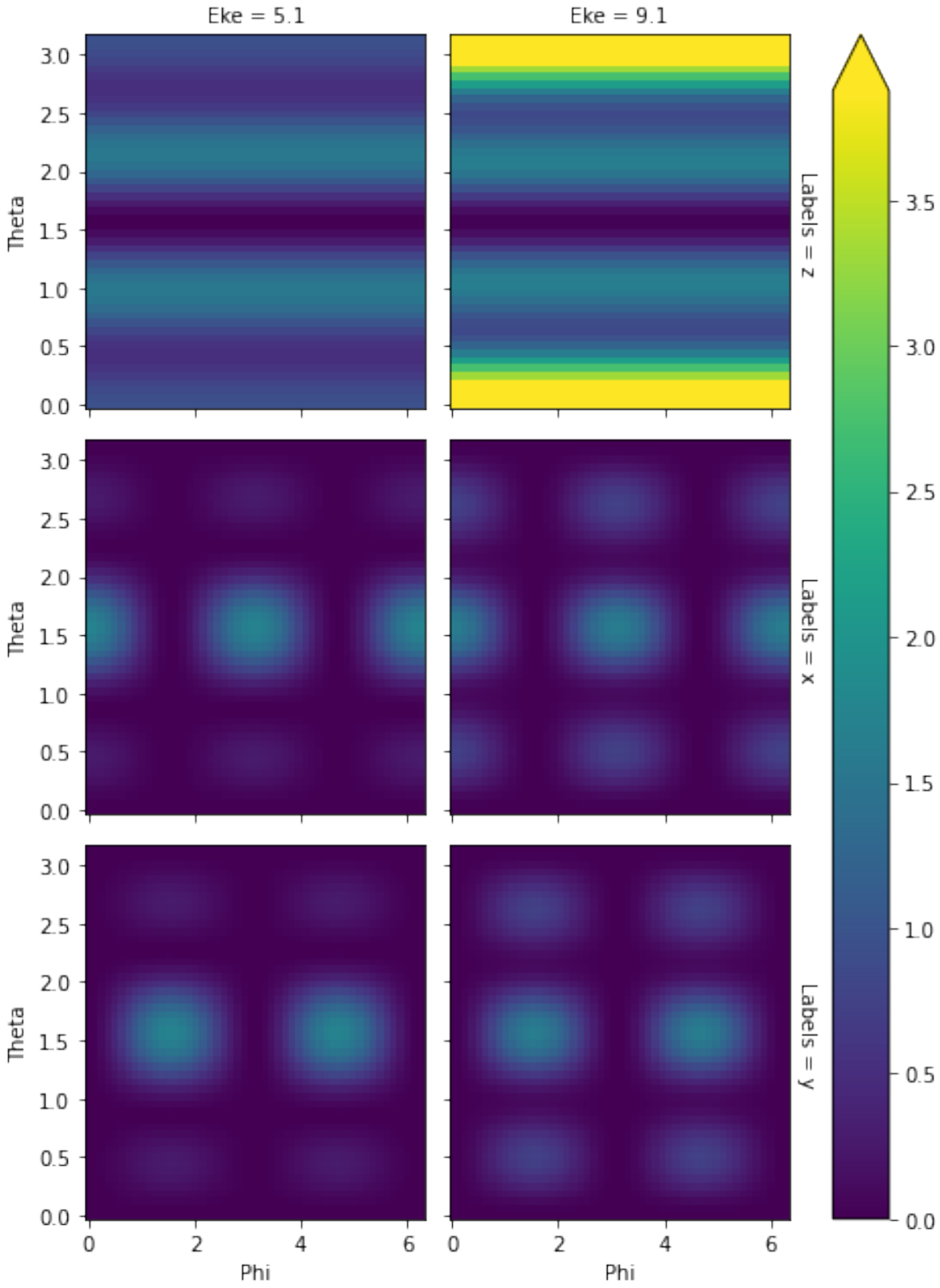

Pol geom: y
Eke: 5.1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0



To view multiple results in a more concise fashion, a Cartesian gridded output is also available.

```
data.padPlot(keys = 'orb5', Erange = [5, 10, 4], pStyle='grid')
```

```
Found dims ('Labels', 'Phi', 'Theta', 'Eke', 'Sym'), summing to reduce for plot.␣
↪Pass selDims to avoid.
Grid plot: 3sg-1
```


Eke = 5.1
Eke = 9.1
Theta
Phi
Labels = z
Labels = x
Labels = y
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
2
4
6
3.5

```
# Various other args can be passed...

# Set a plotting backend, currently 'mpl' (Matplotlib - default) or 'pl' (Plotly -␣
 ↪interactive, but may give issues in some environments)
backend = 'pl'

# Subselect on dimensions, this is set as a dictionary for Xarray selection (see␣
 ↪http://xarray.pydata.org/en/stable/indexing.html#indexing-with-dimension-names)
selDims = {'Labels':'z'}  # Plot z-pol case only.

data.padPlot(Erange = [5, 10, 4], selDims=selDims, backend = backend)
```

```
Found dims ('Phi', 'Theta', 'Eke', 'Sym'), summing to reduce for plot. Pass␣
 ↪selDims to avoid.
Sph plots: 1piu-1
Plotting with pl
```


```
Found dims ('Phi', 'Theta', 'Eke', 'Sym'), summing to reduce for plot. Pass␣
 ↪selDims to avoid.
Sph plots: 3sg-1
Plotting with pl
```

1.2.5 Compute β_{LM} parameters

For computation of β_{LM} parameters the class wraps functions from `epsproc.geom`, which implement a tensor method. This is quite fast, although memory heavy, so may not be suitable for very large problems. (See the method development pages for more info, more concise notes to follow).

- Functions are provided for MF and AF problems (which is the general case, and will equate to the LF case for an unaligned ensemble).
- For the MF the class wraps `ep.geom.mfblmXprod`, see the method development page for more info, more concise notes to follow.
- For the AF the class wraps `ep.geom.afblmXprod`, see the method development page for more info, more concise notes to follow.

Compute MF β_{LM} and PADs

Here's a quick demo for the default MF cases, which will give parameters corresponding to the (z, x, y) polarization geometries computed by the numerical routine above.

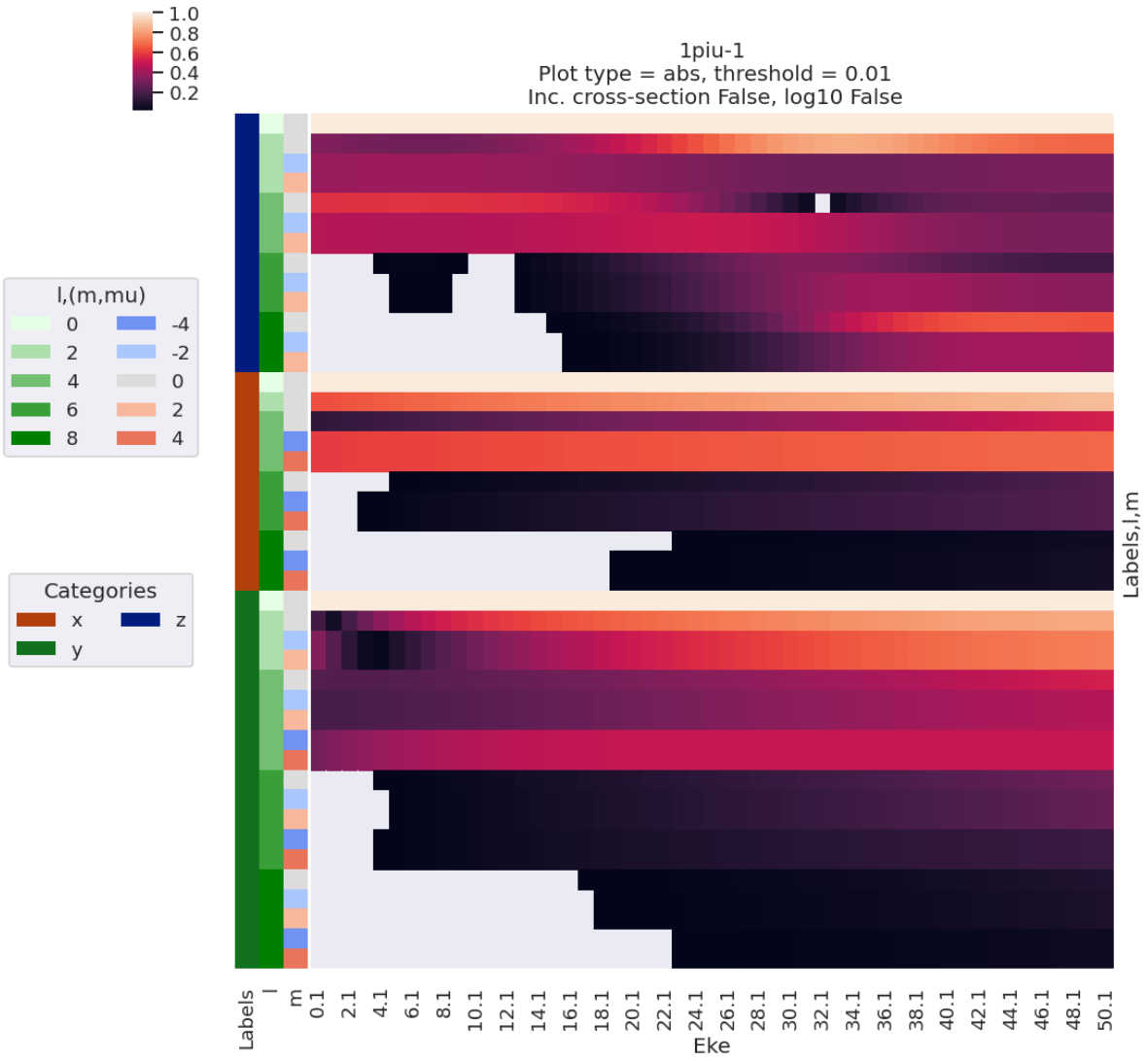
```
data.MFBLM()
```

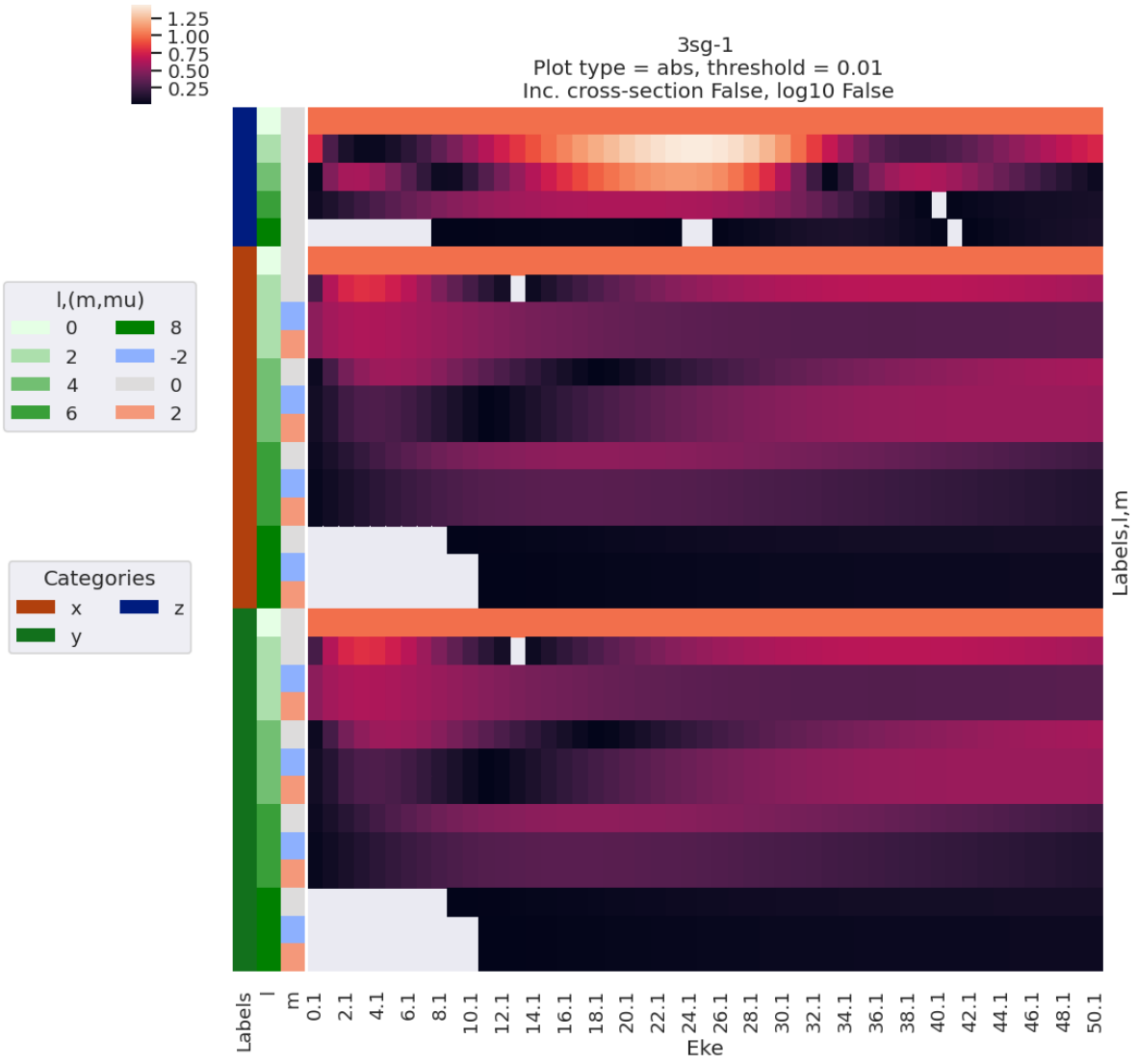
```
Calculating MF-BLMs for job key: orb6
Return type BLM.

Calculating MF-BLMs for job key: orb5
Return type BLM.
```

Plotting still needs to improve… but ep.lmPlot() is a robust way to plot everything.

```
# data.BLMplot(dataType = 'MFBLM')  # HORRIBLE OUTPUT at the moment!!!
data.lmPlot(dataType = 'MFBLM')
```

```
Plotting data n2_1pu_0.1-50.1eV_A2.inp.out, pType=a, thres=0.01, with Seaborn
Plotting data n2_3sg_0.1-50.1eV_A2.inp.out, pType=a, thres=0.01, with Seaborn
```

