
serpentTools Documentation

The serpentTools developer team

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CONTENTS:

1	Project Overview	3
2	Installation	7
3	Changelog	11
4	Examples	21
5	File-parsing API	81
6	Containers	111
7	Samplers	165
8	Settings	183
9	Miscellaneous	189
10	Variable Groups	193
11	Command Line Interface	207
12	Developer's Guide	211
13	License	249
14	Developer Team	251
15	Publications	253
16	Glossary	255
17	Indices and tables	257
	Bibliography	259
	Index	261

A suite of parsers designed to make interacting with *SERPENT* [serpent] output files simple and flawless.

The *SERPENT* Monte Carlo code is developed by VTT Technical Research Centre of Finland, Ltd. More information, including distribution and licensing of *SERPENT* can be found at <http://montecarlo.vtt.fi>

The Annals of Nuclear Energy article should be cited for all work using *SERPENT*.

Preferred citation for attribution

Andrew Johnson, Dan Kotlyar, Stefano Terlizzi, and Gavin Ridley, “serpentTools: A Python Package for Expediting Analysis with Serpent,” *Nuc. Sci. Eng.*, (in press) (2020).

Also, let us know if you publish work using this package! We try and keep an up-to-date list of [works using serpentTools](#), and would be happy to include more.

If you want to refer to a specific version, follow the [Zenodo DOI](#). This will resolve to the latest version, with links to earlier releases.

PROJECT OVERVIEW

The `serpentTools` package contains a variety of parsing utilities, each designed to read a specific output from the *SERPENT* Monte Carlo code [serpent]. Many of the parsing utilities store the outputs in custom container objects, while others store or return a collection of arrays. This page gives an overview of what files are currently supported, including links to examples and relevant documentation.

Unless otherwise noted, all the files listed below can be read using `serpentTools.read()`. For example:

```
>>> import serpentTools
>>> res = serpentTools.read('my_resFile_res.m')
```

would return a *ResultsReader*

Some file-types have an additional reader that is capable of reading multiple files and computing actual uncertainties. These `samplers` are detailed in *Samplers* and listed under the supported files.

Many of the readers have examples present in the *Examples* section. Each example is present as a *Jupyter notebook* at [Github: examples](#). These can be used as a launching point for tutorials or for your own analysis.

1.1 Main output File

- File Description: Primary output file for transport calculation - `[input]_res.m`
- SERPENT wiki: [result wiki](#)
- Primary Reader: *ResultsReader*
- Example - notebook: *ResultsReader*
- Example - manual: *Results Reader*

1.2 Depletion File

- File Description: Output from burnup calculations, showing quantities for various materials - `[input]_dep.m`
- SERPENT wiki: [depletion wiki](#)
- Primary Reader: *DepletionReader*
- Example - notebook: *DepletionReader*
- Example - manual: *Depletion Reader*
- Sampler - `serpentTools.samplers.DepletionSampler`

1.3 Detector/ Tally File

- File Description: Output generated by creating detectors - `[input]_det [N] .m`
- SERPENT wiki: [detector definition](#)
- Primary Reader: *DetectorReader*
- Example - notebook: [Detector](#)
- Example - manual: *Detector Reader*
- Sampler - *serpentTools.samplers.DetectorSampler*

1.4 Sensitivity File

- File Description: Output giving sensitivities of defined responses to perturbations - `[input]_sens [N] .m`
- SERPENT wiki: [sensitivity wiki](#)
- Primary Reader: *SensitivityReader*
- Example - notebook: [Sensitivity](#)
- Example - manual: *Sensitivity Reader*

1.5 Branching Coefficient File

- File Description: Selected homogenized group constants across a variety of defined branch states - `[input] .coe`
- SERPENT wiki: [branching wiki](#)
- Primary Reader: *BranchingReader*
- Secondary Read function: `serpentTools.BranchCollector.fromFile()`
- Example - notebook: [Branching](#)
- Example - manual: *Branching Reader*

1.6 Micro-depletion File

- File Description:
- SERPENT wiki: [microxs wiki](#)
- Primary Reader: *MicroXSReader*
- Example - notebook: [MicroXSReader](#)
- Example - manual: *Micro cross section reader*

1.7 Cross Section Plot File

- File Description: Cross section data and energy grids for various reactions - `[input]_xs0.m`
- SERPENT wiki: [xsplot wiki](#)
- Primary Reader: [*XSPlotReader*](#)
- Example - notebook: [XSPlot](#)
- Example - manual: [*Cross Section Reader/Plotter*](#)

1.8 Depletion Matrix File

- File Description: Data pertaining to depletion for a single burnable material at a single point in time - `depmtx_[material-identifier]-s[step].m`
- Primary Reader: [*DepmtxReader*](#)
- Example - notebook: [DepletionMatrix](#)
- Example - manual: [*Depletion Matrix Reader*](#)

INSTALLATION

In order to properly install this package, you need a version of python that plays well with libraries like *numpy* and *matplotlib*. This is easy or less easy depending on your operating system, but we have a brief walk through at *Obtaining a Python Distribution*.

2.1 Terminal terminology

Commands below that begin with \$ must be run from the terminal containing your preferred python distribution, neglecting the \$. Depending on operating system, this could be the normal terminal, or a modified prompt. See *Obtaining a Python Distribution* for more information if you are not sure.

Commands that begin with >>> should be run inside of a python environment. The following would be a valid set of instructions to pass to your terminal, printing a very basic python command:

```
$ python -m "print('hello world')"  
hello world  
$ python  
>>> print('hello world')  
hello world
```

2.2 Installing from pip

pip is the easiest way to install the latest version of *serpentTools*. First, ensure that you have *numpy* installed, as this is one of the required packages that is tricky to install. You can check by opening up a your preferred terminal and executing

```
$ python -c "import numpy"
```

If this fails, please consult *Obtaining a Python Distribution*.

Next, installation with pip can be completed with:

```
$ python -m pip install --user --upgrade pip serpentTools
```

This installs the dependencies of the package, the latest *serpentTools* release, and upgrades your version of *pip* along the way. When a new release is issued, run the command again to install the updated version.

If you wish to install the development branch to get the latest updates as they happen, use the following command:

```
$ python -m pip install -e git+https://www.github.com/CORE-GATECH-GROUP/serpent-tools.  
→git@develop#egg=serpentTools
```

Note: Changes to the development branch may not always be back-compatible and may cause non-ideal outcomes. Be sure to check the [Changelog](#) before/after updating from the develop branch

See also [pip install from git](#)

2.3 Installing from a Release

1. Download the source code for the latest release from [GitHub releases](#) as a `.zip` or `.tar.gz` compressed file.
2. Extract/decompress the contents somewhere convenient and memorable
3. Open your terminal and navigate to this directory:

```
$ cd path/to/release
```

4. Install using our setup script:

```
$ python setup.py install
```

5. Verify the install by running our test suite:

```
$ python setup.py test
```

2.4 Installing via git

The newest features are available on the `develop` branch before getting pushed to the `master` branch. We try to give decent notice when features are going to change via warning messages and our [Changelog](#), but changes to the API and other functionality can occur across the `develop` branch.

1. Clone the repository and checkout the branch of your choosing. The default is `develop`:

```
$ git clone https://github.com/CORE-GATECH-GROUP/serpent-tools.git
$ cd serpent-tools
$ git checkout master
```

2. Install using our [setup script](#):

```
$ python setup.py install
```

3. Verify the install by running our test suite:

```
$ python setup.py test
```

2.5 Obtaining a Python Distribution

Obtaining a version of python into which `serpent-tools` can be installed varies by operating system, with Windows requiring the most finesse.

2.5.1 Linux/Mac/Unix-like Operating Systems

If you don't have *numpy* installed, you will have to obtain it from your package manager or from pip:

```
# ubuntu
$ sudo apt-get install python-numpy
# pip
$ sudo pip install --upgrade numpy
```

If you already have *numpy*, then the *pip* installation process will take care of our other dependencies.

2.5.2 Windows

The easiest and most painless way to obtain packages like *numpy* on Windows is with either the *Anaconda* or *Mini-conda* distributions. Each of these also includes the *Anaconda Prompt* which is a modified terminal that plays better with Python. The former comes with a few hundred packages, included most of the ones needed for this project, bundled for you. The latter is a very small distribution and requires you to install the packages you want via *conda*. Should you choose this route, then you need to launch the *Anaconda Prompt* and install with:

```
$ conda install setuptools numpy matplotlib pyyaml
```

This prompt is what you should use when following the instructions in *Installation*.

CHANGELOG

Note: Development will be limited to bug fixes for future 0.9.x releases. Release 0.10.0 will introduce new and improved parsers and containers alongside existing structures. For more information, see [Updated Data Model](#)

3.1 0.9.3

- Depletion data now exposed through attributes like *adens* - #390
- Generate a `pandas.DataFrame` with depletion data using `toDataFrame()` - #391
- Dictionary-like item access and iteration for branching, detector, history, depletion, and xsplot readers - #392, #395, #402
- Obtain data from *resdata* with `__getitem__()` and `get()` - #392
- Modify plot legends for `serpentTools.objects.XSData.plot()` for all or some plotted MTs - #402
- Options for plotting sensitivity profiles against energies in MeV - #405

3.1.1 Bug Fixes

- Support xsplot files with branching fractions - #387, #388

3.1.2 Pending Deprecations

- `serpentTools.DepletionReader.metadata`. Prefer attributes like *zais*
- `serpentTools.samplers.DepletionSampler.metadata`. Prefer attributes like *zais*
- `serpentTools.BranchingReader.iterBranches()`. Prefer `items()`
- `serpentTools.XSPlotReader.metadata` and `serpentTools.objects.XSData.metadata`. Prefer attributes like *majorant* or *energies* - #402

3.2 0.9.2

- Officially support installing under Python 3.8
- Support for passing threshold values to hexagonal detector plots - [#351](#)

3.2.1 Bug Fixes

- Detector reader can handle sequential detectors with very similar names - [#374](#).
- `serpentTools` doesn't make any modifications to the logging state, other than introducing package-wide logger - [#380](#)
- Colorbars for mesh plots are placed next to their corresponding plot, rather than near the last drawn plot - [#372](#)

3.3 0.9.1

3.3.1 Bug Fixes

- Sensitivity arrays generated with `sens opt history 1` will no longer overwrite the primary result arrays - [#366](#). These arrays are not currently stored - [#367](#)

3.4 0.9.0

- Python 2 support has been dropped.
- Add support for installing and testing against Python 3.7

3.5 0.8.1

- Use `six>=1.13.0`
- Use `yaml>=5.1.1`

3.5.1 Bug Fixes

- Fix `detector.names` setting

3.6 0.8.0

Warning: Serpent 1 detectors are no longer supported - [#327](#). Version 0.9.0 will remove support for python 2 - [#328](#)

- Better handling of discontinuity factors - [#329](#)
- `HomogUniv` objects no longer automatically convert data to arrays

- Serpent 2.1.31 is the default version for *serpentVersion* setting
- Detectors and related subclasses are now standalone classes that can be imported as `serpentTools.Detector` - #341
- *BranchContainer* now inherits from `dict` - #344
- Keys for universes in `ResultsReader.universes` are *UnivTuple*
- Keys for microscopic cross sections in `MicroXSReader.xsVal` and `MicroXSReader.xsUnc` are *MicroXSTuple*
- Spread plots for sampled detector and depletion containers allow changing how the mean data and sampled data are plotted by passing dictionary of matplotlib commands, e.g. `meanKwargs={"c": "r", "marker": "x"}` would plot the mean data in red with crosses as markers.

3.6.1 Bug Fixes

- Burnup and days are properly set on homogenized universes when reading a result file with multiple universes but no burnup - #346
- Modifications made to detector tally data will be reflected in later plots - #337, #341
- Variable groups for version 2.1.31 are properly expanded - #347

3.6.2 Incompatible API Changes

- Values are stored in array form on *HomogUniv* when it makes sense. For example, values like `infKinf` are stored as scalars.
- Setting `expectGcu` has been removed as #324 fixed how files without group constants are handled.
- Keys to *BranchedUniv* objects stored in `serpentTools.xs.BranchCollector.universes` are stored as strings, rather than integers, e.g. 0 is replaced with "0" - #321
- Keys to *HomogUniv* instances stored on *BranchContainer* are now *UnivTuple*, or tuples with universe, burnup, step, days - #344
- `serpentTools.Detector.indexes` is now a tuple of strings describing each dimension of tallies rather than `OrderedDict` - #341

3.7 0.7.1

- Add `__getitem__()` and `__setitem__()` convenience methods for accessing expected values on *HomogUniv* objects
- Add `thresh` argument to *Detector* `meshPlot` where only data greater than `thresh` is plotted.
- Mitigate pending deprecated imports from `collections` - #313
- Increase required version of *yaml* to 5.1.1
- Include SERPENT 2.1.31 support in *serpentVersion* setting

3.7.1 Bug fixes

- Tally data for detectors with time-bins are properly handled - #312
- Support for generic string universe names for *BranchingReader* and *BranchCollector* - #318

3.7.2 Pending Deprecations

- Keys to *BranchedUniv* objects stored in *serpentTools.xs.BranchCollector.universes* are stored as strings, rather than integers, e.g. 0 is replaced with "0". A workaround is in-place, but will be removed in future versions.
- SERPENT 1 style detectors with additional score column will not be supported starting at version 0.8.0.

3.8 0.7.0

- **Easier construction of *BranchCollector* objects - #276**
 - Directly from the class *FromFile*
 - Don't require passing branch information to *BranchCollector*. Will be inferred from file and set with (p0, p1, ...). State data can be used to determine which index is a given perturbation type.
- Direct *toMatlab* methods for *ResultsReader*, *SensitivityReader*, *DepmtxReader*, *DepletionReader*, *DetectorReader*, *HistoryReader*, and *Detector* objects - #290, #291
- Overhaul, reorganization, and cleanup of documentation

3.8.1 Incompatible API Changes

- *HomogUniv* objects are now stored on *ResultsReader* with zero-based indexing for burnup. The previous first value of burnup step was one. All burnup indices are now decreased by one. Similarly, if no burnup was present in the file, the values of burnup and days for all universes is zero - #288
- When reading Detectors with a single tally, the value of tallies, errors, and scores are stored as floats, rather than *numpy* arrays - #289

3.8.2 Deprecations

- *DepletionReader* *saveAsMatlab* in favor of *toMatlab()*
- SERPENT 2.1.30 is the default version of *serpentVersion*. Will alter some variable groups, like *optimization* and *optimization*, that exist in both versions but are slightly different.

3.8.3 Bug Fixes

- *BranchingReader* is now capable of reading `.coe` files with uncertainties - #272
- Fixed a bug that caused some plots not to return the axes object of the plot - #297
- *HomogUniv* plots are plotted against energy group when no group structure can be determined, and now labeled as such - #299
- Removed a non-zero exit code from a successful use of the *Random Seed Generation* command line command - #300
- *ResultsReader* can process files with assembly discontinuity factors (ADFs) - #305

3.9 0.6.2

- Data files are bundled in source distribution
- CLI interface for converting some output files to matlab files - *Conversion to Binary .mat files*
- Add `serpentTools.io` module for converting objects to other data types. Currently a general function for converting `toMatlab()`
- *DetectorReader* and *Detector* objects can be written to MATLAB files using `serpentTools.io.toMatlab()`
- *ResultsReader* can plot data using `plot()`
- Experimental *BranchCollector* for collecting group constants from coefficient files. Collects group constants in in multi-dimensional matrices according to perturbations, universes, and burnup.
- Plotting routines now use `attach` to the active plot or generate a new plot figure if `ax` argument not given - #267
- *BranchingReader* can read coefficient files with uncertainties - #270

Warning: The API for the *BranchCollector* may be subject to change through revisions until 0.7.0

3.9.1 Pending Deprecations

- `saveAsMatlab()` in favor of `serpentTools.io.toMatlab()` with:

```
>>> from serpentTools.io import toMatlab
>>> toMatlab(depR)
```

- Depletion plot routines will no longer accept `timePoints` arguments, instead plotting against all points in time

3.10 0.6.1

- #256 `serpentTools.settings.rc.loadYaml()` uses `safe_load`
- #257 *DepletionReader* now can utilize `saveAsMatlab()` for exporting data to a binary `.mat` file
- #259 Little more clarity into supported readers through documentation and `serpentTools.read()` function

3.11 0.6.0

- #174 - Added parent object *BaseObject* with basic comparison method from which all objects inherit. Comparison method contains upper and lower bounds for values w/o uncertainties, #191
- #196 - Add comparison methods for *ResultsReader* and *HomogUniv* objects
- #228 - Add comparison methods for *DetectorReader* and *Detector* objects
- #236 - Add comparison methods for *DepletionReader* and *DepletedMaterial* objects
- #241 - Fix a bug in the CLI that rendered the ability to generate files with unique random seeds. `python -m serpentTools seed <input> <N>` can now be properly used.
- #249 - Better sparse support for depletion matrix, `depmtx` files with a *DepmtxReader*
- #252 - Better axis and colorbar labeling for *Detector* mesh plots
- #254 - Better plotting of single concentrations with *DepmtxReader*
- #255 - *DepletionReader* can capture material with underscores now!

3.11.1 Deprecations

- `depmtx()` is deprecated in favor of either `readDepmtx()` or the class-based *DepmtxReader*

3.12 0.5.4

- #239 - Update python dependencies to continue use of python 2

3.13 0.5.3

- #221 - Expanded `utils` module to better assist developers
- #227 - Better documentation of our *Command Line Interface*. Better documentation and testing of functions for generating input files with unique random seeds - `serpentTools.seed`
- #229 - `serpentTools.SensitivityReader.plot()` now respects the option to not set x nor y labels.
- #231 - *ResultsReader* objects can now read files that do not contain group constant data. The setting `results-expectGcu` should be used to inform the reader that no group constant data is anticipated

Note: This setting was removed in *0.8.0* and in #324

3.14 0.5.2

- #198 - Import test and example files using `serpentTools.data`. Load example readers with `serpentTools.data.readDataFile()`
- #199 - Support for structured or unstructured matrix plotting with `serpentTools.plot.cartMeshPlot()`
- #201 - Support for plotting hexagonal meshes with `serpentTools.objects.HexagonalDetector.hexPlot()`
- #204 - Access *Detector* objects directly from *DetectorReader* with `reader[detName]`
- #205 - Access materials from *DepletionReader* and `serpentTools.samplers.DepletionSampler` using key-like indexing, e.g. `reader[matName] == reader.material[matName]`
- #213 - Better default x-axis labels for simple Detector plots

3.14.1 API Changes

- #194 - Some settings in `serpentTools.ResultsReader.metadata` are now stored as `int` or `float`, depending upon their nature. Many of these settings refer to flags of settings used by SERPENT

3.15 0.5.1

- #180 - Add capability to pass isotope `zzaaai` for `getValues()` and associated plot routines
- #187 - Import all readers and samplers from the main package:

```
>>> from serpentTools import ResultsReader
>>> from serpentTools import DetectorSampler
```

- #189 - Support for reading Detectors with hexagonal, cylindrical, and spherical meshes.

3.15.1 API Changes

- `zzaaai` data is stored on `zai` as a list of integers, not strings

3.16 0.5.0

- #131 Updated variable groups between 2.1.29 and 2.1.30 - include poison cross section, kinetic parameters, six factor formula (2.1.30 exclusive), and minor differences
- #141 - Setting `xs.reshapeScatter` can be used to reshape scatter matrices on *HomogUniv* objects to square matrices
- #145 - `hasData()` added to check if *HomogUniv* objects have any data stored on them
- #146 - *HomogUniv* object stores group structure on the object. New dictionaries for storing group constant data that is not INF nor B1 - `gc` and `gcUnc`
- #130 Added the ability to read results file

- #149 - Add the ability to read sensitivity files
- #161 - Add the `utils` module
- #165 - Add the `serpentTools.objects.HomogUniv.plot()` method

3.16.1 API Changes

- #146 removed metadata dictionaries on `HomogUniv` objects.

3.16.2 Deprecation

- Variable group `xs-yields` is removed. Use `poisons` instead
- Branches of a single name are only be accessible through `branches['nom']`, not `branches[('nom'),]` as per #114

3.17 0.4.0

- #95 Add `xsplo` file reader - `XSPloedReader`
- #121 Samplers will raise more warnings/errors if no files are loaded from `*` wildcards
- #122 Better Detector labeling
- #135 Added instructions for better converting Jupyter notebooks to `.rst` files. Plotting guidelines

3.18 0.3.1

- #118 - Support for SERPENT 2.1.30
- #119 - `SampledDepletedMaterial` now respects the value of `xUnits` - #120
- #114 - Standalone branches in the coefficient files are stored and accessed using a single string, rather than a single-entry tuple `branches['myBranch']` vs. `branches[('myBranch',)]`

3.19 0.3.0

- #109 - Capability to read history files
- #107 - `DepletionReader` can now plot data for some or all materials

3.20 0.2.2

- [#82](#) - Command line interface and some sub-commands
- [#88](#) - Pre- and post-check methods for readers
- [#93](#) - Detector and Depletion Samplers
- [#96](#) - Better mesh plotting for Detector
- [#99](#) - Negative universe burnup with branching reader - [#100](#)
- `serpentTools.objects.Detector.indexes` are now zero-indexed
- The PDF manual is no longer tracked in this repository

EXAMPLES

4.1 User Control

The `serpentTools` package is designed to, without intervention, be able to store all the data contained in each of the various output files. However, the `serpentTools.settings` module grants great flexibility to the user over what data is obtained through the `serpentTools.settings.rc` class.

All the settings are given in *Default Settings*, showing their default values and possible options.

4.1.1 Basic Usage

```
>>> import serpentTools
>>> from serpentTools.settings import rc
```

The `serpentTools.settings.rc` object can be used like a dictionary, polling all possible settings with the `.keys` method:

```
>>> rc.keys()
dict_keys(['depletion.processTotal', 'verbosity', 'xs.getInfXS',
'branching.intVariables', 'serpentVersion',
'sampler.raiseErrors', 'xs.getB1XS', 'xs.variableGroups', 'xs.variableExtras',
'depletion.materialVariables', 'depletion.metadataKeys', 'sampler.freeAll',
'sampler.allExist', 'depletion.materials', 'sampler.skipPrecheck',
'xs.reshapeScatter', 'branching.floatVariables', 'detector.names'])
```

Settings such as `depletion.materials` are specific for the `DepletionReader` while settings that are led with `xs` are sent to the `ResultsReader` and `BranchingReader` as well as their specific settings. Updating a setting is similar to setting a value in a dictionary

```
>>> rc['verbosity'] = 'debug'
DEBUG : serpentTools: Updated setting verbosity to debug
```

The `serpentTools.settings.rc` object automatically checks to make sure the value is of the correct type, and is an allowable option, if given.

```
>>> try:
...     rc['depletion.metadataKeys'] = False
>>> except TypeError as te:
...     print(te)
Setting depletion.metadataKeys should be of type <class 'list'>, not <class
'bool'>
>>> try:
```

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```
...     rc['serpentVersion'] = '1.2.3'
>>> except KeyError as ke:
...     print(ke)
'Setting serpentVersion is 1.2.3 and not one of the allowed options: 2.1.29,
2.1.30'
```

The `serpentTools.settings.rc` object can also be used inside a context manager to revert changes.

```
>>> with rc:
...     rc['depletion.metadataKeys'] = ['ZAI', 'BU']
...
DEBUG : serpentTools: Updated setting depletion.metadataKeys to ['ZAI', 'BU']
DEBUG : serpentTools: Updated setting depletion.metadataKeys to ['ZAI', 'NAMES',
↪ 'DAYS', 'BU']
>>> rc['verbosity'] = 'info'
```

Group Constant Variables

Two settings control what group constant data and what variables are extracted from the results and coefficient files.

1. `xs.variableExtras`: Full SERPENT_STYLE variable names, i.e. INF_TOT, FISSION_PRODUCT_DECAY_HEAT
2. `xs.variableGroups`: Select keywords that represent blocks of common variables

These variable groups are described in [Variable Groups](#) and rely upon the SERPENT version to properly expand the groups.

```
>>> rc['serpentVersion']
'2.1.29'
>>> rc['xs.variableGroups'] = ['kinetics', 'xs', 'diffusion']
>>> rc['xs.variableExtras'] = ['XS_DATA_FILE_PATH']
>>> varSet = rc.expandVariables()
>>> print(sorted(varSet))
['ABS', 'ADJ_IFP_ANA_BETA_EFF', 'ADJ_IFP_ANA_LAMBDA', 'ADJ_IFP_GEN_TIME',
'ADJ_IFP_IMP_BETA_EFF', 'ADJ_IFP_IMP_LAMBDA', 'ADJ_IFP_LIFETIME',
'ADJ_IFP_ROSSI_ALPHA', 'ADJ_INV_SPD', 'ADJ_MEULEKAMP_BETA_EFF',
'ADJ_MEULEKAMP_LAMBDA', 'ADJ_NAUCHI_BETA_EFF', 'ADJ_NAUCHI_GEN_TIME',
'ADJ_NAUCHI_LAMBDA', 'ADJ_NAUCHI_LIFETIME', 'ADJ_PERT_BETA_EFF',
'ADJ_PERT_GEN_TIME', 'ADJ_PERT_LIFETIME', 'ADJ_PERT_ROSSI_ALPHA', 'BETA_EFF',
'CAPT', 'CHID', 'CHIP', 'CHIT', 'CMM_DIFFCOEF', 'CMM_DIFFCOEF_X',
'CMM_DIFFCOEF_Y', 'CMM_DIFFCOEF_Z', 'CMM_TRANSPXS', 'CMM_TRANSPXS_X',
'CMM_TRANSPXS_Y', 'CMM_TRANSPXS_Z', 'DIFFCOEF', 'FISS', 'FWD_ANA_BETA_ZERO',
'FWD_ANA_LAMBDA', 'INVV', 'KAPPA', 'LAMBDA', 'NSF', 'NUBAR', 'RABSXS', 'REMXS',
'S0', 'S1', 'S2', 'S3', 'S4', 'S5', 'S6', 'S7', 'SCATT0', 'SCATT1', 'SCATT2',
'SCATT3', 'SCATT4', 'SCATT5', 'SCATT6', 'SCATT7', 'TOT', 'TRANSPXS',
'XS_DATA_FILE_PATH']
```

However, one might see that the full group constant cross sections are not present in this set

```
>>> assert 'INF_SCATT3' not in varSet
```

This is because two additional settings instruct the `BranchingReader` and `ResultsReader` to obtain infinite medium and leakage-corrected cross sections: `xs.getInfXS` and `xs.getBIXS`, respectively. By default, `xs.getInfXS` and `xs.getBIXS` default to True. This, in conjunction with leaving the `xs.variableExtras` and `xs.variableGroups` settings to empty lists, instructs these readers to obtain all the data present in their respective files.

See the [Branching Reader](#) example for more information on using these settings to control scraped data.

Configuration Files

The `serpentTools.settings.rc` object allows for settings to be updated from a yaml configuration file using the `loadYaml()` method. The file is structured with the names of settings as keys and the desired setting value as the values. The loader also attempts to expand nested settings, like reader-specific settings, that may be lumped in a second level:

```
verbosity: warning
xs.getInfXS: False
```

However, the loader can also expand a nested dictionary structure, as:

```
branching:
  floatVariables: [Fhi, Blo]
depletion:
  materials: [fuel*]
  materialVariables:
    [ADENS, MDENS, VOLUME]
```

```
>>> %cat myConfig.yaml
xs.getInfXS: False
xs.getB1XS: True
xs.variableGroups: [gc-meta, kinetics,
xs]
branching:
  floatVariables: [Fhi, Blo]
depletion:
  materials: [fuel*]
  metadataKeys: [NAMES, BU]
materialVariables:
  [ADENS, MDENS, VOLUME]
serpentVersion: 2.1.29
>>> myConf = 'myConfig.yaml'
>>> rc.loadYaml(myConf)
INFO      : serpentTools: Done
>>> rc['xs.getInfXS']
False
```

4.2 Branching Reader

This notebook demonstrates the capability of the `serpentTools` package to read branching coefficient files. The format of these files is structured to iterate over:

1. Branch states, e.g. burnup, material properties
2. Homogenized universes
3. Group constant data

The output files are described in more detail on the [SERPENT Wiki](#)

4.2.1 Basic Operation

Note: The preferred way to read your own output files is with the `serpentTools.read()` function. The `serpentTools.readDataFile()` function is used here to make it easier to reproduce the examples

Note: Without modifying the settings, the `BranchingReader` assumes that all group constant data is presented without the associated uncertainties. See *User Control* for examples on the various ways to control operation

```
>>> import serpentTools
>>> branchFile = 'demo.coe'
>>> r0 = serpentTools.readDataFile(branchFile)
```

The branches are stored in custom dictionary-like `BranchContainer` objects in the `branches` dictionary

```
>>> r0.branches.keys()
dict_keys([
    ('nom', 'nom'),
    ('B750', 'nom'),
    ('B1000', 'nom'),
    ('nom', 'FT1200'),
    ('B750', 'FT1200'),
    ('B1000', 'FT1200'),
    ('nom', 'FT600'),
    ('B750', 'FT600'),
    ('B1000', 'FT600')
])
```

Here, the keys are tuples of strings indicating what perturbations/branch states were applied for each SERPENT solution. Examining a particular case

```
>>> b0 = r0.branches['B1000', 'FT600']
>>> print(b0)
<BranchContainer for B1000, FT600 from demo.coe>
```

SERPENT allows the user to define variables for each branch through `var V1_name V1_value` cards. These are stored in the `stateData` attribute

```
>>> b0.stateData
{'BOR': '1000',
 'DATE': '17/12/19',
 'TFU': '600',
 'TIME': '09:48:54',
 'VERSION': '2.1.29'}
```

The keys `'DATE'`, `'TIME'`, and `'VERSION'` are included by default in the output, while the `'BOR'` and `'TFU'` have been defined for this branch.

Group Constant Data

Note: Group constants are converted from SERPENT_STYLE to mixedCase to fit the overall style of the project.

The *BranchContainer* stores group constant data in *HomogUniv* objects as a dictionary.

```
>>> for key in b0:
...     print(key)
UnivTuple(universe='0', burnup=0.0, step=0, days=None)
UnivTuple(universe='10', burnup=0.0, step=0, days=None)
UnivTuple(universe='20', burnup=0.0, step=0, days=None)
UnivTuple(universe='30', burnup=0.0, step=0, days=None)
UnivTuple(universe='40', burnup=0.0, step=0, days=None)
UnivTuple(universe='0', burnup=1.0, step=1, days=None)
UnivTuple(universe='10', burnup=1.0, step=1, days=None)
UnivTuple(universe='20', burnup=1.0, step=1, days=None)
UnivTuple(universe='30', burnup=1.0, step=1, days=None)
UnivTuple(universe='40', burnup=1.0, step=1, days=None)
UnivTuple(universe='0', burnup=10.0, step=2, days=None)
UnivTuple(universe='10', burnup=10.0, step=2, days=None)
UnivTuple(universe='20', burnup=10.0, step=2, days=None)
UnivTuple(universe='30', burnup=10.0, step=2, days=None)
UnivTuple(universe='40', burnup=10.0, step=2, days=None)
```

The keys here are *UnivTuple* instances indicating the universe ID, and point in the burnup schedule. These universes can be obtained by indexing this dictionary, or by using the *getUniv()* method

```
>>> univ0 = b0["0", 1, 1, None]
>>> print(univ0)
<HomogUniv 0: burnup: 1.000 MWd/kgu, step: 1>
>>> univ0.name, univ0.bu, univ0.step, univ0.day
('0', 1.0, 1, None)
>>> univ1 = b0.getUniv('0', burnup=1)
>>> univ2 = b0.getUniv('0', index=1)
>>> univ0 is univ1 is univ2
True
```

Group constant data is spread out across the following sub-dictionaries:

1. *infExp*: Expected values for infinite medium group constants
2. *infUnc*: Relative uncertainties for infinite medium group constants
3. *b1Exp*: Expected values for leakage-corrected group constants
4. *b1Unc*: Relative uncertainties for leakage-corrected group constants
5. *gc*: Group constant data that does not match the INF nor B1 scheme
6. *gcUnc*: Relative uncertainties for data in *gc*

For this problem, only expected values for infinite and critical spectrum (b1) group constants are returned, so only the *infExp* and *b1Exp* dictionaries contain data

```
>>> univ0.infExp
{'infDiffcoef': array([ 1.83961 ,  0.682022]),
 'infFiss': array([ 0.00271604,  0.059773 ]),
 'infS0': array([ 0.298689 ,  0.00197521,  0.00284247,  0.470054 ]),
```

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```
'infS1': array([ 0.0847372 ,  0.00047366,  0.00062865,  0.106232  ]),
'infTot': array([ 0.310842,  0.618286])}
>>> univ0.infUnc
{}
>>> univ0.blExp
{'blDiffcoef': array([ 1.79892 ,  0.765665]),
'blFiss': array([ 0.00278366,  0.0597712 ]),
'blS0': array([ 0.301766 ,  0.0021261 ,  0.00283866,  0.470114  ]),
'blS1': array([ 0.0856397 ,  0.00051071,  0.00062781,  0.106232  ]),
'blTot': array([ 0.314521,  0.618361])}
>>> univ0.gc
{}
>>> univ0.gcUnc
{}
```

Group constants and their associated uncertainties can be obtained using the `get()` method.

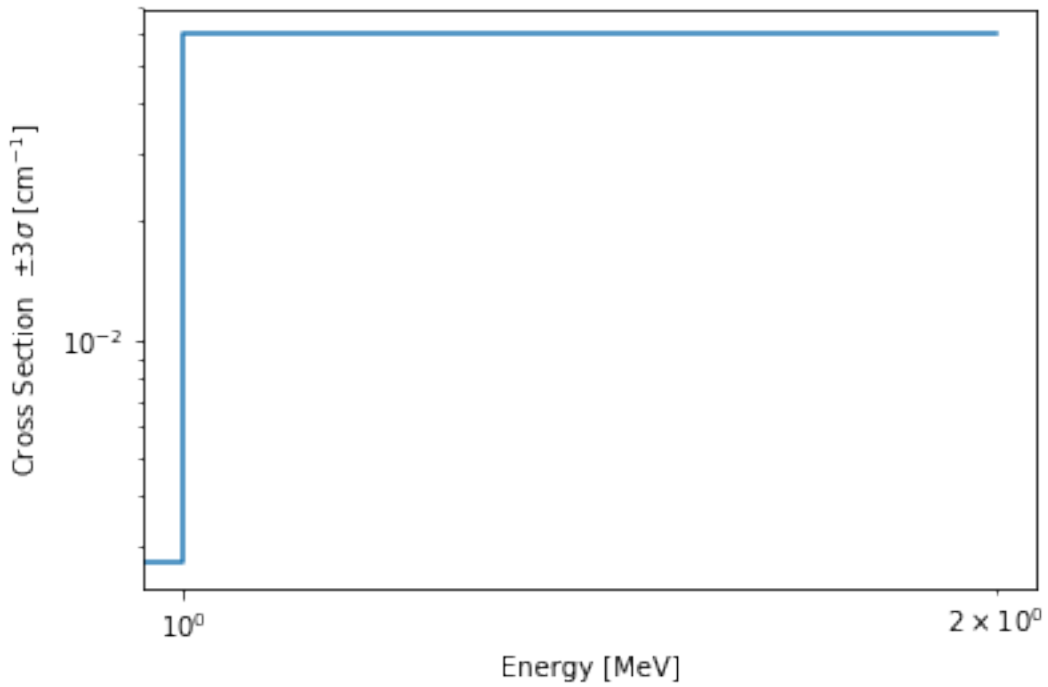
```
>>> univ0.get('infFiss')
array([ 0.00271604,  0.059773  ])

>>> try:
...     univ0.get('infS0', uncertainty=True)
>>> except KeyError as ke: # no uncertainties here
...     print(str(ke))
'Variable infS0 absent from uncertainty dictionary'
```

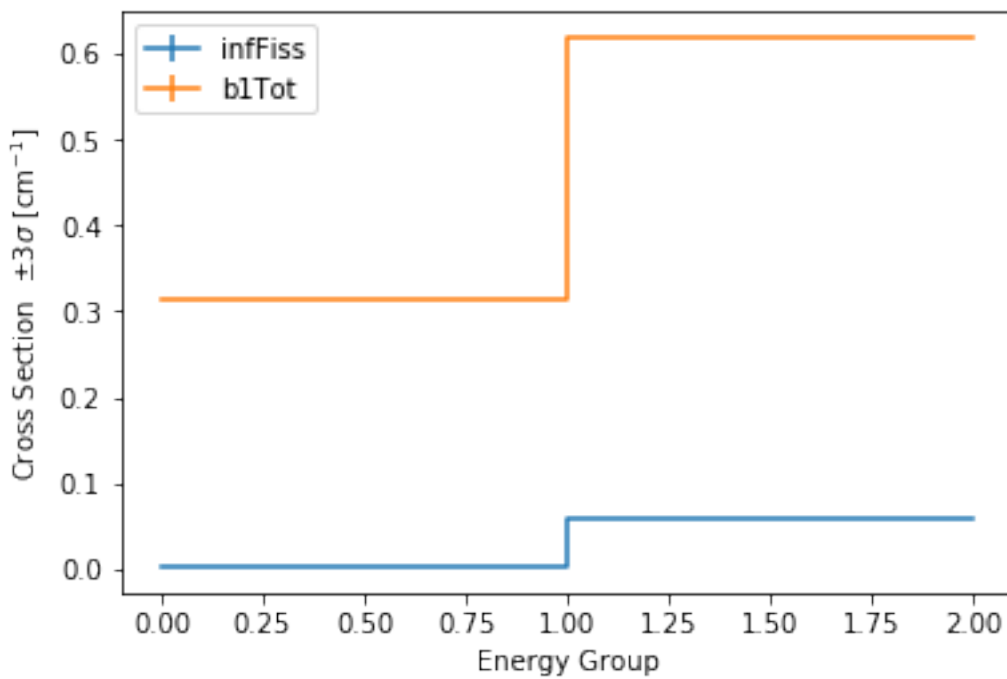
4.2.2 Plotting Universe Data

`HomogUniv` objects are capable of plotting homogenized data using the `plot()` method. This method is tuned to plot group constants, such as cross sections, for a known group structure. This is reflected in the default axis scaling, but can be adjusted on a per case basis. If the group structure is not known, then the data is plotted simply against bin-index.

```
>>> univ0.plot('infFiss');
```



```
>>> univ0.plot(['infFiss', 'b1Tot'], loglog=False);
```



The *ResultsReader* example has a more thorough example of this `plot()` method, including formatting the line labels - *Plotting universes*.