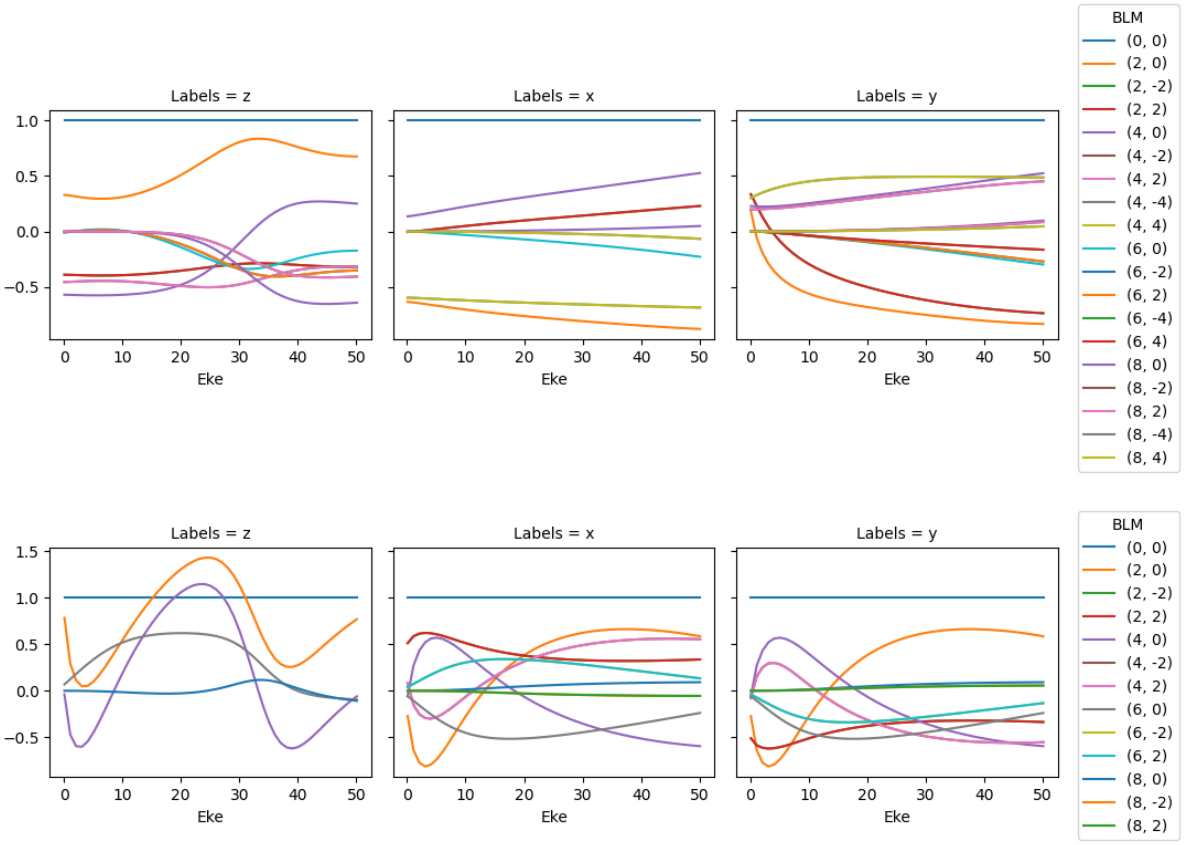

1.0
0.8
0.6
0.4
0.2
1piu-1
Plot type = abs, threshold = 0.01
Inc. cross-section False, log10 False
l,(m,mu)
0
2
4
6
8
-4
-2
0
2
4
Categories
x
y
z
Labels,l,m
Labels
l
m
0.1
2.1
4.1
6.1
8.1
10.1
12.1
14.1
16.1
18.1
20.1
22.1
24.1
26.1
28.1
30.1
32.1
34.1
36.1
38.1
40.1
42.1
44.1
46.1
48.1
50.1
Eke



Line-plots are available with the `BLMplot` method, although this currently only supports the Matplotlib backend, and may have problems with dims in some cases (work in progress!).

```
data.BLMplot(dataType='MFBLM', thres = 1e-2)  # Passing a threshold value here will␣
↪remove any spurious BLM parameters.
```

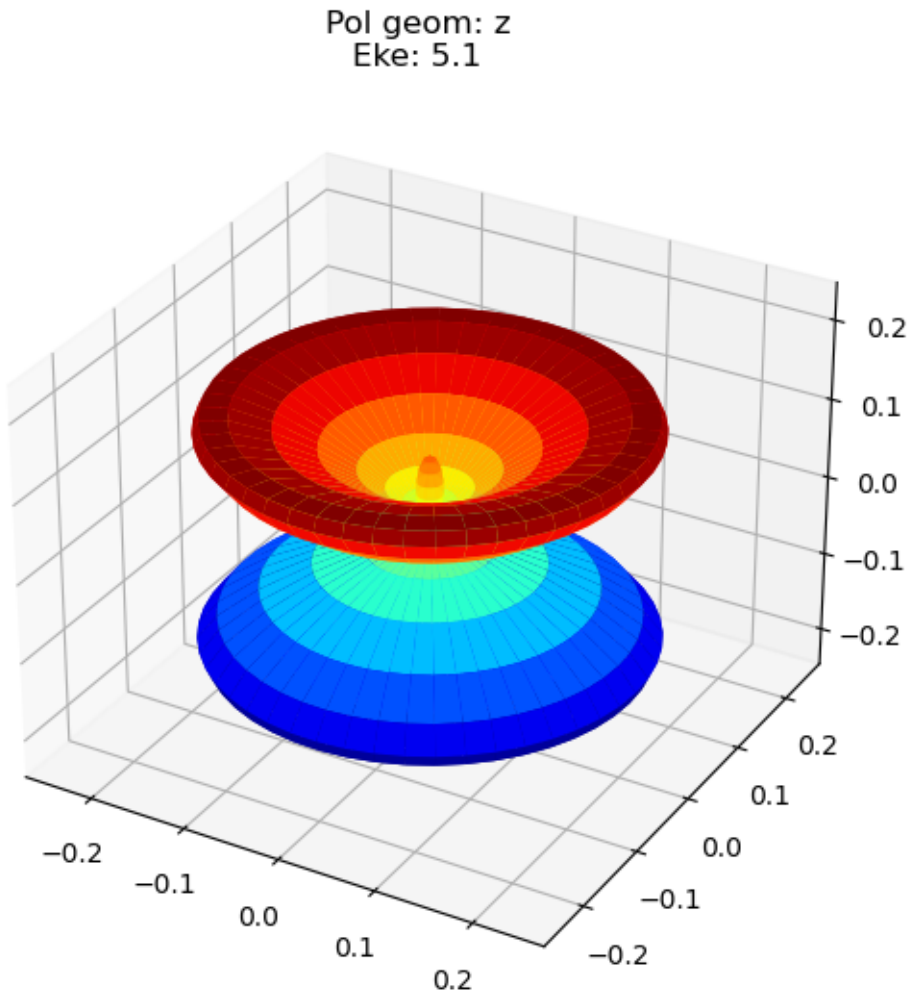
```
Dataset: orb6, 1piu-1, MFBLM
Dataset: orb5, 3sg-1, MFBLM
```

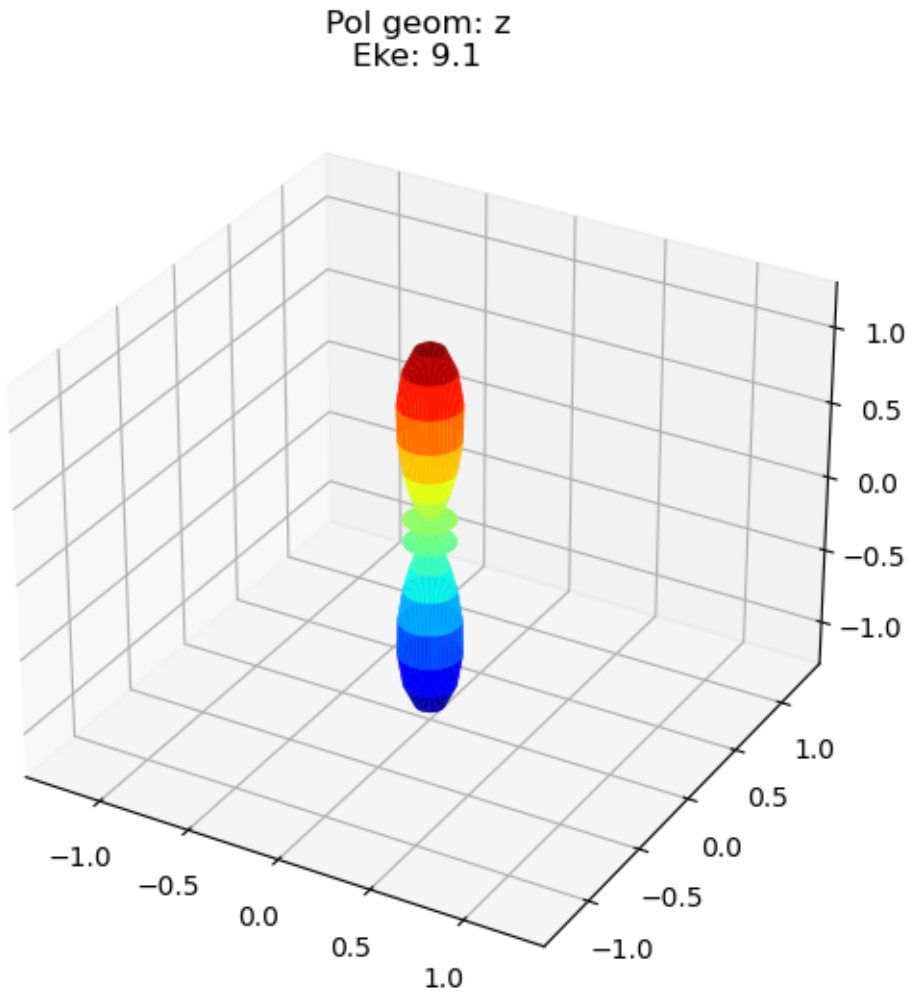


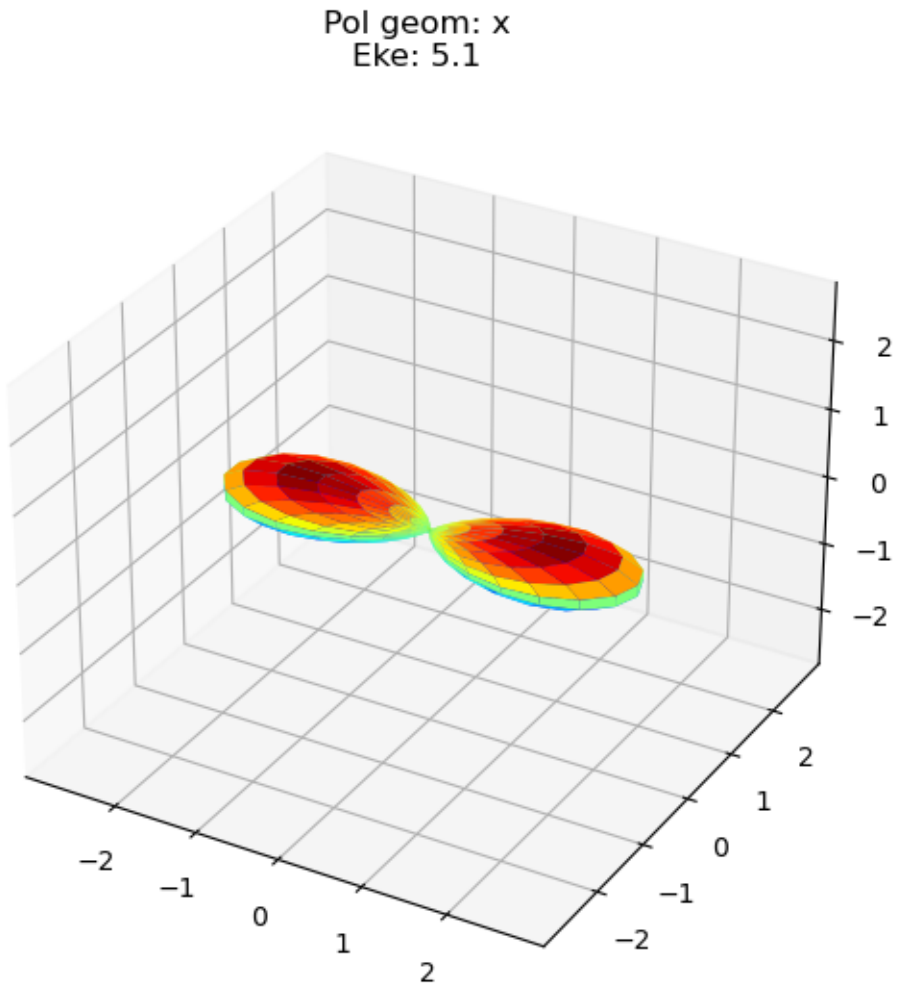
Polar plots are available for these distributions using the `padPlot()` method if the `dataType` is passed.