4.2.3 Iteration

The branching reader has a `iterBranches()` method that works to yield branch names and their associated `BranchContainer` objects. This can be used to efficiently iterate over all the branches presented in the file.

```
>>> for names, branch in r0.iterBranches():
...     print(names, branch)
('nom', 'FT1200') <BranchContainer for nom, FT1200 from demo.coe>
('B1000', 'FT1200') <BranchContainer for B1000, FT1200 from demo.coe>
('B750', 'FT600') <BranchContainer for B750, FT600 from demo.coe>
('nom', 'nom') <BranchContainer for nom, nom from demo.coe>
('B750', 'FT1200') <BranchContainer for B750, FT1200 from demo.coe>
('B1000', 'FT600') <BranchContainer for B1000, FT600 from demo.coe>
('nom', 'FT600') <BranchContainer for nom, FT600 from demo.coe>
('B1000', 'nom') <BranchContainer for B1000, nom from demo.coe>
('B750', 'nom') <BranchContainer for B750, nom from demo.coe>
```

4.2.4 User Control

The SERPENT `set coefpara` card already restricts the data present in the coefficient file to user control, and the `BranchingReader` includes similar control.

- `branching.floatVariables`
- `branching.intVariables`
- `xs.getB1XS`
- `xs.getInfXS`
- `xs.reshapeScatter`
- `xs.variableExtras`
- `xs.variableGroups`

In our example above, the BOR and TFU variables represented boron concentration and fuel temperature, and can easily be cast into numeric values using the `branching.intVariables` and `branching.floatVariables` settings. From the previous example, we see that the default action is to store all state data variables as strings.

```
>>> assert isinstance(b0.stateData['BOR'], str)
```

As demonstrated in the `Group Constant Variables` example, use of `xs.variableExtras` and `xs.variableGroups` controls what data is stored on the `HomogUniv` objects. By default, all variables present in the coefficient file are stored.

```
>>> from serpentTools.settings import rc
>>> rc['branching.floatVariables'] = ['BOR']
>>> rc['branching.intVariables'] = ['TFU']
>>> rc['xs.getB1XS'] = False
>>> rc['xs.variableExtras'] = ['INF_TOT', 'INF_SCATT0']
>>> r1 = serpentTools.readDataFile(branchFile)
>>> b1 = r1.branches['B1000', 'FT600']
>>> b1.stateData
{'BOR': 1000.0,
 'DATE': '17/12/19',
 'TFU': 600,
 'TIME': '09:48:54',
 'VERSION': '2.1.29'}
```

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```
>>> assert isinstance(bl.stateData['BOR'], float)
>>> assert isinstance(bl.stateData['TFU'], int)
```

Inspecting the data stored on the homogenized universes reveals only the variables explicitly requested are present

```
>>> univ4 = bl.getUniv("0", 0)
>>> univ4.infExp
{'infTot': array([ 0.313338,  0.54515 ])}
>>> univ4.blExp
{}
```

4.2.5 Conclusion

The *BranchingReader* is capable of reading coefficient files created by the SERPENT automated branching process. The data is stored according to the branch parameters, universe information, and burnup. This reader also supports user control of the processing by selecting what state parameters should be converted from strings to numeric types, and further down-selection of data.

4.3 Detector Reader

4.3.1 Basic Operation

The *DetectorReader* is capable of reading SERPENT detector files. These detectors can be defined with many binning parameters, listed on the [SERPENT Wiki](#). One could define a detector that has a spatial mesh, $dx/dy/dz$, but also includes reaction and material bins, dr , dm . Detectors are stored on the reader object in the *detectors* dictionary as custom *Detector* objects. Here, all energy and spatial grid data are stored, including other binning information such as reaction, universe, and lattice bins.

Note: The preferred way to read your own output files is with the *serpentTools.read()* function. The *serpentTools.readDataFile()* function is used here to make it easier to reproduce the examples

```
>>> from matplotlib import pyplot
>>> import serpentTools
>>> pinFile = 'fuelPin_det0.m'
>>> bwrFile = 'bwr_det0.m'
>>> pin = serpentTools.readDataFile(pinFile)
>>> bwr = serpentTools.readDataFile(bwrFile)
>>> print(pin.detectors)
{'nodeFlx': <serpentTools.Detector object at 0x7f6df2162b70>}
>>> print(bwr.detectors)
{'xymesh': <serpentTools.Detector object at 0x7f6df2162a90>,
 'spectrum': <serpentTools.Detector object at 0x7f6df2162b00>}
```

These detectors were defined for a single fuel pin with 16 axial layers and a separate BWR assembly, with a description of the detectors provided in below:

Name	Description
nodeFlx	One-group flux tallied in each axial layer
spectrum	CSEWG 239 group structure for flux and U-235 fission cross section
xymesh	Two-group flux for a 20x20 xy grid

For each *Detector* object, the full tally matrix is stored in the *bins* array.

```
>>> nodeFlx = pin.detectors['nodeFlx']
>>> print(nodeFlx.bins.shape)
(16, 12)
>>> nodeFlx.bins[:,3,:].T
array([[1.00000e+00, 2.00000e+00, 3.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [1.00000e+00, 2.00000e+00, 3.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [1.00000e+00, 1.00000e+00, 1.00000e+00],
       [2.34759e-02, 5.75300e-02, 8.47000e-02],
       [4.53000e-03, 3.38000e-03, 2.95000e-03]])
```

Here, only three columns, shown as rows for readability, are changing:

- column 0: universe column
- column 10: tally column
- column 11: errors

Detectors can also be obtained by indexing into the *DetectorReader* like a dictionary.

```
>>> pin["nodeFlx"] is pin.detectors[nodeFlx]
True
>>> bwr.get("spectrum") is bwr.detectors["spectrum"]
```

Tally data is reshaped corresponding to the bin information provided by Serpent. The tally and errors columns are recast into multi-dimensional arrays where each dimension is some unique bin type like energy or spatial bin index. For this case, since the only variable bin quantity is that of the universe, the *tallies* and *errors* attributes will be 1D arrays.

```
>>> assert nodeFlx.tallies.shape == (16, )
>>> assert nodeFlx.errors.shape == (16, )
>>> nodeFlx.tallies
array([0.0234759 , 0.05753   , 0.0847   , 0.102034 , 0.110384 ,
       0.110174 , 0.102934 , 0.0928861 , 0.0810541 , 0.067961 ,
       0.0550446 , 0.0422486 , 0.0310226 , 0.0211475 , 0.0125272 ,
       0.00487726])
>>> nodeFlx.errors
array([0.00453, 0.00338, 0.00295, 0.00263, 0.00231, 0.00222, 0.00238,
       0.00251, 0.00282, 0.00307, 0.00359, 0.00415, 0.00511, 0.00687,
       0.00809, 0.01002])
```

Note: Python and numpy arrays are zero-indexed, meaning the first item is accessed with `array[0]`, rather than `array[1]`.

Bin information is retained through the *indexes* attribute. Each entry indicates what bin type is changing along that dimension of tallies and errors. Here, *universe* is the first item and indicates that the first dimension of tallies and errors corresponds to a changing universe bin.

```
>>> nodeFlx.indexes
('universe', )
```

For detectors that include some grid matrices, such as spatial or energy meshes DET<name>E, these arrays are stored in the *grids* dictionary

```
>>> spectrum = bwr.detectors['spectrum']
>>> print(spectrum.grids['E'][:5])
[[1.00002e-11 4.13994e-07 2.07002e-07]
 [4.13994e-07 5.31579e-07 4.72786e-07]
 [5.31579e-07 6.25062e-07 5.78320e-07]
 [6.25062e-07 6.82560e-07 6.53811e-07]
 [6.82560e-07 8.33681e-07 7.58121e-07]]
```

4.3.2 Multi-dimensional Detectors

The *Detector* objects are capable of reshaping the detector data into an array where each axis corresponds to a varying bin. In the above examples, the reshaped data was one-dimensional, because the detectors only tallied data against one bin, universe and energy. In the following example, the detector has been configured to tally the fission and capture rates (two *dr* arguments) in an XY mesh.

```
>>> xy = bwr.detectors['xymesh']
>>> xy.indexes
('energy', 'ymesh', 'xmesh')
```

Traversing the first axis in the *tallies* array corresponds to changing the value of the energy. The second axis corresponds to changing ymesh values, and the final axis reflects changes in xmesh.

```
>>> print(xy.bins.shape)
(800, 12)
>>> print(xy.tallies.shape)
(2, 20, 20)
>>> print(xy.bins[:5, 10])
[8.19312e+17 7.18519e+17 6.90079e+17 6.22241e+17 5.97257e+17]
>>> print(xy.tallies[0, 0, :5])
[8.19312e+17 7.18519e+17 6.90079e+17 6.22241e+17 5.97257e+17]
```

Slicing

As the detectors produced by SERPENT can contain multiple bin types, obtaining data from the tally data can become complicated. This retrieval can be simplified using the *slice()* method. This method takes an argument indicating what bins (keys in *indexes*) to fix at what position.

If we want to retrieve the tally data for the fission reaction in the *spectrum* detector, you would instruct the *slice()* method to use column 1 along the axis that corresponds to the reaction bin, as the fission reaction corresponded to reaction tally 2 in the original matrix. Since python and *numpy* arrays are zero indexed, the second reaction tally is stored in column 1.

```
>>> spectrum.slice({'reaction': 1})[:20]
array([3.66341e+22, 6.53587e+20, 3.01655e+20, 1.51335e+20, 3.14546e+20,
       7.45742e+19, 4.73387e+20, 2.82554e+20, 9.89379e+19, 9.49670e+19,
       8.98272e+19, 2.04606e+20, 3.58272e+19, 1.44708e+20, 7.25499e+19,
       6.31722e+20, 2.89445e+20, 2.15484e+20, 3.59303e+20, 3.15000e+20])
```

This method also works for slicing the error, or score, matrix

```
>>> spectrum.slice({'reaction': 1}, 'errors')[:20]
array([0.00692, 0.01136, 0.01679, 0.02262, 0.01537, 0.02915, 0.01456,
       0.01597, 0.01439, 0.01461, 0.01634, 0.01336, 0.01549, 0.01958,
       0.02165, 0.0192 , 0.02048, 0.01715, 0.02055, 0.0153 ])
```

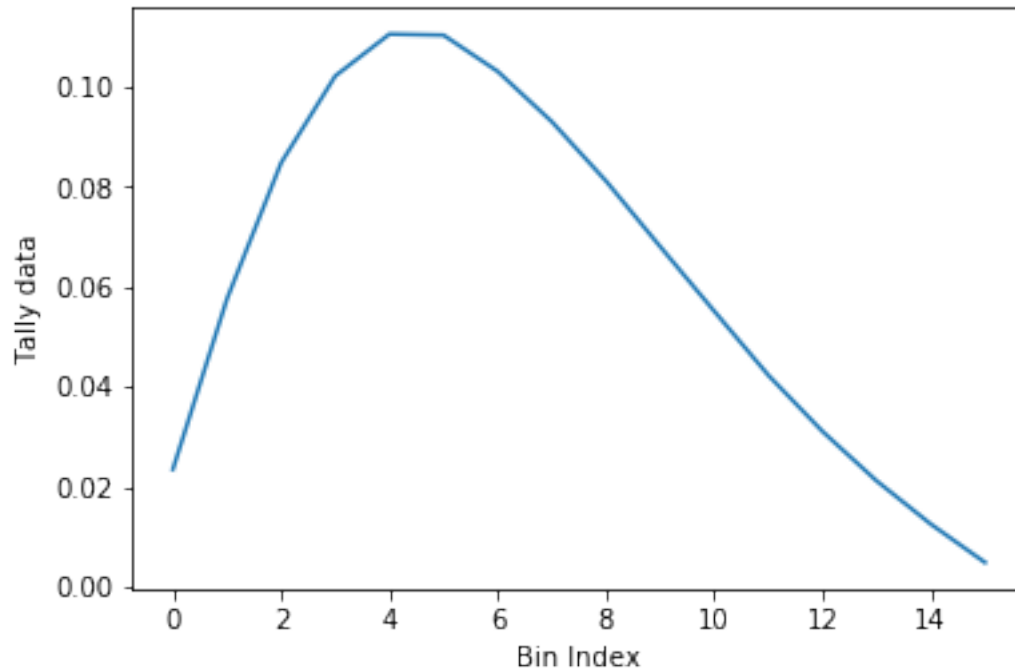
4.3.3 Plotting Routines

Each *Detector* object is capable of simple 1D and 2D plotting routines. The simplest 1D plot method is simply `plot()`, however a wide range of plot options are supported. Below are keyword arguments that can be used to format the plots.

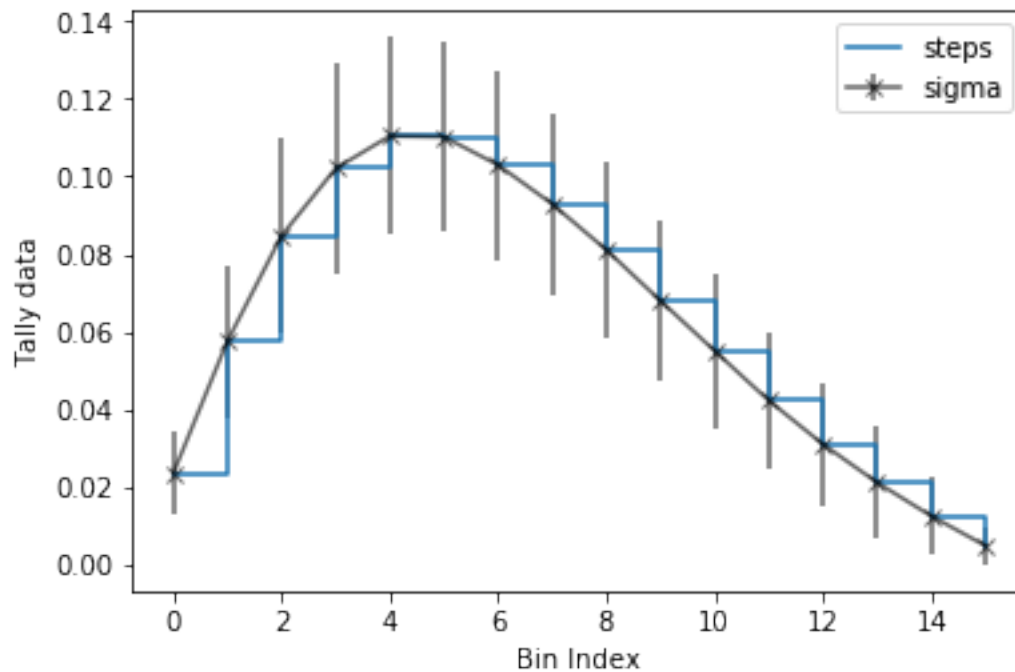
option	description
what	what data to plot
ax	preprepared figure on which to add this plot
xdim	quantity from indexes to use as x-axis
sigma	confidence interval to place on errors - 1d
steps	draw tally values as constant inside bin - 1d
xlabel	label to apply to x-axis
ylabel	label to apply to y-axis
loglog	use a log scaling on both of the axes
logx	use a log scaling on the x-axis
logy	use a log scaling on the y-axis
legend	place a legend on the figure
ncol	number of columns to apply to the legend

The plot routine also accepts various options, which can be found in the [matplotlib.pyplot.plot](#) documentation

```
>>> nodeFlx.plot()
```

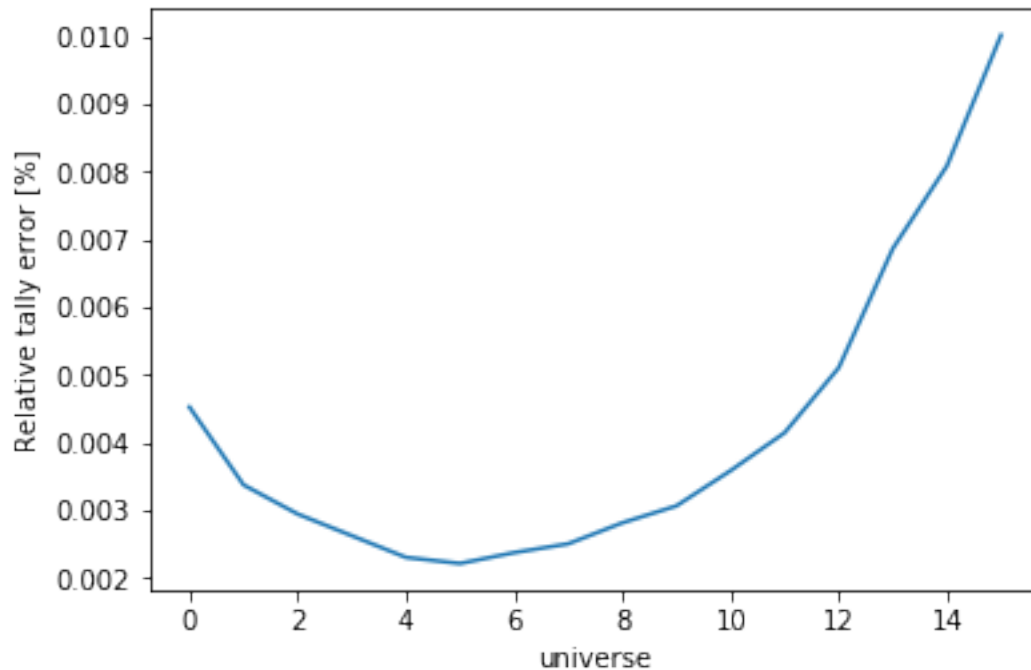


```
>>> ax = nodeFlx.plot(steps=True, label='steps')
>>> ax = nodeFlx.plot(sigma=100, ax=ax, c='k', alpha=0.6,
...                   marker='x', label='sigma')
```



Passing `what='errors'` to the plot method plots the associated relative errors, rather than the tally data on the y-axis. Similarly, passing a key from *indexes* as the `xdim` argument sets the x-axis to be that specific index.

```
>>> nodeFlx.plot(xdim='universe', what='errors',
...              ylabel='Relative tally error [%]')
```



Mesh Plots

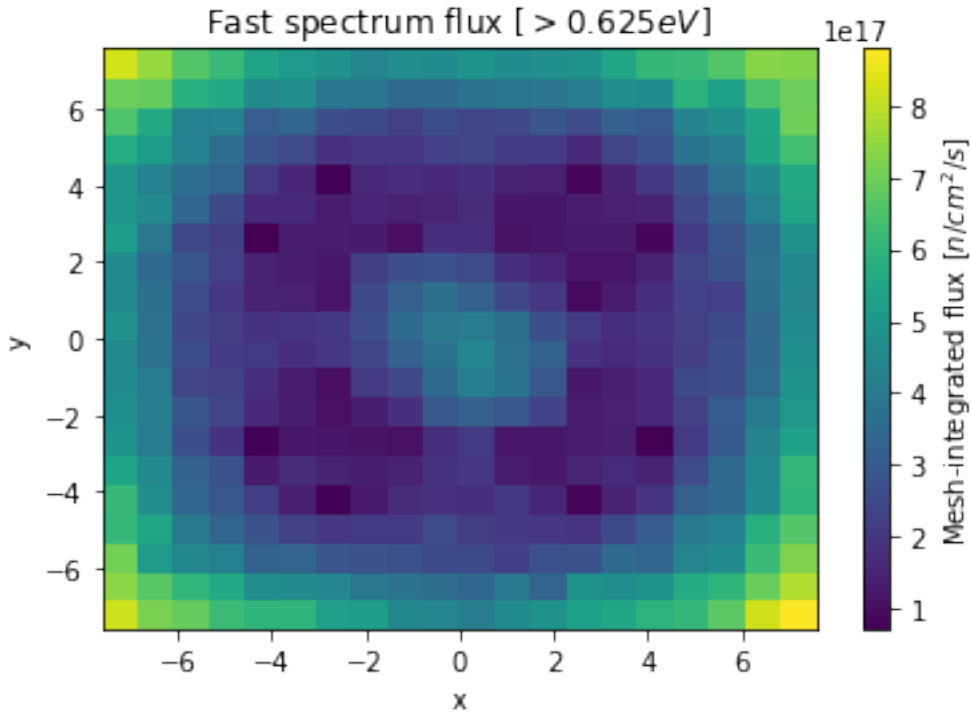
For data with dimensionality greater than one, the `meshPlot()` method can be used to plot some 2D slice of the data on a Cartesian grid. Passing a dictionary as the `fixed` argument restricts the tally data down to two dimensions. The X and Y axis can be quantities from *grids* or *indexes*. If the quantity to be used for an axis is in the *grids* dictionary, then the appropriate spatial or energetic grid from the detector file will be used. Otherwise, the axis will reflect changes in a specific bin type. The following keyword arguments can be used in conjunction with the above options to format the mesh plots.

Option	Action
<code>cmap</code>	Colormap to apply to the figure
<code>cbarLabel</code>	Label to apply to the colorbar
<code>logColor</code>	If true, use a logarithmic scale for the colormap
<code>normalizer</code>	Apply a custom non-linear normalizer to the colormap

The `cmap` argument must be something that `matplotlib` can understand as a valid colormap. This can be a string of any of the colormaps supported by *matplotlib*.

Since the `xymesh` detector is three dimensions, (energy, x, and y), we must pick an energy group to plot.

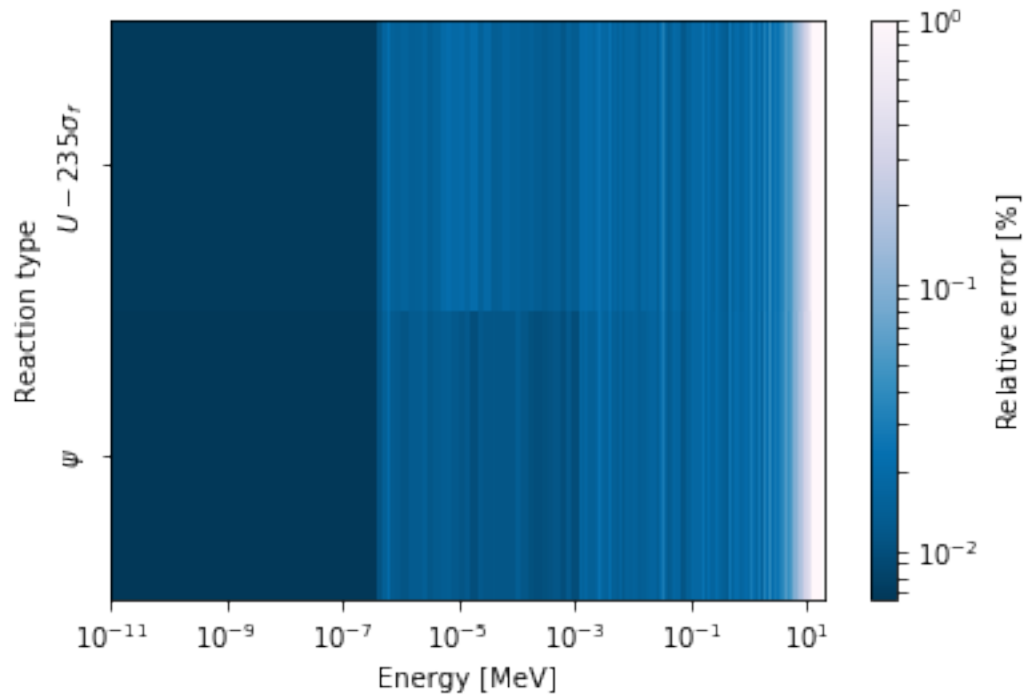
```
>>> xy.meshPlot('x', 'y', fixed={'energy': 0},
...            cbarLabel='Mesh-integrated flux [n/cm^2/s]',
...            title="Fast spectrum flux [>0.625 eV]");
```



The `meshPlot()` also supports a range of labeling and plot options. Here, we attempt to plot the flux and U-235 fission reaction rate errors as a function of energy, with the two reaction rates separated on the y-axis. Passing `logColor=True` applies a logarithmic color scale to all the positive data. Data that is zero is not shown, and errors will be raised if the data contain negative quantities.

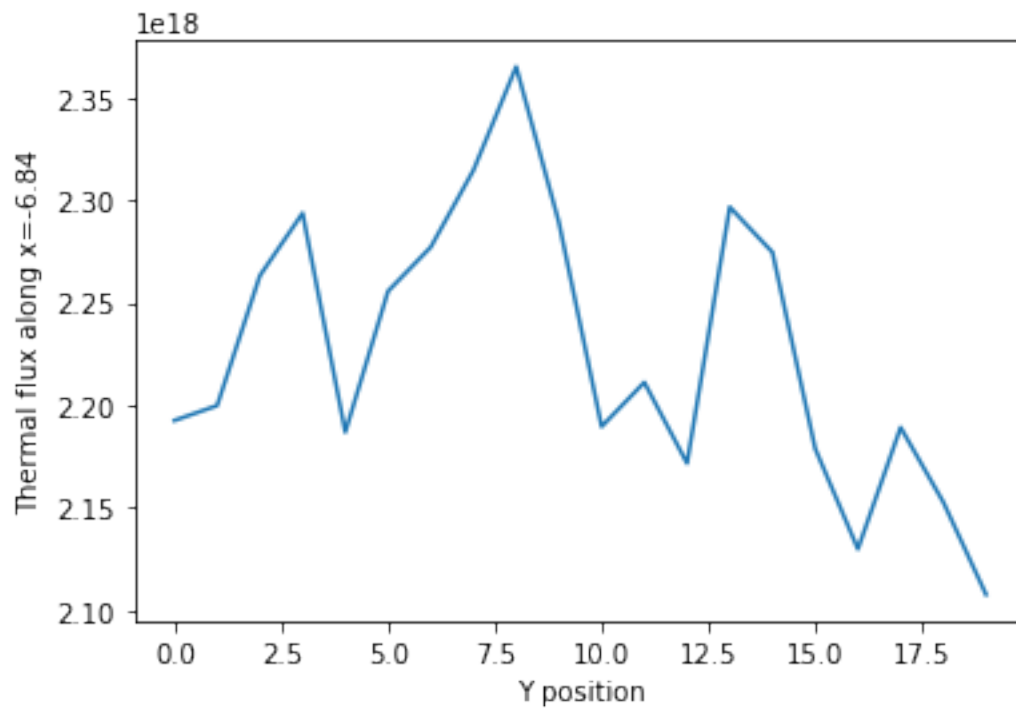
Here we also apply custom y-tick labels to reflect the reaction that is being plotted.

```
>>> ax = spectrum.meshPlot('e', 'reaction', what='errors',
...                        ylabel='Reaction type', cmap='PuBu_r',
...                        cbarLabel="Relative error ${\\%}$",
...                        xlabel='Energy [MeV]', logColor=True,
...                        logx=True);
>>> ax.set_yticks([0.5, 1.5]);
>>> ax.set_yticklabels([r'$\\psi$', r'$U-235 \\sigma_f$'], rotation=90,
>>>                      verticalalignment='center');
```



Using the slicing arguments allows access to the 1D plot methods from before

```
>>> xy.plot(fixed={'energy': 1, 'xmesh': 1},
...         xlabel='Y position',
...         ylabel='Thermal flux along x={}'
...         .format(xy.grids['X'][1, 0]));
```



Spectrum Plots

The `Detector` objects are also capable of energy spectrum plots, if an associated energy grid is given. The `normalize` option will normalize the data per unit lethargy. This plot takes some additional assumptions with the scaling and labeling, but all the same controls as the above line plots.

The `spectrumPlot()` method is designed to prepare plots of energy spectra. Supported arguments for the `spectrumPlot()` method include

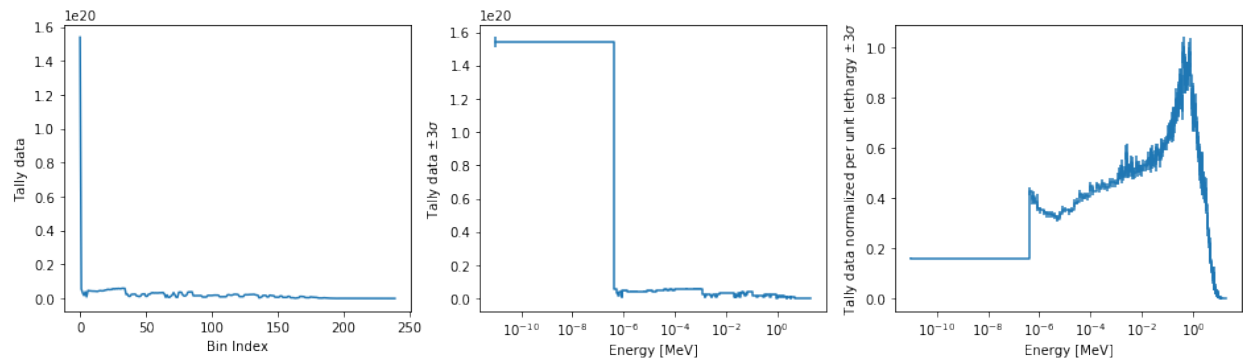
Option	Default	Description
<code>normalize</code>	<code>True</code>	Normalize tallies per unit lethargy
<code>fixed</code>	<code>None</code>	Dictionary that controls matrix reduction
<code>sigma</code>	<code>3</code>	Level of confidence for statistical errors
<code>xscale</code>	<code>'log'</code>	Set the x scale to be log or linear
<code>yscale</code>	<code>'linear'</code>	Set the y scale to be log or linear

The figure below demonstrates the default options and control in this `spectrumPlot()` routine by

1. Using the less than helpful plot routine with no formatting
2. Using `spectrumPlot()` without normalization to show default labels and scaling
3. Using `spectrumPlot()` with normalization

Since our detector has energy bins and reaction bins, we need to reduce down to one-dimension with the `fixed` command.

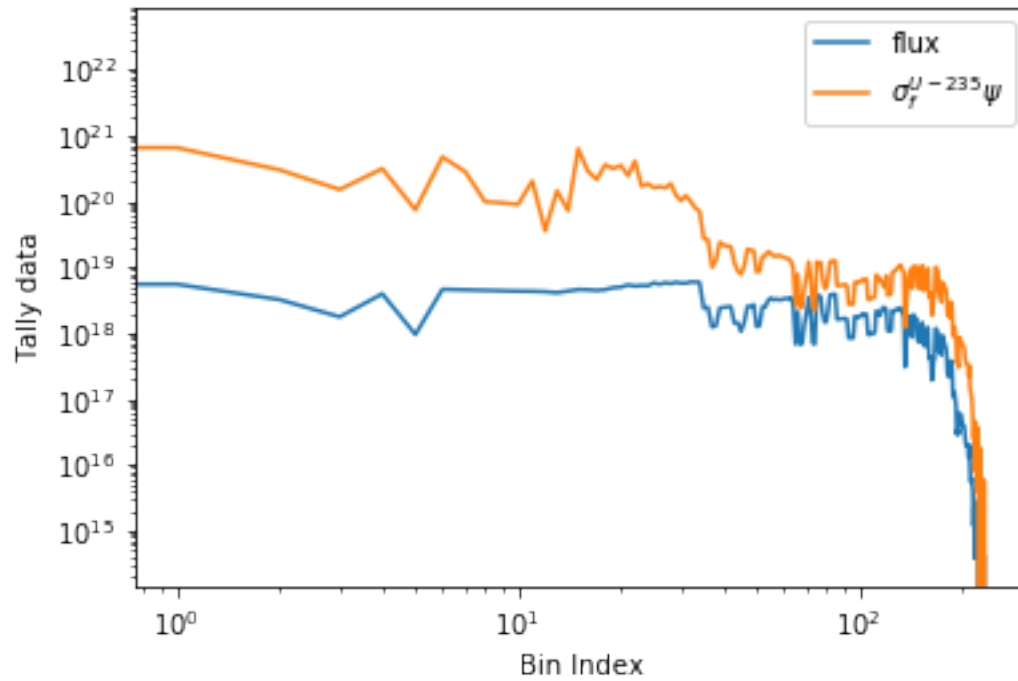
```
>>> fig, axes = pyplot.subplots(1, 3, figsize=(16, 4))
>>> fix = {'reaction': 0}
>>> spectrum.plot(fixed=fix, ax=axes[0]);
>>> spectrum.spectrumPlot(fixed=fix, ax=axes[1], normalize=False);
>>> spectrum.spectrumPlot(fixed=fix, ax=axes[2]);
```



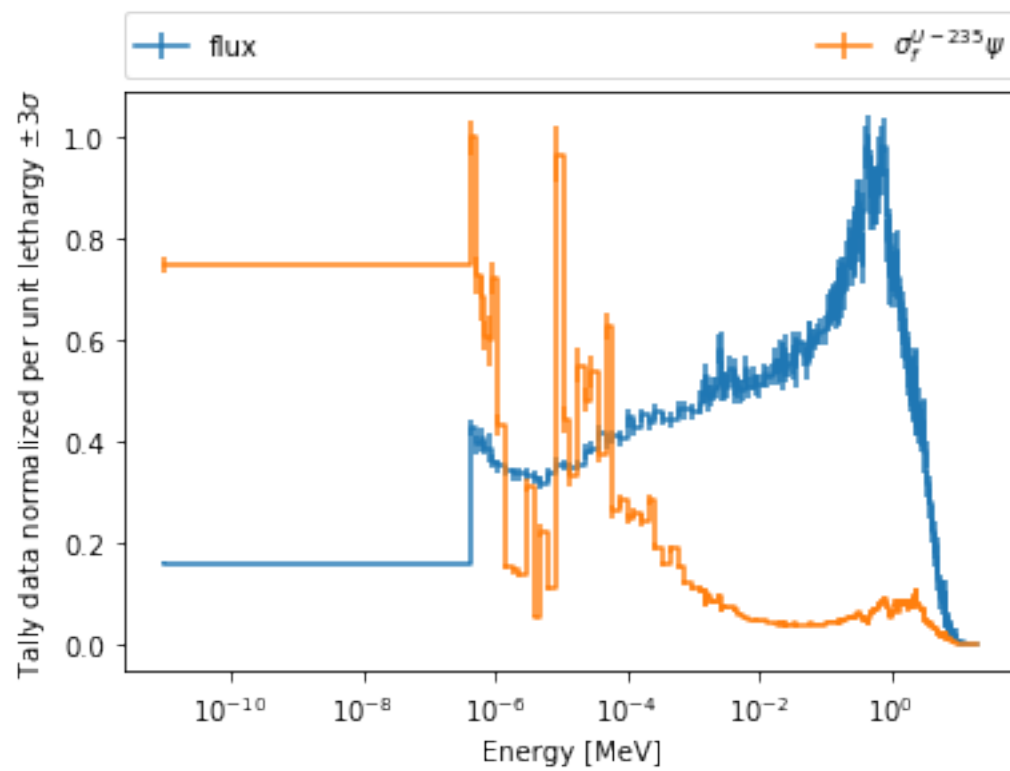
Multiple line plots

Plots can be made against multiple bins, such as spectrum in different materials or reactions, with the `plot()` and `spectrumPlot()` methods. Below is the flux spectrum and spectrum of the U-235 fission reaction rate from the same detector. The `labels` argument is what is used to label each individual plot in the order of the bin index.

```
>>> labels = (
...     'flux',
...     r'$\sigma_f^{U-235}\psi$') # render as mathtype
>>> spectrum.plot(labels=labels, loglog=True);
```



```
>>> spectrum.spectrumPlot(labels=labels, legend='above', ncol=2);
```



4.3.4 Hexagonal Detectors

SERPENT allows the creation of hexagonal detectors with the `dh` card, like:

```
det hex2 2 0.0 0.0 1 5 5 0.0 0.0 1
det hex3 3 0.0 0.0 1 5 5 0.0 0.0 1
```

which would create two hexagonal detectors with different orientations. Type 2 detectors have two faces perpendicular to the x-axis, while type 3 detectors have faces perpendicular to the y-axis. For more information, see the [dh card from SERPENT wiki](#).

`serpentTools` is capable of storing data tallies and grid structures from hexagonal detectors in `HexagonalDetector` objects.

```
>>> hexFile = 'hexplot_det0.m'
>>> hexR = serpentTools.readDataFile(hexFile)
>>> hexR.detectors
{'hex2': <serpentTools.HexagonalDetector at 0x7f1ad03d5da0>,
'hex3': <serpentTools.HexagonalDetector at 0x7f1ad03d5c88>}
```

Here, two `HexagonalDetector` objects are produced, with similar `tallies` and slicing methods as demonstrated above.