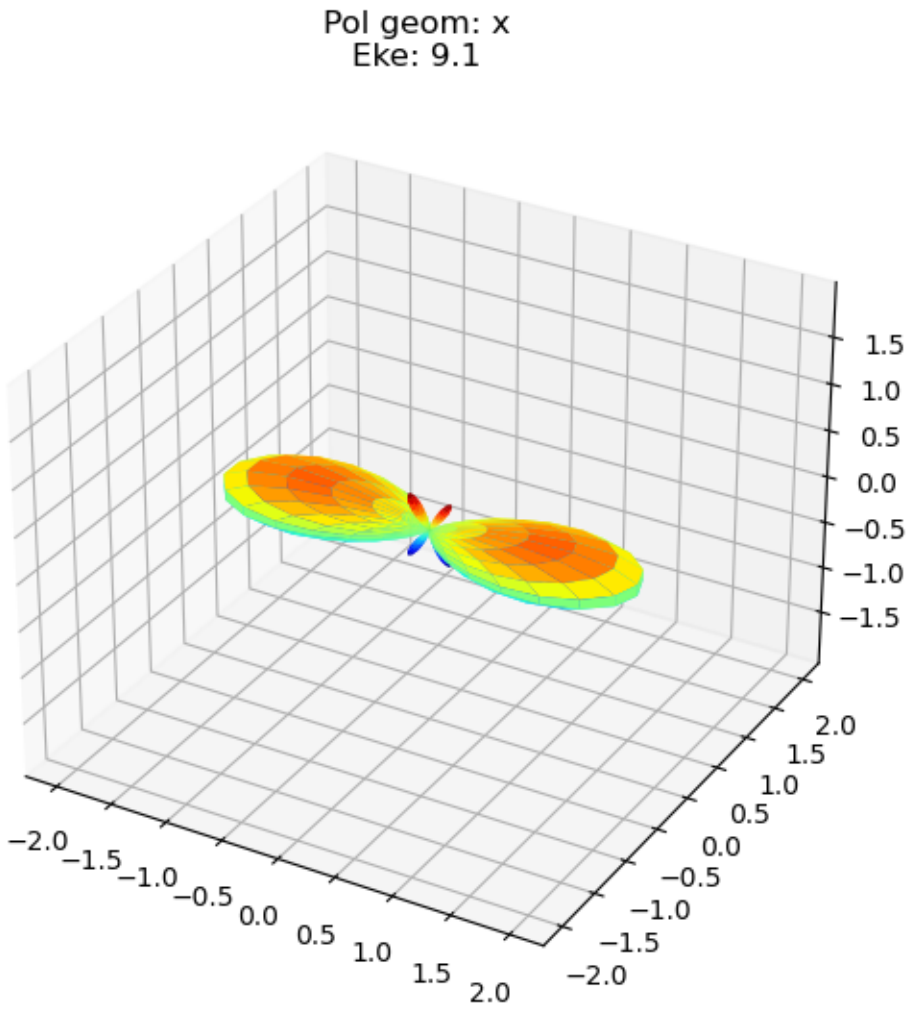
```
data.padPlot(keys = 'orb5', Erange = [5, 10, 4], dataType='MFBLM')
```

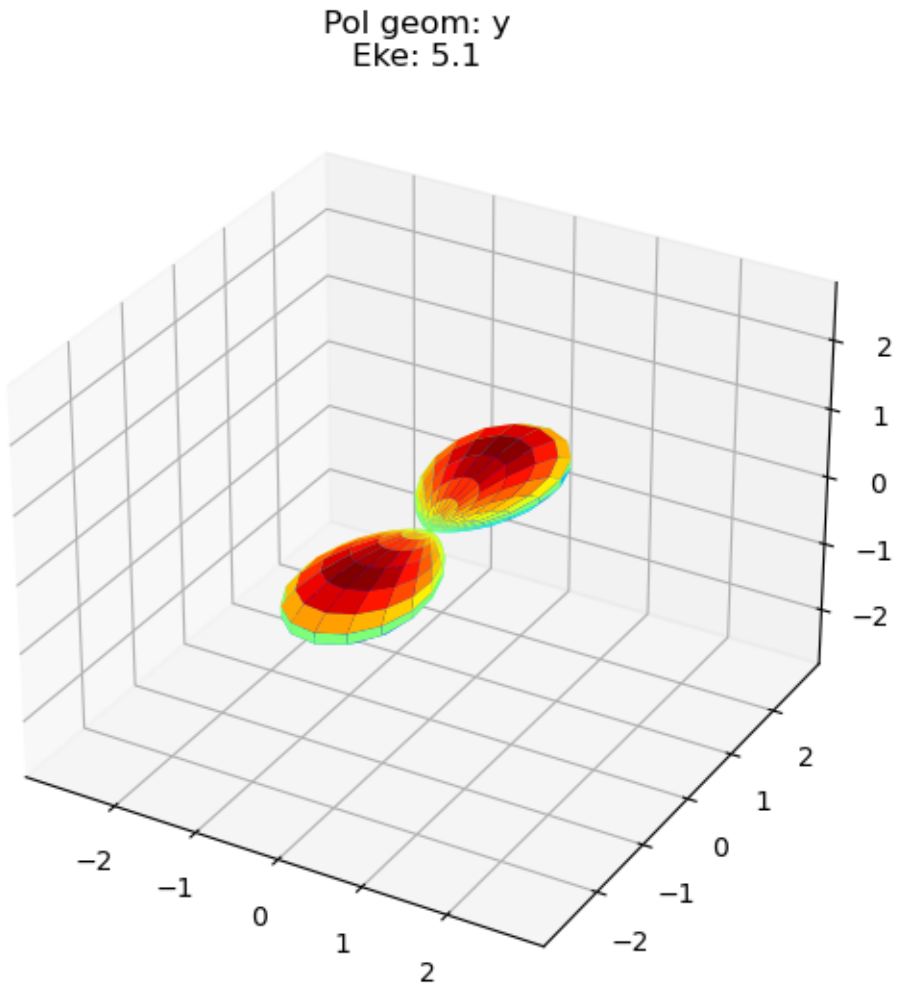
```
Using default sph betas.
Sph plots: Pol geom: z
Plotting with mpl
Data dims: ('Eke', 'Phi', 'Theta'), subplots on Eke
Sph plots: Pol geom: x
Plotting with mpl
Data dims: ('Eke', 'Phi', 'Theta'), subplots on Eke
Sph plots: Pol geom: y
Plotting with mpl
Data dims: ('Eke', 'Phi', 'Theta'), subplots on Eke
```

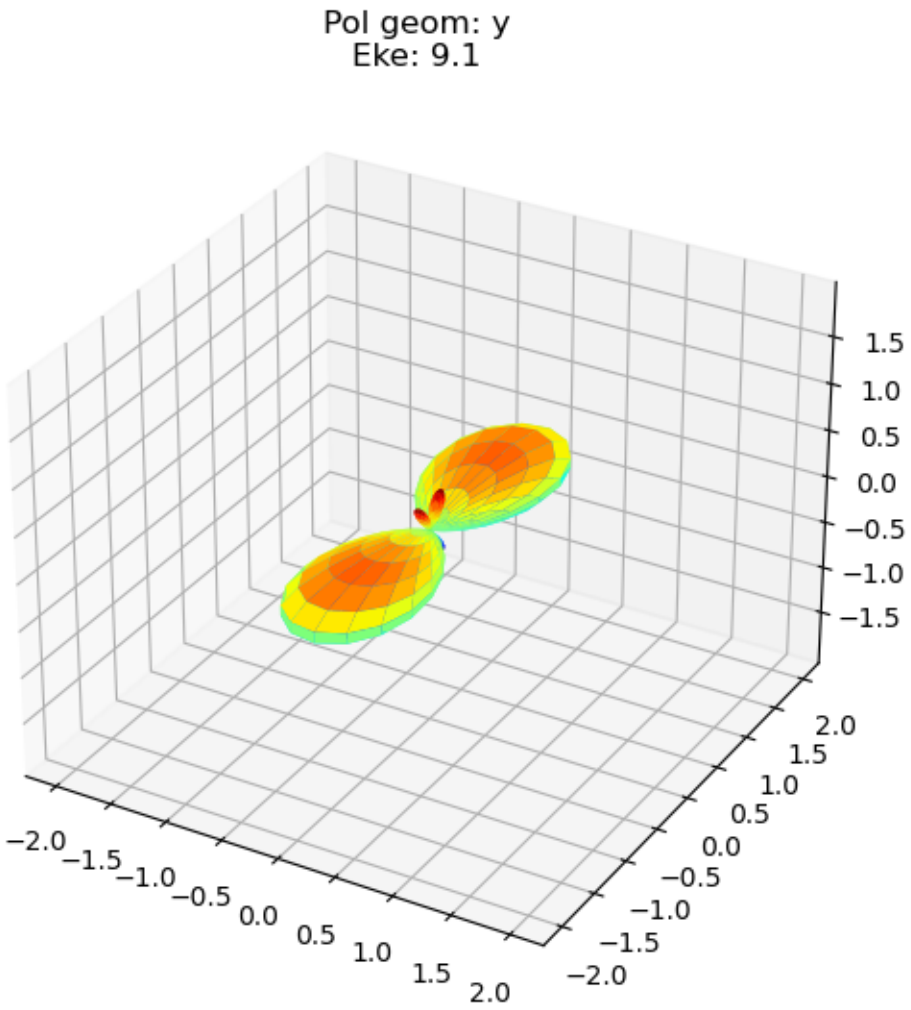

Pol geom: z
Eke: 5.1
0.2
0.1
0.0
−0.1
−0.2
−0.2
−0.1
0.0
0.1
0.2
0.2
0.1
0.0
−0.1
−0.2


Pol geom: z
Eke: 9.1
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
1.0
0.5
0.0
−0.5
−1.0


Pol geom: x
Eke: 5.1
2
1
0
−1
−2
−2
−1
0
1
2
2
1
0
−1
−2


Pol geom: x
Eke: 9.1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


Pol geom: y
Eke: 5.1
2
1
0
−1
−2
−2
−1
0
1
2
2
1
0
−1
−2



Compute LF/AF β_{LM} and PADs

Here's a quick demo for the default AF case (isotropic distribution, hence == LF case).

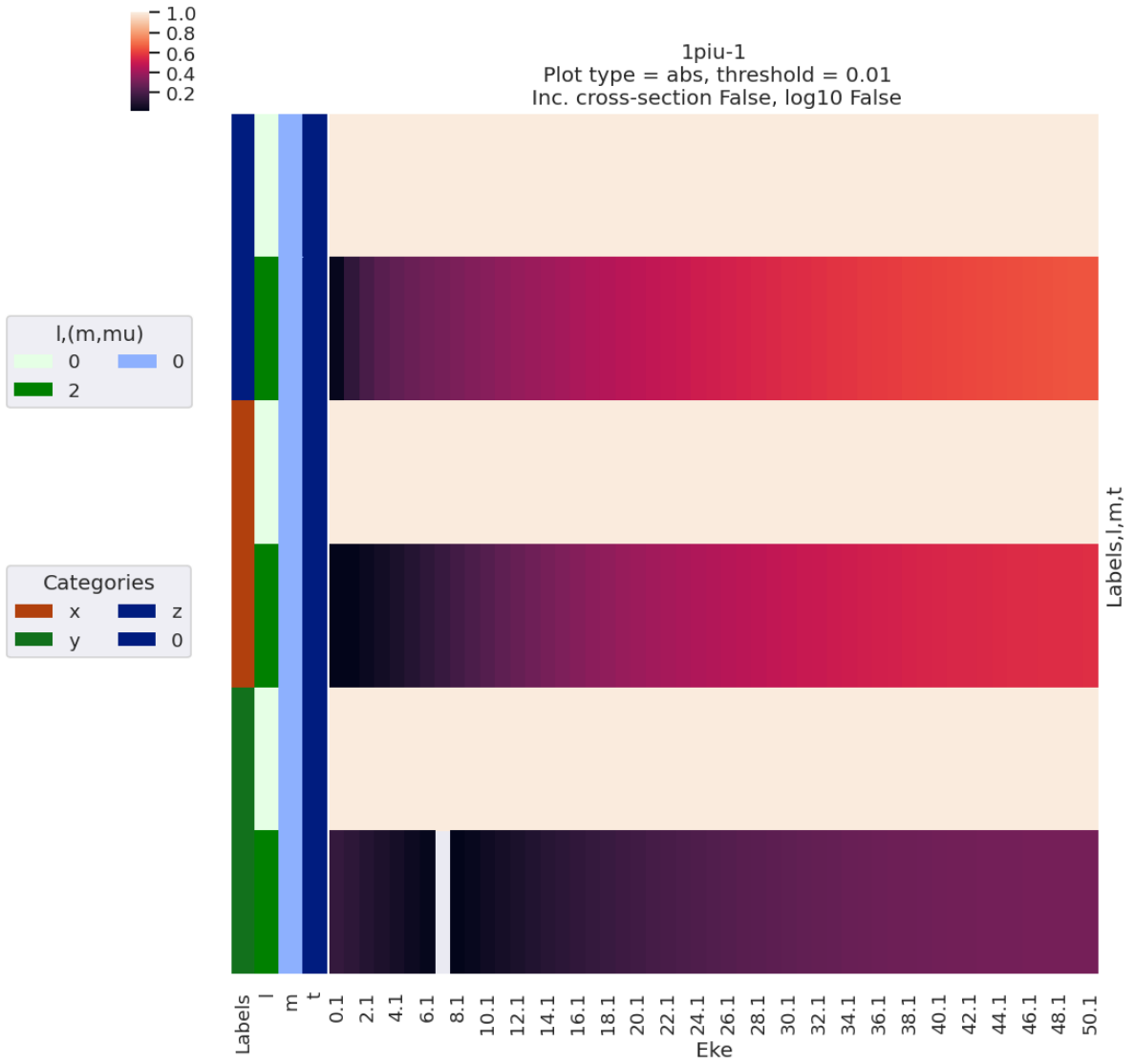
```
data.AFBLM()
```

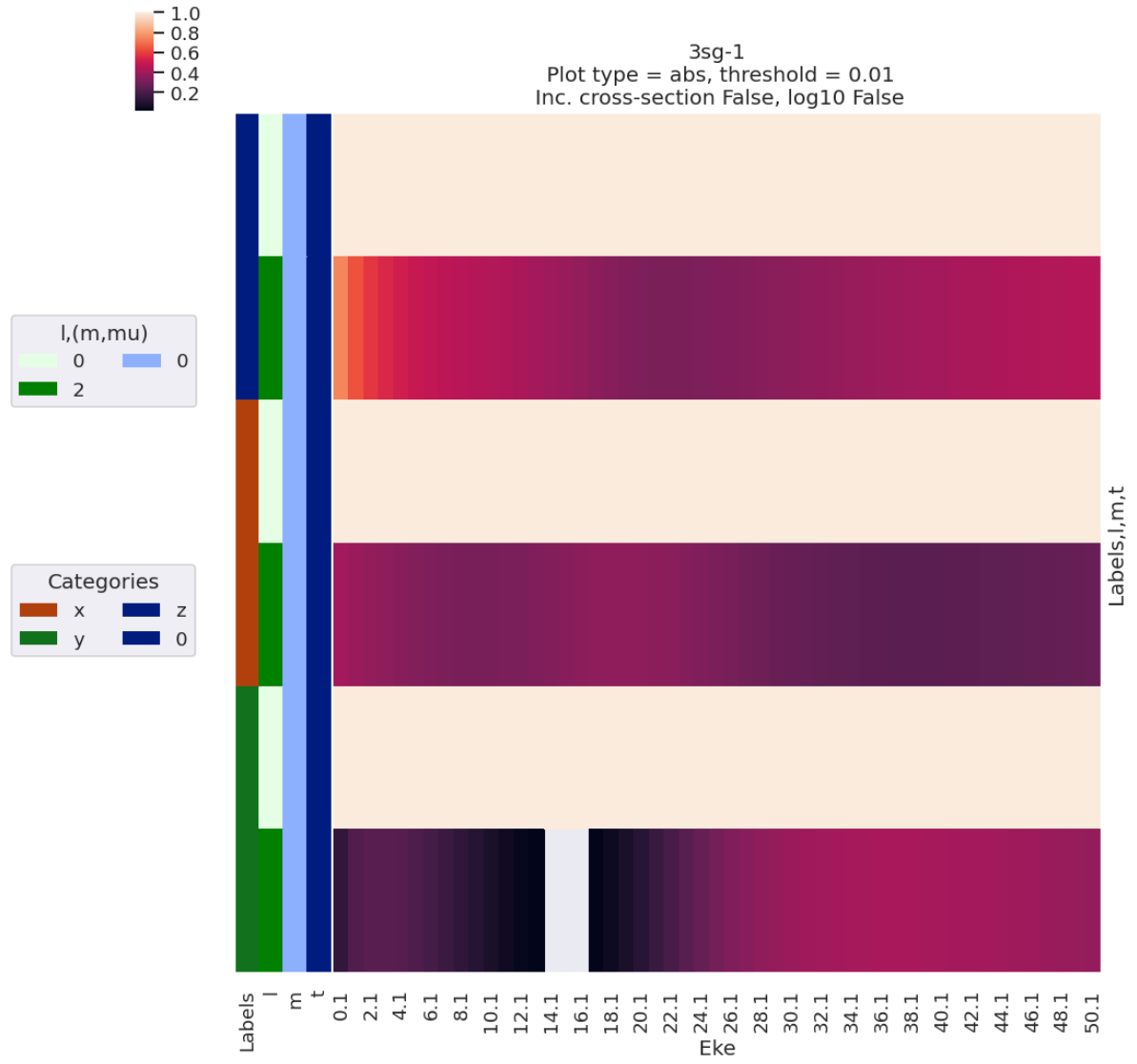
```
Calculating AF-BLMs for job key: orb6

Calculating AF-BLMs for job key: orb5
```

Plotting still needs to improve… but ep.lmPlot() is a robust way to plot everything.

```
# data.BLMplot(dataType = 'MFBLM')  # HORRIBLE OUTPUT at the moment!!!
data.lmPlot(dataType = 'AFBLM')
```

```
Plotting data n2_1pu_0.1-50.1eV_A2.inp.out, pType=a, thres=0.01, with Seaborn
Plotting data n2_3sg_0.1-50.1eV_A2.inp.out, pType=a, thres=0.01, with Seaborn
```

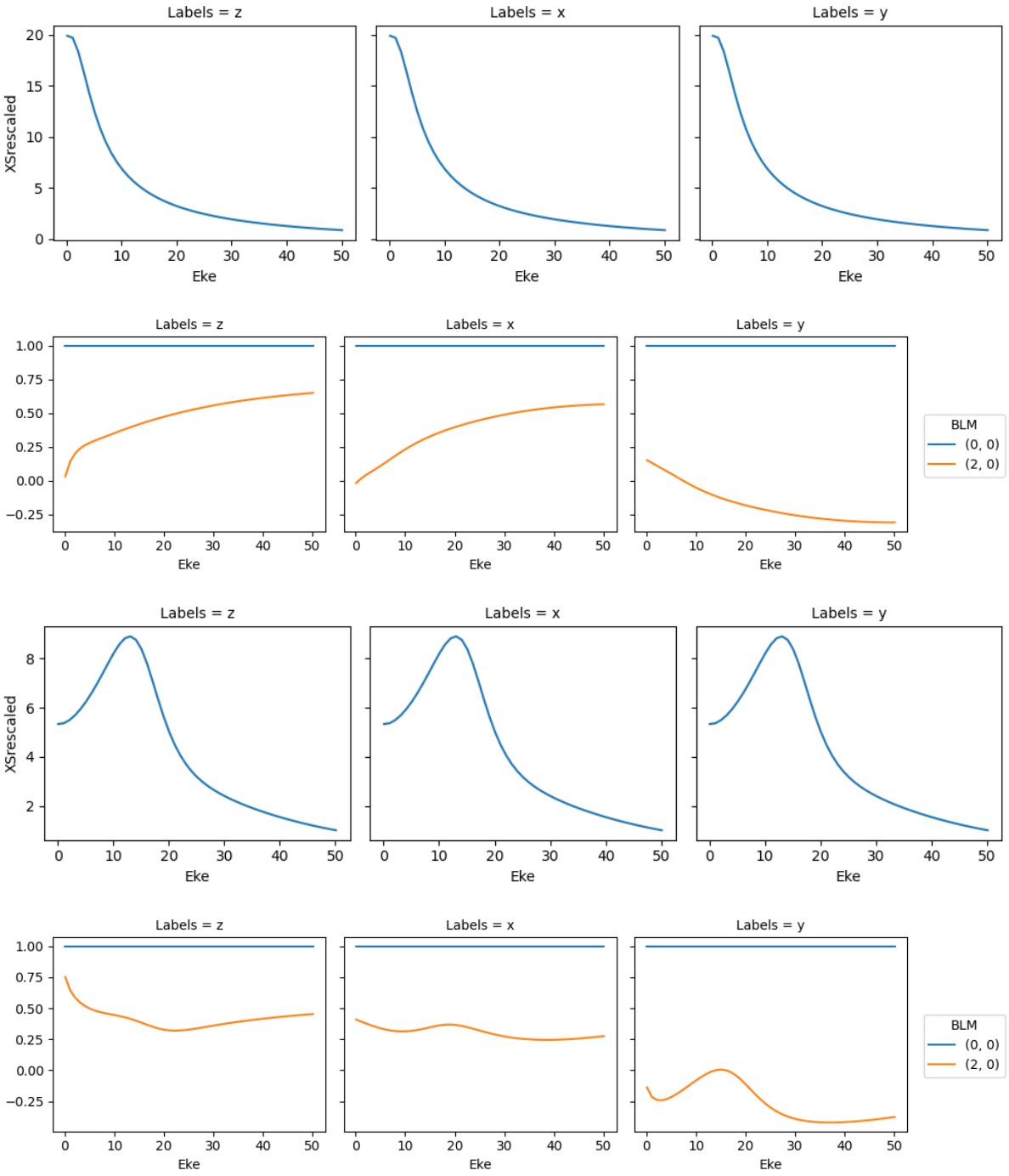

1.0
0.8
0.6
0.4
0.2
1piu-1
Plot type = abs, threshold = 0.01
Inc. cross-section False, log10 False
l,(m,mu)
0
0
2
Categories
x
z
y
0
Labels,l,m,t
Labels
l
m
t
0.1
2.1
4.1
6.1
8.1
10.1
12.1
14.1
16.1
18.1
20.1
22.1
24.1
26.1
28.1
30.1
32.1
34.1
36.1
38.1
40.1
42.1
44.1
46.1
48.1
50.1
Eke



Line-plots are available with the `BLMplot` method, although this currently only supports the Matplotlib backend, and may have problems with dims in some cases (work in progress!).

```
data.BLMplot(dataType='AFBLM', thres = 1e-2)  # Passing a threshold value here will␣
↪remove any spurious BLM parameters.
```

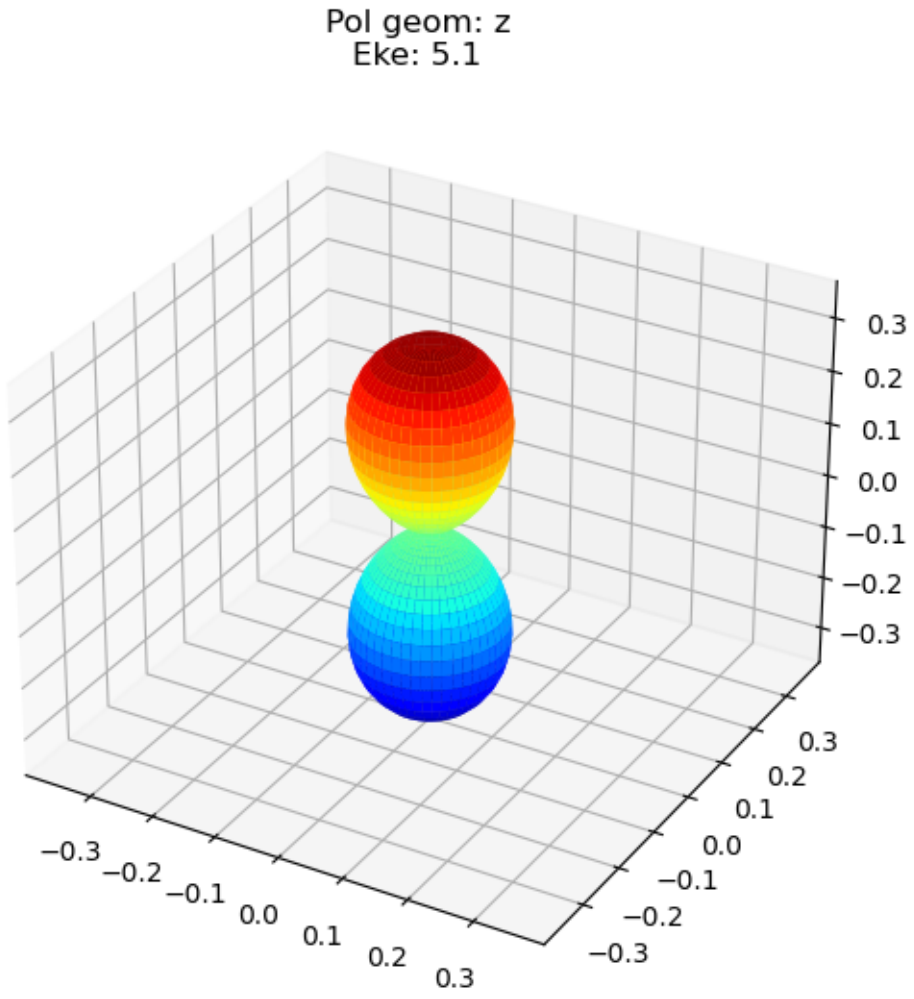
```
Dataset: orb6, 1piu-1, XS
Dataset: orb6, 1piu-1, AFBLM
Dataset: orb5, 3sg-1, XS
Dataset: orb5, 3sg-1, AFBLM
```

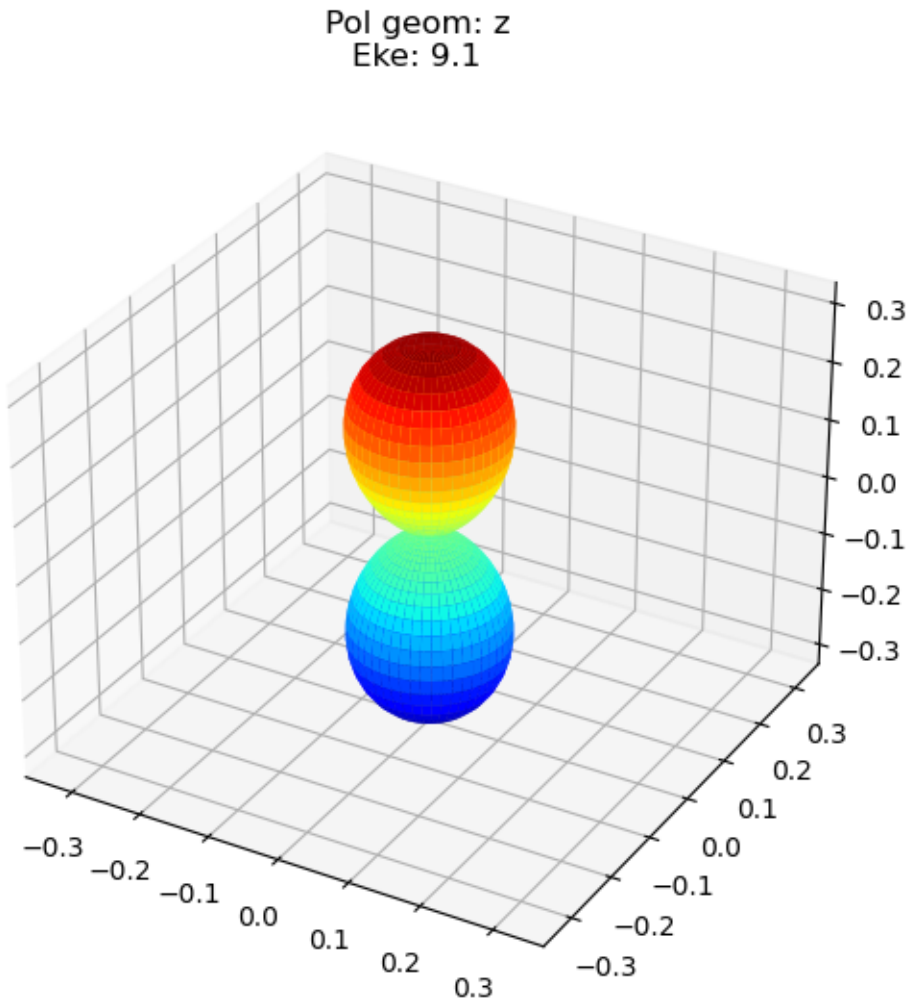


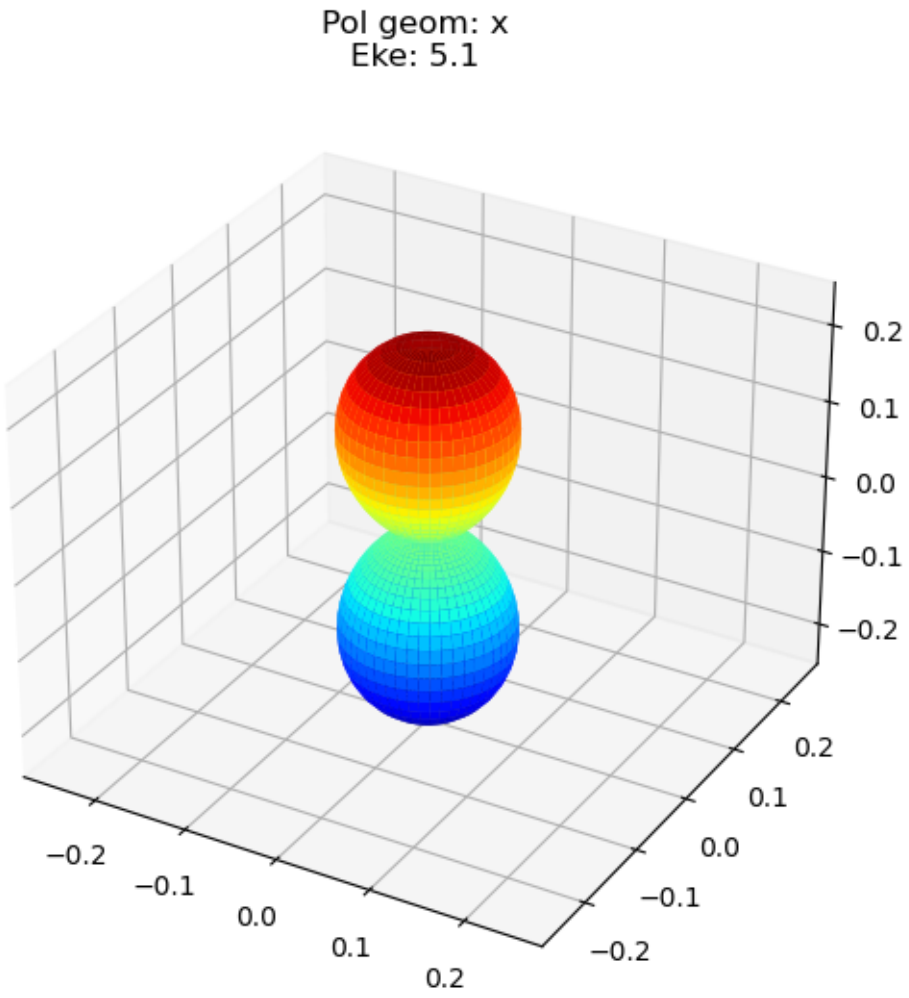
Polar plots are available for these distributions using the `padPlot()` method.