```
>>> hex2 = hexR.detectors['hex2']
>>> hex2.tallies
array([[0.185251, 0.184889, 0.189381, 0.184545, 0.195442],
       [0.181565, 0.186038, 0.193088, 0.195448, 0.195652],
       [0.1856 , 0.190278, 0.192013, 0.193353, 0.184309],
       [0.186249, 0.191939, 0.192513, 0.194196, 0.186953],
       [0.198196, 0.198623, 0.195612, 0.174804, 0.178053]])
>>> hex2.grids
{'COORD': array([[ -3.          , -1.732051 ],
                 [-2.5         , -0.8660254],
                 [-2.         ,  0.          ],
                 [-1.5         ,  0.8660254],
                 [-1.         ,  1.732051 ],
                 [-2.         , -1.732051 ],
                 [-1.5         , -0.8660254],
                 [-1.         ,  0.          ],
                 [-0.5         ,  0.8660254],
                 [ 0.          ,  1.732051 ],
                 [-1.         , -1.732051 ],
                 [-0.5         , -0.8660254],
                 [ 0.          ,  0.          ],
                 [ 0.5         ,  0.8660254],
                 [ 1.          ,  1.732051 ],
                 [ 0.          , -1.732051 ],
                 [ 0.5         , -0.8660254],
                 [ 1.          ,  0.          ],
                 [ 1.5         ,  0.8660254],
                 [ 2.          ,  1.732051 ],
                 [ 1.          , -1.732051 ],
                 [ 1.5         , -0.8660254],
                 [ 2.          ,  0.          ],
                 [ 2.5         ,  0.8660254],
                 [ 3.          ,  1.732051 ]]),
 'Z': array([[0., 0., 0.]])}
```

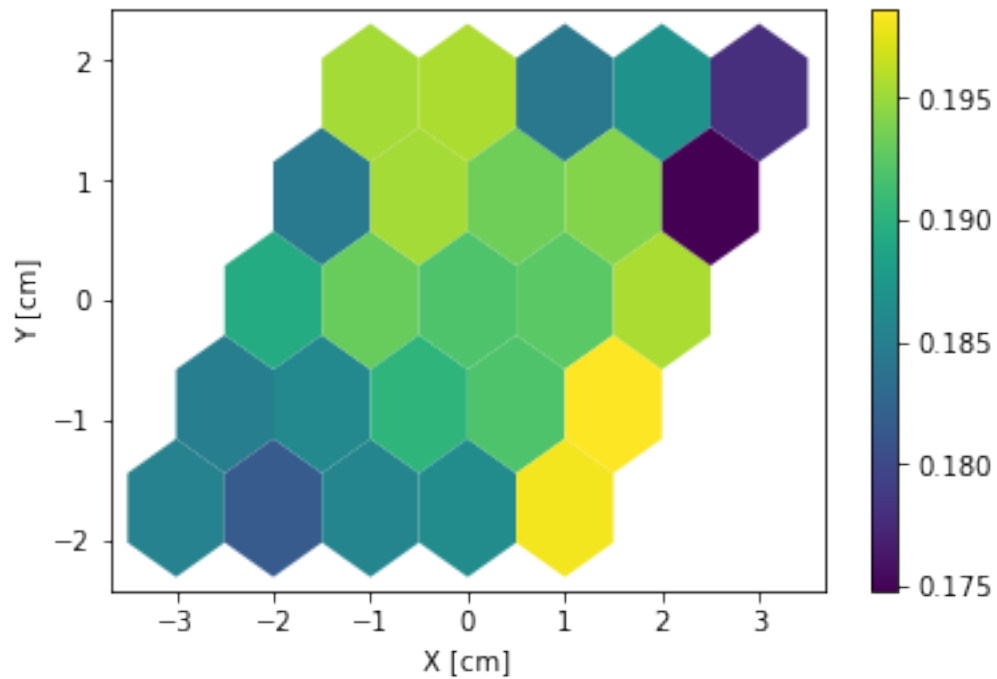
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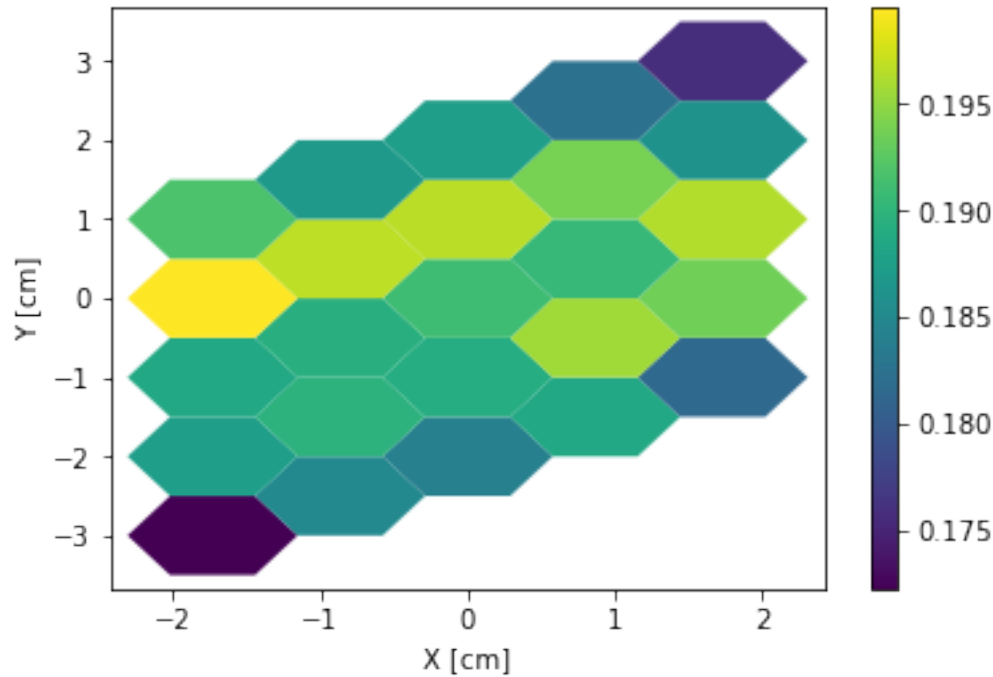
```
>>> hex2.indexes  
( 'ycoord', 'xcoord' )
```

Creating hexagonal mesh plots with these objects requires setting the *pitch* and *hexType* attributes.

```
>>> hex2.pitch = 1  
>>> hex2.hexType = 2  
>>> hex2.hexPlot();
```



```
>>> hex3 = hexR.detectors['hex3']  
>>> hex3.pitch = 1  
>>> hex3.hexType = 3  
>>> hex3.hexPlot();
```



The `thresh` argument can be used to create meshes only above a given value. This works for both Cartesian meshes and hexagonal meshes.

4.3.5 Limitations

`serpentTools` does support reading detector files with hexagonal, cylindrical, and spherical mesh structures. However, creating 2D mesh plots with cylindrical and spherical detectors, and utilizing their mesh structure, is not fully supported. [#169](#) is currently tracking progress for cylindrical plotting.

4.3.6 Conclusion

The `DetectorReader` is capable of reading and storing detector data from SERPENT detector files. The data is stored on custom `Detector` objects, capable of reshaping tally and error matrices into arrays with dimensionality reflecting the detector binning. These `Detector` objects have simple methods for retrieving and plotting detector data.

4.3.7 References

1. [matplotlib plot](#)
2. [Custom colormap normalization](#)
3. [matplotlib 2.0 colormaps](#)

4.4 Depletion Reader

4.4.1 Basic Operation

SERPENT produces a [burned material file](#), containing the evolution of material properties through burnup for all burned materials present in the problem. The [DepletionReader](#) is capable of reading this file, and storing the data inside [DepletedMaterial](#) objects. Each such object has methods and attributes that should ease analysis.

```
>>> import serpentTools
>>> from serpentTools.settings import rc
```

Note: The preferred way to read your own output files is with the `read()` function. The `readDataFile()` function is used here to make it easier to reproduce the examples

```
>>> depFile = 'demo_dep.m'
>>> dep = serpentTools.readDataFile(depFile)
```

The materials read in from the file are stored in the [materials](#) dictionary, where the keys represent the name of specific materials, and the corresponding values are the depleted material.

```
>>> dep.materials
{'fuel0': <serpentTools.objects.materials.DepletedMaterial at 0x7f8f8dccde80>,
 'bglass0': <serpentTools.objects.materials.DepletedMaterial at 0x7f8f8f42f518>,
 'total': <serpentTools.objects.materials.DepletedMaterial at 0x7f8f8dce7940>}
```

Metadata, such as the isotopic vector and depletion schedule are also present on the reader

```
>>> dep.names
['Xe135', 'I135', 'U234', 'U235', 'U236', 'U238', 'Pu238',
 'Pu239', 'Pu240', 'Pu241', 'Pu242', 'Np237', 'Am241', 'Am243',
 'Cm243', 'Cm244', 'Cm245', 'Cs133', 'Nd143', 'Sm147', 'Sm149',
 'Sm150', 'Sm151', 'Sm152', 'Eu153', 'Gd155', 'Mo95', 'Tc99',
 'Ru101', 'Rh103', 'Ag109', 'Cd113', 'lost', 'total']
>>> dep.burnup
array([0. , 0.02, 0.04, 0.06, 0.08, 0.1 , 0.12, 0.14, 0.16, 0.18, 0.2 ,
        0.22, 0.24, 0.26, 0.28, 0.3 , 0.32, 0.34, 0.36, 0.38, 0.4 , 0.42,
        0.44, 0.46, 0.48, 0.5 , 0.52, 0.54, 0.56, 0.58, 0.6 , 0.62, 0.64,
        0.66, 0.68, 0.7 , 0.72, 0.74, 0.76, 0.78, 0.8 , 0.82, 0.84, 0.86,
        0.88, 0.9 , 0.92, 0.94, 0.96, 0.98, 1. , 1.02, 1.04, 1.06, 1.08,
        1.1 , 1.12, 1.14, 1.16, 1.18, 1.2 , 1.22, 1.24, 1.26, 1.28, 1.3 ,
        1.32, 1.34, 1.36, 1.38, 1.4 , 1.42])
>>> dep.zaiss
[541350, 531350, 922340, 922350, 922360, 922380, 942380,
 942390, 942400, 942410, 942420, 932370, 952410, 952430,
 962430, 962440, 962450, 551330, 601430, 621470, 621490,
 621500, 621510, 621520, 631530, 641550, 420950, 430990,
 441010, 451030, 471090, 481130, 666, 0]
```

4.4.2 Depleted Material Objects

As mentioned before, all the material data is stored inside these *DepletedMaterial* objects. These objects share access to the metadata of the reader as well.

```
>>> fuel = dep.materials['fuel0']
>>> fuel.burnup
array([[0.          0.00702676 0.0144405  0.0218803  0.0297245  0.0370823
        0.0447201  0.0513465  0.0590267  0.0671439  0.073392  0.0802637
        0.0887954  0.0974604  0.104807  0.111528  0.119688  0.128006
        0.135704  0.143491  0.150545  0.157608  0.165391  0.172872
        0.180039  0.188011  0.195215  0.202291  0.20963  0.216895
        0.224651  0.232139  0.23904  0.246076  0.25422  0.262011
        0.269681  0.276981  0.284588  0.291835  0.299661  0.30727
        0.314781  0.322364  0.329404  0.336926  0.34438  0.352246
        0.360913  0.367336  0.37415  0.381556  0.388951  0.396286
        0.404159  0.412113  0.419194  0.426587  0.43425  0.442316
        0.449562  0.456538  0.465128  0.472592  0.479882  0.487348
        0.494634  0.502167  0.508326  0.515086  0.522826  0.530643]])
>>> fuel.days is dep.days
True
```

Materials can also be obtained by indexing directly into the reader, with

```
>>> dep["fuel0"] is dep.materials["fuel0"] is dep.get("fuel0")
True
```

All of the variables present in the depletion file for this material are present, stored in the *data* dictionary. A few properties commonly used are accessible as attributes as well.

```
>>> fuel.data.keys()
dict_keys(['volume', 'burnup', 'adens', 'mdens', 'a', 'h', 'sf', 'gsrc', 'ingTox',
↳ 'inhTox'])
>>> print(fuel.adens)
[[0.00000e+00 2.43591e-09 4.03796e-09 ... 4.70133e-09 4.70023e-09
 4.88855e-09]
 [0.00000e+00 6.06880e-09 8.11783e-09 ... 8.05991e-09 8.96359e-09
 9.28554e-09]
 [4.48538e-06 4.48486e-06 4.48432e-06 ... 4.44726e-06 4.44668e-06
 4.44611e-06]
 ...
 [0.00000e+00 3.03589e-11 7.38022e-11 ... 1.62829e-09 1.63566e-09
 1.64477e-09]
 [0.00000e+00 1.15541e-14 2.38378e-14 ... 8.60736e-13 8.73669e-13
 8.86782e-13]
 [6.88332e-02 6.88334e-02 6.88336e-02 ... 6.88455e-02 6.88457e-02
 6.88459e-02]]
>>> print(fuel.adens is fuel.data['adens'])
True
```

Similar to the original file, the rows of the matrix correspond to positions in the isotopic vector, and the columns correspond to positions in burnup/day vectors.

```
>>> fuel.mdens.shape # rows, columns
(34, 72)
>>> fuel.burnup.shape
(72,)
```

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```
>>> len(fuel.names)
34
```

4.4.3 Data Retrieval

At the heart of the *DepletedMaterial* is the *getValues()* method. This method acts as an slicing mechanism that returns data for a select number of isotopes at select points in time. *getValues()* requires two arguments for the units of time requested, e.g. days or burnup, and the name of the data requested. This second value must be a key in the *data* dictionary.

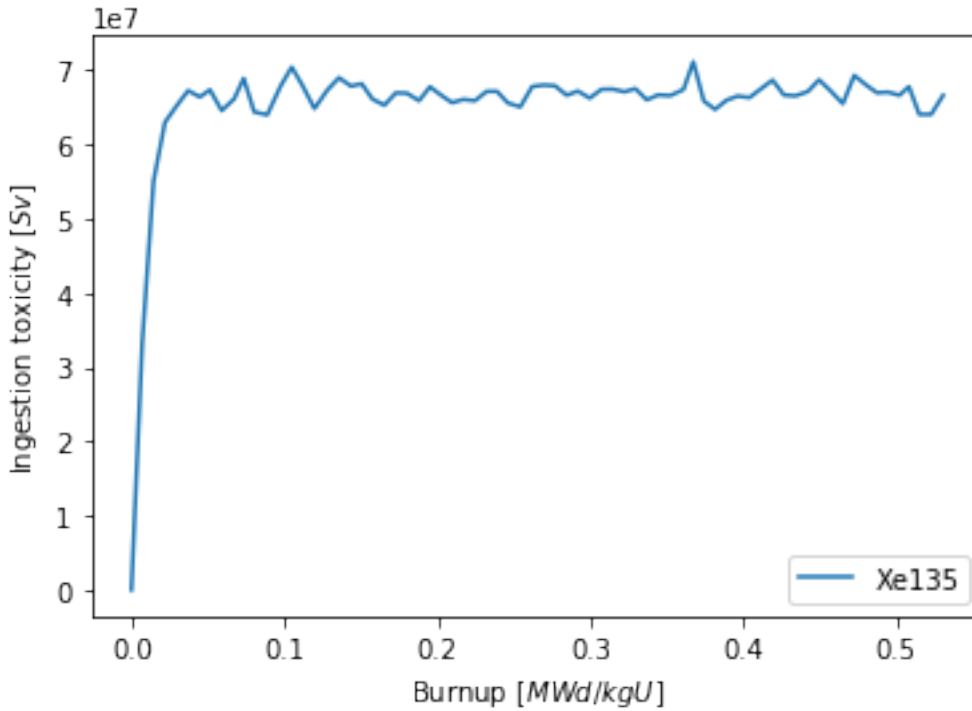
Specific days or values of burnup can be passed with the *timePoints* keyword. This will instruct the slicing tool to retrieve data that corresponds to values of days or burnup in the *timePoints* list. By default the method returns data for every time point on the material unless *timePoints* is given. Similarly, one can pass a string or list of strings as the *names* or *zai* arguments and obtain data for those specific isotopes. Data for every isotope is given if *names* or *zai* are not given.

```
>>> dayPoints = [0, 5, 10, 30]
>>> iso = ['Xe135', 'Sm149']
>>> zai = [541350, 621490]
>>> isoVals = fuel.getValues('days', 'a', dayPoints, iso)
>>> print(isoVals.shape)
>>> zaiVals = fuel.getValues('days', 'a', dayPoints, zai=zai)
print(isoVals - zaiVals)
(2, 4)
[[0.00000e+00 3.28067e+14 3.24606e+14 3.27144e+14]
 [0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00]]
[[ 0.  0.  0.  0.]
 [ 0.  0.  0.  0.]
```

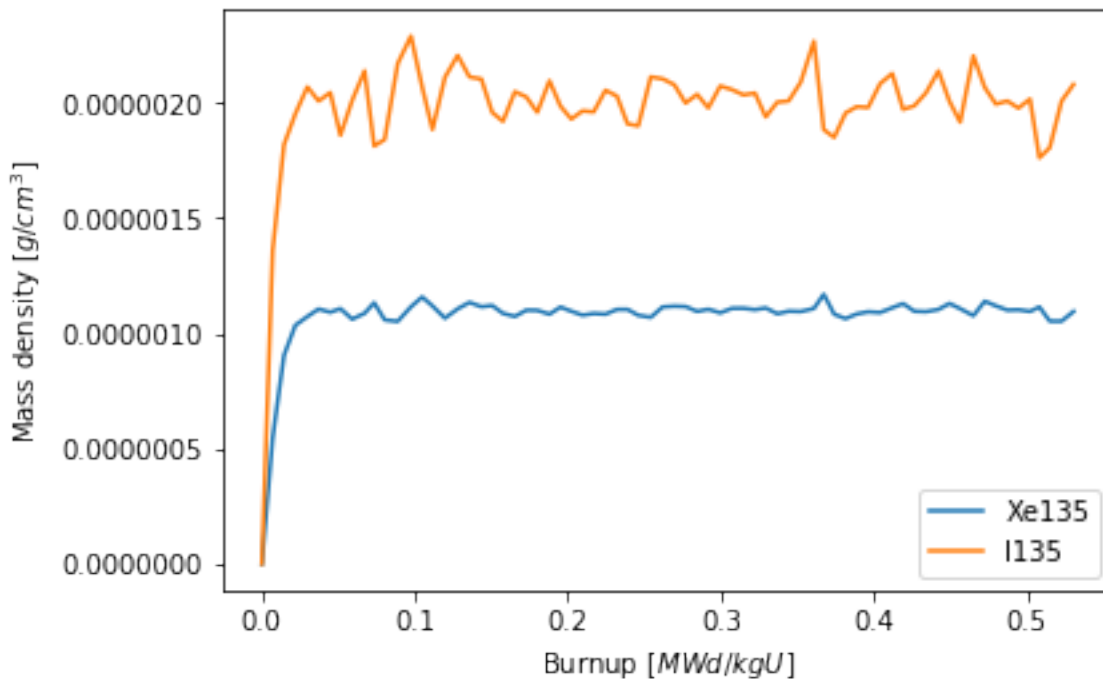
The *DepletedMaterial* uses this slicing for the built-in *plot()* method, which takes similar slicing arguments to *getValues()*.

By default, the plot method will plot data for all isotopes present, leading to very busy plots. The plots can be cleaned up by passing isotope names or ZZAAAI identifiers to the *names* or *zai* arguments, respectively.

```
>>> fuel.plot('burnup', 'ingTox', names='Xe135');
```

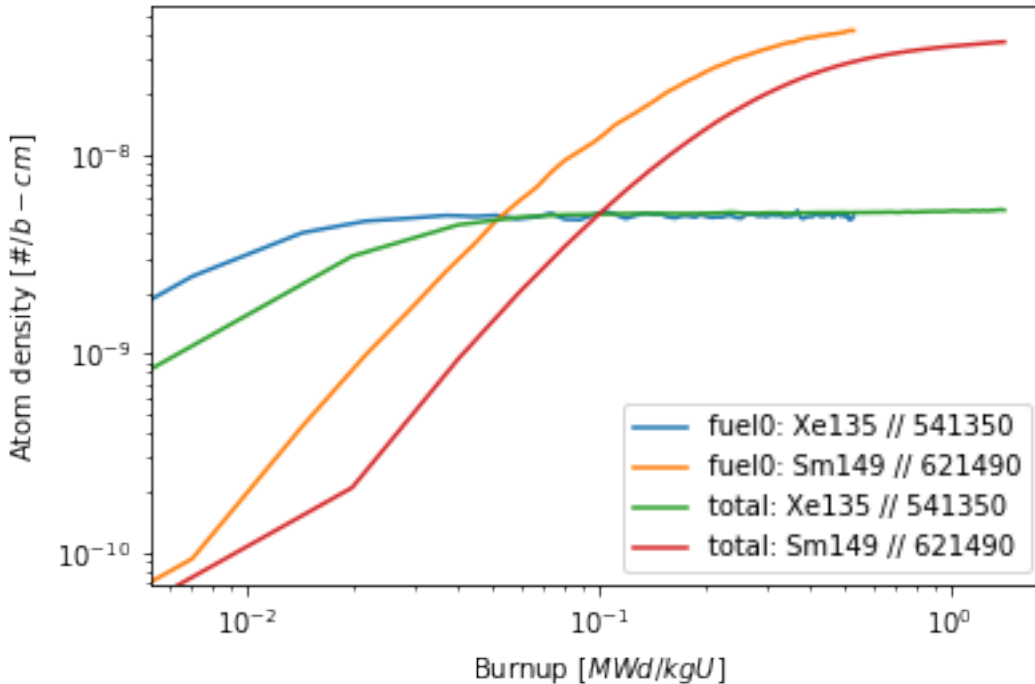
```
>>> fuel.plot('burnup', 'mdens', zai=[541350, 531350]);
```



This type of plotting can also be applied to the *DepletedMaterial* level, with similar options for formatting and retrieving data. The materials to be plotted can be filtered using the `materials` argument. The `labelFmt` argument can be used to apply a consistent label to each unique plot. This argument supports *brace-delimited formatting*, and will automatically replace strings like `{mat}` with the name of the material. The table below contains the special strings and their replacements

String	Replacement
{mat}	Name of the material
{iso}	Name of the isotope, e.g. 'U235'
{zai}	ZZAAAI of the isotope, e.g. 922350

```
>>> dep.plot('burnup', 'adens', names=iso,
...          materials=['fuel0', 'total'],
...          labelFmt="{mat}: {iso} // {zai}", loglog=True);
```



4.4.4 Settings

The *DepletionReader* also has a collection of settings to control what data is stored. If none of these settings are modified, the default is to store all the data from the output file. The settings that control the depletion reader are

- *depletion.materials*
- *depletion.materialVariables*
- *depletion.metadataKeys*
- *depletion.processTotal*

Below is an example of configuring a *DepletionReader* that only stores the burnup days, and atomic density for all materials that begin with bglass followed by at least one integer.

```
>>> rc['depletion.processTotal'] = False
>>> rc['depletion.metadataKeys'] = ['BU']
>>> rc['depletion.materialVariables'] = ['ADENS']
>>> rc['depletion.materials'] = [r'bglass\d+']
>>> bgReader = serpentTools.readDataFile(depFile)
```

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```
>>> bgReader.materials.keys()
dict_keys(['bglass0'])
>>> bglass = bgReader.materials['bglass0']
>>> bglass.data.keys()
dict_keys(['adens'])
```

4.4.5 Integration with pandas

If you have the `pandas` package installed, you can use the `toDataFrame()` method to create tabulated data. The method will retrieve data for all isotopes unless the `names` or `zai` arguments are provided. For compactness, only a few isotopes will be retrieved here.

```
>>> fuel.toDataFrame("adens", names=["U235", "Pu239", "Xe135"]).head()
Isotopes U235 Pu239 Xe135
Time [d]
0.0 0.000558 0.000000e+00 0.000000e+00
0.5 0.000558 6.374580e-09 2.435910e-09
1.0 0.000558 2.590310e-08 4.037960e-09
1.5 0.000558 5.728820e-08 4.620920e-09
2.0 0.000557 9.927160e-08 4.789480e-09
```

Arguments can also be used to control the time values in the index and column structure:

```
>>> fuel.toDataFrame("adens", zai=[922350, 942390, 541350], time="burnup")
Isotope ZAI 922350 942390 541350
Burnup [MWd/kgU]
0.0 0.000558 0.000000e+00 0.000000e+00
0.5 0.000558 6.374580e-09 2.435910e-09
1.0 0.000558 2.590310e-08 4.037960e-09
1.5 0.000558 5.728820e-08 4.620920e-09
2.0 0.000557 9.927160e-08 4.789480e-09
```

4.4.6 Conclusion

The `DepletionReader` is capable of reading and storing all the data from the SERPENT burned materials file. Upon reading, the reader creates custom `DepletedMaterial` objects that are responsible for storing and retrieving the data. These objects also have a handy `plot()` method for quick analysis. Use of the `rc` settings control object allows increased control over the data selected from the output file.

4.4.7 References

1. J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, and T. Kaltiaisenaho. "The Serpent Monte Carlo code: Status, development and applications in 2013." *Ann. Nucl. Energy*, **82** (2015) 142-150

4.5 Sensitivity Reader

As of SERPENT 2.1.29, the ability to compute sensitivities using Generalized Perturbation Theory [gpt]. An overview of the functionality, and how to enable these features is included on the [SERPENT wiki - Sensitivity Calculations](#). Sensitivity calculations produce `_sens.m` or `_sensN.m` files, depending on the version of SERPENT, and contain a collection of arrays and indexes, denoting the sensitivity of a quantity to perturbations in isotopic parameters, such as cross sections or fission spectrum. These perturbations can be applied to specific materials and/or isotopes.

The `SensitivityReader` is capable of reading this file and storing all the arrays and perturbation parameters contained therein. A basic plot method is also contained on the reader. .. note:

The preferred way to read your own output files **is with** the `|read-full|` function. The `|readData|` function **is** used here to make it easier to reproduce the examples

```
>>> import serpentTools
>>> sens = serpentTools.readDataFile('flattop_sens.m')
```

The arrays that are stored in `sensitivities` and `energyIntegratedSens` are stored under converted names. The original names from SERPENT are of the form `ADJ_PERT_KEFF_SENS` or `ADJ_PERT_KEFF_SENS_E_INT`, respectively. Since this reader stores the resulting arrays in unique locations, the names are converted to a succinct form. The two arrays listed above would be stored both as `keff` in `sensitivities` and `energyIntegratedSens`. All names are converted to `mixedCaseNames` to fit the style of the project.

These arrays are quite large, so only their shapes will be shown in this notebook.

```
>>> print(sens.sensitivities.keys(), sens.energyIntegratedSens.keys())
dict_keys(['keff']) dict_keys(['keff'])
>>> print(sens.sensitivities['keff'].shape)
(1, 2, 7, 175, 2)
>>> print(sens.energyIntegratedSens['keff'].shape)
(1, 2, 7, 2)
```

The energy grid structure and lethargy widths are stored on the reader, as `energies` and `lethargyWidths`.

```
>>> print(sens.energies.shape)
(176,)
>>> print(sens.energies[:10])
[1.00001e-11 1.00001e-07 4.13994e-07 5.31579e-07 6.82560e-07 8.76425e-07
 1.12300e-06 1.44000e-06 1.85539e-06 2.38237e-06]
>>> print(sens.lethargyWidths.shape)
(175,)
>>> print(sens.lethargyWidths[:10])
[9.21034 1.42067 0.25      0.249999 0.250001 0.247908 0.248639 0.253452
 0.250001 0.249999]
```

Ordered dictionaries `materials`, `zais`, and `perts` contain keys of the names of their respective data, and the corresponding index, `iSENS_ZAI_zzaaai`, in the sensitivity arrays. These arrays are zero-indexed, so the first item will have an index of zero. The data stored in the `sensitivities` and `energyIntegratedSens` dictionaries has the exact same structure as if the arrays were loaded into MATLAB/Octave, but with zero-indexing.

```
>>> print(sens.materials)
OrderedDict([('total', 0)])
>>> print(sens.zais)
OrderedDict([('total', 0), (922380, 1)])
```

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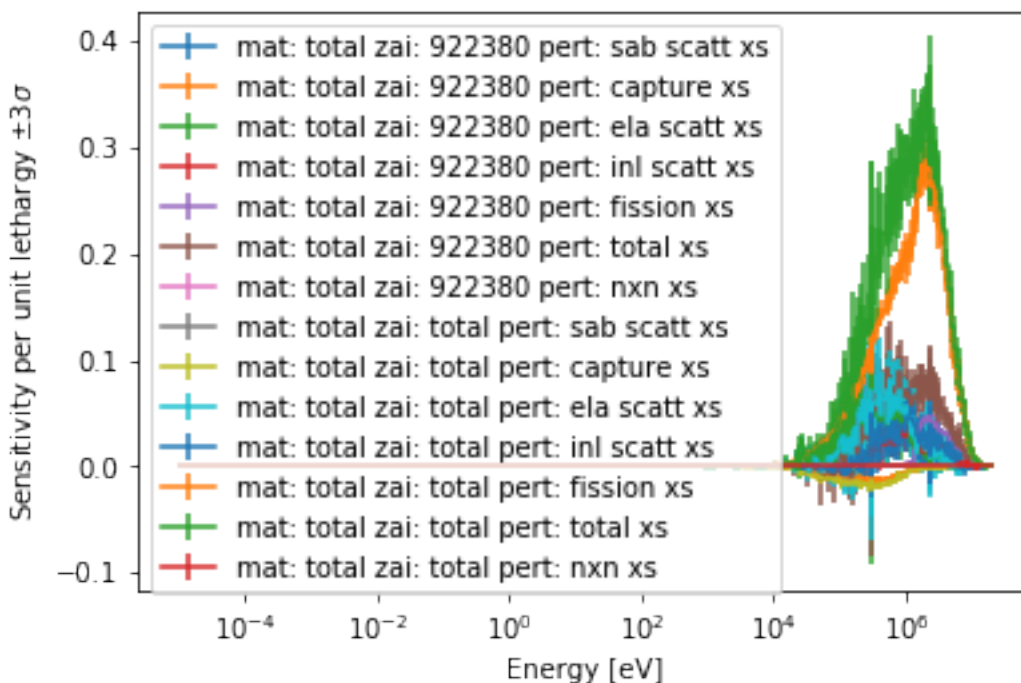
```
>>> print(sens.perts)
OrderedDict([('total xs', 0), ('ela scatt xs', 1), ('sab scatt xs', 2), ('inl
scatt xs', 3), ('capture xs', 4), ('fission xs', 5), ('nxn xs', 6)])
```

4.5.1 Plotting

The *SensitivityReader* has a `plot()` method for visualizing the sensitivities.

Note: Without additional arguments, other than the name of the array, the `plot()` method will plot **all** permutations of materials, isotopes, and isotope perturbations present. This can lead to a very busy plot and legend, so it is recommended that additional arguments are passed.

```
>>> sens.plot('keff');
```



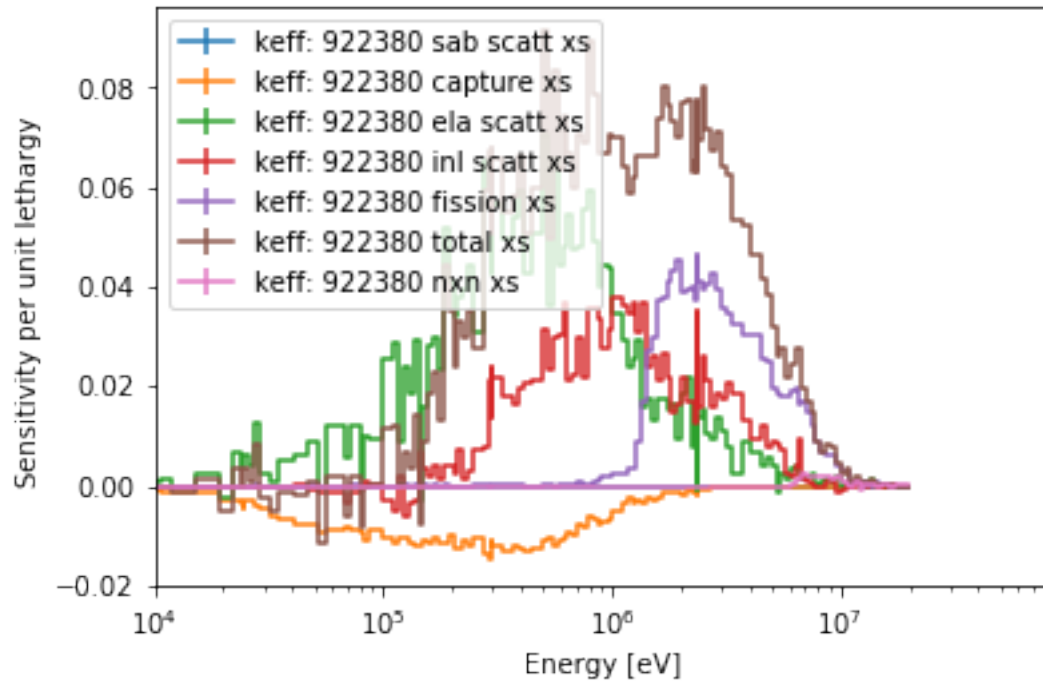
The following arguments can be used to filter the data present:

key	Action
'zai'	Isotopes(s) of interest
'pert'	Perturbation(s) of interest
'mat'	Material(s) of interest

The `sigma` argument can be used to adjust the confidence interval applied to the plot. The `labelFmt` argument can be used to modify the label used for each plot. The following replacements will be made:

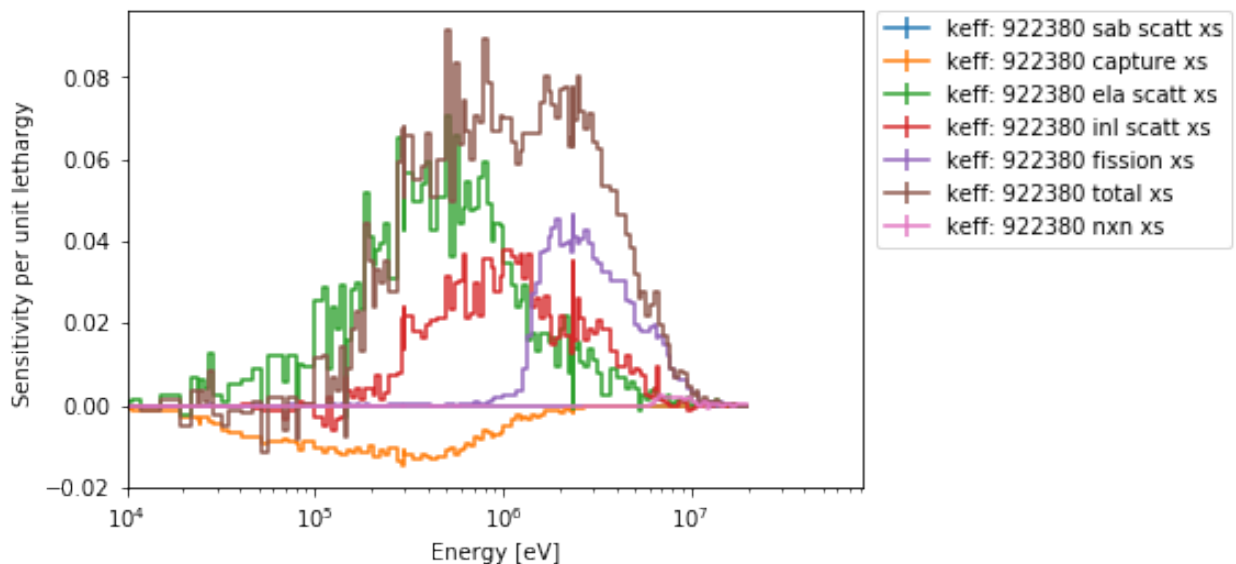
1. {r} - name of the response being plotted 1. {m} - name of the material 1. {z} - isotope zai 1. {p} - specific perturbation

```
>>> ax = sens.plot('keff', 922380, mat='total', sigma=0,
...               labelFmt="{r}: {z} {p}")
>>> ax.set_xlim(1E4); # set the lower limit to be closer to what we care about
```

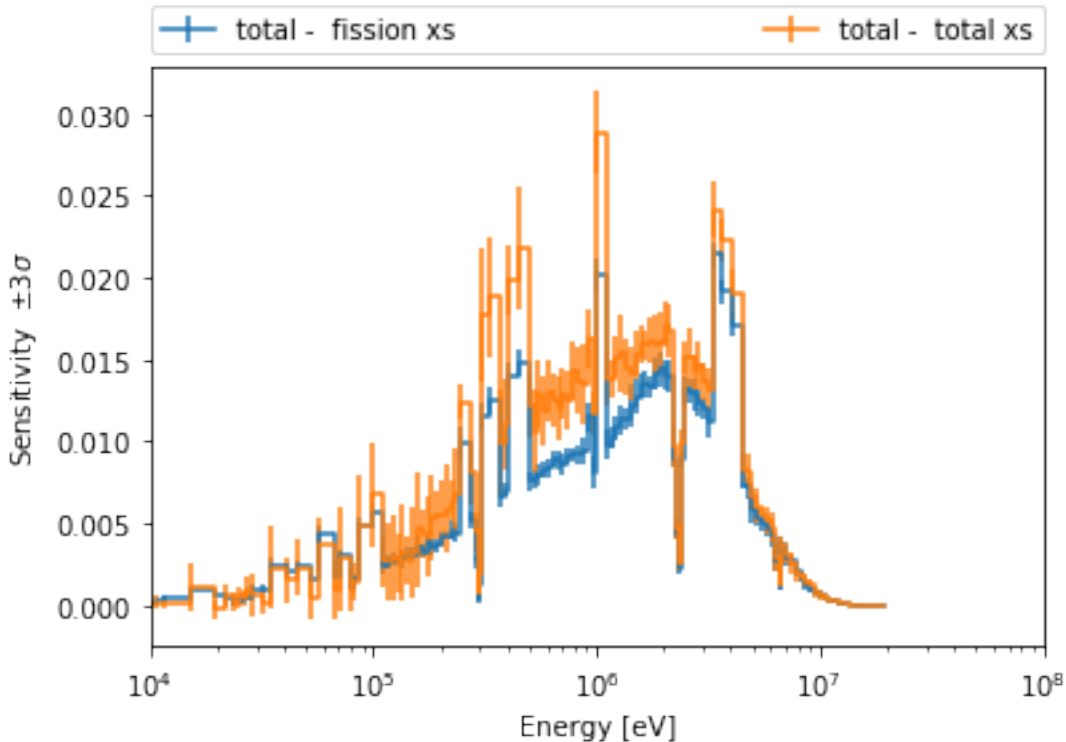


The argument `normalize` is used to turn on/off normalization per unit lethargy, while `legend` can be used to turn off the legend, or set the legend outside the plot.