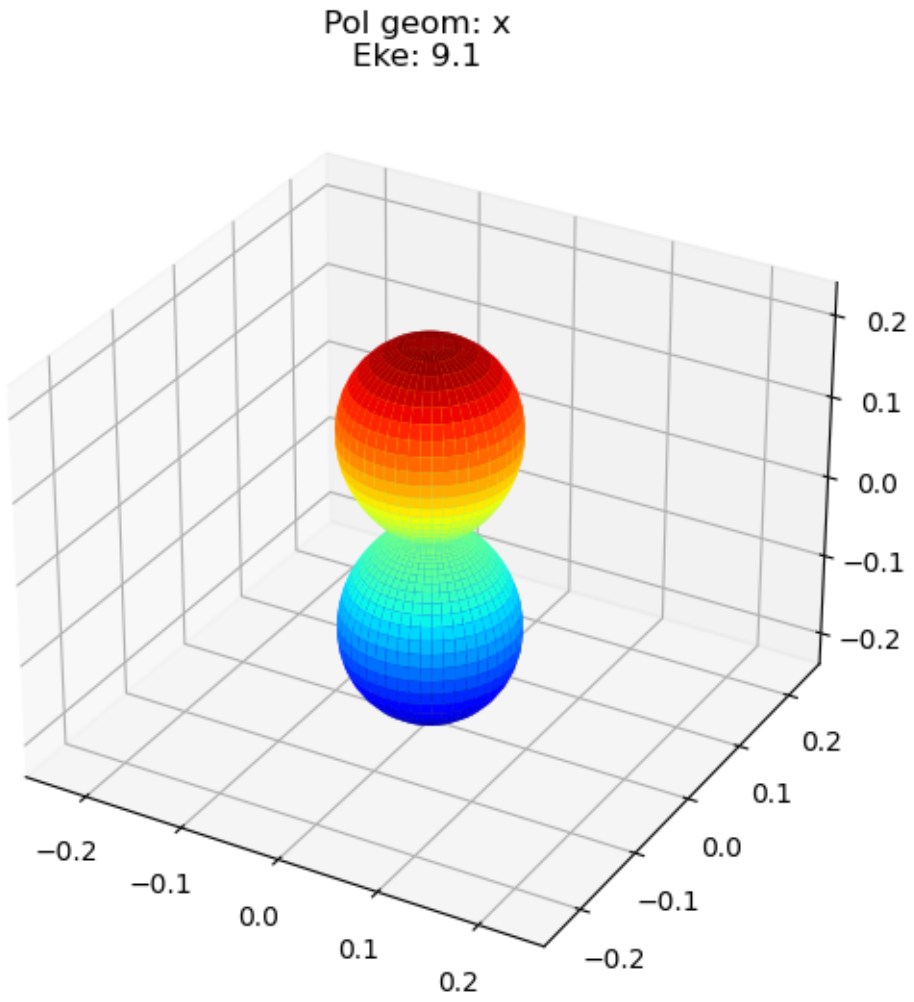
```
data.padPlot(keys = 'orb5', Erange = [5, 10, 4], dataType='AFBLM')

# NOTE - seem to have an inconsistency with (x,y) pol geometries here - should check␣
↪source code & fix. Likely due to mix-up in frame defns., i.e. probably mixing LF␣
↪and MF pol geom defn. - TBC.
```

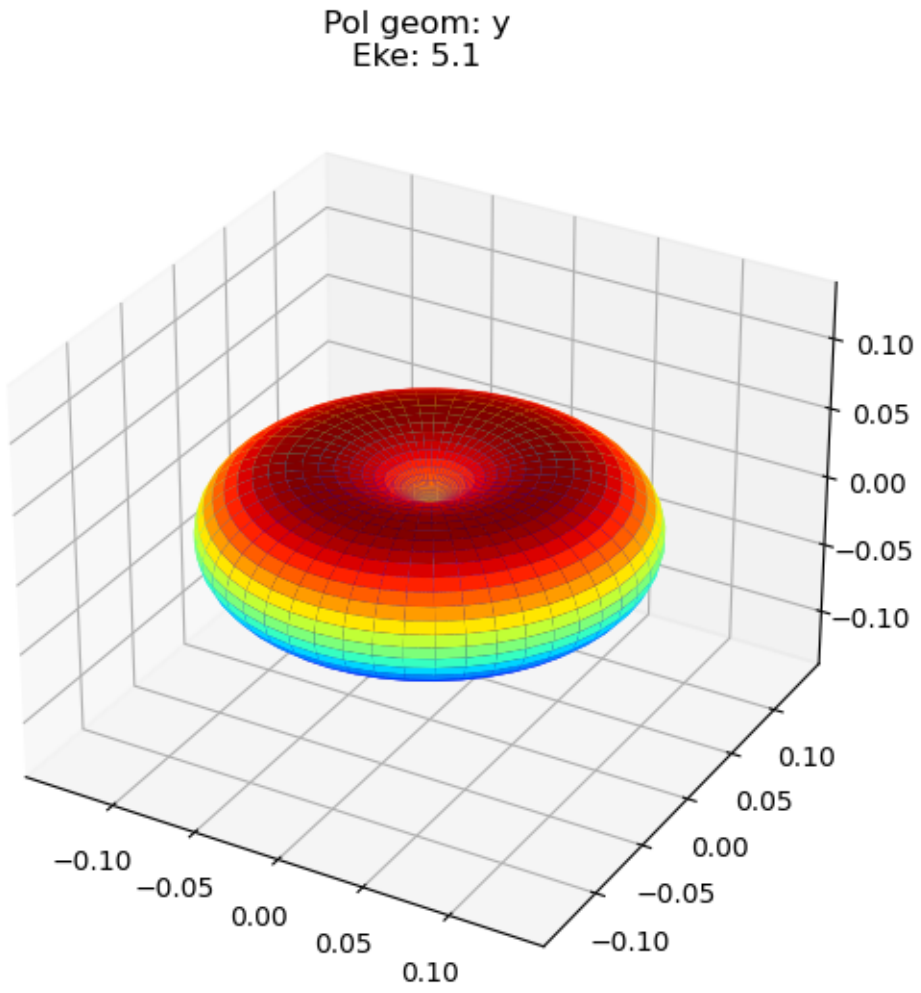
```
Found dims ('Labels', 't', 'Eke', 'BLM'), summing to reduce for plot. Pass selDims␣
↪to avoid.
Using default sph betas.
Sph plots: Pol geom: z
Plotting with mpl
Data dims: ('t', 'Eke', 'Phi', 'Theta'), subplots on Eke
Sph plots: Pol geom: x
Plotting with mpl
Data dims: ('t', 'Eke', 'Phi', 'Theta'), subplots on Eke
Sph plots: Pol geom: y
Plotting with mpl
Data dims: ('t', 'Eke', 'Phi', 'Theta'), subplots on Eke
```

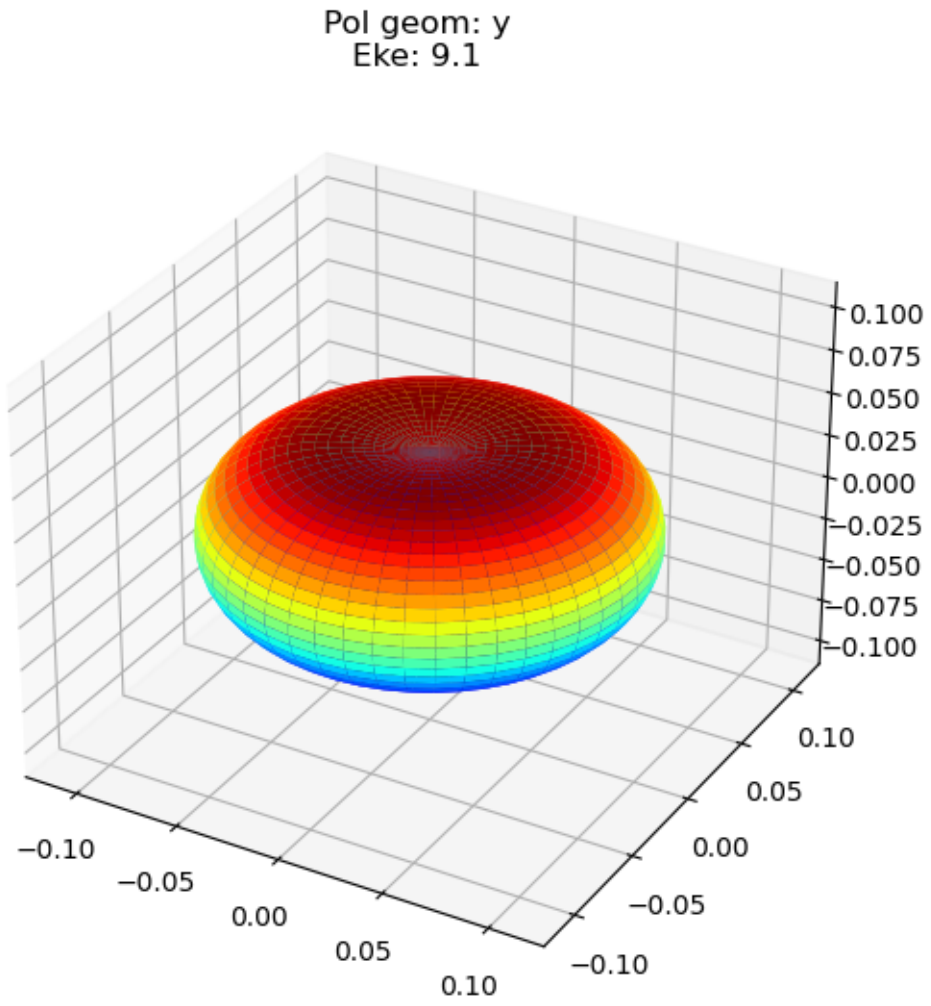



Pol geom: z
Eke: 9.1
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
−0.3
−0.2
−0.1
0.0
0.1
0.2
0.3
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3


Pol geom: x
Eke: 5.1
0.2
0.1
0.0
−0.1
−0.2
−0.2
−0.1
0.0
0.1
0.2
0.2
0.1
0.0
−0.1
−0.2


Pol geom: x
Eke: 9.1
0.2
0.1
0.0
−0.1
−0.2
−0.2
−0.1
0.0
0.1
0.2
0.2
0.1
0.0
−0.1
−0.2


Pol geom: y
Eke: 5.1
0.10
0.05
0.00
−0.05
−0.10
−0.10
−0.05
0.00
0.05
0.10
0.10
0.05
0.00
−0.05
−0.10



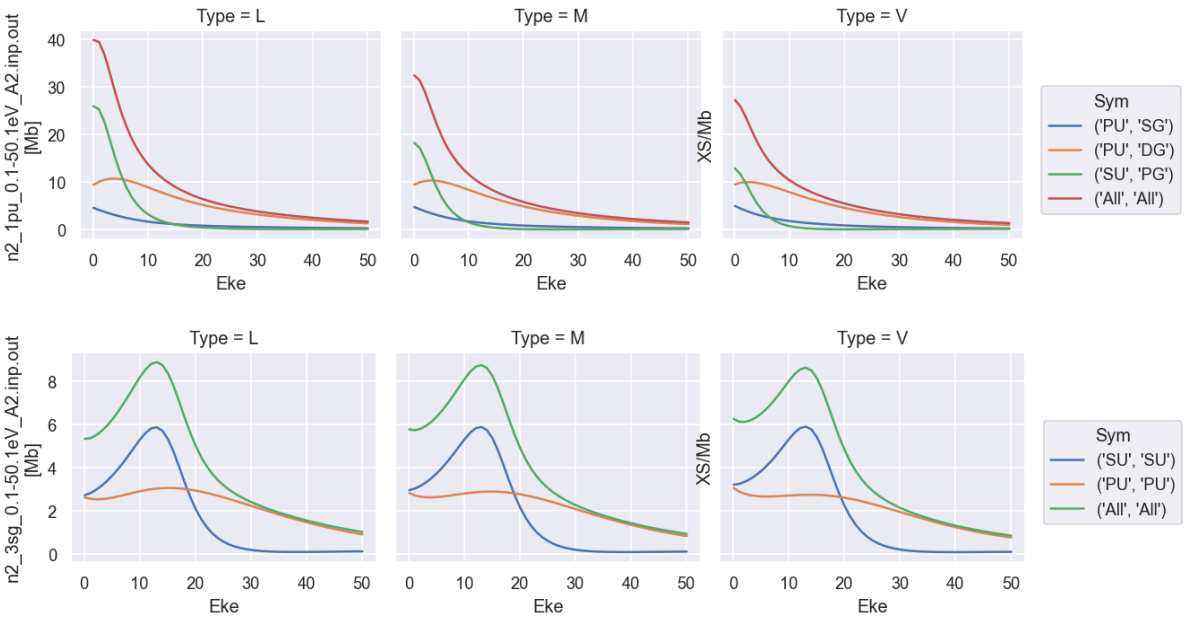
1.3 Additions

1.3.1 Plot styles for line-plots

To set to Seaborn plotting style, use `ep.hvPlotters.setPlotters()` (note this will be set for all plots after loading, unless overriden). Seaborn must be installed for this to function.