```
>>> ax = sens.plot('keff', 922380, mat='total', sigma=0,
...               labelFmt="{r}: {z} {p}", legend='right')
>>> ax.set_xlim(1E4); # set the lower limit to be closer to what we care about
```



```
>>> sens.plot('keff', zai='total', pert=['total xs', 'fission xs'], labelFmt="{z} - {p}",
...           legend='above', ncol=2, normalize=False)
>>> pyplot.xlim(1E4, 1E8);
```



4.5.2 Conclusion

The *SensitivityReader* can quickly read sensitivity files, and stores all data present in the file. A versatile *plot()* method can be used to quickly visualize sensitivities.

4.6 Cross Section Reader/Plotter

4.6.1 Basic Operation

Firstly, to get started plotting some cross sections from Serpent, you generate a *yourInputFileName_xs.m* file using *set xsplot* as documented on the Serpent wiki. *serpentTools* can then read the output, figuring out its file type automatically as with other readers. Let's plot some data used in the *serpentTools* regression suite.

Note: The preferred way to read your own output files is with the *serpentTools.read()* function. The *serpentTools.readDataFile()* function is used here to make it easier to reproduce the examples

```
>>> import serpentTools
>>> xsreader = serpentTools.readDataFile('plut_xs0.m')
```

This file contains some cross sections from a Serpent case containing a chunk of plutonium metal reflected by beryllium. Let's see what cross sections are available from the file:

```
>>> xsreader.xsections.keys()
dict_keys(['i4009_03c', 'i7014_03c', 'i8016_03c', 'i94239_03c', 'mbe',
'mfissile'])
```

Notice that the important part of the reader is the `xsections` attribute, which contains a dictionary of named `XSDData` objects. Entries starting with “i” are isotopes, while “m” preceded names are materials. Notably, materials not appearing in the neutronics calculation, e.g., external tanks in Serpent continuous reprocessing calculations, are not printed in the `yourInputFileName_xs.m` file.

These `XSDData` instances can be obtained by indexing into the `xsections` dictionary or the reader

```
>>> xsreader.xsections["i4009_03c"] is xsreader["i4009_03c"]
True
```

The final bit of useful information stored on the reader are the energy groups and majorant cross sections. The energy groups are shared across all `XSDData` objects stored on the reader

```
>>> xsreader.energies
array([1.00000e-08, 1.03891e-07, 1.07934e-06, 1.12135e-05, 1.16498e-04,
       1.21032e-03, 1.25742e-02, 1.30635e-01, 1.35719e+00, 1.41000e+01])
>>> xsreader.majorant
array([78.4253 , 36.1666 , 2.54417 , 13.0654 , 4.27811 , 0.822536,
       0.781066, 0.598564, 0.34175 , 0.293887])
```

4.6.2 Data Access

Most of the useful information is stored on the `XSDData` instances. These are primarily cross sections provided by Serpent and some descriptive data. The `MT` and `MTdescrip` attributes describe the ordering of the reactions and their descriptions

```
>>> o16 = xsreader["i8016_03c"]
# Make a quick dictionary to show descriptions
>>> dict(zip(o16.MT, o16.MTdescrip))
{1: 'Total',
 101: 'Sum of absorption',
 2: 'elastic scattering',
 ...
 105: '(n,t)',
 23: '(n,n3alpha)',
 16: '(n,2n)'}
```

Cross section data are stored in the `xsdata` array, which has shape `(N_E, N_MT)`

```
>>> o16.xsdata.shape == (len(o16.energies), len(o16.MT))
True
```

The data can be obtained in a few different ways. First, you can index into the array directly

```
>>> o16.xsdata[:, 0]
array([4.16597, 3.88237, 3.85502, 3.8523 , 3.8518 , 3.84938, 3.82434,
       3.58676, 3.19656, 1.593  ])
```

This does require you to know the position of your reaction. Alternatively, you can index into the `XSDData` object using the reaction `MT` as a key


```
>>> o16[1]
array([4.16597, 3.88237, 3.85502, 3.8523 , 3.8518 , 3.84938, 3.82434,
       3.58676, 3.19656, 1.593  ])
```

The `tabulate` method can be used to create a `pandas.DataFrame` for nice tabular representation.

```
>>> xsreader.xsections['mfissile'].tabulate()
```

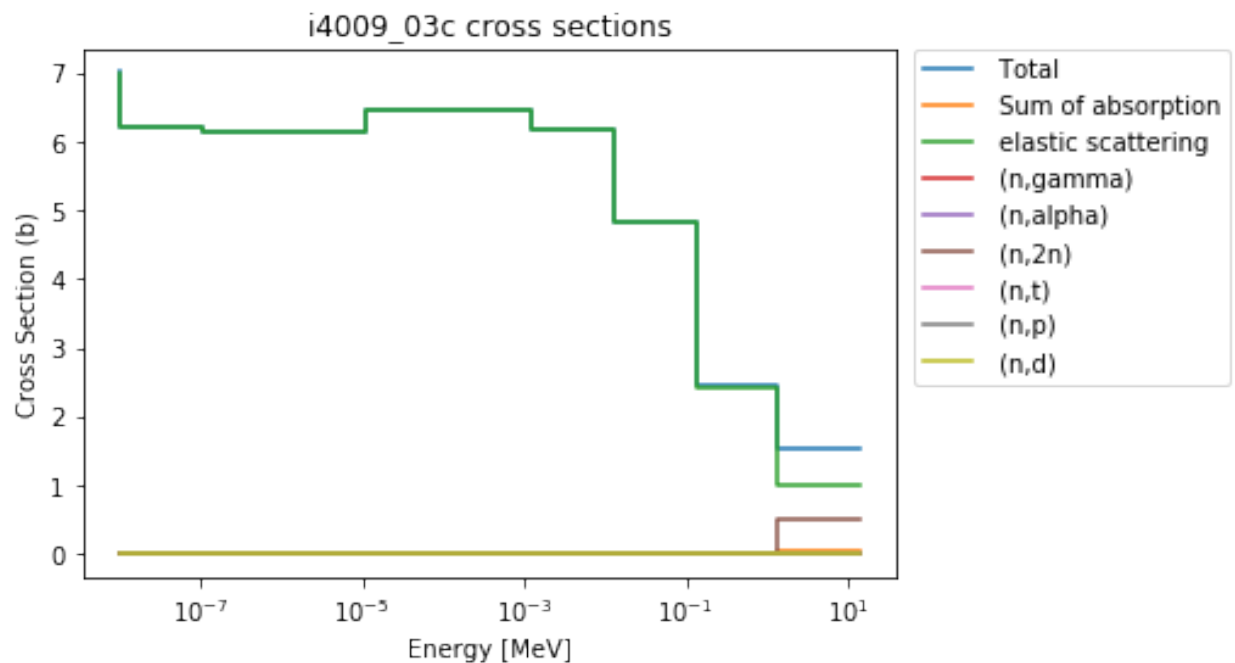
Lastly, the descriptions for each reaction can be found in `MTdescrip` or using `describe`

```
>>> o16.MTdescrip[0]
'Total'
>>> o16.describe(1)
'Total'
```

4.6.3 Plotting

Plotting reactions is provided through the `plot()` method. With no MTs provided, all reactions are plotted and labeled

```
>>> be9 = xsreader['i4009_03c']
>>> be9.plot(legend='right');
```



This is nice to have an automatically generated legend, but gets somewhat busy quickly. So, it's easy to check which MT numbers are available, and plot only a few:

```
>>> be9.showMT()
MT numbers available for i4009_03c:
-----
1      Total
101    Sum of absorption
```

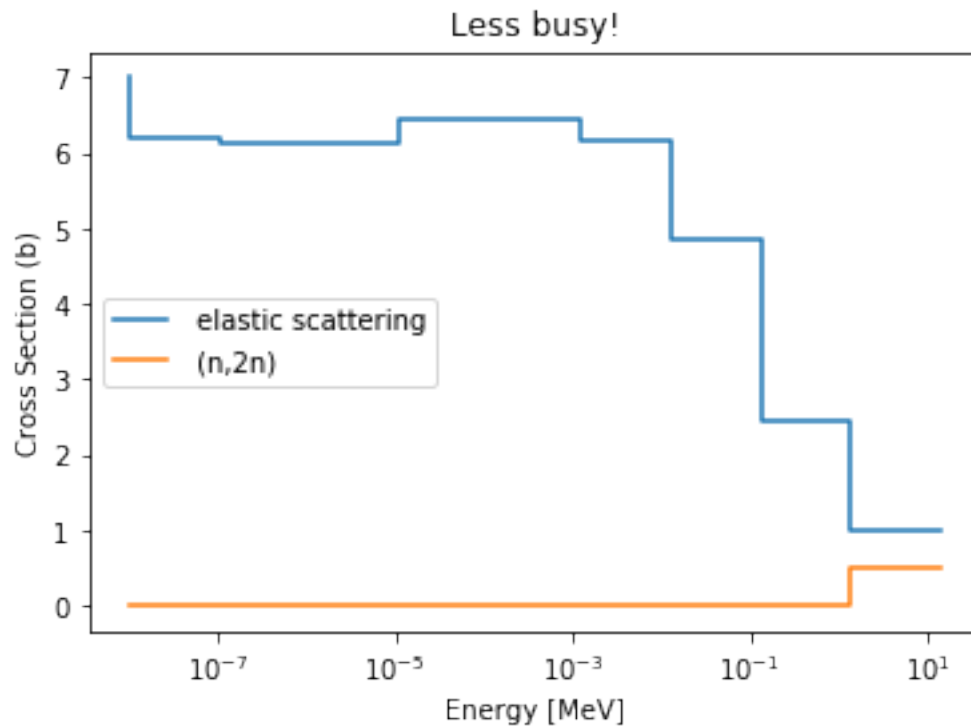
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```

2      elastic scattering
102    (n,gamma)
107    (n,alpha)
16     (n,2n)
105    (n,t)
103    (n,p)
104    (n,d)
>>> be9.plot(mts=[2, 16], title='Less busy!');

```



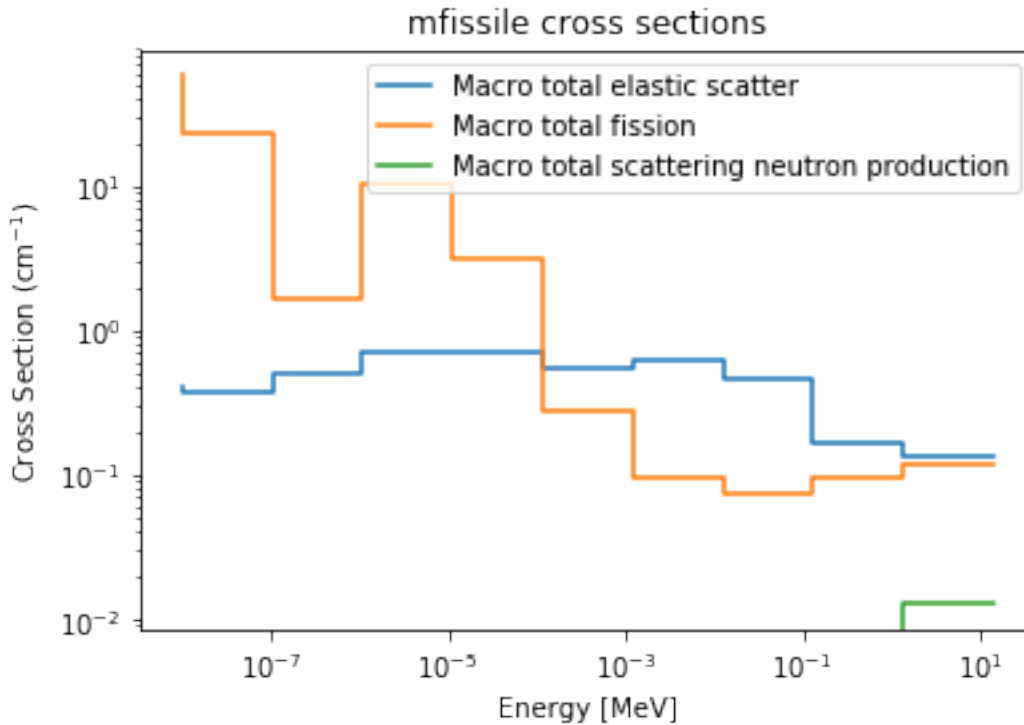
Of course, the same process can be applied to materials, but Serpent has some special unique negative MT numbers. The code will give you their meaning without requiring your reference back to the wiki.

```

>>> xsreader['mfissile'].showMT()
MT numbers available for mfissile:
-----
-1    Macro total
-3    Macro total elastic scatter
-2    Macro total capture
-6    Macro total fission
-7    Macro total fission neutron production
-16   Macro total scattering neutron production

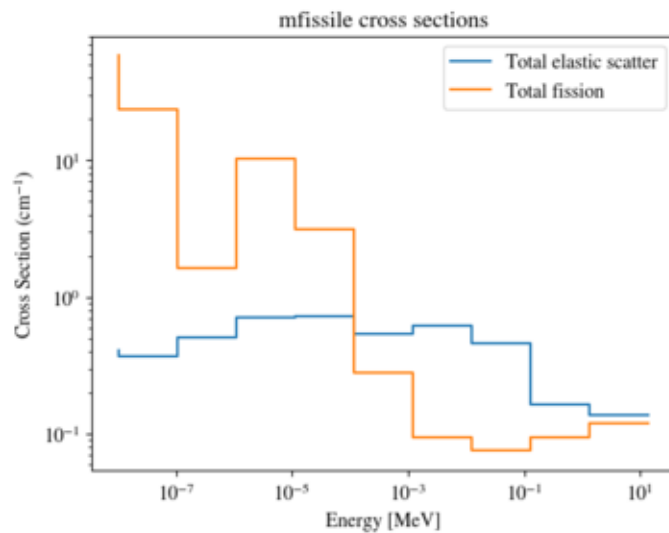
>>> xsreader['mfissile'].plot(mts=[-3, -6, -16], loglog=True)

```



Labels can be configured through the `labels` argument

```
>>> xsreader['mfissile'].plot(
...     mts=[-3, -6], loglog=True,
...     labels=["Total elastic scatter", "Total fission"])
```



4.6.4 Conclusions

serpentTools can plot your Serpent XS data in a friendly way. We're always looking to improve the feel of the code though, so let us know if there are changes you would like.

Keep in mind that setting an energy grid with closer to 10000 points makes far prettier XS plots however. There were none in this example to not clog up the repository.

4.7 Results Reader

4.7.1 Basic operations

This notebook demonstrates the capabilities of the serpentTools to read Serpent results files. SERPENT [serpent] produces a result file (i.e. `_res.m`), containing general results (e.g. `k-eff`), metadata (e.g. `title`) and homogenized cross-sections. The homogenized cross-section sets are printed in the results file for all the requested universes. The `ResultsReader` is capable of reading this file, and storing the data inside `HomogUniv` objects. Each such object has methods and attributes that should ease the analyses.

Note: The preferred way to read your own output files is with the `serpentTools.read()` function. The `serpentTools.readDataFile()` function is used here to make it easier to reproduce the examples

```
>>> import numpy as np
>>> import serpentTools
>>> from serpentTools.settings import rc

>>> resFile = 'InnerAssembly_res.m'
>>> res = serpentTools.readDataFile(resFile)
```

Metadata

`metadata` is a collective data that describes the problem. These are values that do not change over burnup and across homogenized universes. The following data is included: titles, data paths, and other descriptive data exist on the reader

```
>>> print(res.metadata['version'])
Serpent 2.1.30
>>> print(res.metadata['decayDataFilePath'])
/nv/hp22/dkotlyar6/data/Codes/DATA/endfb7/sss_endfb7.dec
>>> print(res.metadata['inputFileName'])
InnerAssembly
>>> res.metadata.keys()
dict_keys(['version', 'compileDate', 'debug', 'title', 'confidentialData',
'inputFileName', 'workingDirectory', 'hostname', 'cpuType', 'cpuMhz',
'startDate', 'completeDate', 'pop', 'cycles', 'skip', 'batchInterval',
'srcNormMode', 'seed', 'ufsMode', 'ufsOrder', 'neutronTransportMode',
'photonTransportMode', 'groupConstantGeneration', 'blCalculation',
'blBurnupCorrection', 'implicitReactionRates', 'optimizationMode',
'reconstructMicroxs', 'reconstructMacroxs', 'doubleIndexing', 'mgMajorantMode',
'spectrumCollapse', 'mpiTasks', 'ompThreads', 'mpiReproducibility',
'ompReproducibility', 'ompHistoryProfile', 'shareBufArray', 'shareRes2Array',
'xsDataFilePath', 'decayDataFilePath', 'sfyDataFilePath', 'nfyDataFilePath',
'braDataFilePath'])
```

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```
>>> res.metadata['startDate']
'Sat Apr 28 06:09:54 2018'
>>> res.metadata['pop'], res.metadata['skip'], res.metadata['cycles']
(5000, 10, 50)
```

Results Data

Results are stored as a function of time/burnup/index and include integral parameters of the system. Results, such as k-eff, total flux, and execution times are included in *resdata*. Some results include values and uncertainties (e.g. criticality) and some just the values (e.g. CPU resources).

```
>>> sorted(res.resdata.keys())[0:5]
['absKeff', 'absKinf', 'actinideActivity', 'actinideDecayHeat', 'actinideIngTox']
```

Values are presented in similar fashion as if they were read in to Matlab, with one exception. Serpent currently appends a new row for each burnup step, but also for each set of homogenized universe. This results in repetition of many quantities as Serpent loops over group constant data. The *ResultsReader* understands Serpent outputs and knows when to append “new” data to avoid repetition.

The structure of the data is otherwise identical to Matlab. For many quantities, the first column contains expected values, and the second column contains relative uncertainties.

```
>>> res.resdata['absKeff']
array([[ 1.29160000e+00,  9.00000000e-04],
       [ 1.29500000e+00,  9.30000000e-04],
       [ 1.29172000e+00,  9.10000000e-04],
       [ 1.29172000e+00,  7.80000000e-04],
       [ 1.29312000e+00,  6.80000000e-04],
       [ 1.29140000e+00,  7.80000000e-04]])
>>> res.resdata['absKeff'][:,0]
array([ 1.2916,  1.295,  1.29172,  1.29172,  1.29312,  1.2914])

>>> res.resdata['burnup']
array([[ 0.,  0.],
       [ 0.1,  0.100001],
       [ 1.,  1.00001],
       [ 2.,  2.00001],
       [ 3.,  3.00003],
       [ 4.,  4.00004]])
>>> res.resdata['burnDays']
[[ 0.],
 [ 1.20048],
 [ 12.0048],
 [ 24.0096],
 [ 36.0144],
 [ 48.0192]]
```

Data in the *resdata* can be obtained directly by indexing into the reader:

```
>>> res["burnup"]
array([[ 0.,  0.],
       [ 0.1,  0.100001],
       [ 1.,  1.00001],
       [ 2.,  2.00001],
       [ 3.,  3.00003],
```

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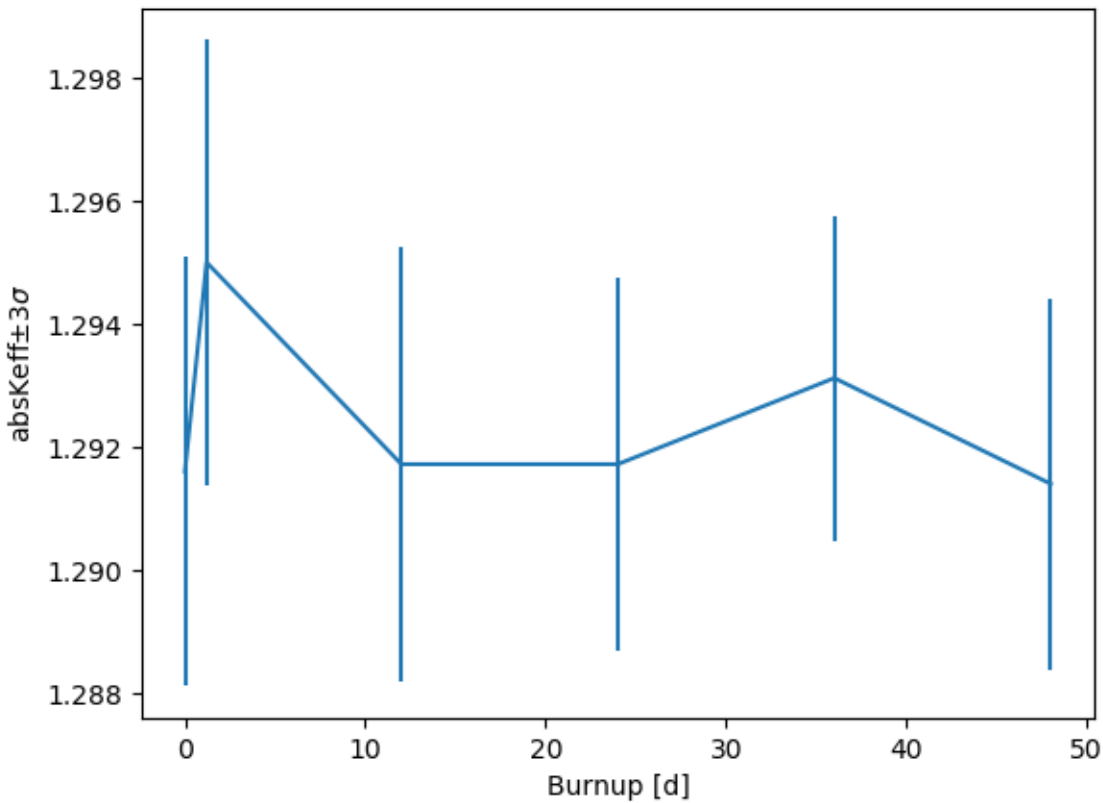
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```
[ 4.          , 4.00004  ]
>>> res.resdata.get('absKeff')
array([[ 1.29160000e+00,  9.00000000e-04],
       [ 1.29500000e+00,  9.30000000e-04],
       [ 1.29172000e+00,  9.10000000e-04],
       [ 1.29172000e+00,  7.80000000e-04],
       [ 1.29312000e+00,  6.80000000e-04],
       [ 1.29140000e+00,  7.80000000e-04]])
```

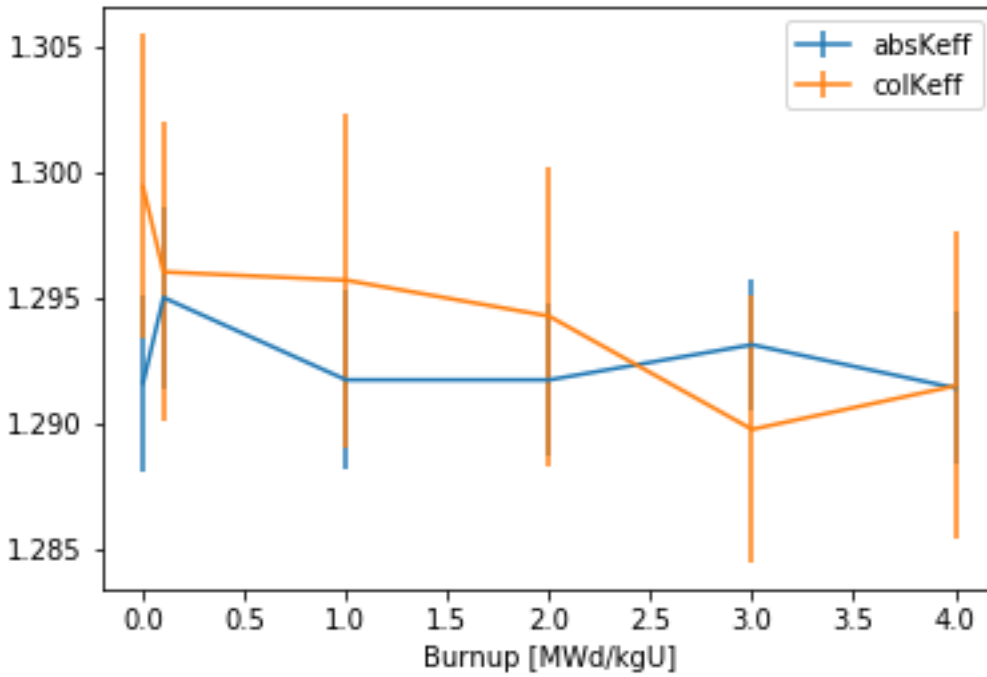
4.7.2 Plotting Results Data

The *ResultsReader* has a versatile `plot()` method, used to plot primary time-dependent data from the result file. One can plot data from one or more quantities against various metrics of time. Control over axis formatting, legend placement, and label formatting is easily yielded to the user.

```
>>> res.plot('absKeff')
```

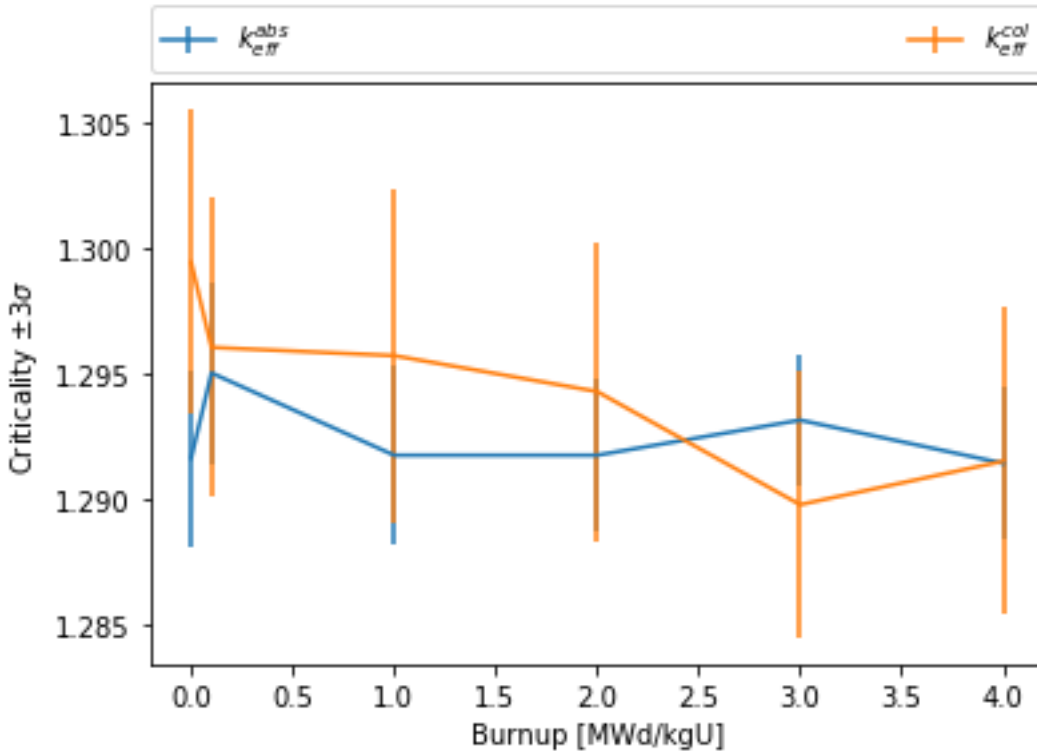


```
>>> res.plot('burnup', ['absKeff', 'colKeff'])
```



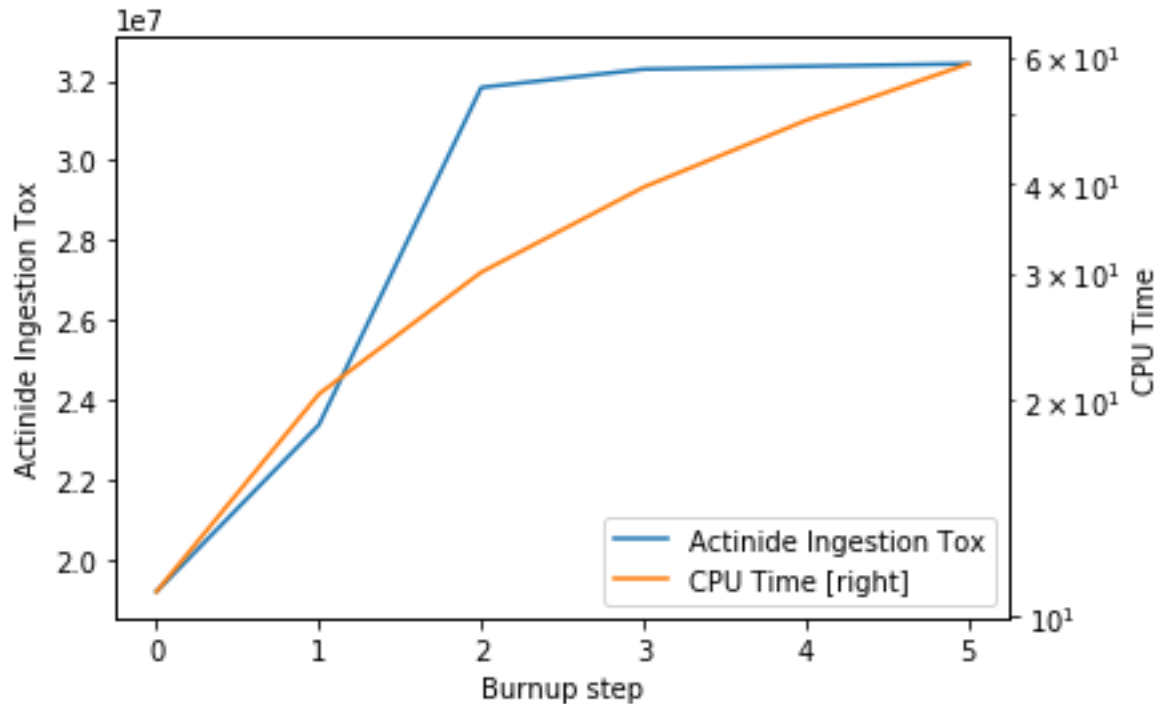
Pass a dictionary of variable: label pairs to set plot labels.

```
>>> res.plot(
>>>   'burnup', {
>>>     'absKeff': '$k_{eff}^{abs}$',
>>>     'colKeff': '$k_{eff}^{col}$',},
>>>   ylabel=r'Criticality $\pm 3\sigma$',
>>>   legend='above', ncol=2,
>>> )
```



Using the `right` argument, quantities can be plotted using the left and right y-axis. Similar formatting options are available.

```
>>> res.plot(
>>> 'burnStep',
>>> {'actinideIngTox': 'Actinide Ing. Tox'},
>>> right={'totCpuTime': 'CPU Time [right]'},
>>> sigma=0, rightlabel="CPU Time",
>>> # set the yscale to log only of right axis
>>> logy=[False, True],
>>> )
```

Universe Data

Universe data is stored for each state point in the `universes` dictionary. Keys are `UnivTuple` representing ('univ', burnup, burnupIdx, time)

- 'univ': universe ID (e.g., '0')
- burnup: in MWd/kg,
- burnupIdx: step index
- time: in days

and can be indexed by attribute or by position.

```
>>> for key in sorted(res.universes):
...     break
>>> key
UnivTuple(universe='0', burnup=0.0, step=0, days=0.0)
>>> key[0]
'0'
>>> key.burnup == key[1]
True
```

Results, such as infinite cross-sections, b1-leakage corrected cross-sections, kinetic parameters, are included in `universes`. All the results include values and uncertainties.

```
>>> res.universes.keys()
dict_keys([
    UnivTuple(universe='3101', burnup=0.0, step=0, days=0.0),
    UnivTuple(universe='3102', burnup=0.0, step=0, days=0.0),
    UnivTuple(universe='0', burnup=0.0, step=0, days=0.0),
```

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```
UnivTuple(universe='3101', burnup=0.1, step=1, days=1.20048),
UnivTuple(universe='3102', burnup=0.1, step=1, days=1.20048),
...
UnivTuple(universe='3101', burnup=4.0, step=5, days=48.0192),
UnivTuple(universe='3102', burnup=4.0, step=5, days=48.0192),
UnivTuple(universe='0', burnup=4.0, step=5, days=48.0192)])
```

One can directly index into *universes* to obtain a specific *HomogUniv* object:

```
>>> print(res.universes['0', 0, 0, 0])
<HomogUniv 0: burnup: 0.00000E+00 MWd/kgU, 0.00000E+00 days>
```

However, this requires knowledge of all four parameters, which may be difficult. The *getUniv()* method retrieves the first universe that matches a set of parameters, the universe and at least one point in time. While all four identifiers (universe id, burnup, step, and time) can be provided, the latter three are usually redundant.

```
>>> univ0 = res.getUniv('0', timeDays=24.0096)
>>> print(univ0)
<HomogUniv 0: burnup: 0.00000E+00 MWd/kgU, 0.00000E+00 days>
>>> univ3101 = res.getUniv('3101', index=3)
>>> print(univ3101)
<HomogUniv 3101: burnup: 2.00000E+00 MWd/kgU, 2.40096E+01 days>
>>> univ3102 = res.getUniv('3102', burnup=0.1)
>>> print(univ3102)
<HomogUniv 3102: burnup: 1.00000E-01 MWd/kgU, 1.20048E+00 days>
```

4.7.3 Working with homogenized universe data

Each state contains the same data fields, which can be obtained by using the following attributes on the *HomogUniv* object:

- *infExp*: infinite values, e.g. INF_ABS
- *infUnc*: infinite uncertainties
- *b1Exp*: b1 (leakage corrected) values, e.g. B1_ABS
- *b1Unc*: b1 (leakage corrected) uncertainties
- *gc*: variables that are not included in inf or b1, e.g. BETA
- *gcUnc*: uncertainties for quantities in *gc*
- *groups*: macro energy group structure, MeV
- *microGroups*: micro energy group structure, MeV

The parser reads all the variables by default. The values are all energy dependent in the order they would appear in the results file:

```
>>> univ0.infExp.keys()
dict_keys(['infMicroFlx', 'infKinfl', 'infFlx', 'infFissFlx', 'infTot',
'infCapt', 'infAbs', 'infFiss', 'infNsf', 'infNubar', 'infKappa', 'infInnv',
'infScatt0', 'infScatt1', 'infScatt2', 'infScatt3', 'infScatt4', 'infScatt5',
'infScatt6', 'infScatt7', 'infScattp0', 'infScattp1', 'infScattp2',
'infScattp3', 'infScattp4', 'infScattp5', 'infScattp6', 'infScattp7',
'infTranspxs', 'infDiffcoef', 'infRabsxs', 'infRemxs', 'infI135Yield',
'infXe135Yield', 'infPm147Yield', 'infPm148Yield', 'infPm148mYield',
```

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```
'infPm149Yield', 'infSm149Yield', 'infI135MicroAbs', 'infXe135MicroAbs',
'infPm147MicroAbs', 'infPm148MicroAbs', 'infPm148mMicroAbs',
'infPm149MicroAbs', 'infSm149MicroAbs', 'infXe135MacroAbs', 'infSm149MacroAbs',
'infChit', 'infChip', 'infChid', 'infS0', 'infS1', 'infS2', 'infS3', 'infS4',
'infS5', 'infS6', 'infS7', 'infSp0', 'infSp1', 'infSp2', 'infSp3', 'infSp4',
'infSp5', 'infSp6', 'infSp7'])

>>> univ0.infExp['infAbs']
array([ 0.0170306 , 0.0124957 , 0.00777066, 0.00773255, 0.00699608,
        0.00410746, 0.00334604, 0.00296948, 0.0030725 , 0.00335412,
        0.00403133, 0.00506587, 0.00651475, 0.00737292, 0.00907442,
        0.0113446 , 0.0125896 , 0.0164987 , 0.0181642 , 0.0266464 ,
        0.0292439 , 0.0315338 , 0.0463069 , 0.0807952 ])

>>> univ0.infExp['infFlx']
array([ 1.10460000e+15, 1.72386000e+16, 7.78465000e+16,
        1.70307000e+17, 2.85783000e+17, 4.61226000e+17,
        8.04999000e+17, 1.17536000e+18, 1.17488000e+18,
        1.26626000e+18, 1.03476000e+18, 7.58885000e+17,
        4.95687000e+17, 5.85369000e+17, 2.81921000e+17,
        1.16665000e+17, 8.06833000e+16, 2.26450000e+16,
        6.51541000e+16, 2.79929000e+16, 8.87468000e+15,
        1.70822000e+15, 8.87055000e+14, 6.22266000e+13])
```

Uncertainties can be obtained in a similar way by using the *infUnc* field:

```
>>> univ0.infUnc['infFlx']
array([0.02125, 0.0287 , 0.00901, 0.00721, 0.00441, 0.00434, 0.00448,
        0.0007 , 0.00369, 0.00071, 0.00045, 0.00133, 0.00061, 0.00341,
        0.00674, 0.00197, 0.00802, 0.00368, 0.00127, 0.00046, 0.02806,
        0.0491 , 0.19529, 0.16476])
```

Serpent also outputs the B1 cross-sections. However, the user must enable the B1 option by setting the *fum* card: http://serpent.vtt.fi/mediawiki/index.php/Input_syntax_manual#set_fum If this card is not enabled by the user, the B1_ variables will all be zeros.

```
>>> univ0.b1Exp.keys()
dict_keys(['b1MicroFlx', 'b1Kinfl', 'b1Keff', 'b1B2', 'b1Err', 'b1Flx',
'b1FissFlx', 'b1Tot', 'b1Capt', 'b1Abs', 'b1Fiss', 'b1Nsf', 'b1Nubar',
'b1Kappa', 'b1Innv', 'b1Scatt0', 'b1Scatt1', 'b1Scatt2', 'b1Scatt3',
'b1Scatt4', 'b1Scatt5', 'b1Scatt6', 'b1Scatt7', 'b1Scattp0', 'b1Scattp1',
'b1Scattp2', 'b1Scattp3', 'b1Scattp4', 'b1Scattp5', 'b1Scattp6', 'b1Scattp7',
'b1Transpxs', 'b1Diffcoef', 'b1Rabsxs', 'b1Remxs', 'b1I135Yield',
'b1Xe135Yield', 'b1Pm147Yield', 'b1Pm148Yield', 'b1Pm148mYield',
'b1Pm149Yield', 'b1Sm149Yield', 'b1I135MicroAbs', 'b1Xe135MicroAbs',
'b1Pm147MicroAbs', 'b1Pm148MicroAbs', 'b1Pm148mMicroAbs', 'b1Pm149MicroAbs',
'b1Sm149MicroAbs', 'b1Xe135MacroAbs', 'b1Sm149MacroAbs', 'b1Chit', 'b1Chip',
'b1Chid', 'b1S0', 'b1S1', 'b1S2', 'b1S3', 'b1S4', 'b1S5', 'b1S6', 'b1S7',
'b1Sp0', 'b1Sp1', 'b1Sp2', 'b1Sp3', 'b1Sp4', 'b1Sp5', 'b1Sp6', 'b1Sp7'])

>>> univ3101.b1Exp['b1Flx']
array([ 1.20660000e+15, 1.65202000e+16, 7.47956000e+16,
        1.62709000e+17, 2.74814000e+17, 4.22295000e+17,
        7.04931000e+17, 9.70795000e+17, 9.11899000e+17,
        9.33758000e+17, 7.23255000e+17, 5.00291000e+17,
        3.16644000e+17, 3.52049000e+17, 1.62308000e+17,
```

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```
6.68674000e+16, 4.47932000e+16, 1.23599000e+16,
3.51299000e+16, 1.46504000e+16, 4.38516000e+15,
7.96971000e+14, 3.54233000e+14, 2.11013000e+13])
```

Data that does not contain the prefix `INF_` or `B1_` is stored under the `gc` and `gcUnc` fields. Criticality, kinetic, and other variables are stored under this field.

```
>>> univ3101.gc.keys()
dict_keys(['cmmTranspxs', 'cmmTranspxsX', 'cmmTranspxsY', 'cmmTranspxsZ',
'cmmDiffcoef', 'cmmDiffcoefX', 'cmmDiffcoefY', 'cmmDiffcoefZ', 'betaEff',
'lambda'])
>>> univ3101.gc['betaEff']
array([ 3.04272000e-03,  8.93131000e-05,  6.59324000e-04,
        5.62858000e-04,  1.04108000e-03,  5.67326000e-04,
        1.22822000e-04])
```

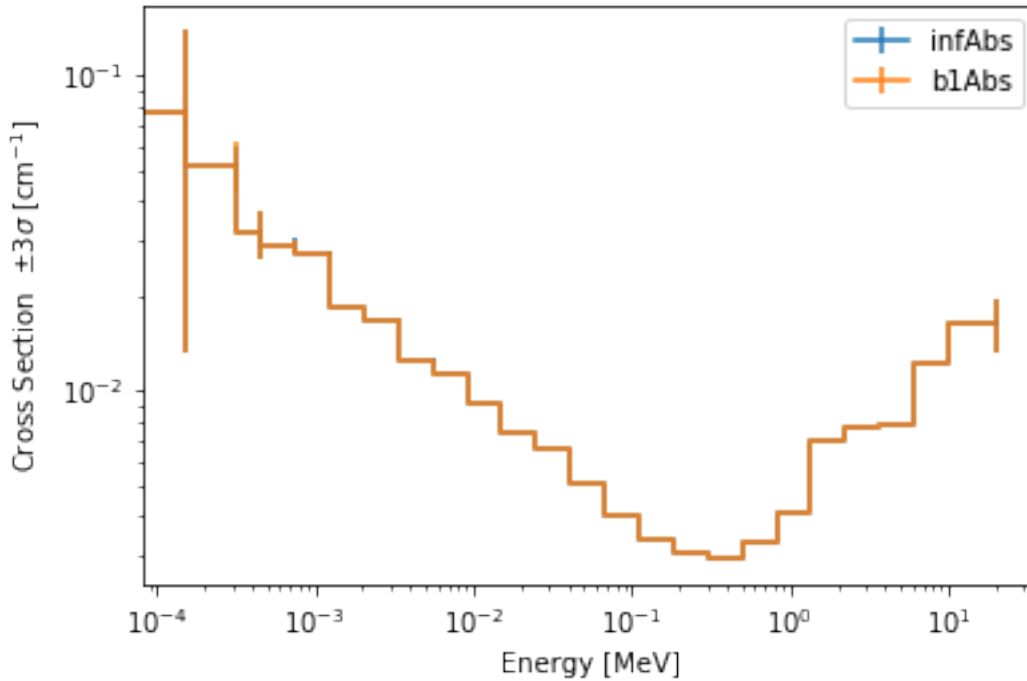
Macro- and micro- group structures are stored directly on the universe in MeV as they appear in Serpent output files. This means that the macro-group structure is in order of descending energy, while micro-group are in order of increasing energy:

```
>>> univ3101.groups
array([ 1.00000000e+37,  1.00000000e+01,  6.06530000e+00,
        3.67880000e+00,  2.23130000e+00,  1.35340000e+00,
        8.20850000e-01,  4.97870000e-01,  3.01970000e-01,
        1.83160000e-01,  1.11090000e-01,  6.73800000e-02,
        4.08680000e-02,  2.47880000e-02,  1.50340000e-02,
        9.11880000e-03,  5.53090000e-03,  3.35460000e-03,
        2.03470000e-03,  1.23410000e-03,  7.48520000e-04,
        4.54000000e-04,  3.12030000e-04,  1.48940000e-04,
        0.00000000e+00])
>>> univ3101.microGroups[:5:]
array([ 1.00000000e-10,  1.48940000e-04,  1.65250000e-04,
        1.81560000e-04,  1.97870000e-04])
```

4.7.4 Plotting universes

`HomogUniv` objects can plot group constants using their `plot()` method. This method has a range of formatting options, with defaults corresponding to plotting macroscopic cross sections. This is manifested in the default y axis label, but can be easily adjusted.

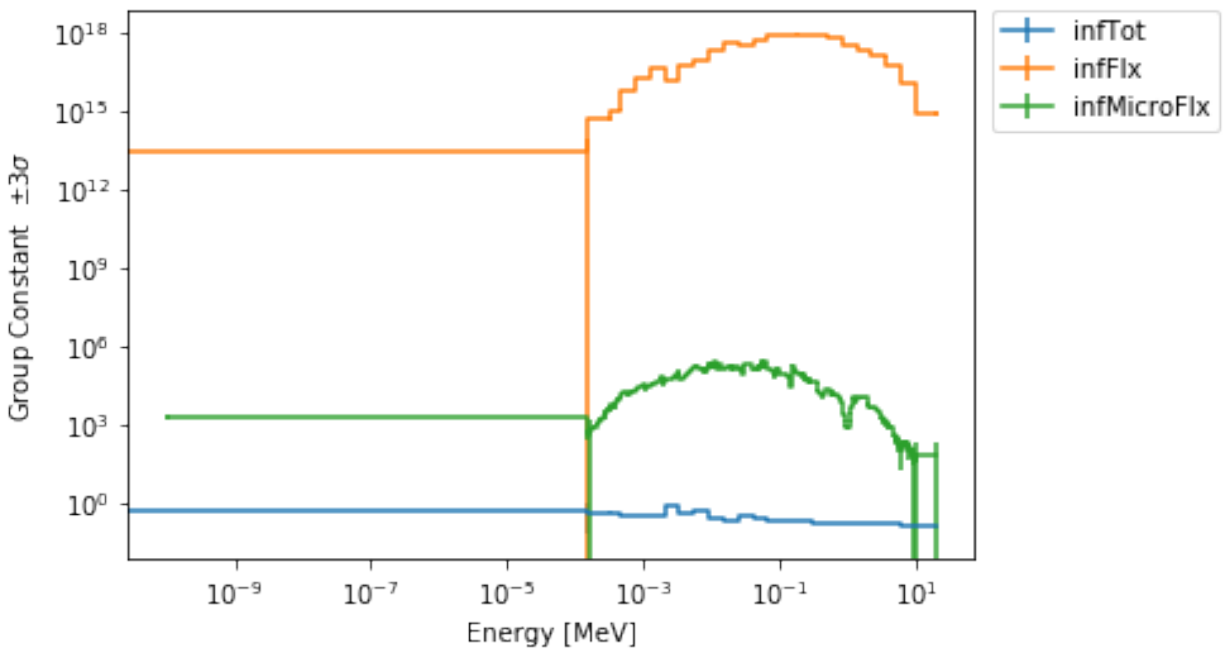
```
>>> univ3101.plot(['infAbs', 'b1Abs']);
```



Macroscopic and microscopic quantities, such as micro-group flux, can be plotted on the same figure.

Note: The units and presentation of the micro- and macro-group fluxes are dissimilar, and the units do not agree with that of the assumed group constants. This will adjust the default y-label, as demonstrated below.

```
>>> univ3101.plot(['infTot', 'infFlx', 'infMicroFlx'], legend='right');
```

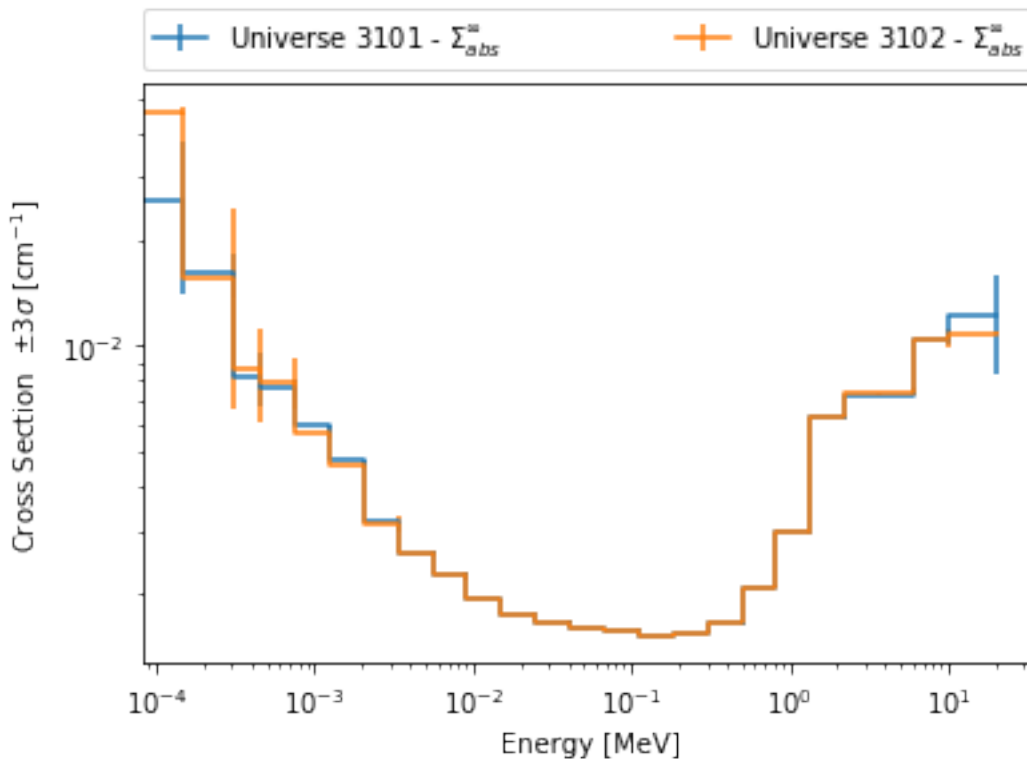


For plotting data from multiple universes, pass the returned `matplotlib.axes.Axes` object, on which the plot was drawn, into the plot method for the next universe. The `labelFmt` argument can be used to differentiate between plotted data. The following strings are replaced when creating the labels:

String	Replaced value
{k}	Name of variable plotted
{u}	Name of this universe
{b}	Value of burnup in MWd/kgU
{d}	Value of burnup in days
{i}	Burnup index

These can be used in conjunction with the \LaTeX rendering system .

```
>>> fmt = r"Universe {u} -  $\Sigma_{abs}^{\infty}$ "
>>> ax = univ3101.plot('infFiss', labelFmt=fmt)
>>> univ3102.plot('infFiss', ax=ax, labelFmt=fmt, legend='above', ncol=2);
```



4.7.5 User Defined Settings

The user is able to filter the required information by using the `serpentTools.settings.rc` settings object. A detailed description on how to use the settings can be found on: [Default Settings](#).

```
>>> from serpentTools.settings import rc
>>> rc.keys()
dict_keys(['branching.areUncsPresent', 'branching.intVariables',
'branching.floatVariables', 'depletion.metadataKeys',
'depletion.materialVariables', 'depletion.materials', 'depletion.processTotal',
```

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```
'detector.names', 'verbosity', 'sampler.allExist', 'sampler.freeAll',
'sampler.raiseErrors', 'sampler.skipPrecheck', 'serpentVersion', 'xs.getInfXS',
'xs.getB1XS', 'xs.reshapeScatter', 'xs.variableGroups', 'xs.variableExtras']])
```

The `serpentTools.settings.rc` object and various `xs.*` settings can be used to control the `ResultsReader`. Specifically, these settings can be used to store only specific pieces of information. Here, we will store the version of Serpent, various cross sections, eigenvalues, and burnup data:

```
>>> rc['xs.variableGroups'] = ['versions', 'xs', 'eig', 'burnup-coeff']
```

Furthermore, we instruct the read to no read critical spectrum cross sections:

```
>>> rc['xs.getB1XS'] = False

>>> resFilt = serpentTools.readDataFile(resFile)
>>> resFilt.metadata.keys()
dict_keys(['version', 'compileDate', 'debug', 'title', 'confidentialData',
'inputFileName', 'workingDirectory', 'hostname', 'cpuType', 'cpuMhz',
'startDate', 'completeDate'])
>>> resFilt.resdata.keys()
dict_keys(['burnMaterials', 'burnMode', 'burnStep', 'burnup', 'burnDays',
'nubar', 'anaKeff', 'impKeff', 'colKeff', 'absKeff', 'absKinf', 'geomAlbedo'])
>>> univ0Filt = resFilt.getUniv('0', burnup=0.0, index=0, timeDays=0.0)
>>> univ0Filt.infExp.keys()
dict_keys(['infCapt', 'infAbs', 'infFiss', 'infNsf', 'infNubar', 'infKappa',
'infInvv', 'infScatt0', 'infScatt1', 'infScatt2', 'infScatt3', 'infScatt4',
'infScatt5', 'infScatt6', 'infScatt7', 'infTranspxs', 'infDiffcoef',
'infRabsxs', 'infRemxs', 'infChit', 'infChip', 'infChid', 'infS0', 'infS1',
'infS2', 'infS3', 'infS4', 'infS5', 'infS6', 'infS7'])
>>> univ0Filt.b1Exp
{}
```

4.7.6 Conclusion

The `ResultsReader` is capable of reading and storing all the data from the `SERPENT_res.m` file. Upon reading, the reader creates custom `HomogUniv` objects that are responsible for storing the universe related data. In addition, `metadata` and `resdata` are stored on the reader. These objects also have a handy `getUniv()` method for quick analysis of results corresponding to a specific universe and time point. Use of the `serpentTools.settings.rc` settings control object allows increased control over the data selected from the output file.

4.7.7 References

1. J. Leppanen, M. Pusa, T. Viitanen, V. Valtavirta, and T. Kaltiaisenaho. “The Serpent Monte Carlo code: Status, development and applications in 2013.” Ann. Nucl. Energy, 82 (2015) 142-150

4.8 Micro cross section reader

4.8.1 Basic Operation

This notebook demonstrates the capabilities of the `serpentTools` in regards to reading group micro cross-section files. SERPENT [1] produces a `micro depletion file`, containing independent and cumulative fission yields as well as group cross-sections for the isotopes and reactions defined by the user. The `MicroXSReader` is capable of reading this file, and storing the data directly on the reader. The `MicroXSReader` has two methods to retrieve the data and ease the analysis. Note: in order to obtain the micro depletion files, the user must set the `mdep` card in the input file.

Note: The preferred way to read your own output files is with the `serpentTools.read()` function. The `serpentTools.readDataFile()` function is used here to make it easier to reproduce the examples

```
>>> import serpentTools
>>> mdxFile = 'ref_mdx0.m'
>>> mdx = serpentTools.readDataFile(mdxFile)
```

The fission yields read in from the file are stored in the `nfy` dictionary, where the keys represent a specific (parent, energy) pair and the corresponding values is a dictionary with fission products ids and corresponding fission yield values.

```
>>> # All the (parent, energy) pairs can be obtained by using '.keys()'
>>> pairs = mdx.nfy.keys()
>>> list(pairs)[0:5] # list only the first five pairs
[(902270, 2.53e-08),
 (902280, 2.53e-08),
 (902280, 0.5),
 (902280, 14.0),
 (902290, 2.53e-08)]
```

Each pair represents the isotope undergoing fission and the impending neutron energy in MeV.

```
>>> pair = list(pairs)[0] # obtain the first (isotope, energy) pair
>>> print('Isotope= {: 1.0f}'.format(pair[0]))
Isotope= 902270
>>> print('Energy= {} MeV'.format(pair[1]))
Energy= 2.53e-08 MeV
```

The results for each pair are dictionaries that contain three fields:

1. `fissProd` list of fission products ids
2. `indYield` corresponding list of independent fission yields
3. `cumYield` corresponding list of cumulative fission yields

```
>>> # Obtain the keys in the nfy dictionary
>>> mdx.nfy[pair].keys()
```

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```
dict_keys(['fissProd', 'indYield', 'cumYield'])
>>> # Print only the five first fission products
>>> print(mdx.nfy[pair]['fissProd'][0:5])
[ 250660. 250670. 250680. 260660. 260670.]
>>> # Print only the five first fission independent yields
>>> print(mdx.nfy[pair]['indYield'][0:5])
[ 6.97001000e-13 1.35000000e-13 1.01000000e-14 2.57000000e-10
1.13000000e-10]
>>> # Print only the five first fission cumulative yields
>>> print(mdx.nfy[pair]['cumYield'][0:5])
[ 6.97001000e-13 1.35000000e-13 1.01000000e-14 2.58000000e-10
1.13000000e-10]
```

Fluxes ratios and uncertainties are stored in the *fluxRatio* and *fluxUnc* dictionaries, where the keys represent a specific universe and the corresponding values are group fluxes values.

```
>>> # obtain the universes
>>> print(mdx.fluxRatio.keys())
dict_keys(['0'])
```

Cross sections and their uncertainties are stored in the *xsVal* and *xsUnc* dictionaries, where the keys represent a specific universe and the corresponding values are dictionaries. The keys within the nested dictionary describe the isotope, reaction and special flag:

```
>>> print(mdx.xsVal['0'].keys())
dict_keys([(10010, 102, 0), (982490, 18, 0), (982510, 102, 0), (982510, 16, 0),
(982510, 17, 0), (982510, 18, 0), (40090, 107, 0)])
```

Each key has three entries (isotope, reaction, flag)

1. isotope ID of the isotope (ZZAAA0/1), int or float
2. reaction MT e.g., 102 representing (n,gamma)
3. flag special flag to describe isomeric state or fission yield distribution number

For each such key (isotope, reaction, flag) the *xsVal* and *xsUnc* store the group-wise flux values and uncertainties respectively.

```
>>> val = mdx.xsVal['0']
>>> unc = mdx.xsUnc['0']
>>> # Print flux values
>>> print(val[(10010, 102, 0)])
[ 3.09753000e-05 3.33901000e-05 3.57054000e-05 3.70926000e-05
3.61049000e-05 3.39464000e-05 3.39767000e-05 3.98315000e-05
5.38962000e-05 7.96923000e-05 1.18509000e-04 1.73915000e-04
2.54571000e-04 3.38540000e-04 4.52415000e-04 5.98190000e-04
7.69483000e-04 1.04855000e-03 1.31149000e-03 1.67790000e-03
2.15195000e-03 2.70125000e-03 3.44635000e-03 5.04611000e-03]
>>> # Print flux uncertainties
>>> print(unc[(10010, 102, 0)])
[ 1.10000000e-04 2.00000000e-05 1.00000000e-05 0.00000000e+00
0.00000000e+00 0.00000000e+00 0.00000000e+00 1.00000000e-05
1.00000000e-05 2.00000000e-05 2.00000000e-05 2.00000000e-05
2.00000000e-05 1.00000000e-05 1.00000000e-05 2.00000000e-05
2.00000000e-05 3.00000000e-05 2.00000000e-05 3.00000000e-05
4.00000000e-05 5.00000000e-05 1.70000000e-04 6.90000000e-04]
```

4.8.2 Data Retrieval

The *MicroXSReader* object has two `get` methods: 1. `getFY()` method obtains the independent and cumulative fission yields for a specific parent (ZZAAA0/1), daughter (ZZAAA0/1), neutron energy (MeV). If no parent or daughter is found, the method raises an exception. The method also has a special flag that indicates whether the user wants to obtain the value corresponding to the nearest energy. 2. `getXS()` method to obtain the group-wise cross-sections for a specific universe, isotope and reaction.

```
>>> indYield, cumYield = mdx.getFY(parent=922350, energy=2.53e-08, daughter=541350 )
>>> print('Independent yield = {}'.format(indYield))
Independent yield = 0.000785125
>>> print('Cumulative yield = {}'.format(cumYield))
Cumulative yield = 0.065385
```

By default, the method includes a flag that allows to obtain the values for the closest energy defined by the user.

```
>>> indYield, cumYield = mdx.getFY(parent=922350, energy=1e-06, daughter=541350 )
>>> print('Independent yield = {}'.format(indYield))
Independent yield = 0.000785125
>>> print('Cumulative yield = {}'.format(cumYield))
Cumulative yield = 0.065385
```

The user can set this boolean flag to `False` if only the values at existing energies are of interest.

```
>>> indYield, cumYield = mdx.getFY(parent=922350, energy=2.53e-08, daughter=541350,
↳flagEnergy=False )
```

`getXS()` method is used to obtain the group cross-sections for a specific universe, isotope and reaction. The method returns the values and uncertainties.

```
>>> # Obtain the group cross-sections
>>> vals, unc = mdx.getXS(universe='0', isotope=10010, reaction=102)
>>> # Print group flux values
>>> print(vals)
[ 3.09753000e-05  3.33901000e-05  3.57054000e-05  3.70926000e-05
 3.61049000e-05  3.39464000e-05  3.39767000e-05  3.98315000e-05
 5.38962000e-05  7.96923000e-05  1.18509000e-04  1.73915000e-04
 2.54571000e-04  3.38540000e-04  4.52415000e-04  5.98190000e-04
 7.69483000e-04  1.04855000e-03  1.31149000e-03  1.67790000e-03
 2.15195000e-03  2.70125000e-03  3.44635000e-03  5.04611000e-03]
>>> # Print group flux uncertainties values
>>> print(unc)
[ 1.10000000e-04  2.00000000e-05  1.00000000e-05  0.00000000e+00
 0.00000000e+00  0.00000000e+00  0.00000000e+00  1.00000000e-05
 1.00000000e-05  2.00000000e-05  2.00000000e-05  2.00000000e-05
 2.00000000e-05  1.00000000e-05  1.00000000e-05  2.00000000e-05
 2.00000000e-05  3.00000000e-05  2.00000000e-05  3.00000000e-05
 4.00000000e-05  5.00000000e-05  1.70000000e-04  6.90000000e-04]
```

The method includes a special flag `isomeric`, which is set to zero by default. The special flag either describes the isomeric state or fission yield distribution number.

```
>>> # Example of how to use the isomeric flag
>>> vals, unc = mdx.getXS(universe='0', isotope=10010, reaction=102, isomeric=0)
```

If the universe exist, but the isotope or reaction do not exist, the method raises an error.

4.8.3 Settings

The *MicroXSReader* also has a collection of *serpentTools.settings.rc* to control what data is stored. If none of these settings are modified, the default is to store all the data from the output file.

```
>>> from serpentTools.settings import rc
>>> rc['microxs.getFY'] = False # True/False only
>>> rc['microxs.getXS'] = True # True/False only
>>> rc['microxs.getFlx'] = True # True/False only
```

- *microxs.getFY*: True or False, store fission yields
- *microxs.getXS*: True or False, store group cross-sections and uncertainties
- *microxs.getFlx*: True or False, store flux ratios and uncertainties

```
>>> mdx = serpentTools.readDataFile(mdxFile)
>>> # fission yields are not stored on the reader
>>> mdx.nfy.keys()
dict_keys([])
```

4.8.4 Conclusion

The *MicroXSReader* is capable of reading and storing all the data from the SERPENT micro depletion file. Fission yields, cross-sections and flux ratios are stored on the reader. The reader also includes two methods *getFY()* and *getXS()* to retrieve the data. Use of *serpentTools.settings.rc* settings control object allows increased control over the data selected from the output file.

4.8.5 References

1. J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, and T. Kaltiaisenaho. “The Serpent Monte Carlo code: Status, development and applications in 2013.” *Ann. Nucl. Energy*, 82 (2015) 142-150

4.9 Depletion Matrix Reader

The *serpentTools* package supports reading depletion matrix files, generated when `set depmtx 1` is added to the input file. As of SERPENT 2.1.30, these files contain

1. The length of time for a depletion interval
2. Vector of initial concentrations for all isotopes present in the depletion problem
3. ZAI vector
4. Depletion matrix governing destruction and transmutation of isotopes
5. Vector of final concentrations following one depletion event

Files such as this are present for each burnable material tracked by SERPENT and at each time step in the problem.

This document will demonstrate the *DepmtxReader*, designed to store such data.

Note: The depletion matrices can be very large for most problems, ~1000 x 1000 elements. For this reason, the `DepmtxReader` can store matrices in `Compressed Sparse Column` or full `numpy` arrays. The reader will use the sparse format if `scipy` is installed unless explicitly told to use dense arrays.

4.9.1 Basic Operation

Note: The preferred way to read your own output files is with the `serpentTools.read()` function. The `serpentTools.readDataFile()` function is used here to make it easier to reproduce the examples

```
>>> import serpentTools
>>> reader = serpentTools.readDataFile('depmtx_ref.m')
>>> reader
<serpentTools.parsers.depmtx.DepmtxReader at 0x7f0b1a9702b0>
```

We not have access to all the data present in the file directly on the reader.

```
>>> reader.n0
array([[1.17344222e-07, 6.10756908e-12, 7.48053806e-13, 7.52406757e-16,
        1.66113020e-34, 1.67580185e-09, 1.19223790e-36, 1.89040622e-26,
        5.09195054e-16, 7.91142112e-34, 1.68989876e-22, 6.92676695e-12,
        7.52406345e-16, 8.52076751e-13, 4.52429540e-02, 1.71307881e-12,
        1.86228871e-51, 2.32287315e-50, 1.15352152e-55, 7.72524686e-50,
        5.74084741e-44, 1.55414063e-42, 3.10757266e-40, 9.12566461e-40,
        6.82216144e-39, 9.71825616e-56, 1.59237444e-51, 1.14764875e-46,
        1.15203415e-43, 5.66072799e-41, 4.49411601e-34, 8.99210202e-31,
        8.65694179e-29, 5.96910982e-28, 1.06642058e-26, 9.10883647e-27,
        7.56006632e-36, 6.08157358e-33, 7.93562601e-40, 1.67857401e-29,
        2.76995718e-26, 2.42939173e-30, 6.93658246e-27, 3.21960435e-20,
        4.14863808e-17, 6.02145579e-16, 3.68254657e-15, 2.25927183e-15,
        2.85992932e-15, 5.34540710e-28, 2.34532631e-25, 1.36140065e-17,
        4.17935379e-16, 4.61527247e-15, 2.15346589e-15, 2.90307762e-15,
        4.90358169e-16, 3.62499544e-13, 4.61691784e-05, 2.96919439e-04,
        4.13730091e-04, 3.14746134e-04, 4.98296713e-04, 4.37637914e-04,
        3.84679634e-17, 6.87038906e-14, 4.29307714e-06, 5.62156587e-04,
        2.98288610e-08, 1.45634092e-09, 2.05487374e-02, 2.10836706e-07,
        9.84180195e-12, 8.05226656e-16], dtype=float128)
```

This specific input file did not include `fission yield libraries` and thus only tracks 74 isotopes, rather than 1000+, through depletion. This was intentionally done to reduce the size of files tracked in this project.

Number densities and entries in the depletion matrix are stored using the `numpy.longfloat` data type to preserve the precision present in the output files.

```
>>> reader.zai
array([[-1, 10010, 10020, 10030, 20030, 20040, 30060, 30070,
        40090, 50100, 50110, 60120, 70140, 70150, 80160, 80170,
        561380, 561400, 581380, 581390, 581400, 581410, 581420, 581430,
        581440, 591410, 591420, 591430, 601420, 601430, 601440, 601450,
        601460, 601470, 601480, 601500, 611470, 611480, 611481, 611490,
        611510, 621470, 621480, 621490, 621500, 621510, 621520, 621530,
        621540, 631510, 631520, 631530, 631540, 631550, 631560, 631570,
        641520, 641530, 641540, 641550, 641560, 641570, 641580, 641600,
```

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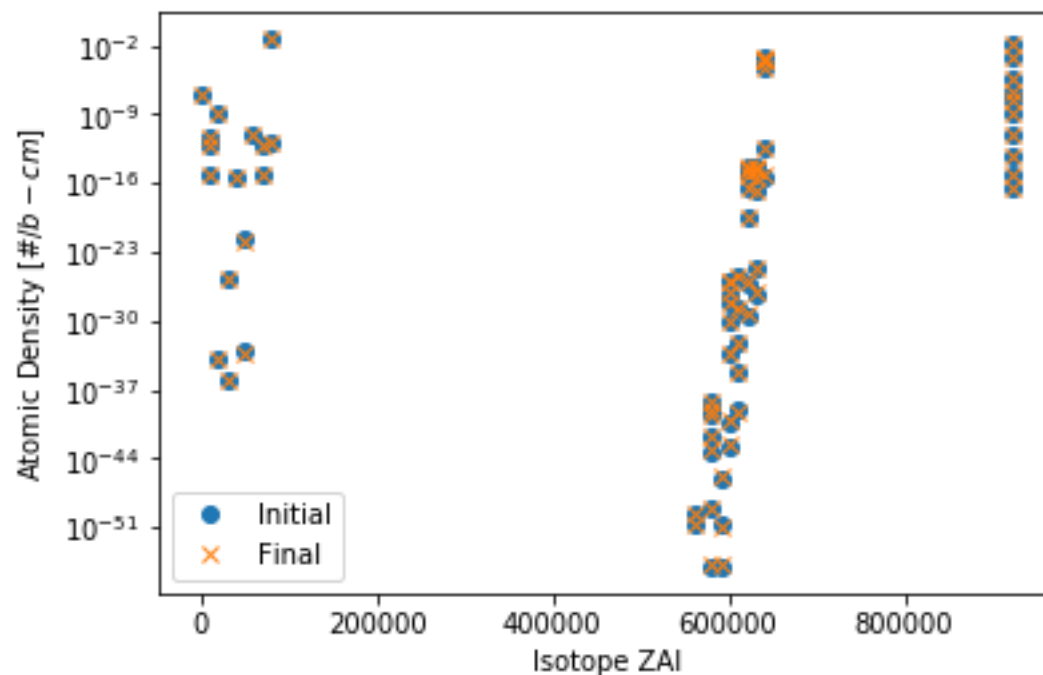
```
922320, 922330, 922340, 922350, 922360, 922370, 922380, 922390,
922400, 922410])
```

One can easily check if the depletion matrix is stored in a sparse or dense structure using the `sparse` attribute:

```
>>> reader.sparse
True
>>> reader.depmtx
<74x74 sparse matrix of type '<class 'numpy.float128'>'
  with 633 stored elements in Compressed Sparse Column format>
```

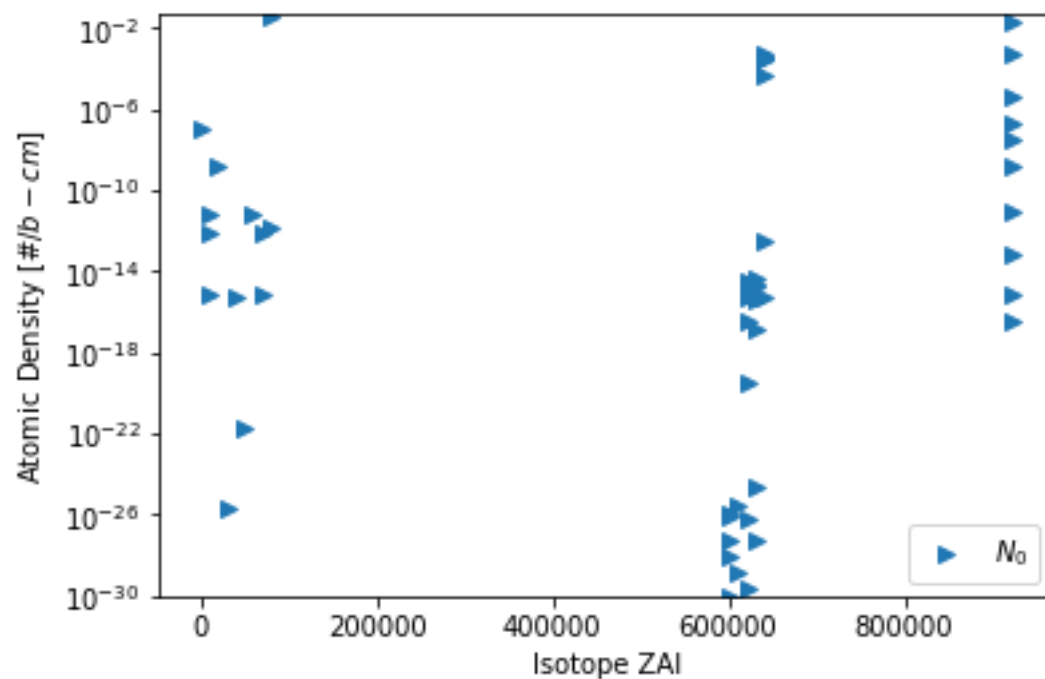
A simple plot method can be used to plot initial concentrations, final concentrations, or both:

```
>>> reader.plotDensity()
```

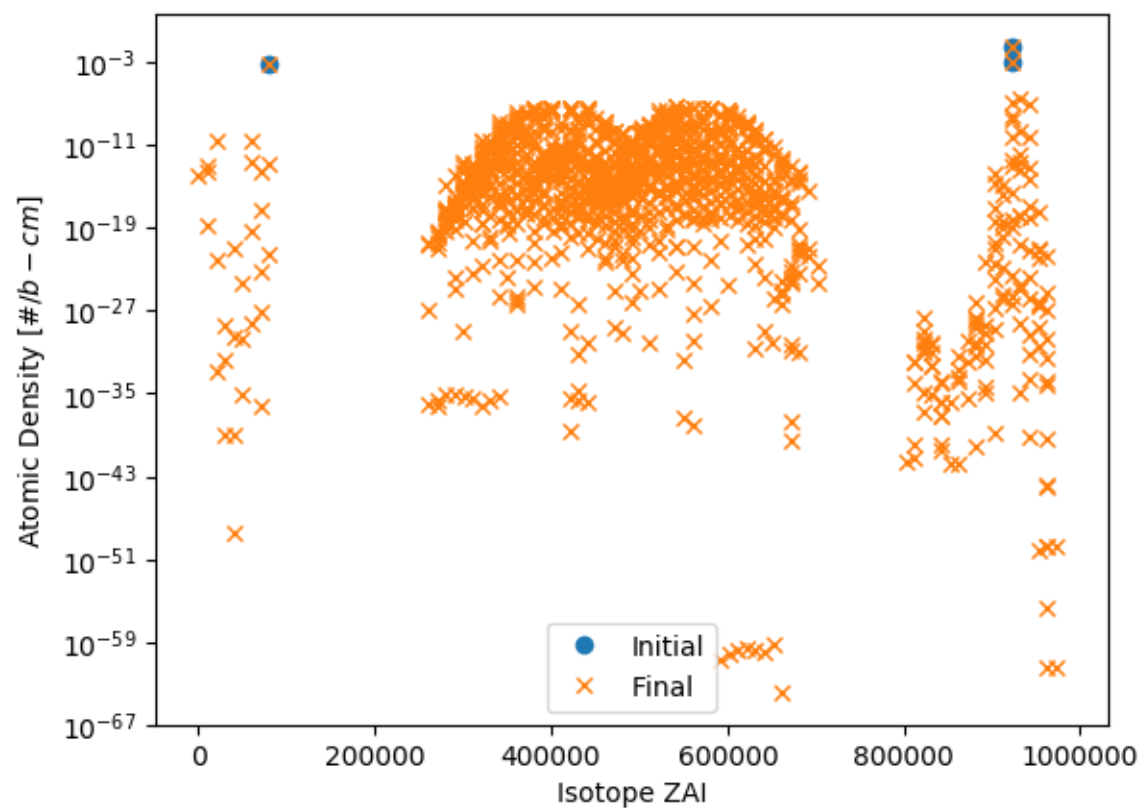


Some options can be passed to alter the formatting of the plot:

```
>>> reader.plotDensity(
    what='n0', # plot only initial concentration
    markers='>', # marker for scatter plot
    labels='$N_0$' # label for each plotted entry
    ylim=1E-30, # set the lower y-axis limit
)
```



We can see that there is not a lot of change in the isotopic concentration in this depletion step. Furthermore, the classical fission yield distributions are not present due to the lack of fission yield data. Using a more complete, and typical data set, one can view the distribution of fission products more clearly, demonstrated in the below plot.



4.10 Coefficient file to nodal diffusion cross sections

A recent feature of SERPENT is the ability to performing branching calculations using the [automated burnup sequence](#). `serpentTools` can read these coefficient files using the [BranchingReader](#). This automated burnup sequence is ideal for generating group constant data for nodal diffusion codes, that often include some multi-physics features, criticality searches, or other control mechanisms. A criticality search could be performed by tweaking the boron concentration in the coolant or adjusting control rod insertions. Similarly, some codes may include coupled TH analysis to convert power profiles to temperature profiles and adjust cross sections accordingly. Each code has a unique flavor for utilizing a set of group constants across these perturbations, and this notebook will demonstrate using the [BranchCollector](#) to gather and write a simple set of cross sections.