For more on Seaborn styles, see the Seaborn docs.

```
from epsproc.plot import hvPlotters
hvPlotters.setPlotters()

data.plotGetCro()
```

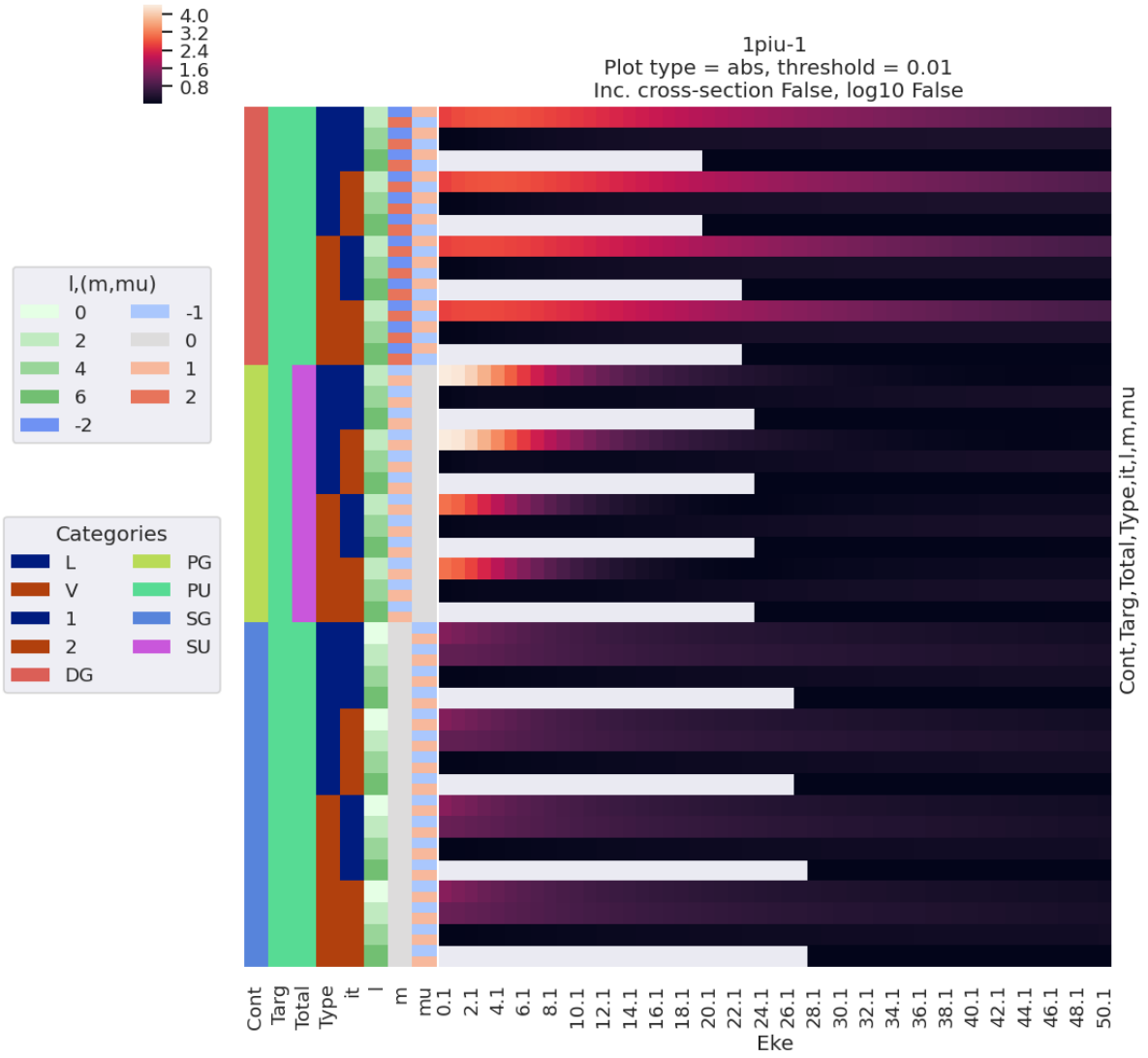


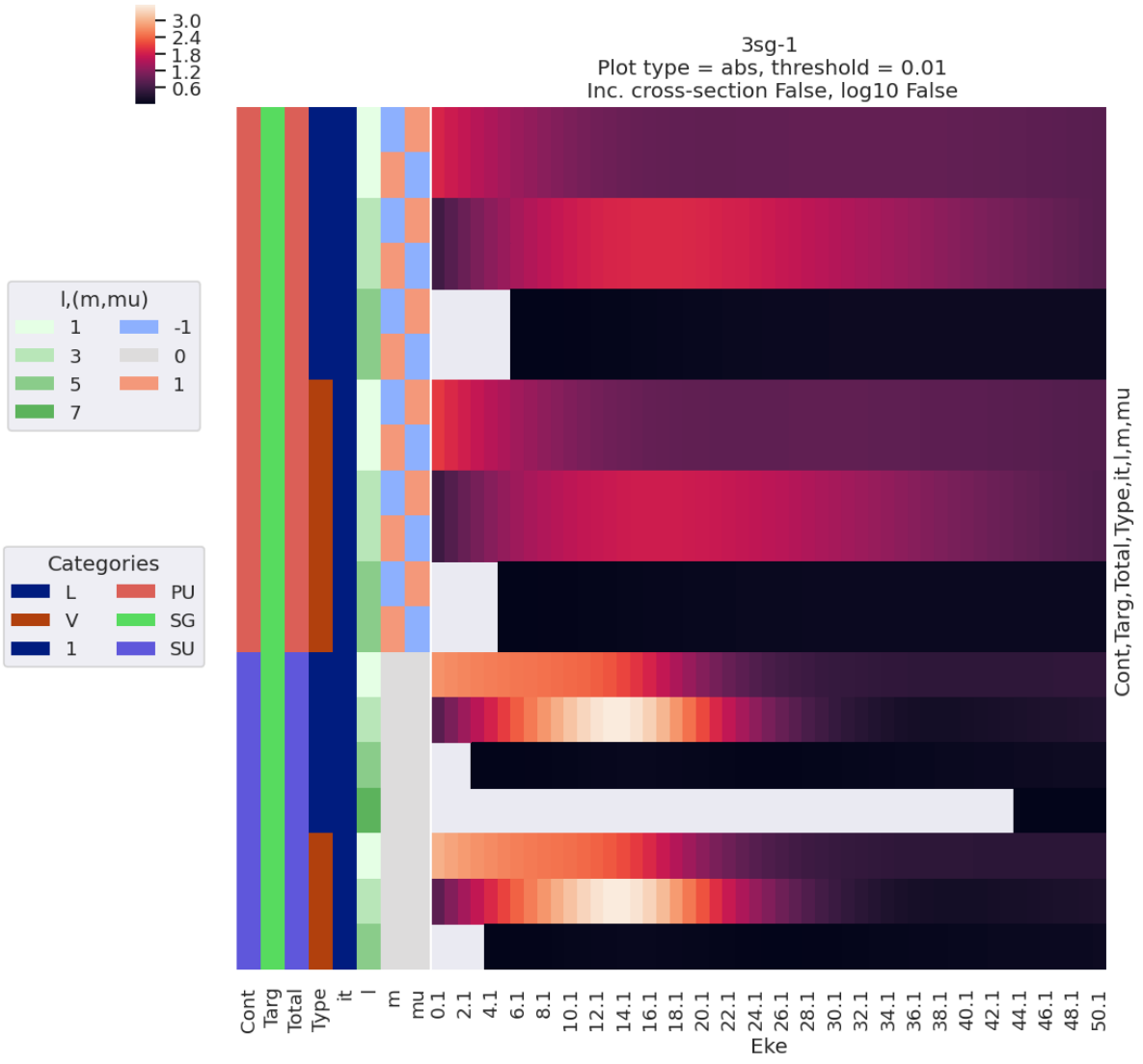
1.3.2 Matrix element plotting

For a full view of the computational results, use the `lmPlot()` method with the default, which correspond to `dataType=matE`.

```
data.lmPlot()
```

```
Plotting data n2_1pu_0.1-50.1eV_A2.inp.out, pType=a, thres=0.01, with Seaborn
Plotting data n2_3sg_0.1-50.1eV_A2.inp.out, pType=a, thres=0.01, with Seaborn
```

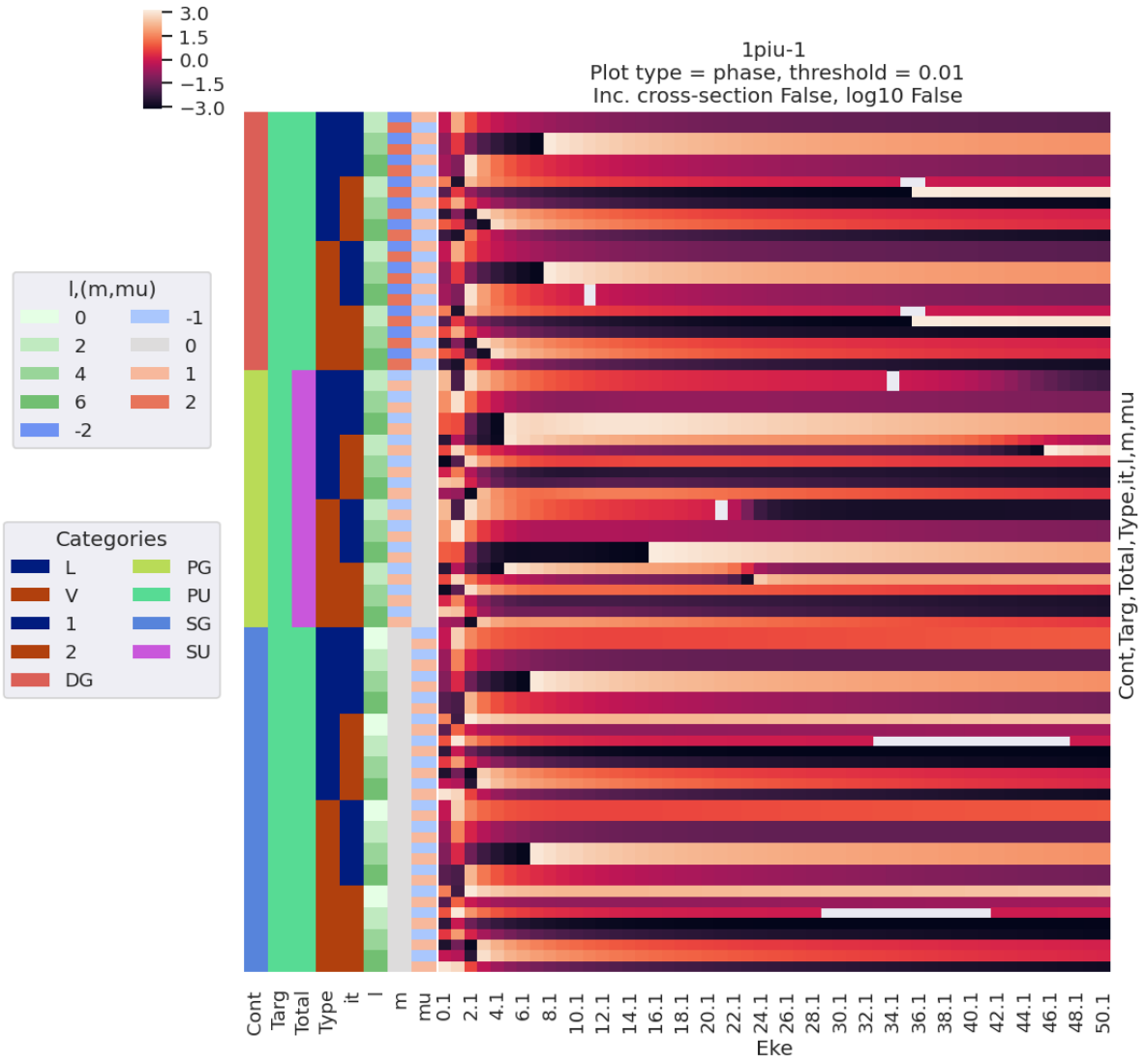

4.0
3.2
2.4
1.6
0.8
1piu-1
Plot type = abs, threshold = 0.01
Inc. cross-section False, log10 False
l,(m,mu)
0
2
4
6
-2
-1
0
1
2
Categories
L
V
1
2
DG
PG
PU
SG
SU
Cont,Targ,Total,Type,it,l,m,mu
Cont
Targ
Total
Type
it
l
m
mu
0.1
2.1
4.1
6.1
8.1
10.1
12.1
14.1
16.1
18.1
20.1
22.1
24.1
26.1
28.1
30.1
32.1
34.1
36.1
38.1
40.1
42.1
44.1
46.1
48.1
50.1
Eke

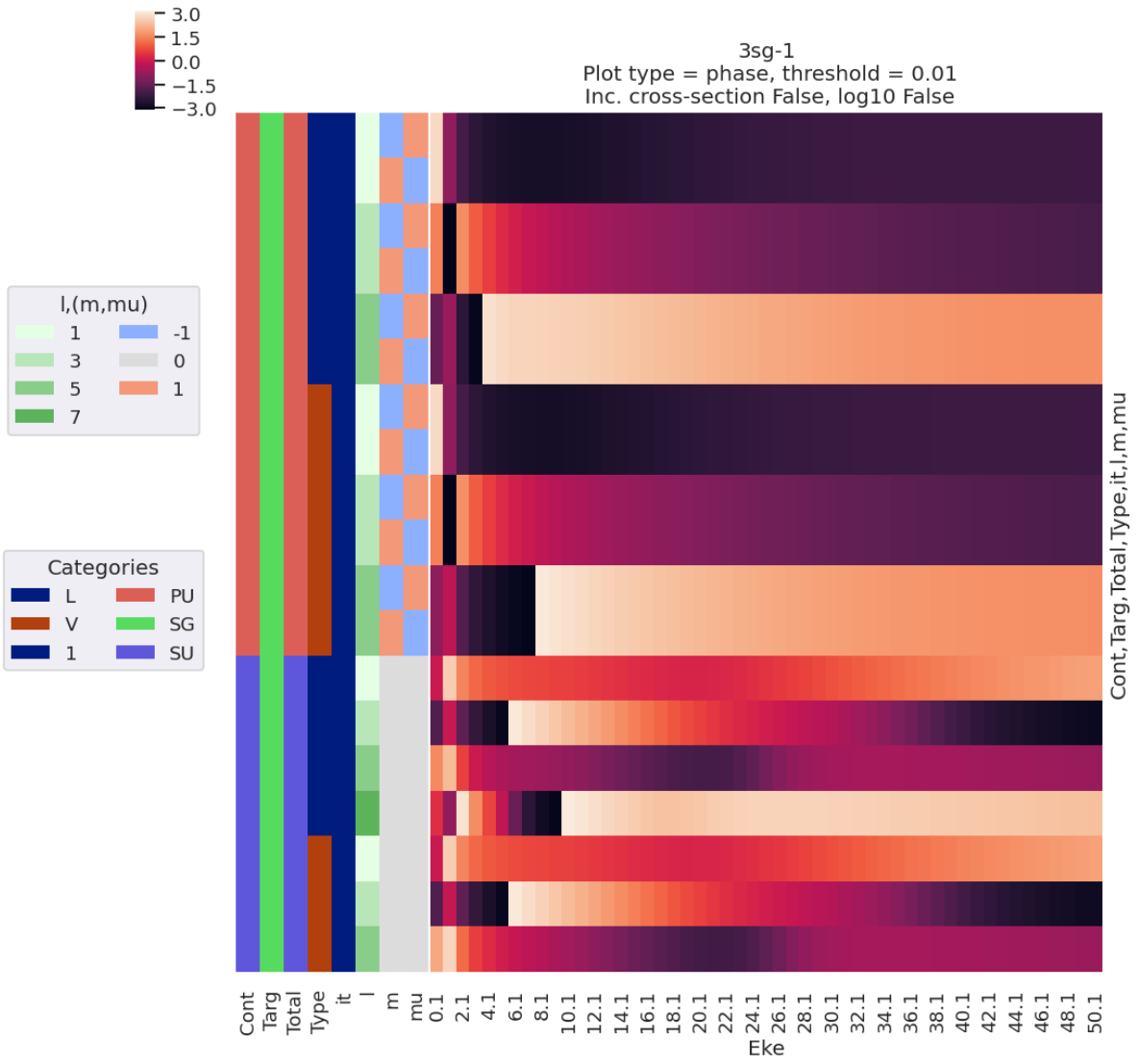


The default here plots abs values, but the same routine can be set for phase plotting.

```
data.lmPlot(pType='phase')
```

```
Plotting data n2_1pu_0.1-50.1eV_A2.inp.out, pType=phase, thres=0.01, with Seaborn
Plotting data n2_3sg_0.1-50.1eV_A2.inp.out, pType=phase, thres=0.01, with Seaborn
```


3.0
1.5
0.0
−1.5
−3.0
1piu-1
Plot type = phase, threshold = 0.01
Inc. cross-section False, log10 False
l,(m,mu)
0
2
4
6
-2
-1
0
1
2
Categories
L
V
1
2
DG
PG
PU
SG
SU
Cont
Targ
Total
Type
it
l
m
mu
0.1
2.1
4.1
6.1
8.1
10.1
12.1
14.1
16.1
18.1
20.1
22.1
24.1
26.1
28.1
30.1
32.1
34.1
36.1
38.1
40.1
42.1
44.1
46.1
48.1
50.1
Eke
Cont,Targ,Total,Type,it,l,m,mu



1.4 Versions

```
import scooby
scooby.Report(additional=['epsproc', 'xarray', 'jupyter'])
```

```
--------------------------------------------------------------------------------
  Date: Tue Oct 20 15:57:33 2020 Eastern Daylight Time

                OS : Windows
            CPU(s) : 32
           Machine : AMD64
      Architecture : 64bit
               RAM : 63.9 GB
       Environment : Jupyter
```

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```
  Python 3.7.3 (default, Apr 24 2019, 15:29:51) [MSC v.1915 64 bit (AMD64)]

           epsproc : 1.3.0-dev
            xarray : 0.15.0
           jupyter : Version unknown
             numpy : 1.19.2
             scipy : 1.3.0
           IPython : 7.12.0
        matplotlib : 3.3.1
            scooby : 0.5.6

  Intel(R) Math Kernel Library Version 2020.0.0 Product Build 20191125 for
  Intel(R) 64 architecture applications
--------------------------------------------------------------------------------
```

1.5 ePSproc Matlab demo

As noted in the main readme/intro doc, ePSproc originally started as a set of Matlab routines, before migration to Python in 2019. Although no longer maintained/updated since ~2018, the Matlab routines are still available as part of the ePSproc distribution. This notebook demos the routines, following the demo script `ePSproc_NO2_MFPADs_demo.m` (to run this code in a Jupyter environment, a Matlab kernel is required, e.g. Calysto's Matlab kernel).

Functionality:

- Read raw photoionization matrix elements from ePS output files with "dumpIdy" segments
- Calculate MF-PADs from the matrix elements (ePSproc_MFPAD.m, see also ePSproc_NO2_MFPADs_demo.m)
- Plot MF-PADs
- Plot X-sects
- (Beta testing): Calculate MF-BLMs from matrix elements, see ePSproc_MFBLM.m
- (Under development): Calculate AF-BLMs from matrix elements.

Source:

- /matlab: stable matlab code (as per `release v1.0.1 <https://github.com/phockett/ePSproc/releases>__`).
  - a set of functions for processing (ePSproc*.m files)
  - a script showing demo calculations, `ePSproc_NO2_MFPADs_demo.m`
- /docs/additional contains:
  - the benchmark results from these calculations, `ePSproc_NO2_testing_summary_250915.pdf`
  - additional notes on ePS photoionization matrix elements, `ePSproc_scattering_theory_ePS_notes_011015.pdf`.

See `ePSproc: Post-processing suite for ePolyScat electron-molecule scattering calculations <https://www.authorea.com/users/71114/articles/122402/_show_article>_` for more details.

1.5.1 Setup

```
cd('~/github/ePSproc')  % Change to ePSproc root dir.
```

```
ans =

    '9.4.0.813654 (R2018a)'
```

```
%% *** SETTINGS
%  Set up basic environment

% Name & path to ePS output file. In this version set full file name here, and␣
 ↪working directory below.
% fileName='no2_demo_ePS.out'  % OK for MFPAD testing, but only single E point
fileName='n2_3sg_0.1-50.1eV_A2.inp.out'

% Set paths for Linux or Win boxes (optional!)
if isunix
    dirSlash='/';
else
    dirSlash='\';
end

filePath=[pwd dirSlash 'data' dirSlash 'photoionization'];                    %␣
 ↪Root to working directory, here set as current dir/data/photoionization
fileBase=[filePath dirSlash fileName];   % Full path to ePS results file, here set as␣
 ↪current working direcory

scriptPath=[pwd dirSlash 'matlab' dirSlash];  % Add path to ePSproc scrips to Matlab␣
 ↪path list, here set as current dir/matlab
path(path,[scriptPath]);
```

```
fileName =

    'n2_3sg_0.1-50.1eV_A2.inp.out'
```

```
%% *** Read data
%  Variables:
%       rlAll contains matrix elements (from DumpIdy segments)
%       params contains various calculation parameters
%       getCro contains cross-section (from GetCro segments), if present

[rlAll, params, getCro]=ePSproc_read(fileBase);

params.fileBase=fileBase;
params.fileName=fileName;
```

```
*** Reading ePS output file
/home/paul/github/ePSproc/data/photoionization/n2_3sg_0.1-50.1eV_A2.inp.out
Found 102 sets of matrix elements
Read 102 sets of matrix elements (0 blank records)
Found 2 symmetries
    'SU'    'PU'
```

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```
Found 51 energies
Found 2 atoms
Found 18 data records
Found 3 sets of cross sections
```

```
% Matrix elements are stored in a structure
rlAll
```

```
rlAll =

  2x51 struct array with fields:

    eKE
    PE
    symm
    symmSet
    MbNorm
    rawIdyHead
    rawIdy1
    rlnlHead
    rlnl1
    rawIdy2
    rlnl2
    pWaveAll
```

```
% GetCro outputs (total cross-secions, LF betas)
getCro
```

```
getCro =

  1x3 struct array with fields:

    GetCro
```

```
% General calculation params
params
```

```
params =

  struct with fields:

        symmList: {'SU'  'PU'  'All'}
             eKE: [1x51 double]
         symmAll: {1x102 cell}
            eAll: [1x102 double]
        nRecords: 102
       nEnergies: 51
          nSymms: 2
           gLmax: 11
        blankRec: 0
        missingE: [1x0 double]
```

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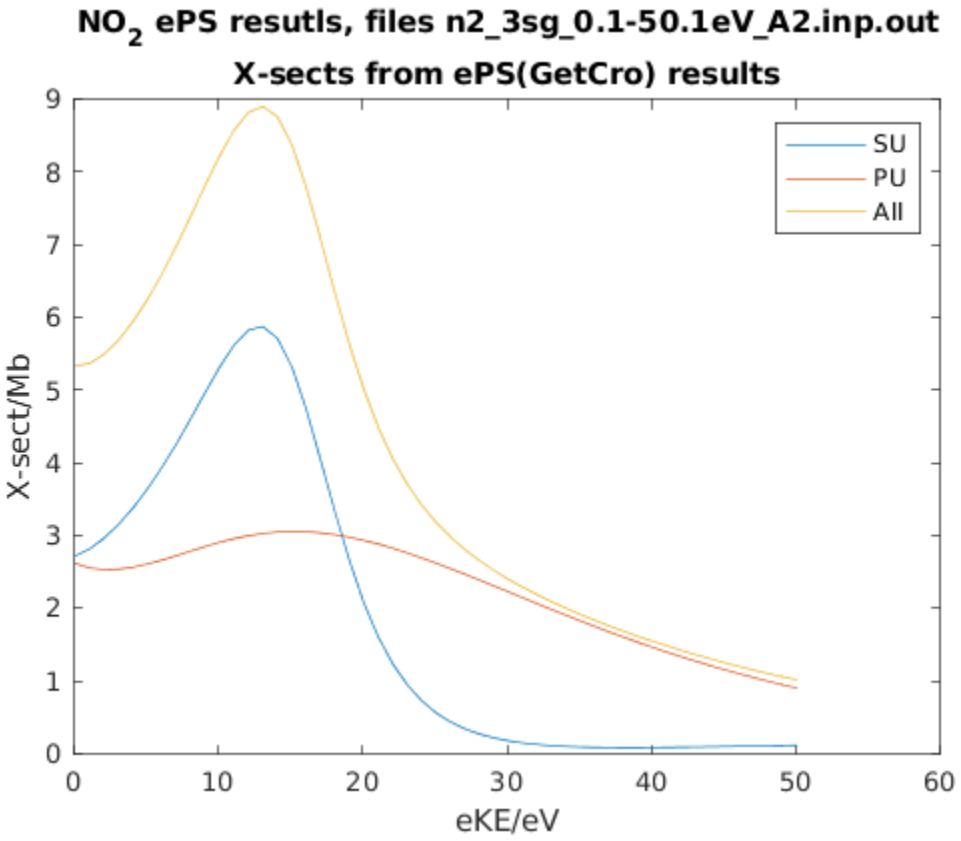
```
        pWaveAll: [144x51x3 double]
      pWaveAllMb: [144x51x3 double]
        LMallInd: [144x2 double]
          coords: {1x5 cell}
     dataRecords: {18x2 cell}
              IP: 15.5800
    GetCroHeader: {{1x1 cell}}
        fileBase: '/home/paul/github/ePSproc/data/photoionization/n2_3sg_0.1-50.
↪1eV_A2.inp.out'
        fileName: 'n2_3sg_0.1-50.1eV_A2.inp.out'
```

1.5.2 Plot cross-sections and betas

These are taken from the `GetCro` segments in the ePS output files, and correspond to results for an isotropic ensemble of molecules, i.e. observables in the lab frame (LF) for 1-photon ionization (see the ePS tutorial for more details).

```
%% Plot GetCro results for each symm & total

col=2;  % Select column from getCro output (see params.GetCroHeader)

figure('color',[1 1 1],'name','GetCro outputs');

for n=1:length(getCro)
    plot(getCro(n).GetCro(:,1)-params.IP,getCro(n).GetCro(:,col));
    hold on;
end

title({['NO_2 ePS resutls, files ' strrep(fileName,'_','\_')]; 'X-sects from␣
↪ePS(GetCro) results'});
xlabel('eKE/eV');
ylabel('X-sect/Mb');

legend([params.symmList 'Sum']);
```

```
Warning: MATLAB has disabled some advanced graphics rendering features by␣
↪switching to software OpenGL. For more information, click <a href="matlab:opengl(
↪'problems')">here</a>.
Warning: Ignoring extra legend entries.
> In legend>set_children_and_strings (line 646)
  In legend>make_legend (line 316)
  In legend (line 259)
```



1.5.3 MFPADs

These are calculated numerically from the matrix elements, for a given polarization geometry and symmetry (the method is the same as the python version of the routine).

```
%% *** Calculate MFPADs - single polarization geometry, all energies and symmetries
%  Calculate for specified Euler angles (polarization geometry) & energies

% Set resolution for calculated I(theta,phi) surfaces
res=100;

% ip components to use from ePS output (1=length gauge, 2=velocity gauge)
ipComponents=1;

% it components to use from ePS output (for degenerate cases), set an array here for␣
 ↪as many components as required, e.g. it=1, it=[1 2] etc.
it=1;

% Set light polarization and axis rotations LF -> MF
p=0;                % p=0 for linearly pol. light, +/-1 for L/R circ. pol.
eAngs=[0 0 0];      % Eugler angles for rotation of LF->MF, set as [0 0 0] for z-pol,␣
 ↪[0 pi/2 0] for x-pol, [pi/2 pi/2 0] for y-pol
polLabel='z';

% Run calculation - outputs are D, full set of MFPADs (summed over symmetries); Xsect,
 ↪ calculated X-sects; calcsAll, structure with results for all symmetries.
```