```
>>> import numpy
>>> import serpentTools
>>> from serpentTools.xs import BranchCollector
>>> # use serpentTools.read for everything except following along with examples
>>> coe = serpentTools.readDataFile('demo.coe')
```

This specific input file contained two perturbations: boron concentration and fuel temperature. Boron concentration had three branches: `nom` with no boron, then `B1000` and `B750`, with 1000 and 750 ppm boron in coolant. Fuel temperature had a nominal branch at 900 K, with 1200 and 600 K perturbations as well. These can be confirmed by observing the [branches](#) dictionary on the [BranchingReader](#).

```
>>> list(coe.branches.keys())
[('nom', 'nom'),
 ('B750', 'nom'),
 ('B1000', 'nom'),
 ('nom', 'FT1200'),
 ('B750', 'FT1200'),
 ('B1000', 'FT1200'),
 ('nom', 'FT600'),
 ('B750',
 'FT600'),
 ('B1000', 'FT600')]
```

Cross sections are spread out through this [BranchingReader](#) across branches, burnup, and universes. The job of the [BranchCollector](#) is to place that data into multi-dimensional matrices that represent the perturbations chosen by the user. A single group constant, say total cross section, has unique values for each universe, at each burnup point, for each perturbed state, and each energy group. Such a matrix would then contain five dimensions for this case.

First, we create the [BranchCollector](#) from the [BranchingReader](#) and instruct the reader what perturbations are present in the file. The ordering is not important at this point, as it can be changed later.

```
>>> collector = BranchCollector(coe)
>>> collector.collect(('BOR', 'TFU'))
```

Now we can inspect the perturbation states, `states` found by the collector.

```
>>> collector.states
(('B1000', 'B750', 'nom'), ('FT1200', 'FT600', 'nom'))
```

The group constants are stored in the `xsTables` dictionary. Here we select the total cross section, `infTot` for further exploration.

```
>>> list(collector.xsTables.keys())
['infTot', 'infFiss', 'infS0', 'infS1',
 'infDiffcoef', 'b1Tot', 'b1Fiss', 'b1S0',
```

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```
'b1S1', 'b1Diffcoef']
>>> infT = collector.xsTables['infTot']
>>> infT.shape
(5, 3, 3, 3, 2)
```

Five dimensions as mentioned above. But how are they ordered? Inspecting the `axis` attribute tells us that the dimensions are universe, boron concentration, fuel temperature, burnup, and energy group.

```
>>> collector.axis
('Universe', 'BOR', 'TFU', 'Burnup', 'Group')
```

The ordering of each of these dimensions is found by examining the `univIndex`, `states` and `burnups` attributes.

```
>>> collector.univIndex
(0, 10, 20, 30, 40)
>>> collector.states
(('B1000', 'B750', 'nom'), ('FT1200', 'FT600', 'nom'))
>>> collector.burnups
array([ 0.,  1., 10.])
```

For example, if we wanted the total cross section for universe 10, at 1000 ppm boron, nominal fuel temperature, and 10 MWd/kgU burnup, we would request

```
>>> infT[1, 0, 2, 2]
array([0.324746, 0.864346])
```

For this example, the scattering matrices were not reshaped from vectors to matrices and we would observe slightly different behavior in the 'Group' dimension.

```
>>> collector.xsTables['infS1'].shape
(5, 3, 3, 3, 4)
```

Four items in the last axis as the vectorized matrix represents fast to fast, fast to thermal, thermal to fast, and thermal to thermal scattering.

```
>>> collector.xsTables['infS1'][1, 0, 2, 2]
array([0.087809 , 0.00023068, 0.00073939, 0.123981  ])
```

Many nodal diffusion codes request group constants on a per universe basis, or per assembly type. As we saw above, the first dimension of the `xsTables` matrices corresponds to universe. One can view group constants for specific universes with the `universes` dictionary.

```
>>> collector.universes
{"0": <serpentTools.BranchedUniv at 0x7fb62f749a98>, 10:
<serpentTools.BranchedUniv at 0x7fb62f731b88>, 20:
<serpentTools.BranchedUniv at 0x7fb62f749e08>, 30:
<serpentTools.BranchedUniv at 0x7fb62f749e58>, 40:
<serpentTools.BranchedUniv at 0x7fb62f749ea8>}
>>> u0 = collector.universes["0"]
```

These `BranchedUniv` objects store views into the underlying collectors `xsTables` data corresponding to a single universe. The structuring is identical to that of the collector, with the first axis removed.

```
>>> u0.perturbations
('BOR', 'TFU')
>>> u0.axis
```

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```
( 'BOR', 'TFU', 'Burnup', 'Group')
>>> u0.states
(( 'B1000', 'B750', 'nom'), ( 'FT1200', 'FT600', 'nom'))
```

The contents of the `xsTables` dictionary are `numpy.array` views into the data stored on the collector.

```
>>> list(u0.xsTables.keys())
['infTot', 'infFiss', 'infS0', 'infS1',
 'infDiffcoef', 'b1Tot', 'b1Fiss', 'b1S0',
 'b1S1', 'b1Diffcoef']
>>> u0Tot = u0.xsTables['infTot']
>>> u0Tot.shape
(3, 3, 3, 2)
>>> u0Tot
array([[[[0.313696, 0.544846],
          [0.311024, 0.617734],
          [0.313348, 0.614651]],

        [[0.313338, 0.54515 ],
          [0.310842, 0.618286],
          [0.31299 , 0.614391]],

        ...

        [[0.210873, 0.223528],
          [0.208646, 0.        ],
          [0.206532, 0.        ]]]])
```

4.10.1 Changing perturbation values

The values of states and perturbations can be easily modified, so long as the structures are preserved. For example, as the current states are string values, and of equal perturbations (three boron concentrations, three fuel temperatures), we can set the states to be a single 2x3 array

```
>>> collector.states = numpy.array([
...     [1000, 750, 0],
...     [1200, 600, 900]],
...     dtype=float)
>>> collector.states
array([[1000., 750., 0.],
       [1200., 600., 900.]])
```

Some error checking is performed to make sure the passed perturbations match the structure of the underlying data. Here, we attempt to pass the wrong number of fuel temperature perturbations.

```
>>> try:
...     collector.states = numpy.array([
...         [1000, 750, 0],
...         [1200, 600], # wrong
...     ])
>>> except ValueError as ve:
...     print(str(ve))

Current number of perturbations for state TFU is 3, not 2
```

If the specific perturbations were not known when creating the collector, the value of `perturbations` can also be changed, with similar error checking.

```
>>> collector.perturbations = ['boron conc', 'fuel temperature']
>>> collector.perturbations
['boron conc', 'fuel temperature']
>>> try:
...     collector.perturbations = ['boron', 'fuel', 'ctrl'] # wrong
>>> except ValueError as ve:
...     print(str(ve))
Current number of perturbations is 2, not 3
```

4.10.2 Example nodal diffusion writer

As each nodal diffusion code has its own required data structure, creating a general writer is a difficult task. The intent with the *BranchCollector* is to provide a framework where the data is readily available, and such a writer can be created with ease. Here, an example writer is demonstrated, one that writes each cross section. The writer first writes a table of the perturbations at the top of the input file, showing the ordering and values of the perturbations. Options are also provided for controlling formatting.

The full file is available for download: [nodal_writer.py](#)

```
>>> from nodal_writer import Writer
>>> print(Writer.__doc__.strip())
Class for writing an example cross section file.

Parameters
-----
collector: Collector
    Object that read the branching file and stored
the cross sections
    along the perturbation vector
xsPerLine: int
    Number of cross sections / group constants to write per line
floatFmt: str
    Formattable string used when writing floating point values
strFmt: str
    Formattable string used when writing the names of the perturbations
xsRemap: None or dict
    Dictionary used to find a replacement name for
cross sections when
    writing. Between each cross section block, the
name of cross
    section and group will be written as ``# {name} group
{g}``.
    When ``xsRemap`` is ``None``, the names are ``mixedCase`` as
they appear in ``HomogUniv`` objects, e.g. ``'infTot'``,
``'diffCoeff'``, etc. If ``xsRemap`` is a dictionary, it can
be used to
write a different name. Passing ``{'infTot': 'Total
cross section'}``
would write ``'Total cross section'``
instead of ``'infTot'``, but all
other names would be unchanged.

>>> writer = Writer(collector)
```

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```

>>> print(writer.write.__doc__.strip())
Write the contents of a single universe

Parameters
-----
universe: int or key
            Key of universe that exists in
            ``self.collector``. Typically
            integer values of homogenized
            universes from coefficient file
stream: None or str or writeable
If ``None``, return a string containing what would have been
written to file. If a string, then write to this file. Otherwise,
ensure that the object has a ``write`` method and write to this
object
mode: {'a', 'w'}
            Write or append to file. Only
            needed if stream is a string

>>> # write to a file "in memory"
>>> out = writer.write(0)
>>> print(out[:1000])
# Cross sections for universe 0
boron conc          1.00000000E+03
7.50000000E+02 0.00000000E+00
fuel temperature    1.20000000E+03
6.00000000E+02 9.00000000E+02
Burnup [MWd/kgU]    0.00000000E+00
1.00000000E+00 1.00000000E+01
# infTot group 1
3.13696000E-01 3.11024000E-01
3.13348000E-01 3.13338000E-01
3.10842000E-01 3.12990000E-01 3.16730000E-01
3.13987000E-01
3.16273000E-01 3.13772000E-01 3.11335000E-01 3.13311000E-01
3.13437000E-01 3.10967000E-01 3.13160000E-01 3.16688000E-01
3.14245000E-01
3.16392000E-01 2.08020000E-01 2.05774000E-01
2.03646000E-01 2.07432000E-01
2.05326000E-01 2.03533000E-01
2.10873000E-01 2.08646000E-01 2.06532000E-01
#
infTot group 2
5.44846000E-01 6.17734000E-01 6.14651000E-01 5.45150000E-01
6.18286000E-01 6.14391000E-01 5.48305000E-01 6.21804000E-01
6.18120000E-01
5.41505000E-01 6.09197000E-01 6.08837000E-01
5.42373000E-01 6.09192000E-01
6.08756000E-01 5.45294000E-01
6.12767000E-01 6.12985000E-01 2.28908000E-01
1.07070000E-01
0.00000000E+00 3.1

```


FILE-PARSING API

This page contains links to the full documentation for the readers used by `serpentTools`.

5.1 Functions

The core of `serpentTools` is the `read()` function. This function attempts to determine the file type based on the extension and use the correct reader to parse the file. Below are links to primary reader functions that accept a file path argument and will process the file accordingly.

<code>read</code>	Simple entry point to read a file and obtain the processed reader.
<code>readDepmtx</code>	Simple entry point to obtain data from depletion matrix files

5.1.1 `serpentTools.read`

`serpentTools.read(filePath, reader='infer')`

Simple entry point to read a file and obtain the processed reader.

Parameters

- **filePath** (*str*) – Path to the file to be reader
- **reader** (*str or callable*) – Type of reader to use. If a string is given, then the actions described below will happen. If callable, then that function will be used with the file path as the first argument.

String argument	Action
infer	Infer the correct reader based on the file
branch	BranchingReader
bumat	BumatReader
dep	DepletionReader
det	DetectorReader
fission	FissionMatrixReader
history	HistoryReader
microxs	MdxReader
results	ResultsReader
sensitivity	SensitivityReader
xsplo	XSPloReader

Returns Correct subclass corresponding to the file type

Return type `serpentTools.objects.base.BaseReader`

Raises

- **AttributeError** – If the object created by the reader through `reader(filePath)` does not have a `read` method.
- **SerpentToolsException** – If the reader could not be inferred or if the requested reader string is not supported
- **NotImplementedError** – This has the ability to load in readers that may not be complete, and thus the `read` method may raise this error.

5.1.2 `serpentTools.readDepmtx`

`serpentTools.readDepmtx(filePath, sparse=True)`

Simple entry point to obtain data from depletion matrix files

Parameters

- **filePath** (*str*) – Path of file to be read
- **sparse** (*bool*) – If this is `True`, attempt to construct a sparse depletion matrix, rather than a dense matrix. Requires `scipy`. If `scipy` is not installed, a full matrix will be returned

Returns

- **dt** (*float*) – Length of depletion interval
- **n0** (`numpy.ndarray`) – 1D vector of initial isotopics. Ordered according to `zai` vector
- **zai** (`numpy.ndarray`) – 1D vector of ZZAAAI isotope identifiers
- **A** (`numpy.ndarray` or `scipy.sparse.csc_matrix`) – Depletion matrix governing decay/production of isotopics. Will be a sparse matrix if `sparse` was passed as `True` and `scipy` is installed.
- **n1** (`numpy.ndarray`) – 1D vector of isotopics after depletion event.

5.2 Classes

The `read()` function relies heavily on the following parsers which can be created and used outside of the function. These classes are also the returned types for `read()`.

<i>BumatReader</i>	Parser responsible for reading and working with burned material files.
<i>BranchingReader</i>	Parser responsible for reading and working with automated branching files.
<i>DepletionReader</i>	Parser responsible for reading and working with depletion files.
<i>DepmtxReader</i>	Reader for processing depletion matrix files
<i>DetectorReader</i>	Parser responsible for reading and working with detector files.
<i>HistoryReader</i>	Class responsible for reading history files

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Table 2 – continued from previous page

<i>MicroXSReader</i>	Parser responsible for reading and working with microxs (mdx) files.
<i>ResultsReader</i>	Parser responsible for reading and working with result files.
<i>SensitivityReader</i>	Class for reading sensitivity files
<i>XSPlotReader</i>	Parser responsible for reading and working with xsplot output files.

5.2.1 serpentTools.BumatReader

class `serpentTools.BumatReader` (*filePath*)

Parser responsible for reading and working with burned material files.

..note:

This **is** experimental **and** will be subject to change depending upon the implementation of GH Issue [#12](#)

Parameters `filePath` (*str*) – path to the depletion file

materials

Dictionary of materials with keys as names and values being a dictionary of parameters. **The storage of materials is subject to change**

Type `dict`

burnup

Burnup [MWd/kgU] for this file

Type `float`

days

Burnup [days] for this file

Type `float`

__getitem__ (*key*)

Return a material from *materials*

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the upper and lower arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised

- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

read()

The main method for reading that not only parses data, but also runs pre and post checks.

5.2.2 serpentTools.BranchingReader

class `serpentTools.BranchingReader` (*filePath*)

Parser responsible for reading and working with automated branching files.

Parameters `filePath` (*str*) – path to the depletion file

branches

Dictionary of branch names and their corresponding *BranchContainer* objects

Type `dict`

__contains__ (*key*)

Check if a branch is stored on the reader

Parameters `key` (*str or iterable of str*) – Name of the branch as defined in the Serpent input file

Returns Flag indicating the presence of key

Return type `bool`

__getitem__ (*key*)

Return a specific branch from *branches*

Parameters `key` (*str or iterable of str*) – Branch name as defined in Serpent input

Returns Branch corresponding to key

Return type *serpentTools.objects.BranchContainer*

__iter__ ()

Iterate over all branch names

__len__ ()

Number of branches stored on the reader

compare (*other, lower=0, upper=10, sigma=2, verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the `upper` and `lower` arguments control what passes and what messages get raised. If a quantity in `other` is less than `lower` percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than `upper` percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float or int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

get (*key, default=None*)

Return a branch that may or may not exist in *branches*

Parameters

- **key** (*str or iterable of str*) – Branch name as defined in Serpent input
- **default** (*object, optional*) – Item to return if `key` is not found

Returns *BranchContainer* if `key` is found. `default` if not

Return type `object`

property hasUncs

boolean if uncertainties are present in the file

items ()

Iterate over key, branch pairs from *branches*

iterBranches ()

Iterate over branches yielding paired branch IDs and containers

Deprecated since version 0.9.3: Use *items* () instead

read ()

The main method for reading that not only parses data, but also runs pre and post checks.

5.2.3 serpentTools.DepletionReader

class `serpentTools.DepletionReader` (*filePath*)
 Parser responsible for reading and working with depletion files.

Note: `metadata` is now a deprecated property, generated at each call. Additional keys added will not be retained. Prefer using `names`, `burnup`, `days`, and `zais`

Parameters `filePath` (*str*) – path to the depletion file

days

Vector of points in time

Type `numpy.ndarray` or `None`

burnup

Nominal burnup in MWd/kgU

Type `numpy.ndarray` or `None`

names

Names of isotopes corresponding to each row in the 2D arrays

Type list of str or `None`

zais

ZZAAAI identifiers for isotopes

Type list of int or `None`

metadata

Dictionary with zai and names

Deprecated since version 0.9.3.

Type dict of str to list

materials

Materials from the file. Keys will be the names as they appear in the file

Type dict of str to `serpentTools.objects.Material`

settings

names and values of the settings used to control operations of this reader

Type `dict`

__contains__ (*name*)

Check if a material is stored

__getitem__ (*name*)

Retrieve a material from `materials`.

__iter__ ()

Iterate over material names

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the upper and lower arguments control what passes and what messages get raised. If a quantity in `other` is less than `lower` percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than `upper` percent different

will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

compareMaterials (*other, lower=0, upper=10, sigma=2*)

Return the result of comparing all materials on two readers

Parameters

- **other** (*DepletionReader*) – Reader to compare against
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail

Returns `True` if all materials agree to the given tolerances

Return type `bool`

Raises **TypeError** – If `other` is not of the same class as this class nor a subclass of this class

compareMetadata (*other, lower=0, upper=10, sigma=2*)

Return the result of comparing metadata on two readers

Parameters

- **other** (*DepletionReader*) – Object to compare against
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **header** (*bool*) – Print/log an `info` message about this comparison.

Returns True if the metadata agree within the given tolerances

Return type `bool`

Raises `TypeError` – If `other` is not of the same class as this class nor a subclass of this class

get (*key*, *default=None*)

Retrieve a material from the dictionary if it exists

Parameters

- **key** (*str*) – Name of a material that may or may not exist in *materials*
- **default** (*optional*) – Item to return if `key` isn't found

Returns A `serpentTools.objects.DepletedMaterial` if it is stored under `key`. Otherwise return `default`

Return type `object`

items ()

Iterate over name, material pairs

keys ()

Key-view into material dictionary

plot (*xUnits*, *yUnits=None*, *timePoints=None*, *names=None*, *zai=None*, *materials=None*, *ax=None*, *legend=None*, *logx=False*, *logy=False*, *loglog=False*, *labelFmt=None*, *xlabel=None*, *ylabel=None*, *ncol=1*, ***kwargs*)

Plot properties for all materials in this file together.

Parameters

- **xUnits** (*str*) – If `xUnits` is given and `yUnits` is `None`, then the plotted data will be `xUnits` against 'days' name of x value to obtain, e.g. 'days', 'burnup'
- **yUnits** (*str*) – name of y value to return, e.g. 'adens', 'ingTox'
- **timePoints** (*list or None*) – If given, select the time points according to those specified here. Otherwise, select all points
- **names** (*str or list or None*) – If given, plot values corresponding to these isotope names. Otherwise, plot values for all isotopes.
- **zai** (*int or list or None*) – If given, plot values corresponding to these isotope ZAAAI values. Otherwise, plot for all isotopes

New in version 0.5.1.

- **materials** (*None or list*) – Selection of materials from `self.materials` to plot. If `None`, plot all materials, potentially including `tot`
- **ax** (`matplotlib.axes.Axes`, *optional*) – Ax on which to plot the data. If not provided, create a new plot
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label. Otherwise, use `xUnits`

- **ylabel** (*str* or *bool*, *optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label. Otherwise, use `yUnits`
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **labelFmt** (*str*, *optional*) – Formattable string for labeling the individual plots. If not given, just label as isotope name, e.g. 'U235'. Will make the following substitutions on the `labelFmt` string, if given:

Keyword	Replacement
'mat'	name of this material
'iso'	specific isotope name
'zai'	specific isotope ZZAAAI

- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **kwargs** (*dict*, *optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()`

Returns `Ax` on which the data was plotted.

Return type `matplotlib.axes.Axes`

See also:

- `getValues()`
- `str.format()` - used for formatting labels
- `plot()`

Raises

- **KeyError** – If x axis units are not 'days' nor 'burnup'
- **SerpentToolsException** – If the materials dictionary does not contain any items

read()

The main method for reading that not only parses data, but also runs pre and post checks.

saveAsMatlab (*fileP*, *reconvert=True*, *metadata=None*, *append=True*, *format='5'*, *longNames=True*, *compress=True*, *oned='row'*)

Write a binary MATLAB file from the contents of this reader

Deprecated since version 0.7.0: Use `toMatlab()`

Parameters

- **fileP** (*str* or *file-like object*) – Name of the file to write
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file, e.g. `MAT_TOTAL_ING_TOX`. Otherwise, maintain the `mixedCase` style, `total_ingTox`.
- **metadata** (*bool* or *str* or *list of strings*) – If this evaluates to true, then write all metadata to the file as well.

- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{ '5', '4' }*) – Format of file to write. '5' for MATLAB 5 to 7.2, '4' for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{ 'row', 'col' }*) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

`scipy.io.savemat()`

toMatlab (*fileP, reconvert=True, append=True, format='5', longNames=True, compress=True, oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str or file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{ '5', '4' }*) – Format of file to write. '5' for MATLAB 5 to 7.2, '4' for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{ 'row', 'col' }*) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

values ()

Values-view into material dictionary

5.2.4 serpentTools.DepmtxReader

class `serpentTools.DepmtxReader` (*filePath*, *sparse=None*)

Reader for processing depletion matrix files

Parameters

- **filePath** (*str*) – Path to file to be read
- **sparse** (bool or None) – Use *scipy* sparse matrices if True. If passed as None, only use sparse if *scipy* is installed

deltaT

Length of depletion interval

Type `float`

n0

Vector of original isotopics

Type `numpy.ndarray`

zai

Integer vector of isotope ZAI (zzaai) identifiers

Type `numpy.ndarray`

depmtx

Depletion matrix for this material. Will be `scipy.sparse.csc_matrix` if *scipy* is installed and the sparse-engine option is either not specified (None) during `read()` or passed as True. Otherwise, will be a `numpy.ndarray`

Type `numpy.ndarray` or

n1

Vector for isotopics after depletion

Type `numpy.ndarray`

checkSparse()

Return True if the object is configured for sparse support

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the upper and lower arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail

- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

plotDensity (*what='both', ax=None, logx=False, logy=True, loglog=None, legend=None, title=None, labels=None, markers=None, xlabel=None, ylabel=None, ylim=None*)
Plot initial, final, or both number densities.

Parameters

- **what** (*str*) – Concentrations to plot.
 1. 'both': plot initial and final
 2. 'n0' or 'initial': only initial
 3. 'n1' or 'final': only final
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **legend** (*bool* or *str* or *None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **title** (*str*) – Title to apply to the figure.
- **labels** (*None* or *str* or *list of strings*) – Labels to apply to concentration plot(s). If given, must have length equal to the number of quantities plotted, e.g. plotting both concentrations and passing a single string for `labels` is not allowed
- **markers** (*None* or *str* or *list of strings*) – Markers to apply to each plot. Must be a valid matplotlib marker such as 'o', '>', etc. If given, the number of markers given must equal the number of quantities to plot.
- **xlabel** (*str* or *bool*, optional) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **ylabel** (*str* or *bool*, optional) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **ylim** (*None* or *float* or *list of floats*) – If a single value is given, set the lower y-axis limit to this value. If two values are given, set the upper and lower y-axis limits to this value

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

read()

The main method for reading that not only parses data, but also runs pre and post checks.

toMatlab (*filePath*, *reconvert=True*, *append=True*, *format='5'*, *longNames=True*, *compress=True*, *oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **filePath** (*str* or *file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{'5', '4'}*) – Format of file to write. `'5'` for MATLAB 5 to 7.2, `'4'` for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{'row', 'col'}*) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises `ImportError` – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

5.2.5 serpentTools.DetectorReader

class `serpentTools.DetectorReader` (*filePath*)

Parser responsible for reading and working with detector files.

Parameters **filePath** (*str*) – path to the depletion file

detectors

Dictionary where key, value pairs correspond to detector names and their respective *Detector* instances

Type `dict`

__contains__ (*key*)

Check if a detector key is stored

__getitem__ (*name*)

Retrieve a detector from *detectors*

__iter__ ()

Iterate over detector names

__len__ ()

Number of detectors stored

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the upper and lower arguments control what passes and what messages get raised. If a quantity in `other` is less than `lower` percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than `upper` percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

get (*key, default=None*)

Retrieve a detector from the dictionary if it exists

Parameters

- **key** (*str*) – Name of a detector that may or may not exist in *detectors*
- **default** (*optional*) – Item to return if `key` isn't found

Returns A *serpentTools.Detector* if it is stored under `key`. Otherwise return `default`

Return type `object`

items ()

Iterate over key, detector pairs

iterDets ()

Yield name, detector pairs by iterating over *detectors*.

Deprecated since version 0.9.3: Use *items* ()

read ()

The main method for reading that not only parses data, but also runs pre and post checks.

toMatlab (*fileP, reconvert=True, append=True, format='5', longNames=True, compress=True, oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str or file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`

- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (`{ '5', '4' }`) – Format of file to write. '5' for MATLAB 5 to 7.2, '4' for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (`{ 'row', 'col' }`) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

5.2.6 serpentTools.HistoryReader

class `serpentTools.HistoryReader` (*filePath*)

Class responsible for reading history files

Arrays can be accessed through either the `arrays` dictionary, or with `his[key]`, where `key` is the name of an array in `arrays`.

Parameters `filePath` (*str*) – path pointing towards the file to be read

arrays

Dictionary of all the arrays produced in the file. These arrays do not have the index column that is presented in the file.

Type `dict`

numInactive

Number of inactive cycles used in this calculation

Type `int`

__contains__ (*key*)

Return True if key is in `arrays`, otherwise False

__getitem__ (*key*)

Return an item from `arrays`

__iter__ ()

Iterate over keys in `arrays`

__len__ ()

Return number of entries in `arrays`.

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the upper and lower arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different

will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

get (*key, default=None*)

Return an array or default if not found

static ioConvertName (*name*)

Convert a variable name to `camelCase` for exporting.

static ioReconvertName (*name*)

Reconvert a variable name to `SERPENT_STYLE` for exporting

items ()

Iterate over (*key, value*) pairs from *arrays*

read ()

The main method for reading that not only parses data, but also runs pre and post checks.

toMatlab (*fileP, reconvert=True, append=True, format='5', longNames=True, compress=True, oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str or file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{ '5', '4' }*) – Format of file to write. `'5'` for MATLAB 5 to 7.2, `'4'` for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters

- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{'row', 'col'}*) – Write one-dimensional arrays as row vectors if oned=='row' (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

5.2.7 serpentTools.MicroXSReader

class `serpentTools.MicroXSReader` (*filePath*)

Parser responsible for reading and working with micro-xs (mdx) files.

Parameters **filePath** (*str*) – path to the *mdx[n].m file

nfy

Nested dictionary with tuples (parent, energy) as keys. Parent is the isotope undergoing fission, e.g. 922350 and energy is the impending neutron energy causing fission in MeV. The values are nested dictionaries with the following structure:

```
"fissProd": list of fission product ZAI ids, e.g. [541350, 551350, ...]
"indYield": list of independent yields
"cumYield": list of cumulative yields
```

Type `dict`

fluxRatio

Dictionary with universes id as keys and the corresponding group-wise flux values. e.g.,
`fluxRatio['0'] = [9.91938E+14, 1.81729E+15]`

Type `dict`

fluxUnc

Dictionary with universes id as keys and the corresponding group-wise flux uncertainty values. e.g.,
`fluxRatio['0'] = [0.00023, 0.00042]`

Type `dict`

xsVal

Expected value on microscopic cross sections, sorted by universe then by isotope, reaction, and metastable flag. Nested dictionary with universes as keys, e.g. '0'. The values are nested dictionary with `MicroXSTuple` as keys (isotope, reaction, flag) and group xs as values. e.g., (922350, 18, 0)

Type `dict`

xsUnc

Uncertainties on microscopic cross sections, sorted by universe then by isotope, reaction, and metastable flag. Nested dictionary with universes as keys, e.g. '0'. The values are nested dictionary with `MicroXSTuple` as keys (isotope, reaction, flag) and group xs as values. e.g., (922350, 18, 0)

Type `dict`

Raises **SerpentToolsException** – No results exist in the file, or no results are collected

compare (*other*, *lower*=0, *upper*=10, *sigma*=2, *verbosity*=None)

Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have an error message printed and the comparison will return `False`, but continue. Quantities with a difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable.
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and error messages will be raised.
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail.
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified.

Return type `bool`

Raises

- **TypeError** – If *other* is not of the same class as this class nor a subclass of this class.
- **ValueError** – If *upper* > *lower*, If *sigma*, *lower*, or *upper* are negative.

getFY (*parent*, *energy*, *daughter*, *flagEnergy*=`True`)

Return a specific fission yield given the parent ID, neutron energy and daughter ID

If the energy does not exist in the results, the fission yield corresponding to the closest energy is returned.

Parameters

- **parent** (*int* or *float*) – ID of the parent undergoing fission.
- **energy** (*float*) – neutron energy in MeV.
- **daughter** (*int* or *float*) – ID of the fission product.
- **flagEnergy** (*boolean*) – If set to `true`, the function will return the fission yield that matches to the closest energy given by the user.

Returns

- **indYield** (*float*) – Independent fission yield.
- **cumYield** (*float*) – Cumulative fission yield.

Raises **SerpentToolsException**: – If *energy* is a negative number. If *parent* or *fission product* are not found.

getXS (*universe*, *isotope*, *reaction*, *isomeric*=0)

Return the group-wise micro cross-sections for a specific isotope, and reaction.

Parameters

- **universe** (*string*) – universe ID, e.g., 0
- **isotope** (*int or float*) – ID of the isotope (ZZAAA0/1)
- **reaction** (*int*) – MT reaction, e.g., 102 → (n,gamma)
- **flag** (*Special*) – Isomeric state or fission yield distribution number Default is zero

Returns

- **xsVal** (*numpy.ndarray*) – Group-wise cross-section values
- **xsUnc** (*numpy.ndarray*) – Group-wise uncertainty values

Raises `SerpentToolsException`: – If the universe does not exist If the isotope's format is incorrect (not ZZAAA0/1)

read()

The main method for reading that not only parses data, but also runs pre and post checks.

5.2.8 `serpentTools.ResultsReader`

class `serpentTools.ResultsReader` (*filePath*)

Parser responsible for reading and working with result files.

When inspecting keys of `universes`, it is preferable to use an attribute based approach rather than positional. For example:

```
>>> for key in res.universes:
...     break
>>> key.universe
# rather than
>>> key[0]
```

metadata

Dictionary with serpent descriptive variables as keys and the corresponding description. Within the `_res.m` file this data is printed multiple times, but contains the same description and thus is stored only once. e.g., 'version': 'Serpent 2.1.29'

Type `dict`

resdata

Dictionary with serpent time-dependent variables as keys and the corresponding values. The data is unique for each burnup step. Some variables also contain uncertainties. e.g., 'absKeff': [[9.91938E-01, 0.00145],[1.81729E-01, 0.00240]]

Type `dict`

universes

Dictionary of universe identifiers `UnivTuple` and their corresponding `HomogUniv` objects. The keys describe a unique state: 'universe', burnup (MWd/kg), burnup index, time (days) ('0', 0.0, 0, 0.0). Burnup indexes are zero-indexed, meaning the first step is index 0.

Type `dict`

Parameters `filePath` (*str*) – path to the results file

Raises

- **`SerpentToolsException`** – Serpent version is not supported, No universes are found in the file, No results are collected, Corrupted results

- **IOError** – file is unexpectedly closes while reading:

__getitem__ (*key*)

Retrieve an item from *resdata* only

Universes data like group constants should be pulled from universes directly with *getUniv()*

Parameters *key* (*str*) – mixedCase variable name like "absKeff" that may exist in *resdata*

Returns Requested quantity

Return type *numpy.ndarray*

Raises **KeyError** – If *key* does not exist in *resdata*

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have a error messages printed and the comparison will return *False*, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns *True* if the objects are in agreement with each other according to the parameters specified

Return type *bool*

Raises

- **TypeError** – If *other* is not of the same class as this class nor a subclass of this class
- **ValueError** – If *upper* > *lower*, If *sigma*, *lower*, or *upper* are negative

compareMetadata (*other*, *header=False*)

Return *True* if the metadata (settings) are identical.

Parameters

- **other** (*ResultsReader*) – Class against which to compare
- **header** (*bool*) – Print/log an *info* message about this comparison.

Returns If the metadata are identical

Return type *bool*

Raises **TypeError** – If *other* is not of the same class as this class nor a subclass of this class

compareResults (*other*, *lower=0*, *upper=10*, *sigma=2*, *header=False*)

Compare the contents of the results dictionary

Parameters

- **other** (*ResultsReader*) – Class against which to compare
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **header** (*bool*) – Print/log an info message about this comparison.

Returns If the results data agree to given tolerances

Return type `bool`

Raises `TypeError` – If *other* is not of the same class as this class nor a subclass of this class

compareUniverses (*other*, *lower=0*, *upper=10*, *sigma=2*)

Compare the contents of the universes dictionary

Parameters

- **other** (*ResultsReader*) – Reader by which to compare
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail

Returns If the contents of the universes agree to given tolerances

Return type `bool`

Raises `TypeError` – If *other* is not of the same class as this class nor a subclass of this class

get (*key*, *default=None*)

Retrieve an item from *resdata* or default

Parameters

- **key** (*str*) – mixedCase variable name that may or may not exist in *resdata*
- **default** (*optional*) – Object to be returned in key is not found

Returns `numpy.ndarray` if key is found. Otherwise *default* is returned

Return type `object`

getUniv (*univ*, *burnup=None*, *index=None*, *timeDays=None*)

Return a specific universe given the ID and time of interest

Parameters

- **univ** (*str*) – Unique str for the desired universe
- **burnup** (*float or int, optional*) – Burnup [MWd/kgU] of the desired universe

- **timeDays** (*float or int, optional*) – Time [days] of the desired universe
- **index** (*int, optional*) – Point of interest in the burnup/days index

Returns Requested universe

Return type *serpentTools.objects.HomogUniv*

Raises

- **KeyError** – If the requested universe could not be found
- **ValueError** – If burnup, days and index are not given

plot (*x, y=None, right=None, sigma=3, ax=None, legend=None, ncol=None, xlabel=True, ylabel=None, logx=False, logy=False, loglog=False, rightlabel=None*)
 Plot quantities over time

Parameters

- **x** (*str or iterable of strings*) – *y* is not given, then plot these quantities against burnup in days. Otherwise, plot this quantity as the *x* axis with same rules as if called by `plot('burndays', x)`. Burnup options are {'burnup', 'days', 'burnDays', 'burnStep'}
- **y** (*str or iterable of strings*) – Quantity or quantities to plot. For all entries, only the first column, with respect to time, will be plotted. If the second column exists, and *sigma* is > 0, that column will be treated as the relative uncertainty for an errorbar plot. If a dictionary is passed, then plots will be labeled by the values of that dictionary, e.g. {'anaKeff': '\$k_{eff}\$'} would plot the first column of *anaKeff* with a LaTeX-ready k_{eff}
- **right** (*str or iterable of strings*) – Quantities to plot on the same plot, but with a different *y* axis and common *x* axis. Same rules apply as for arguments to *y*. Each label will be modified to have a unique identifier indicating the plot uses the right *y*-axis
- **ax** (*matplotlib.axes.Axes, optional*) – *Ax* on which to plot the data. If not provided, create a new plot
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **xlabel** (*str or bool, optional*) – Label to apply to the *x*-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the *y*-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **logx** (*bool*) – Apply a log scale to *x* axis.
- **logy** (*bool or list or tuple*) – Apply a log scale to the *y*-axis. If passing values to *right*, this can be a two item list or tuple, corresponding to log-scaling the left and right axis, respectively.
- **loglog** (*bool*) – Apply a log scale to both axes.

- **rlabel** (*str* or *None*) – If given and passing values to *right*, use this to label the y-axis.

Returns If *right* is not given, then only the primary axes object is returned. Otherwise, the primary and the “right” axes object are returned

Return type `matplotlib.axes.Axes` or tuple of axes

read()

The main method for reading that not only parses data, but also runs pre and post checks.

toMatlab (*fileP*, *reconvert=True*, *append=True*, *format='5'*, *longNames=True*, *compress=True*, *oned='row'*)

Write a binary MATLAB file from the contents of this reader

The group constant data will be presented as a multi-dimensional array, rather than a stacked 2D matrix. The axis are ordered *burnup*, *universeIndex*, *group*, *value/uncertainty*

The ordering of the universes can be found in the 'UNIVERSES' vector if *reconvert==True*, otherwise 'universes'. Each universe ID is present in this vector, ordered to their position along the second axis in the matrix.

Parameters

- **fileP** (*str* or *file-like object*) – Name of the file to write
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under *output*, append to that file. Otherwise the file will be overwritten
- **format** (*{'5', '4'}*) – Format of file to write. '5' for MATLAB 5 to 7.2, '4' for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{'row', 'col'}*;) – Write one-dimensional arrays as row vectors if *oned=='row'* (default), or column vectors

Examples

```
>>> import serpentTools
>>> from scipy.io import loadmat
>>> r = serpentTools.readDataFile('pwr_res.m')
# convert to original variable names
>>> r.toMatlab('pwr_res.mat', True)
>>> loaded = loadmat('pwr_res.mat')
>>> loaded['ABS_KEFF']
array([[0.991938, 0.00145 ],
       [0.181729, 0.0024  ]])
>>> kinf = loaded['INF_KINF']
>>> kinf.shape
(2, 1, 1, 2)
>>> kinf[:, 0, 0, 0]
array([0.993385, 0.181451])
>>> tot = loaded['INF_TOT']
>>> tot.shape
```

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```
(2, 1, 2, 2)
>>> tot[:, 0, :, 0]
array([[0.496553, 1.21388 ],
       [0.481875, 1.30993 ]])
# use the universes key to identify ordering of universes
>>> loaded['UNIVERSES']
array([0])
```

Raises `ImportError` – If `scipy` is not installed

See also:

- `scipy.io.savemat()`

5.2.9 serpentTools.SensitivityReader

class `serpentTools.SensitivityReader` (*filePath*)

Class for reading sensitivity files

The arrays that are stored in `sensitivities` and `energyIntegratedSens` are stored under converted names. The original names from SERPENT are of the form `ADJ_PERT_KEFF_SENS` or `ADJ_PERT_KEFF_SENS_E_INT`, respectively. Since this reader stores the resulting arrays in unique locations, the names are converted to a succinct form. The two arrays listed above would be stored both as `keff` in `sensitivities` and `energyIntegratedSens`. All names are converted to `mixedCaseNames` to fit the style of the project.

Ordered dictionaries `materials`, `zais` and `perts` contain keys of the names of their respective data, and the corresponding index, `iSENS_ZAI_zzaai`, in the sensitivity arrays. These arrays are zero-indexed, so the first item will have an index of zero. The data stored in the `sensitivities` and `energyIntegratedSens` dictionaries has the exact same structure as if the arrays were loaded into MATLAB/Octave, but with zero-indexing.

The matrices in `sensitivities` are ordered as they would be in MATLAB. The five dimensions correspond to:

1. `materials` that were contained perturbed isotopes
2. `zais` that were perturbed
3. `perts` - reactions that were perturbed, e.g. 'total xs'
4. `energies` - which energy group contained the perturbation. Will have one fewer dimensions than the number of values in `energies`, corresponding to the number of energy groups.
5. [value, relative uncertainty] pairs

The matrices in `energyIntegratedSens` will have the same structure, but with the `energies` dimension removed.

Note: Arrays generated using the history option `sens opt history 1` are not currently stored on the reader. See feature request [#367](#)

Parameters `filePath` (*str*) – Path to sensitivity file

nMat
Number of materials
Type `None` or `int`

nZai
Number of perturbed isotopes
Type `None` or `int`

nPert
Number of perturbations
Type `None` or `int`

nEne
Number of energy groups
Type `None` or `int`

nMu
Number of perturbed materials
Type `None` or `int`

materials
Ordered dictionary of materials that have been perturbed.
Type `OrderedDict`

zais
Ordered dictionary of nuclides that have been perturbed
Type `OrderedDict`

perts
Ordered dictionary of reactions that have been perturbed, e.g. *'total xs'*
Type `OrderedDict`

latGen
Number of latent generations used to generate these sensitivities
Type `int`

energies
Array of energy bounds for the sensitivities, from lowest to highest
Type `None` or `numpy.array`

lethargyWidths
Array of lethargy widths of each energy group.
Type `None` or `numpy.array`

sensitivities
Dictionary of names of sensitivities and their corresponding arrays.
Type `dict`

energyIntegratedSens
Dictionary of names of the sensitivities that have been integrated against energy, and their corresponding arrays
Type `dict`

compare (*other*, *lower*=0, *upper*=10, *sigma*=2, *verbosity*=None)

Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have an error message printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable.
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and error messages will be raised.
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail.
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified.

Return type `bool`

Raises

- **TypeError** – If *other* is not of the same class as this class nor a subclass of this class.
- **ValueError** – If *upper* > *lower*, If *sigma*, *lower*, or *upper* are negative.

plot (*resp*, *zai*=None, *pert*=None, *mat*=None, *mevscale*=False, *egrid*=None, *sigma*=3, *normalize*=True, *ax*=None, *labelFmt*=None, *title*=None, *logx*=True, *logy*=False, *loglog*=False, *xlabel*=None, *ylabel*=None, *legend*=None, *ncol*=1)

Plot sensitivities due to some or all perturbations.

Note: Without passing *zai*, *pert*, or *mat* arguments, this method will plot all permutations of sensitivities for a given response.

Parameters

- **resp** (*str*) – Name of the specific response to be examined. Must be a key in `sensitivities` and `energyIntegratedSens`.
- **zai** (*None* or *str* or *int* or *iterable*) – Plot sensitivities due to these isotopes. Passing `None` will plot against all isotopes.
- **pert** (*None* or *str* or *list of strings*) – Plot sensitivities due to these perturbations. Passing `None` will plot against all perturbations.
- **mat** (*None* or *str* or *list of strings*) – Plot sensitivities due to these materials. Passing `None` will plot against all materials.
- **mevscale** (*bool*, *optional*) – Flag for plotting energy grid in MeV units. If `True`, the energy axis is expressed in MeV. Default is `False`.

- **egrid** (*numpy.array, optional*) – User-defined energy grid boundaries displayed on the sensitivities as vblack, dashed vertical lines. Default is `None`.
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **normalize** (*True*) – Normalize plotted data per unit lethargy
- **ax** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **labelFmt** (*None or str*) – Formattable string to be applied to the labels. The following entries will be formatted for each plot permutation:

```
{m} - name of the material
{z} - isotope zai
{p} - specific perturbation
{r} - response being plotted
```

- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: `above`, `right`
- **ncol** (*int*) – Integer number of columns to apply to the legend.

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises **KeyError** – If response or any passed perturbation settings are not present on the object

See also:

- `str.format()` - used for formatting labels

read()

The main method for reading that not only parses data, but also runs pre and post checks.

toMatlab (*fileP, reconvert=True, append=True, format='5', longNames=True, compress=True, oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str or file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.

- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (`{ '5', '4' }`) – Format of file to write. '5' for MATLAB 5 to 7.2, '4' for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (`{ 'row', 'col' }`) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

5.2.10 serpentTools.XSPlotReader

class `serpentTools.XSPlotReader` (*filePath*)

Parser responsible for reading and working with xsplot output files. These files can be generated using:

http://serpent.vtt.fi/mediawiki/index.php/Input_syntax_manual#set_xsplot

Parameters `filePath` (*str*) – path to the xsplot result file

xsections

Contains *XSData* objects with keys given by their names. There should be one *XSData* instance for each isotope and material present in the problem.

Type `dict`

energies

Array of energy grids, shared across all *XSData* instances

Type `numpy.ndarray` or `None`

majorant

L-inf norm among all macroscopic cross sections used in the problem.

Type `numpy.ndarray` or `None`

metadata

Alias for accessing *energies* and *majorant*. Attribute-based access is preferred, as this property will likely be removed in the future

Type `dict`

__contains__ (*key*)

Return true or false if *key* in *xsections*

__getitem__ (*key*)

Return item corresponding to *key* in *xsections*

__iter__ ()

Iterate over all keys in *xsections*

__len__ ()

Number of *xsdata* objects stored

compare (*other*, *lower*=0, *upper*=10, *sigma*=2, *verbosity*=None)

Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If *other* is not of the same class as this class nor a subclass of this class
- **ValueError** – If *upper* > *lower*, If *sigma*, *lower*, or *upper* are negative

get (*key*, *default*=None)

Return the value of *key* from *xsections* or *default*

Parameters

- **key** (*str*) – Name of isotope or material that may or may not exist in *xsections*
- **default** (*object*) – Item to return if *key* not found

Returns *XSDData* that corresponds to *key* if *key* is found. Otherwise return *default*

Return type `object`

items ()

Item-view (*k*, *v*) into *xsections*

keys ()

Key-view into *xsections*

read ()

The main method for reading that not only parses data, but also runs pre and post checks.

values ()

Values-view into *xsections*

CONTAINERS

Many of the readers provided in this project and by `read()` rely on custom classes for storing physically-similar data. This includes detector data, where tallies can be stored next to underlying spatial and/or energy grids, or depleted material data with isotopes and burnup data. Below are links to reference documentation for all of the helper classes used in `serpentTools`

Note: With the exception of the detectors, these classes are not well suited to be created and populated outside of the readers. Much of the data accessing methods are stable, but providing data may change in future versions

6.1 Detectors

Warning: Serpent 1 detectors are not supported as of 0.8.0

Note: Energy grids are stored in order of increasing energy, exactly as they appear in the output file. The three columns of this array correspond to lower bound, upper bound, and mid-point of that energy group

<i>Detector</i>	Class for storing detector data with multiple bins
<i>CartesianDetector</i>	Class for storing detector data with Cartesian grid
<i>HexagonalDetector</i>	Class for storing detector data with a hexagonal grid
<i>CylindricalDetector</i>	Class for storing detector data with a cylindrical mesh
<i>SphericalDetector</i>	Class for storing detector data with multiple bins

6.1.1 `serpentTools.Detector`

class `serpentTools.Detector` (*name*, *bins=None*, *tallies=None*, *errors=None*, *indexes=None*,
grids=None)

Class for storing detector data with multiple bins

For detectors with spatial meshes, including rectilinear, hexagonal, cylindrical, or spherical meshes, refer to companion classes `serpentTools.CartesianDetector`, `serpentTools.HexagonalDetector`, `serpentTools.CylindricalDetector`, or `serpentTools.SphericalDetector`

If simply the tally bins are available, it is recommended to use the `fromTallyBins()` class method. This will reshape the data and separate the mean tally [second to last column] and relative errors [last column].

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray, optional*) – Full 2D tally data from detector file, including tallies and errors in last two columns
- **tallies** (*numpy.ndarray, optional*) – Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.
- **errors** (*numpy.ndarray, optional*) – Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin. Note: this is a relative error as it would appear in the output file
- **indexes** (*iterable of string, optional*) – Iterable naming the bins that correspond to reshaped tally and *errors*.
- **grids** (*dict, optional*) – Supplemental grids that may be supplied to this detector, including energy points or spatial coordinates.

name

Name of this detector

Type *str*

bins

Full 2D tally data from detector file, including tallies and errors in last two columns

Type *numpy.ndarray* or *None*

tallies

Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.

Type *numpy.ndarray* or *float* or *None*

errors

Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin. Note: this is a relative error as it would appear in the output file

Type *numpy.ndarray* or *float* or *None*

indexes

Iterable naming the bins that correspond to reshaped tally and *errors*. The tuple (*energy*, *ymesh*, *xmesh*) indicates that *tallies* should have three dimensions corresponding to various energy, y-position, and x-position bins. Must be set after *tallies* or *errors* and agree with the shape of each

Type *tuple* or *None*

grids

Dictionary containing grid information for binned quantities like energy or time.

Type *dict*

energy

Potential underlying energy grid in MeV. Will be (*n_ene*, 3), where *n_ene* is the number of values in the energy grid. Each row *energy[j]* will be the low point, high point, and mid point of the energy bin *j*.

Type *numpy.ndarray* or *None*

Raises

- **ValueError** – If some spatial grid is found in `indexes` during creation. This class is ill-suited for these problems. Refer to the companion classes mentioned above.
- **IndexError** – If the shapes of `bins`, `tallies`, and `errors` are inconsistent

compare (*other*, *lower*=0, *upper*=10, *sigma*=2, *verbosity*=None)

Compare the results of this reader to another.

For values without uncertainties, the `upper` and `lower` arguments control what passes and what messages get raised. If a quantity in `other` is less than `lower` percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than `upper` percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper` > `lower`, If `sigma`, `lower`, or `upper` are negative

classmethod fromTallyBins (*name*, *bins*, *grids*=None)

Create a detector instance from 2D detector data

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*) – 2D array taken from Serpent. Expected to have either 12 or 13 columns, where the latter indicates a time bin has been added.
- **grids** (*dict, optional*) – Dictionary of underlying energy, space, and/or time data.

Returns

Return type `Detector`

Raises **ValueError** – If the tally data does not appear to be Serpent 2 tally data

meshPlot (*xdim*, *ydim*, *what*='tallies', *fixed*=None, *ax*=None, *cmap*=None, *cbarLabel*=None, *logColor*=False, *xlabel*=None, *ylabel*=None, *logx*=False, *logy*=False, *loglog*=False, *title*=None, *thresh*=None, ***kwargs*)

Plot tally data as a function of two bin types on a cartesian mesh.

Parameters

- **xdim** (*str*) – Primary dimension - will correspond to x-axis on plot
- **ydim** (*str*) – Secondary dimension - will correspond to y-axis on plot
- **what** (*{'tallies', 'errors'}*) – Color meshes from tally data or uncertainties
- **fixed** (*None or dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **cmap** (*str, optional*) – Valid Matplotlib colormap to apply to the plot.
- **logColor** (*bool*) – If true, apply a logarithmic coloring to the data positive data
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **title** (*str*) – Title to apply to the figure.
- **thresh** (*float*) – Do not plot data less than or equal to this value.
- **cbarLabel** (*str*) – Label to apply to colorbar. If not given, infer from what
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `pcolormesh()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **serpentTools.SerpentToolsException** – If data to be plotted, with or without constraints, is not 1D
- **KeyError** – If `fixed` is given and `xdim` or `ydim` are contained in `fixed`
- **AttributeError** – If the data set by `what` not in the allowed selection
- **ValueError** – If the data contains negative quantities and `logColor` is True

See also:

- `slice()`
- `matplotlib.pyplot.pcolormesh()`

plot (*xdim=None, what='tallies', sigma=None, fixed=None, ax=None, xlabel=None, ylabel=None, steps=False, labels=None, logx=False, logy=False, loglog=False, legend=None, ncol=1, title=None, **kwargs*)

Simple plot routine for 1- or 2-D data

Parameters

- **xdim** (*str*, *optional*) – Plot the data corresponding to changing this bin, e.g. "energy". Must exist in *indexes*
- **what** ({'tallies', 'errors'}) – Primary data to plot
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **fixed** (*None* or *dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes*, *optional*) – Ax on which to plot the data. If not provided, create a new plot
- **xlabel** (*str* or *bool*, *optional*) – Label to apply to the x-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label. If *xdim* is given and *xlabel* is *None*, then *xdim* will be applied to the x-axis.
- **ylabel** (*str* or *bool*, *optional*) – Label to apply to the y-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **steps** (*bool*) – If true, plot the data as constant inside the respective bins. Sets *drawstyle* to be *steps-post* unless *drawstyle* given in *kwargs*
- **labels** (*None* or *iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **legend** (*bool* or *str* or *None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict*, *optional*) – Addition keyword arguments to pass to *plot()* or *errorbar()* function.

Returns Ax on which the data was plotted.

Return type *matplotlib.axes.Axes*

Raises

- **SerpentToolsException** – If data contains more than 2 dimensions
- **AttributeError** – If plot data or *indexes* set up.

See also:

- *slice()*
- *spectrumPlot()* better options for plotting energy spectra

reshapedBins()

Obtain multi-dimensional tally, error, and index data

Returns

- **tallies** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally data along each bin index
- **errors** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally relative error along each bin index
- **indexes** (*list of str*) – Ordering of named bin information, e.g. "xmesh", "energy", corresponding to axis in **tallies** and **errors**

Examples

A detector is created with a single bin with two bins values. These could represent tallying two different reaction rates

```
>>> import numpy
>>> from serpentTools import Detector
>>> bins = numpy.ones((2, 12))
>>> bins[1, 0] = 2
>>> bins[1, 4] = 2
>>> bins[:, -2:] = [
...     [5.0, 0.1],
...     [10.0, 0.2]]
>>> det = Detector("reshape", bins=bins)
>>> tallies, errors, indexes = det.resapedBins()
>>> tallies
array([5.0, 10.0])
>>> errors
array([0.1, 0.2])
>>> indexes
["reaction", ]
```

slice (*fixed*, *data*='tallies')

Return a view of the reshaped array where certain axes are fixed

Parameters

- **fixed** (*dict*) – dictionary to aid in the restriction on the multidimensional array. Keys correspond to the various grids present in *indexes* while the values are used to
- **data** (*{'tallies', 'errors'}*) – Which data set to slice

Returns View into the respective data where certain dimensions have been removed

Return type *numpy.ndarray*

Raises **AttributeError** – If data is not supported

spectrumPlot (*fixed=None*, *ax=None*, *normalize=True*, *xlabel=None*, *ylabel=None*, *steps=True*, *logx=True*, *logy=False*, *loglog=False*, *sigma=3*, *labels=None*, *legend=None*, *ncol=1*, *title=None*, ***kwargs*)

Quick plot of the detector value as a function of energy.

Parameters

- **fixed** (*None* or *dict*) – Dictionary controlling the reduction in data
- **ax** (*matplotlib.axes.Axes*, optional) – Ax on which to plot the data. If not provided, create a new plot
- **normalize** (*bool*) – Normalize quantities per unit lethargy

- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **steps** (*bool*) – Plot tally as constant inside bin
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **labels** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()` or `matplotlib.pyplot.errorbar()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises `SerpentToolsException` – if number of rows in data not equal to number of energy groups

See also:

- `slice()`

toMatlab (*fileP, reconvert=True, append=True, format='5', longNames=True, compress=True, oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str or file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{ '5', '4' }*) – Format of file to write. `'5'` for MATLAB 5 to 7.2, `'4'` for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters

- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{'row', 'col'}*) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

6.1.2 serpentTools.CartesianDetector

class `serpentTools.CartesianDetector` (*name, bins=None, tallies=None, errors=None, indexes=None, grids=None, x=None, y=None, z=None*)

Class for storing detector data with Cartesian grid

If simply the tally bins are available, it is recommended to use the `fromTallyBins()` class method. This will reshape the data and separate the mean tally [second to last column] and relative errors [last column].

Note: In order to get full functionality from this class, *x*, *y*, and *z* must be set. All grids are expected to be (*N*, 3) arrays, not necessarily of equal shape.

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*) – Full 2D tally data from detector file, including tallies and errors in last two columns
- **tallies** (*numpy.ndarray*) – Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.
- **errors** (*numpy.ndarray*) – Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin. Note: this is a relative error as it would appear in the output file
- **indexes** (*dict or None*) – Dictionary mapping the bin name to its corresponding axis in *tallies* and *errors*, e.g. `{"energy": 0}`. Optional
- **x** (*numpy.ndarray, optional*) – Directly set the *x* grid
- **y** (*numpy.ndarray, optional*) – Directly set the *y* grid
- **z** (*numpy.ndarray, optional*) – Directly set the *z* grid
- **grids** (*dict, optional*) – Supplemental grids that may be supplied to this detector, including energy points or spatial coordinates. If spatial grids are not provided directly with the *x*, *y*, or *z* arguments, the grids will be pulled from this dictionary in the following manner.
 - Key "X" denotes the *x* grid
 - Key "Y" denotes the *y* grid
 - Key "Z" denotes the *z* grid

If the keys are not present, or the grids are directly provided, no actions are taken.

name
Name of this detector
Type `str`

bins
Full 2D tally data from detector file, including tallies and errors in last two columns
Type `numpy.ndarray` or `None`

tallies
Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.
Type `numpy.ndarray` or `None`

errors
Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin.
Note: this is a relative error as it would appear in the output file
Type `numpy.ndarray` or `None`

indexes
Dictionary mapping the bin name to its corresponding axis in *tallies* and *errors*, e.g. `{"energy": 0}`.
Type `dict`

energy
Potential underlying energy grid in MeV. Will be `(n_ene, 3)`, where `n_ene` is the number of values in the energy grid. Each row `energy[j]` will be the low point, high point, and mid point of the energy bin `j`.
Type `numpy.ndarray` or `None`

x
X grid
Type `numpy.ndarray` or `None`

y
Y grid
Type `numpy.ndarray` or `None`

z
Z grid
Type `numpy.ndarray` or `None`

Raises **ValueError** – If the values for `x`, `y`, and `z` are not 2D arrays with 3 columns

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)
Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.

- **lower** (*float or int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

classmethod `fromTallyBins` (*name, bins, grids=None*)

Create a detector instance from 2D detector data

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*) – 2D array taken from Serpent. Expected to have either 12 or 13 columns, where the latter indicates a time bin has been added.
- **grids** (*dict, optional*) – Dictionary of underlying energy, space, and/or time data.

Returns

Return type *Detector*

Raises **ValueError** – If the tally data does not appear to be Serpent 2 tally data

meshPlot (*xdim='x', ydim='y', what='tallies', fixed=None, ax=None, cmap=None, cbarLabel=None, logColor=False, xlabel=None, ylabel=None, logx=False, logy=False, loglog=False, title=None, thresh=None, **kwargs*)

Plot tally data as a function of two bin types on a cartesian mesh.

Parameters

- **xdim** (*str*) – Primary dimension - will correspond to x-axis on plot. Defaults to “x”
- **ydim** (*str*) – Secondary dimension - will correspond to y-axis on plot. Defaults to “y”
- **what** (*{'tallies', 'errors'}*) – Color meshes from tally data or uncertainties
- **fixed** (*None or dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **cmap** (*str, optional*) – Valid Matplotlib colormap to apply to the plot.
- **logColor** (*bool*) – If true, apply a logarithmic coloring to the data positive data
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.

- **ylabel** (*str* or *bool*, *optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **title** (*str*) – Title to apply to the figure.
- **thresh** (*float*) – Do not plot data less than or equal to this value.
- **cbarLabel** (*str*) – Label to apply to colorbar. If not given, infer from what
- **kwargs** (*dict*, *optional*) – Addition keyword arguments to pass to `pcolormesh()`

Returns `Ax` on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **serpentTools.SerpentToolsException** – If data to be plotted, with or without constraints, is not 1D
- **KeyError** – If `fixed` is given and `xdim` or `ydim` are contained in `fixed`
- **AttributeError** – If the data set by `what` not in the allowed selection
- **ValueError** – If the data contains negative quantities and `logColor` is `True`

See also:

- `slice()`
- `matplotlib.pyplot.pcolormesh()`

plot (*xdim=None*, *what='tallies'*, *sigma=None*, *fixed=None*, *ax=None*, *xlabel=None*, *ylabel=None*, *steps=False*, *labels=None*, *logx=False*, *logy=False*, *loglog=False*, *legend=None*, *ncol=1*, *title=None*, ***kwargs*)

Simple plot routine for 1- or 2-D data

Parameters

- **xdim** (*str*, *optional*) – Plot the data corresponding to changing this bin, e.g. "energy". Must exist in `indexes`
- **what** (`{'tallies', 'errors'}`) – Primary data to plot
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **fixed** (*None* or *dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (`matplotlib.axes.Axes`, *optional*) – `Ax` on which to plot the data. If not provided, create a new plot
- **xlabel** (*str* or *bool*, *optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label. If `xdim` is given and `xlabel` is `None`, then `xdim` will be applied to the x-axis.

- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **steps** (*bool*) – If true, plot the data as constant inside the respective bins. Sets `drawstyle` to be `steps-post` unless `drawstyle` given in `kwargs`
- **labels** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: `above`, `right`
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `plot()` or `errorbar()` function.

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **SerpentToolsException** – If data contains more than 2 dimensions
- **AttributeError** – If plot data or `indexes` set up.

See also:

- `slice()`
- `spectrumPlot()` better options for plotting energy spectra

reshapedBins()

Obtain multi-dimensional tally, error, and index data

Returns

- **tallies** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally data along each bin index
- **errors** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally relative error along each bin index
- **indexes** (*list of str*) – Ordering of named bin information, e.g. `"xmesh"`, `"energy"`, corresponding to axis in `tallies` and `errors`

Examples

A detector is created with a single bin with two bins values. These could represent tallying two different reaction rates

```
>>> import numpy
>>> from serpentTools import Detector
>>> bins = numpy.ones((2, 12))
>>> bins[1, 0] = 2
>>> bins[1, 4] = 2
>>> bins[:, -2:] = [
...     [5.0, 0.1],
...     [10.0, 0.2]]
>>> det = Detector("reshape", bins=bins)
>>> tallies, errors, indexes = det.resapedBins()
>>> tallies
array([5.0, 10.0])
>>> errors
array([0.1, 0.2])
>>> indexes
["reaction", ]
```

slice (*fixed*, *data*='tallies')

Return a view of the reshaped array where certain axes are fixed

Parameters

- **fixed** (*dict*) – dictionary to aid in the restriction on the multidimensional array. Keys correspond to the various grids present in *indexes* while the values are used to
- **data** ({'tallies', 'errors'}) – Which data set to slice

Returns View into the respective data where certain dimensions have been removed

Return type `numpy.ndarray`

Raises `AttributeError` – If data is not supported

spectrumPlot (*fixed*=None, *ax*=None, *normalize*=True, *xlabel*=None, *ylabel*=None, *steps*=True, *logx*=True, *logy*=False, *loglog*=False, *sigma*=3, *labels*=None, *legend*=None, *ncol*=1, *title*=None, ***kwargs*)

Quick plot of the detector value as a function of energy.

Parameters

- **fixed** (None or *dict*) – Dictionary controlling the reduction in data
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **normalize** (*bool*) – Normalize quantities per unit lethargy
- **xlabel** (*str* or *bool*, optional) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **ylabel** (*str* or *bool*, optional) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **steps** (*bool*) – Plot tally as constant inside bin
- **logx** (*bool*) – Apply a log scale to x axis.

- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **labels** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()` or `matplotlib.pyplot.errorbar()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises **SerpentToolsException** – if number of rows in data not equal to number of energy groups

See also:

- `slice()`

toMatlab (*fileP, reconvert=True, append=True, format='5', longNames=True, compress=True, oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str or file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{ '5', '4' }*) – Format of file to write. `'5'` for MATLAB 5 to 7.2, `'4'` for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{ 'row', 'col' }*) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If `scipy` is not installed

See also:

- `scipy.io.savemat()`

6.1.3 serpentTools.HexagonalDetector

class serpentTools.HexagonalDetector (*name*, *bins=None*, *tallies=None*, *errors=None*, *indexes=None*, *z=None*, *centers=None*, *pitch=None*, *hexType=None*, *grids=None*)

Class for storing detector data with a hexagonal grid

If simply the tally bins are available, it is recommended to use the `fromTallyBins()` class method. This will reshape the data and separate the mean tally [second to last column] and relative errors [last column].

Note: In order to get full functionality from this class, *z*, *centers*, *pitch*, and *hexType* must be set. This can be done by having "Z" and "COORDS" as keys in *grids* and passing *pitch* and *hexType* directly, or by setting the attributes directly. Z grid is expected to be (N, 3) array.

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*, *optional*) – Full 2D tally data from detector file, including tallies and errors in last two columns
- **tallies** (*numpy.ndarray*, *optional*) – Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.
- **errors** (*numpy.ndarray*, *optional*) – Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin. Note: this is a relative error as it would appear in the output file
- **indexes** (*dict*, *optional*) – Dictionary mapping the bin name to its corresponding axis in *tallies* and *errors*, e.g. {"energy": 0}
- **centers** (*numpy.ndarray*, *optional*) – (N, 2) array with centers of each hexagonal element
- **pitch** (*float*, *optional*) – Center to center distance between adjacent hexagons
- **hexType** ({2, 3}, *optional*) – Integer orientation, identical to Serpent detector structure. 2 corresponds to a hexagon with flat faces perpendicular to y-axis. 3 corresponds to a flat faces perpendicular to x-axis
- **grids** (*dict*, *optional*) – Supplemental grids that may be supplied to this detector, including energy points or spatial coordinates.

name

Name of this detector

Type *str*

bins

Full 2D tally data from detector file, including tallies and errors in last two columns

Type *numpy.ndarray* or *None*

tallies

Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.

Type *numpy.ndarray* or *None*

pitch

Center to center distance between hexagons. Must be set before calling `hexPlot()`

Type `float` or `None`

hexType

Integer orientation, identical to Serpent detector structure. 2 corresponds to a hexagon with flat faces perpendicular to y-axis. 3 corresponds to a flat faces perpendicular to x-axis

Type `{2, 3}` or `None`

errors

Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin. Note: this is a relative error as it would appear in the output file

Type `numpy.ndarray` or `None`

indexes

Dictionary mapping the bin name to its corresponding axis in *tallies* and *errors*, e.g. `{"energy": 0}`.

Type `dict` or `None`

energy

Potential underlying energy grid in MeV. Will be `(n_ene, 3)`, where `n_ene` is the number of values in the energy grid. Each row `energy[j]` will be the low point, high point, and mid point of the energy bin `j`.

Type `numpy.ndarray` or `None`

coords

Centers of hexagonal meshes in XY plane

Type `numpy.ndarray` or `None`

z

Z Grid

Type `numpy.ndarray` or `None`

compare (*other*, *lower*=0, *upper*=10, *sigma*=2, *verbosity*=None)

Compare the results of this reader to another.

For values without uncertainties, the upper and lower arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

classmethod `fromTallyBins` (*name*, *bins*, *grids=None*)

Create a detector instance from 2D detector data

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*) – 2D array taken from Serpent. Expected to have either 12 or 13 columns, where the latter indicates a time bin has been added.
- **grids** (*dict*, *optional*) – Dictionary of underlying energy, space, and/or time data.

Returns

Return type *Detector*

Raises **ValueError** – If the tally data does not appear to be Serpent 2 tally data

hexPlot (*what='tallies'*, *fixed=None*, *ax=None*, *cmap=None*, *thresh=None*, *logColor=False*, *xlabel=None*, *ylabel=None*, *logx=False*, *logy=False*, *loglog=False*, *title=None*, *normalizer=None*, *cbarLabel=None*, *borderpad=2.5*, ***kwargs*)

Create and return a hexagonal mesh plot.

Parameters

- **what** (*{'tallies', 'errors'}*, *optional*) – Quantity to plot. Defaults to "tallies"
- **fixed** (*dict*, *optional*.) – Dictionary of slicing arguments to pass to `slice()`. If not provided, detector must be defined with a 2D grid.
- **ax** (*matplotlib.axes.Axes*, *optional*) – Ax on which to plot the data. If not provided, create a new plot
- **thresh** (*float*, *optional*) – Threshold value for plotting values. A hexagon must have a value greater than this quantity in order to be drawn.
- **cmap** (*str*, *optional*) – Valid Matplotlib colormap to apply to the plot.
- **{logColor}** –
- **xlabel** (*str or bool*, *optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **ylabel** (*str or bool*, *optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **title** (*str*) – Title to apply to the figure.

- **borderpad** (*int or float, optional*) – Percentage of total plot to apply as a border. A value of zero means that the extreme edges of the hexagons will touch the x and y axis.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.patches.RegularPolygon`

Raises **AttributeError** – If *pitch* and *hexType* are not set.

meshPlot (*xdim, ydim, what='tallies', fixed=None, ax=None, cmap=None, logColor=False, xlabel=None, ylabel=None, logx=False, logy=False, loglog=False, title=None, **kwargs*)
Plot tally data as a function of two bin types on a cartesian mesh.

Parameters

- **xdim** (*str*) – Primary dimension - will correspond to x-axis on plot
- **ydim** (*str*) – Secondary dimension - will correspond to y-axis on plot
- **what** (*{'tallies', 'errors'}*) – Color meshes from tally data or uncertainties
- **fixed** (*None or dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **cmap** (*str, optional*) – Valid Matplotlib colormap to apply to the plot.
- **logColor** (*bool*) – If true, apply a logarithmic coloring to the data positive data
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **title** (*str*) – Title to apply to the figure.
- **thresh** (*float*) – Do not plot data less than or equal to this value.
- **cbarLabel** (*str*) – Label to apply to colorbar. If not given, infer from what
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `pcolormesh()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **serpentTools.SerpentToolsException** – If data to be plotted, with or without constraints, is not 1D
- **KeyError** – If *fixed* is given and *xdim* or *ydim* are contained in *fixed*
- **AttributeError** – If the data set by *what* not in the allowed selection
- **ValueError** – If the data contains negative quantities and *logColor* is True

See also:

- `slice()`
- `matplotlib.pyplot.pcolormesh()`

plot (*xdim=None, what='tallies', sigma=None, fixed=None, ax=None, xlabel=None, ylabel=None, steps=False, labels=None, logx=False, logy=False, loglog=False, legend=None, ncol=1, title=None, **kwargs*)

Simple plot routine for 1- or 2-D data

Parameters

- **xdim** (*str, optional*) – Plot the data corresponding to changing this bin, e.g. "energy". Must exist in *indexes*
- **what** (*{'tallies', 'errors'}*) – Primary data to plot
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **fixed** (*None or dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label. If xdim is given and xlabel is None, then xdim will be applied to the x-axis.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **steps** (*bool*) – If true, plot the data as constant inside the respective bins. Sets drawstyle to be steps-post unless drawstyle given in kwargs
- **labels** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `plot()` or `errorbar()` function.

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **SerpentToolsException** – If data contains more than 2 dimensions
- **AttributeError** – If plot data or *indexes* set up.

See also:

- *slice()*
- *spectrumPlot()* better options for plotting energy spectra

reshapedBins()

Obtain multi-dimensional tally, error, and index data

Returns

- **tallies** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally data along each bin index
- **errors** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally relative error along each bin index
- **indexes** (*list of str*) – Ordering of named bin information, e.g. "xmesh", "energy", corresponding to axis in **tallies** and **errors**

Examples

A detector is created with a single bin with two bins values. These could represent tallying two different reaction rates