(continues on next page)

(continued from previous page)

```
[Xsect, calcsAll, pWaves]=ePSproc_MFPAD(rlAll,p,eAngs,it,ipComponents,res);

% Add pol labels - currently expected in plotting routine, but not set in MFPAD␣
↪routine
for n=1:size(calcsAll,2)
    for symmIn=1:size(calcsAll,1)
        calcsAll(symmInd,n).polLabel=polLabel;
    end
end
```

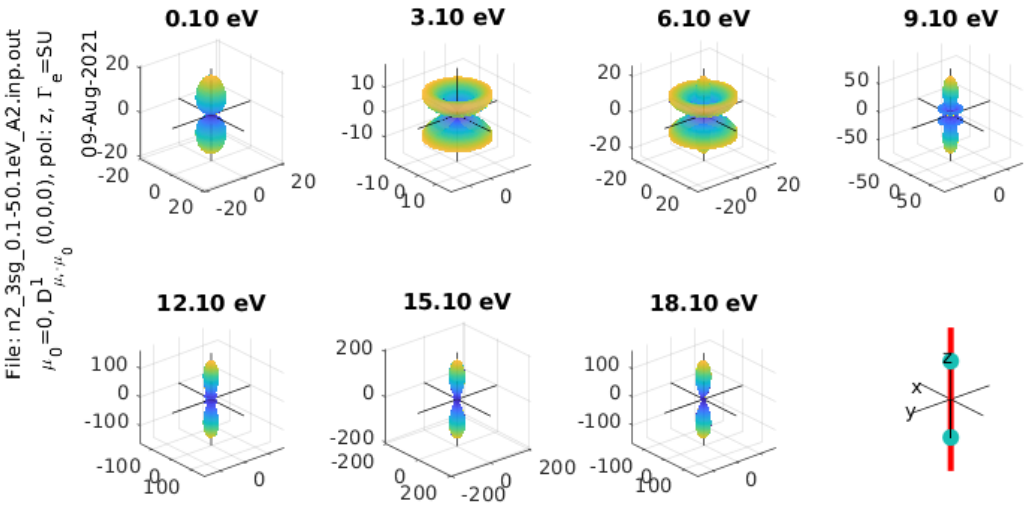
```
% Results are output as a structure, dims (symmetries, energies).
calcsAll
```

```
calcsAll =

  3x51 struct array with fields:

    D
    C
    Cthres
    eKE
    symm
    euler
    Xsect
    XsectD
    Rlf
    p
    Cind
```

```
%plot -s 800,400
```

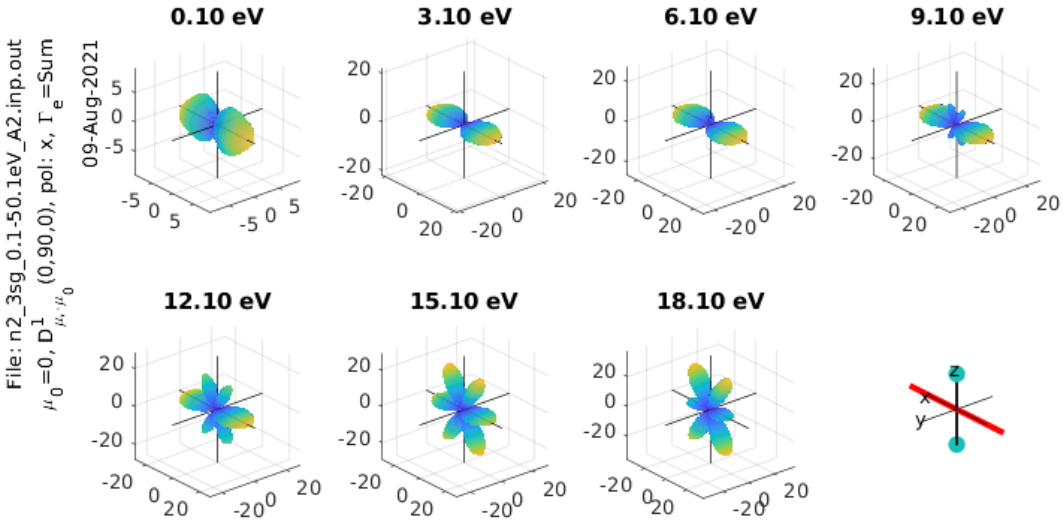
(Above is a line-magic for setting displayed plot size with the Calysto kernel - see the demo notebook for more.)

```
%% Plotting - MFPAD panel plots

% Set plot ranges
symmInd=1;      % Select symmetry (by index into calcsAll rows). Final symmetry state␣
↪is set as sum over all symmetries
% eRange=1;      % Select energies (by index into calcsAll cols)
eRange=1:3:20;

% Additional options (optional)
sPlotSet=[2 4];             % Set [rows cols] for subplot panels. The final panel␣
↪will be replaced with a diagram of the geometry
% titlePrefix='NO2 testing';  % Set a title prefix for the figure
titlePrefix='';

ePSproc_MFPAD_plot(calcsAll,eRange,symmInd,params,sPlotSet,titlePrefix);
% ePSproc_MFPAD_plot(calcsAll,eRange,symmInd,params,sPlotSet,'','n','off');
% ePSproc_MFPAD_plot(calcsAll,eRange,symmInd,params,[2 4],'','n','off');
```

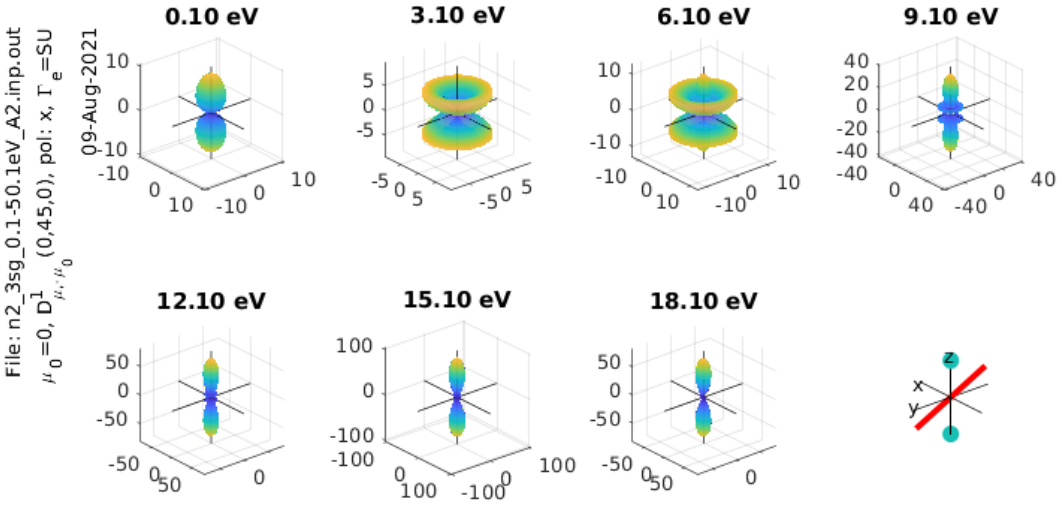


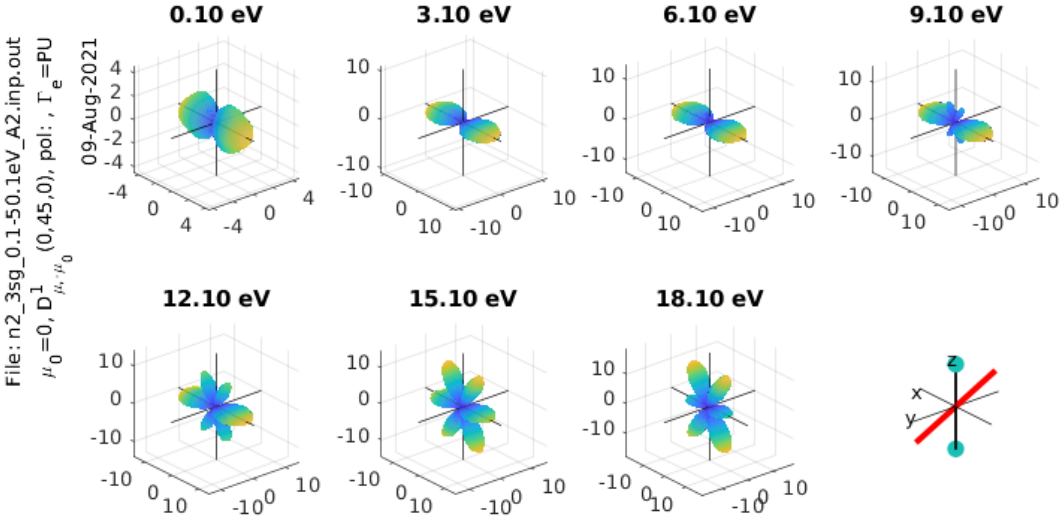

```
% Calculate & plot for a different polarization state
eAngs = [0 pi/2 0];  % x-pol case
polLabel = 'x';

[Xsect, calcsAll, pWaves]=ePSproc_MFPAD(rlAll,p,eAngs,it,ipComponents,res);

% Add pol labels - currently expected in plotting routine, but not set in MFPAD␣
↪routine
for n=1:size(calcsAll,2)
    for symmIn=1:size(calcsAll,1)
        calcsAll(symmInd,n).polLabel=polLabel;
    end
end

symmInd=3;
ePSproc_MFPAD_plot(calcsAll,eRange,symmInd,params,sPlotSet,titlePrefix);
```

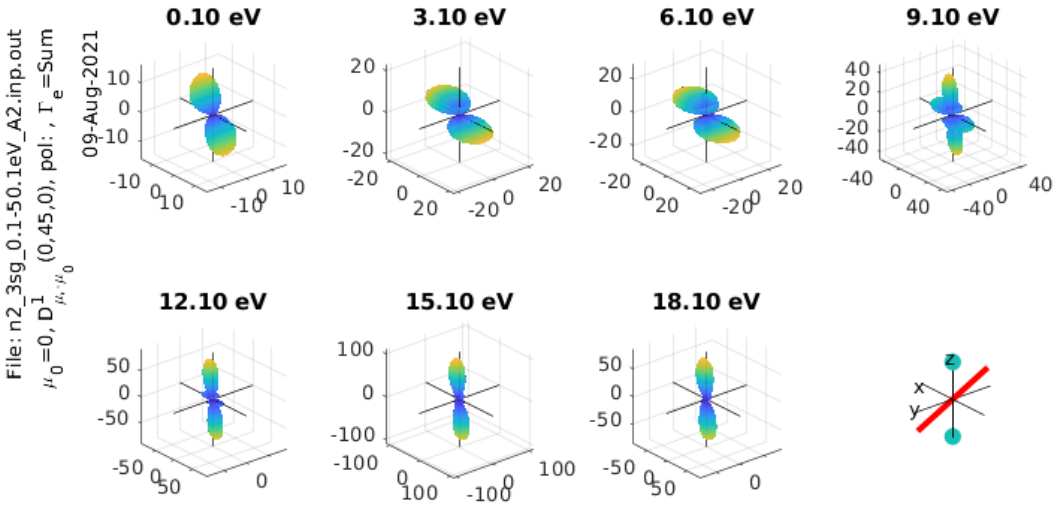
```
symmInd =

     3
```




```
% Calculate & plot for a different polarization state
eAngs = [0 pi/4 0];  % Diagonal pol case
polLabel = 'x';

[Xsect, calcsAll, pWaves]=ePSproc_MFPAD(rlAll,p,eAngs,it,ipComponents,res);

% Add pol labels - currently expected in plotting routine, but not set in MFPAD␣
↪routine
for n=1:size(calcsAll,2)
    for symmIn=1:size(calcsAll,1)
        calcsAll(symmInd,n).polLabel=polLabel;
    end
end

% Plot all symmetries
for symmInd = 1:3
    ePSproc_MFPAD_plot(calcsAll,eRange,symmInd,params,sPlotSet,titlePrefix);

end
```


File: n2_3sg_0.1-50.1eV_A2.inp.out
μ_0=0, D^1_{μ,μ_0} (0,45,0), pol: x, Γ_e=SU
09-Aug-2021
0.10 eV
3.10 eV
6.10 eV
9.10 eV
12.10 eV
15.10 eV
18.10 eV
z
x
y


File: n2_3sg_0.1-50.1eV_A2.inp.out
μ_0=0, D^1_{μ,μ_0} (0,45,0), pol: , Γ_e=PU
09-Aug-2021
0.10 eV
3.10 eV
6.10 eV
9.10 eV
12.10 eV
15.10 eV
18.10 eV
z
x
y



1.5.4 MF β_{LM}

```
%% *** Calculate MFPADs - single polarization geometry, all energies and symmetries
%  Calculate for specified Euler angles (polarization geometry) & energies

% Set resolution for calculated I(theta,phi) surfaces
res=100;

% ip components to use from ePS output (1=length gauge, 2=velocity gauge)
ipComponents=1;

% it components to use from ePS output (for degenerate cases), set an array here for␣
 ↪as many components as required, e.g. it=1, it=[1 2] etc.
it=1;

% Set light polarization and axis rotations LF -> MF
p=0;                % p=0 for linearly pol. light, +/-1 for L/R circ. pol.
eAngs=[0 0 0];      % Eugler angles for rotation of LF->MF, set as [0 0 0] for z-pol,␣
 ↪[0 pi/2 0] for x-pol, [pi/2 pi/2 0] for y-pol
polLabel='z';

% Run calculation - outputs are D, full set of MFPADs (summed over symmetries); Xsect,
 ↪ calculated X-sects; calcsAll, structure with results for all symmetries.
calcsAll=ePSproc_MFPAD(rlAll,p,eAngs,it,ipComponents,res);

% Add pol labels - currently expected in plotting routine, but not set in MFPAD␣
 ↪routine
% for n=1:size(calcsAll,2)
%     for symmIn=1:size(calcsAll,1)
%         calcsAll(symmInd,n).polLabel=polLabel;
%     end
% end
```

```
plot(calcsAll.')
```