```
>>> import numpy
>>> from serpentTools import Detector
>>> bins = numpy.ones((2, 12))
>>> bins[1, 0] = 2
>>> bins[1, 4] = 2
>>> bins[:, -2:] = [
...     [5.0, 0.1],
...     [10.0, 0.2]]
>>> det = Detector("reshape", bins=bins)
>>> tallies, errors, indexes = det.reshapedBins()
>>> tallies
array([5.0, 10.0])
>>> errors
array([0.1, 0.2])
>>> indexes
["reaction", ]
```

slice (*fixed*, *data*='tallies')

Return a view of the reshaped array where certain axes are fixed

Parameters

- **fixed** (*dict*) – dictionary to aid in the restriction on the multidimensional array. Keys correspond to the various grids present in *indexes* while the values are used to
- **data** (*{'tallies', 'errors'}*) – Which data set to slice

Returns View into the respective data where certain dimensions have been removed

Return type *numpy.ndarray*

Raises **AttributeError** – If data is not supported

spectrumPlot (*fixed=None, ax=None, normalize=True, xlabel=None, ylabel=None, steps=True, logx=True, logy=False, loglog=False, sigma=3, labels=None, legend=None, ncol=1, title=None, **kwargs*)

Quick plot of the detector value as a function of energy.

Parameters

- **fixed** (*None* or *dict*) – Dictionary controlling the reduction in data
- **ax** (*matplotlib.axes.Axes*, optional) – Ax on which to plot the data. If not provided, create a new plot
- **normalize** (*bool*) – Normalize quantities per unit lethargy
- **xlabel** (*str* or *bool*, optional) – Label to apply to the x-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **ylabel** (*str* or *bool*, optional) – Label to apply to the y-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **steps** (*bool*) – Plot tally as constant inside bin
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **labels** (*None* or *iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **legend** (*bool* or *str* or *None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict*, optional) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()` or `matplotlib.pyplot.errorbar()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises `SerpentToolsException` – if number of rows in data not equal to number of energy groups

See also:

- `slice()`

toMatlab (*fileP, reconvert=True, append=True, format='5', longNames=True, compress=True, oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str* or *file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (`{ '5', '4' }`) – Format of file to write. `'5'` for MATLAB 5 to 7.2, `'4'` for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (`{ 'row', 'col' }`) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

6.1.4 serpentTools.CylindricalDetector

class `serpentTools.CylindricalDetector` (*name*, *bins=None*, *tallies=None*, *errors=None*, *indexes=None*, *grids=None*)

Class for storing detector data with a cylindrical mesh

If simply the tally bins are available, it is recommended to use the `fromTallyBins()` class method. This will reshape the data and separate the mean tally [second to last column] and relative errors [last column].

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray, optional*) – Full 2D tally data from detector file, including tallies and errors in last two columns
- **tallies** (*numpy.ndarray, optional*) – Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.
- **errors** (*numpy.ndarray, optional*) – Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin. Note: this is a relative error as it would appear in the output file
- **indexes** (*collections.OrderedDict, optional*) – Dictionary mapping the bin name to its corresponding axis in *tallies* and *errors*, e.g. `{"energy": 0}`
- **grids** (*dict, optional*) – Supplemental grids that may be supplied to this detector, including energy points or spatial coordinates.

name

Name of this detector

Type *str*

bins

Full 2D tally data from detector file, including tallies and errors in last two columns

Type `numpy.ndarray`

tallies

Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.

Type `numpy.ndarray`

errors

Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin.
Note: this is a relative error as it would appear in the output file

Type `numpy.ndarray`

indexes

Dictionary mapping the bin name to its corresponding axis in `tallies` and `errors`, e.g. `{"energy": 0}`.

Type `collections.OrderedDict`

energy

Potential underlying energy grid in MeV. Will be `(n_ene, 3)`, where `n_ene` is the number of values in the energy grid. Each row `energy[j]` will be the low point, high point, and mid point of the energy bin `j`.

Type `numpy.ndarray` or `None`

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the `upper` and `lower` arguments control what passes and what messages get raised. If a quantity in `other` is less than `lower` percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than `upper` percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

classmethod **fromTallyBins** (*name*, *bins*, *grids=None*)

Create a detector instance from 2D detector data

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*) – 2D array taken from Serpent. Expected to have either 12 or 13 columns, where the latter indicates a time bin has been added.
- **grids** (*dict, optional*) – Dictionary of underlying energy, space, and/or time data.

Returns

Return type *Detector*

Raises **ValueError** – If the tally data does not appear to be Serpent 2 tally data

meshPlot (*xdim, ydim, what='tallies', fixed=None, ax=None, cmap=None, logColor=False, xlabel=None, ylabel=None, logx=False, logy=False, loglog=False, title=None, **kwargs*)
 Plot tally data as a function of two bin types on a cartesian mesh.

Parameters

- **xdim** (*str*) – Primary dimension - will correspond to x-axis on plot
- **ydim** (*str*) – Secondary dimension - will correspond to y-axis on plot
- **what** (*{'tallies', 'errors'}*) – Color meshes from tally data or uncertainties
- **fixed** (*None or dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **cmap** (*str, optional*) – Valid Matplotlib colormap to apply to the plot.
- **logColor** (*bool*) – If true, apply a logarithmic coloring to the data positive data
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **title** (*str*) – Title to apply to the figure.
- **thresh** (*float*) – Do not plot data less than or equal to this value.
- **cbarLabel** (*str*) – Label to apply to colorbar. If not given, infer from what
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `pcolormesh()`

Returns Ax on which the data was plotted.

Return type *matplotlib.axes.Axes*

Raises

- **serpentTools.SerpentToolsException** – If data to be plotted, with or without constraints, is not 1D

- **KeyError** – If `fixed` is given and `xdim` or `ydim` are contained in `fixed`
- **AttributeError** – If the data set by `what` not in the allowed selection
- **ValueError** – If the data contains negative quantities and `logColor` is `True`

See also:

- `slice()`
- `matplotlib.pyplot.pcolormesh()`

plot (`xdim=None`, `what='tallies'`, `sigma=None`, `fixed=None`, `ax=None`, `xlabel=None`, `ylabel=None`, `steps=False`, `labels=None`, `logx=False`, `logy=False`, `loglog=False`, `legend=None`, `ncol=1`, `title=None`, `**kwargs`)

Simple plot routine for 1- or 2-D data

Parameters

- **xdim** (`str`, *optional*) – Plot the data corresponding to changing this bin, e.g. "energy". Must exist in `indexes`
- **what** (`{'tallies', 'errors'}`) – Primary data to plot
- **sigma** (`int`) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **fixed** (`None` or `dict`) – Dictionary controlling the reduction in data down to one dimension
- **ax** (`matplotlib.axes.Axes`, *optional*) – Ax on which to plot the data. If not provided, create a new plot
- **xlabel** (`str` or `bool`, *optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label. If `xdim` is given and `xlabel` is `None`, then `xdim` will be applied to the x-axis.
- **ylabel** (`str` or `bool`, *optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **steps** (`bool`) – If true, plot the data as constant inside the respective bins. Sets `drawstyle` to be `steps-post` unless `drawstyle` given in `kwargs`
- **labels** (`None` or *iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **logx** (`bool`) – Apply a log scale to x axis.
- **logy** (`bool`) – Apply a log scale to y axis.
- **loglog** (`bool`) – Apply a log scale to both axes.
- **legend** (`bool` or `str` or `None`) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: `above`, `right`
- **ncol** (`int`) – Integer number of columns to apply to the legend.
- **title** (`str`) – Title to apply to the figure.
- **kwargs** (`dict`, *optional*) – Addition keyword arguments to pass to `plot()` or `errorbar()` function.

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **SerpentToolsException** – If data contains more than 2 dimensions
- **AttributeError** – If plot data or *indexes* set up.

See also:

- *slice()*
- *spectrumPlot()* better options for plotting energy spectra

reshapedBins()

Obtain multi-dimensional tally, error, and index data

Returns

- **tallies** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally data along each bin index
- **errors** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally relative error along each bin index
- **indexes** (*list of str*) – Ordering of named bin information, e.g. "xmesh", "energy", corresponding to axis in *tallies* and *errors*

Examples

A detector is created with a single bin with two bins values. These could represent tallying two different reaction rates

```
>>> import numpy
>>> from serpentTools import Detector
>>> bins = numpy.ones((2, 12))
>>> bins[1, 0] = 2
>>> bins[1, 4] = 2
>>> bins[:, -2:] = [
...     [5.0, 0.1],
...     [10.0, 0.2]]
>>> det = Detector("reshape", bins=bins)
>>> tallies, errors, indexes = det.reshapedBins()
>>> tallies
array([5.0, 10.0])
>>> errors
array([0.1, 0.2])
>>> indexes
["reaction", ]
```

slice (*fixed*, *data*='tallies')

Return a view of the reshaped array where certain axes are fixed

Parameters

- **fixed** (*dict*) – dictionary to aid in the restriction on the multidimensional array. Keys correspond to the various grids present in *indexes* while the values are used to
- **data** (*{'tallies', 'errors'}*) – Which data set to slice

Returns View into the respective data where certain dimensions have been removed

Return type `numpy.ndarray`

Raises `AttributeError` – If data is not supported

spectrumPlot (*fixed=None, ax=None, normalize=True, xlabel=None, ylabel=None, steps=True, logx=True, logy=False, loglog=False, sigma=3, labels=None, legend=None, ncol=1, title=None, **kwargs*)

Quick plot of the detector value as a function of energy.

Parameters

- **fixed** (*None* or *dict*) – Dictionary controlling the reduction in data
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **normalize** (*bool*) – Normalize quantities per unit lethargy
- **xlabel** (*str* or *bool*, optional) – Label to apply to the x-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **ylabel** (*str* or *bool*, optional) – Label to apply to the y-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **steps** (*bool*) – Plot tally as constant inside bin
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **labels** (*None* or *iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **legend** (*bool* or *str* or *None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict*, optional) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()` or `matplotlib.pyplot.errorbar()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises `SerpentToolsException` – if number of rows in data not equal to number of energy groups

See also:

- `slice()`

toMatlab (*fileP*, *reconvert=True*, *append=True*, *format='5'*, *longNames=True*, *compress=True*, *oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str* or *file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{ '5', '4' }*) – Format of file to write. `'5'` for MATLAB 5 to 7.2, `'4'` for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{ 'row', 'col' }*) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

6.1.5 serpentTools.SphericalDetector

class `serpentTools.SphericalDetector` (*name*, *bins=None*, *tallies=None*, *errors=None*, *indexes=None*, *grids=None*)

Class for storing detector data with multiple bins

If simply the tally bins are available, it is recommended to use the `fromTallyBins()` class method. This will reshape the data and separate the mean tally [second to last column] and relative errors [last column].

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*) – Full 2D tally data from detector file, including tallies and errors in last two columns
- **tallies** (*numpy.ndarray*) – Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.
- **errors** (*numpy.ndarray*) – Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin. Note: this is a relative error as it would appear in the output file
- **indexes** (*dict*) – Dictionary mapping the bin name to its corresponding axis in `tallies` and `errors`, e.g. `{"energy": 0}`. Optional
- **grids** (*dict*) – Supplemental grids that may be supplied to this detector, including energy points or spatial coordinates.

name

Name of this detector

Type `str`

bins

Full 2D tally data from detector file, including tallies and errors in last two columns

Type `numpy.ndarray`

tallies

Reshaped tally data such that each dimension corresponds to a unique bin, such as energy or spatial bin.

Type `numpy.ndarray`

errors

Reshaped error data such that each dimension corresponds to a unique bin, such as energy or spatial bin.

Note: this is a relative error as it would appear in the output file

Type `numpy.ndarray`

indexes

Dictionary mapping the bin name to its corresponding axis in *tallies* and *errors*, e.g. {"energy": 0}.

Type `dict`

energy

Potential underlying energy grid in MeV. Will be `(n_ene, 3)`, where `n_ene` is the number of values in the energy grid. Each row `energy[j]` will be the low point, high point, and mid point of the energy bin `j`.

Type `numpy.ndarray` or `None`

compare (*other*, *lower*=0, *upper*=10, *sigma*=2, *verbosity*=None)

Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If *other* is not of the same class as this class nor a subclass of this class

- **ValueError** – If upper > lower, If sigma, lower, or upper are negative

classmethod fromTallyBins (*name, bins, grids=None*)

Create a detector instance from 2D detector data

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*) – 2D array taken from Serpent. Expected to have either 12 or 13 columns, where the latter indicates a time bin has been added.
- **grids** (*dict, optional*) – Dictionary of underlying energy, space, and/or time data.

Returns

Return type *Detector*

Raises **ValueError** – If the tally data does not appear to be Serpent 2 tally data

meshPlot (*xdim, ydim, what='tallies', fixed=None, ax=None, cmap=None, logColor=False, xlabel=None, ylabel=None, logx=False, logy=False, loglog=False, title=None, **kwargs*)
 Plot tally data as a function of two bin types on a cartesian mesh.

Parameters

- **xdim** (*str*) – Primary dimension - will correspond to x-axis on plot
- **ydim** (*str*) – Secondary dimension - will correspond to y-axis on plot
- **what** (*{'tallies', 'errors'}*) – Color meshes from tally data or uncertainties
- **fixed** (*None or dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **cmap** (*str, optional*) – Valid Matplotlib colormap to apply to the plot.
- **logColor** (*bool*) – If true, apply a logarithmic coloring to the data positive data
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **title** (*str*) – Title to apply to the figure.
- **thresh** (*float*) – Do not plot data less than or equal to this value.
- **cbarLabel** (*str*) – Label to apply to colorbar. If not given, infer from what
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `pcolormesh()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **`serpentTools.SerpentToolsException`** – If data to be plotted, with or without constraints, is not 1D
- **`KeyError`** – If `fixed` is given and `xdim` or `ydim` are contained in `fixed`
- **`AttributeError`** – If the data set by `what` not in the allowed selection
- **`ValueError`** – If the data contains negative quantities and `logColor` is `True`

See also:

- `slice()`
- `matplotlib.pyplot.pcolormesh()`

plot (*xdim=None, what='tallies', sigma=None, fixed=None, ax=None, xlabel=None, ylabel=None, steps=False, labels=None, logx=False, logy=False, loglog=False, legend=None, ncol=1, title=None, **kwargs*)

Simple plot routine for 1- or 2-D data

Parameters

- **`xdim`** (*str, optional*) – Plot the data corresponding to changing this bin, e.g. "energy". Must exist in `indexes`
- **`what`** (*{'tallies', 'errors'}*) – Primary data to plot
- **`sigma`** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **`fixed`** (*None or dict*) – Dictionary controlling the reduction in data down to one dimension
- **`ax`** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **`xlabel`** (*str or bool, optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label. If `xdim` is given and `xlabel` is `None`, then `xdim` will be applied to the x-axis.
- **`ylabel`** (*str or bool, optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **`steps`** (*bool*) – If true, plot the data as constant inside the respective bins. Sets `drawstyle` to be `steps-post` unless `drawstyle` given in `kwargs`
- **`labels`** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **`logx`** (*bool*) – Apply a log scale to x axis.
- **`logy`** (*bool*) – Apply a log scale to y axis.
- **`loglog`** (*bool*) – Apply a log scale to both axes.
- **`legend`** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: `above`, `right`
- **`ncol`** (*int*) – Integer number of columns to apply to the legend.

- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict*, *optional*) – Addition keyword arguments to pass to `plot()` or `errorbar()` function.

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **SerpentToolsException** – If data contains more than 2 dimensions
- **AttributeError** – If plot data or *indexes* set up.

See also:

- `slice()`
- `spectrumPlot()` better options for plotting energy spectra

reshapedBins()

Obtain multi-dimensional tally, error, and index data

Returns

- **tallies** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally data along each bin index
- **errors** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally relative error along each bin index
- **indexes** (*list of str*) – Ordering of named bin information, e.g. "xmesh", "energy", corresponding to axis in *tallies* and *errors*

Examples

A detector is created with a single bin with two bins values. These could represent tallying two different reaction rates

```
>>> import numpy
>>> from serpentTools import Detector
>>> bins = numpy.ones((2, 12))
>>> bins[1, 0] = 2
>>> bins[1, 4] = 2
>>> bins[:, -2:] = [
...     [5.0, 0.1],
...     [10.0, 0.2]]
>>> det = Detector("reshape", bins=bins)
>>> tallies, errors, indexes = det.reshapedBins()
>>> tallies
array([5.0, 10.0])
>>> errors
array([0.1, 0.2])
>>> indexes
["reaction", ]
```

slice (*fixed*, *data*='tallies')

Return a view of the reshaped array where certain axes are fixed

Parameters

- **fixed** (*dict*) – dictionary to aid in the restriction on the multidimensional array. Keys correspond to the various grids present in *indexes* while the values are used to
- **data** ({'tallies', 'errors'}) – Which data set to slice

Returns View into the respective data where certain dimensions have been removed

Return type `numpy.ndarray`

Raises `AttributeError` – If data is not supported

spectrumPlot (*fixed=None, ax=None, normalize=True, xlabel=None, ylabel=None, steps=True, logx=True, logy=False, loglog=False, sigma=3, labels=None, legend=None, ncol=1, title=None, **kwargs*)

Quick plot of the detector value as a function of energy.

Parameters

- **fixed** (*None or dict*) – Dictionary controlling the reduction in data
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **normalize** (*bool*) – Normalize quantities per unit lethargy
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **steps** (*bool*) – Plot tally as constant inside bin
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **labels** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()` or `matplotlib.pyplot.errorbar()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises `SerpentToolsException` – if number of rows in data not equal to number of energy groups

See also:

- `slice()`

toMatlab (*fileP*, *reconvert=True*, *append=True*, *format='5'*, *longNames=True*, *compress=True*, *oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str* or *file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{'5', '4'}*) – Format of file to write. `'5'` for MATLAB 5 to 7.2, `'4'` for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{'row', 'col'}*) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises **ImportError** – If *scipy* is not installed

See also:

- `scipy.io.savemat()`

6.2 Supporting Classes

<i>BranchContainer</i>	Class that stores data for a single branch.
<i>DepletedMaterial</i>	Base class for storing material data from a depleted material file
<i>HomogUniv</i>	Class for storing homogenized universe specifications and retrieving them
<i>UnivTuple</i>	Convenient identifier for universes
<i>XSDData</i>	Base class for storing cross section data an xsplot file

6.2.1 serpentTools.objects.BranchContainer

class `serpentTools.objects.BranchContainer` (*filePath*, *branchID*, *branchNames*, *stateData*)

Class that stores data for a single branch.

This container acts like a dictionary, mapping *UnivTuple* to *HomogUniv* corresponding to a specific branch state. As such, there is no need for the *universes* dictionary that previously served this purpose. However, it is provided for compatibility but will be removed after 0.9.0

The *BranchingReader* stores branch variables and branched group constant data inside these container objects. These are used in turn to create *HomogUniv* objects for storing group constant data.

Parameters

- **filePath** (*str*) – Path to input file from which this container was connected
- **branchID** (*int*) – Index for the run for this branch
- **branchNames** (*tuple*) – Name of branches provided for this universe
- **stateData** (*dict*) – key: value pairs for branch variables

stateData

Name: value pairs for the variables defined on each branch card

Type *dict*

universes

Deprecated since version 0.8.0: Treat this object as the universes dictionary instead

Type *dict*

__contains__ ()

True if D has a key k, else False.

__getitem__ ()

x.__getitem__(y) <==> x[y]

__iter__ ()

Implement iter(self).

__len__ ()

Return len(self).

__setitem__ (*key, value*)

Set self[key] to value.

clear () → None. Remove all items from D.

copy () → a shallow copy of D

fromkeys ()

Returns a new dict with keys from iterable and values equal to value.

get (*k*, *d*) → D[k] if k in D, else d. d defaults to None.

getUniv (*univID*, *burnup=None*, *index=None*, *days=None*)

Return a specific universe given the ID and time of interest

Parameters

- **univID** (*str*) – Unique ID for the desired universe
- **burnup** (*float*, *optional*) – Burnup [MWd/kgU] of the desired universe
- **index** (*int*, *optional*) – Point of interest in the burnup index
- **days** (*float*, *optional*) – Point in time [d] for the desired universe

Returns Requested universe

Return type *HomogUniv*

Raises

- **KeyError** – If the requested universe could not be found
- **serpentTools.SerpentToolsException** – If neither burnup nor index are given

items () → a set-like object providing a view on D's items

keys () → a set-like object providing a view on D's keys

property orderedUniv

Universe keys sorted by ID and by burnup

pop (*k*, *d*) → *v*, remove specified key and return the corresponding value.

If key is not found, *d* is returned if given, otherwise `KeyError` is raised

popitem () → (*k*, *v*), remove and return some (key, value) pair as a

2-tuple; but raise `KeyError` if *D* is empty.

setdefault (*k*, *d*) → *D.get(k,d)*, also set *D[k]=d* if *k* not in *D*

update (*other*)

Update with contents of another `BranchContainer`

values () → an object providing a view on *D*'s values

6.2.2 serpentTools.objects.DepletedMaterial

class `serpentTools.objects.DepletedMaterial` (*name*, *metadata*)

Base class for storing material data from a depleted material file

Many of the instance attributes are shortcuts for accessing data in the underlying dictionary. For example, the following command fetch the same data:

```
>>> m.data["adens"]
>>> m["adens"]
>>> m.adens
```

With one exception: the attribute-based accessing is guaranteed to not raise an error if the data has not been loaded into the dictionary. This may be the case if a file was read using filtering settings and `adens` was not read.

Parameters

- **name** (*str*) – Name of this material
- **metadata** (*dict*) – Dictionary with file metadata

data

Main dictionary of arrays from the output file

Type `dict`

zai

Isotopic ZZAAAI identifiers like 922350. Ordered like the rows of the data arrays

Type list of int

names

Isotope names like "U235". Ordered like the rows of the data arrays

Type list of str

days

Time in days for each column in the data arrays

Type `numpy.ndarray`

burnup

Burnup vector for this specific material

Type `numpy.ndarray` or `None`

volume

Volume of this material over time

Type `numpy.ndarray` or `None`

adens

2D array of atom densities in atoms/b-cm

Type `numpy.ndarray` or `None`

mdens

2D array of mass densities in g/cm³

Type `numpy.ndarray` or `None`

activity

2D array of activities in Bq

Type `numpy.ndarray` or `None`

decayHeat

2D array of decay heats in W

Type `numpy.ndarray` or `None`

spontaneousFissionRate

2D array of spontaneous fission rate in fission per second

Type `numpy.ndarray` or `None`

photonProdRate

2D array of photon emission rate in photons per second

Type `numpy.ndarray` or `None`

ingTox

2D array of ingestion toxicity in sieverts

Type `numpy.ndarray` or `None`

inhTox

2D array of inhalation toxicity in sieverts

Type `numpy.ndarray` or `None`

__getitem__ (*item*)

Retrieve a value from the data dictionary

addData (*variable*, *rawData*)

Add data straight from the file onto a variable.

Parameters

- **variable** (*str*) – Name of the variable directly from SERPENT
- **rawData** (*list*) – List of strings corresponding to the raw data from the file

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the upper and lower arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have an error message printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float or int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

get (*key, default=None*)

Retrieve a value from the dictionary, or default if not found

Parameters

- **key** (*str*) – Name of a quantity that may or may not exist in `data`
- **default** (*object, optional*) – Item to return if `key` is not found

Returns `numpy.ndarray` if `key` was found, otherwise `default`

Return type `object`

getValues (*xUnits, yUnits, timePoints=None, names=None, zai=None*)

Return material variable data at specified time points and isotopes

If the quantity `yUnits` corresponds to a vector in the data dictionary, e.g. `burnup` or `volume`, and not something that varies by isotope, then `names` does not have to be given

Parameters

- **xUnits** (*str*) – name of x value to obtain, e.g. `'days'`, `'burnup'`
- **yUnits** (*str*) – name of y value to return, e.g. `'adens'`, `'burnup'`
- **timePoints** (*list or None*) – If given, select the time points according to those specified here. Otherwise, select all points
- **names** (*str or list or None*) – If given, return y values corresponding to these isotope names. Otherwise, return values for all isotopes.
- **zai** (*str or list or None*) – If given, return y values corresponding to isotopes with these ZZAAAI as would be present in `self.zai`. Otherwise, return values for all isotopes.

New in version 0.5.1.

Returns Array of values.

Return type `numpy.array`

Raises

- **AttributeError** – If the names of the isotopes have not been obtained and specific isotopes have been requested
- **KeyError** – If at least one of the days requested is not present
- **TypeError** – If both `names` and `zai` arguments are passed
- **ValueError** – If one isotope cannot be found

plot (*xUnits*, *yUnits=None*, *timePoints=None*, *names=None*, *zai=None*, *ax=None*, *legend=None*, *xlabel=None*, *ylabel=None*, *logx=False*, *logy=False*, *loglog=False*, *labelFmt=None*, *ncol=1*, *title=None*, ***kwargs*)

Plot some data as a function of time for some or all isotopes.

Note: `kwargs` will be passed to the plot for all isotopes. If `c='r'` is passed, to make a plot red, then data for all isotopes plotted will be red and potentially very confusing.

Parameters

- **xUnits** (*str*) – name of x value to obtain, e.g. 'days', 'burnup' If `xUnits` is given and `yUnits` is `None`, then the plotted data will be `xUnits` against 'days'
- **yUnits** (*str*) – name of y value to return, e.g. 'adens', 'burnup'
- **timePoints** (*list or None*) – If given, select the time points according to those specified here. Otherwise, select all points
- **names** (*str or list or None*) – If given, plot values corresponding to these isotope names. Otherwise, plot values for all isotopes.
- **zai** (*int or list or None*) – If given, plot values corresponding to these isotope ZZZAAI values. Otherwise, plot for all isotopes

New in version 0.5.1.

- **ax** (*matplotlib.axes.Axes*, optional) – Ax on which to plot the data. If not provided, create a new plot
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label. Otherwise, use `xUnits`
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label. Otherwise, use `yUnits`
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **labelFmt** (*str, optional*) – Formattable string for labeling the individual plots. If not given, just label as isotope name, e.g. 'U235'. Will make the following substitutions on the `labelFmt` string, if given:

Keyword	Replacement
'mat'	name of this material
'iso'	specific isotope name
'zai'	specific isotope ZZAAAI

- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

See also:

- `getValues()`
- `matplotlib.pyplot.plot()`
- `str.format()` - used for formatting labels

Raises

- **KeyError** – If x axis units are not 'days' nor 'burnup'
- **TypeError** – If both names and zai are given

toDataFrame (*quantity, names=None, zai=None, time='days', multiIndex=False*)

Create a pandas DataFrame for a property of interest

If names and zai are not provided, then the isotope names will be used as the columns.

Parameters

- **quantity** (*str*) – Either a key in *data* or the string name of an attribute like `photonProdRate` for *photonProdRate*
- **names** (*sequence of str, optional*) – Specific isotope names to obtain. Not compatible with *zai*
- **zai** (*sequence of int, optional*) – Specific isotope zai to obtain. Not compatible with *names*
- **time** (*{ "days", "burnup", "step" }, optional*) – What array to use for the index or rows of the DataFrame. Defaults to using *days*, but "burnup" can be passed to use *burnup*, if it is present. The value of "step" will simply create a basic index that starts at 0 and increments by one per row

Returns 2D tabulated representation of the requested array. Columns reflect isotopes, rows represent points in time

Return type `pandas.DataFrame`

6.2.3 serpentTools.objects.HomogUniv

class `serpentTools.objects.HomogUniv` (*name, bu, step, day*)

Class for storing homogenized universe specifications and retrieving them

Parameters

- **name** (*str*) – name of the universe
- **bu** (*float*) – burnup value
- **step** (*float*) – temporal step
- **day** (*float*) – depletion day

name

name of the universe

Type *str*

bu

non-negative burnup value

Type *float* or *int*

step

temporal step

Type *int*

day

non-negative depletion day

Type *float* or *int*

infExp

Expected values for infinite medium group constants

Type *dict*

infUnc

Relative uncertainties for infinite medium group constants

Type *dict*

b1Exp

Expected values for leakage corrected group constants

Type *dict*

b1Unc

Relative uncertainties for leakage-corrected group constants

Type *dict*

gc

Expected values for group constants that do not fit the `INF_` nor `B1_` pattern

Type *dict*

gcUnc

Relative uncertainties for group constants that do not fit the `INF_` nor `B1_` pattern

Type *dict*

reshaped

True if scattering matrices have been reshaped to square matrices. Otherwise, these matrices are stored as vectors.

Type `bool`

groups

Group boundaries from highest to lowest

Type `None` or `numpy.array`

numGroups

Number of energy groups bounded by `groups`

Type `None` or `int`

microGroups

Micro group structure used to produce group constants. Listed from lowest to highest

Type `None` or `numpy.array`

Raises `serpentTools.messages.SerpentToolsException` – If a negative value of burnup, step, or burnup days is passed

__getitem__ (*gcname*)

Return just the group constant with this name, no uncertainty

To return data with uncertainties, or to return uncertainties, use `get()`.

__setitem__ (*gckey, gcvalue*)

Set the expected value of `gckey` to be `gcvalue`

No conversions are placed on the variable name. What you pass is what gets set. For uncertainties, or to convert variable names to `mixedCase`, use `addData()`.

Much like a dictionary, this will overwrite existing data.

Parameters

- **gckey** (*str*) – Group constant name. If it begins with `inf`, value will be placed in `infExp`. If it begins with `b1`, the value will be placed in `b1Exp`. Otherwise it will be placed in `gc`
- **gcvalue** (*numpy.ndarray*) – Corresponding group constant

addData (*variableName, variableValue, uncertainty=False*)

Sets the value of the variable and, optionally, the associate s.d.

New in version 0.5.0: Reshapes scattering matrices according to setting `xs.reshapeScatter`. Matrices are of the form $S[i, j] = \sum_{s, i \rightarrow j}$

Warning: This method will overwrite data for variables that already exist

Parameters

- **variableName** (*str*) – Variable Name
- **variableValue** – Variable Value
- **uncertainty** (*bool*) – Set to `True` if this data is an uncertainty

Raises `TypeError` – If the uncertainty flag is not boolean

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have an error message printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable.
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and error messages will be raised.
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail.
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified.

Return type `bool`

Raises

- **TypeError** – If *other* is not of the same class as this class nor a subclass of this class.
- **ValueError** – If *upper* > *lower*, If *sigma*, *lower*, or *upper* are negative.

compareAttributes (*other*, *lower=0*, *upper=10*, *sigma=2*)

Compare attributes like group structure and burnup. Return the result.

Parameters

- **other** (*HomogUniv*) – Universe against which to compare.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable.
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and error messages will be raised.
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail.

Returns `True` if the attributes agree within specifications.

Return type `bools`

Raises **TypeError** – If *other* is not of the same class as this class nor a subclass of this class.

compareB1Data (*other*, *sigma*)

Return `True` if contents of *b1Exp* and *b1Unc* agree.

Parameters

- **other** (*HomogUniv*) – Object from which to grab group constant dictionaries.

- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **Returns** –
- **bool** – If the dictionaries contain identical values with uncertainties, and if those values have overlapping confidence intervals

Raises **TypeError** – If *other* is not of the same class as this class nor a subclass of this class

compareGCData (*other*, *sigma*)

Return True if contents of *gcExp* and *gcUnc* agree

Parameters

- **other** (*HomogUniv*) – Object from which to grab group constant dictionaries
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **Returns** –
- **bool** – If the dictionaries contain identical values with uncertainties, and if those values have overlapping confidence intervals

Raises **TypeError** – If *other* is not of the same class as this class nor a subclass of this class

compareInfData (*other*, *sigma*)

Return True if contents of *infExp* and *infUnc* agree

Parameters

- **other** (*HomogUniv*) – Object from which to grab group constant dictionaries
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **Returns** –
- **bool** – If the dictionaries contain identical values with uncertainties, and if those values have overlapping confidence intervals

Raises **TypeError** – If *other* is not of the same class as this class nor a subclass of this class

get (*variableName*, *uncertainty=False*)

Gets the value of the variable *VariableName* from the dictionaries

Parameters

- **variableName** (*str*) – Variable Name
- **uncertainty** (*bool*, *optional*) – Boolean Variable- set to True in order to retrieve the uncertainty associated to the expected values

Returns

- *x* – Variable Value
- *dx* – Associated uncertainty if *uncertainty*

Raises

- **TypeError** – If the uncertainty flag is not boolean
- **KeyError** – If the variable requested is not stored on the object

See also:

`__getitem__()`

hasData()

Return True if data is stored on the object.

plot (*qtys*, *limitE=True*, *ax=None*, *logx=None*, *logy=None*, *loglog=None*, *sigma=3*, *xlabel=None*, *ylabel=None*, *legend=None*, *ncol=1*, *steps=True*, *labelFmt=None*, *labels=None*)
Plot homogenized data as a function of energy.

Parameters

- **qtys** (*str* or *iterable*) – Plot this or these value against energy.
- **limitE** (*bool*) – If given, set the maximum energy value to be that of the micro group structure. By default, SERPENT macro group structures can reach 1E37, leading for a very large tail on the plots.
- **ax** (*matplotlib.axes.Axes*, optional) – Ax on which to plot the data. If not provided, create a new plot
- **labels** (*None* or *iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **xlabel** (*str* or *bool*, optional) – Label to apply to the x-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **ylabel** (*str* or *bool*, optional) – Label to apply to the y-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label.
- **legend** (*bool* or *str* or *None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **steps** (*bool*) – If *True*, plot values as constant within energy bins.
- **labelFmt** (*str*, optional) – Formattable string for labeling the individual plots.

String	Replaced value
{k}	Name of variable plotted
{u}	Name of this universe
{b}	Value of burnup in MWd/kgU
{d}	Value of burnup in days
{i}	Burnup index

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

6.2.4 serpentTools.objects.UnivTuple

class serpentTools.objects.UnivTuple

Convenient identifier for universes

Properties can be accessed by position or by attribute name. The latter is preferable as it will be consistent across potential API changes

Parameters

- **universe** (*str*) – Universe from Serpent input
- **burnup** (*float or None*) – Burnup for this universe [MWd/kgU]
- **step** (*int*) – Burnup step
- **days** (*float or None*) – Burnup day

Example

```
>>> x = UnivTuple("0", 0.1, 1, 10.0)
>>> x.universe
"0"
>>> x[0] == x.universe
True
```

__contains__()
Return key in self.

__getitem__()
Return self[key].

__iter__()
Implement iter(self).

__len__()
Return len(self).

property burnup
Alias for field number 1

count (*value*) → integer -- return number of occurrences of value

property days
Alias for field number 3

index (*value* [, *start* [, *stop*]]) → integer -- return first index of value.
Raises ValueError if the value is not present.

property step
Alias for field number 2

property universe
Alias for field number 0

6.2.5 serpentTools.objects.XSData

class `serpentTools.objects.XSData` (*name*, *metadata*, *isIso=False*)

Base class for storing cross section data an xsplot file

Parameters

- **name** (*str*) – Name of this material
- **metadata** (*dict*) – Dictionary with file metadata. Expects `egrid` as a key at least
- **isIso** (*bool*, *optional*) – Flag indicating if this data section is for a single isotope or for a material

isIso

Whether this describes individual isotope XS, or whole-material XS

Type `bool`

MT

Macroscopic cross section integers

Type `list`

MTdescrip

Descriptions of reactions in MT

Type `list`

xsdata

Array of xs data. Rows correspond to items in *MT*

Type `numpy.ndarray`

hasNuData

True if nu data is present

Type `bool`

energies

Energy grid [MeV]

Type `numpy.ndarray`

metadata

File-wide metadata from the reader. Alias for accessing *energies*. Will be removed in the future

Type `dict`

__getitem__

 (*mt*)

Return data corresponding to a given mt

Parameters **mt** (*int*) – Integer MT reaction number

Returns Cross section data for this mt

Return type `numpy.ndarray`

Raises

- **AttributeError** – If *xsdata* is empty
- **KeyError** – If *mt* not found in *MT*

__len__

 ()

Number of reactions stored

compare (*other*, *lower=0*, *upper=10*, *sigma=2*, *verbosity=None*)

Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have an error message printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent. Differences below this will be considered allowable.
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and error messages will be raised.
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail.
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified.

Return type `bool`

Raises

- **TypeError** – If *other* is not of the same class as this class nor a subclass of this class.
- **ValueError** – If *upper* > *lower*, If *sigma*, *lower*, or *upper* are negative.

describe (*mt*)

Return the description for any reaction MT.

Parameters *mt* (*int*) – Integer reaction number, e.g. 102 or -8. Assumes neutrons only.

Returns Description for this reaction.

Return type `str`

get (*mt*, *default=None*)

Return data corresponding to a given *mt* or a default.

Parameters

- **mt** (*int*) – Integer MT reaction number.
- **default** (*object*) – Object to be returned if *mt* is not found.

Returns `numpy.ndarray` if *mt* is found. Otherwise *default*.

Return type `object`

Raises **AttributeError** – If *xldata* is empty.

hasExpectedData ()

Check that the expected data (MT numbers, an energy grid, etc) were collected.

static negativeMTDescription (*mt*)

Descriptions for Serpent negative MT numbers.

These correspond to macroscopic properties, like fission energy production, and for neutrons only. From Serpent Wiki

Parameters `mt` (*int*) – Macroscopic reaction MT. Must be negative

Returns Description

Return type *str*

plot (*mts='all', ax=None, loglog=False, xlabel=None, ylabel=None, logx=True, logy=False, title=None, legend=None, ncol=1, labels=None, **kwargs*)
Plot XS corresponding to their MTs.

Parameters

- **mts** (*int, string, or list of ints*) – If it's a string, it should be 'all'. A single int indicates one MT reaction number. A list should be a list of MT numbers to plot.
- **ax** (*matplotlib.axes.Axes, optional*) – Ax on which to plot the data. If not provided, create a new plot
- **loglog** (*bool*) – Apply a log scale to both axes.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **title** (*str*) – Title to apply to the figure.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **labels** (*str or list of str or dict {int: str}*) – Labels to apply to the plot. Defaults to labeling by MT description. If a string, then mts must be a single integer. If a list of strings, each label will be applied to each entry in mts. If a dictionary, keys must be mts and their labels as values. The number of keys do not have to align with the number of MTs
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises `TypeError` – If MT numbers that don't make sense come up

setData (*chunk*)

Parse data from chunk to np array.

setMTs (*chunk*)

Parse chunk to MT numbers and descriptions

setNuData (*chunk*)

Add fission neutrons per fission data

showMT (*retstring=False*)

Create a pretty-print style string of the MT values available

Parameters **retstring** (*bool*) – Return a string if true. Otherwise, print it

tabulate (*mts='all', colnames=None*)

Returns a pandas table, for pretty tabulation in Jupyter notebooks.

Parameters

- **mts** (*int, string, or list of ints*) – If it's a string, it should be 'all', which is default. A single int indicates one MT reaction number. A list should be a list of MT numbers to plot.
- **colnames** (*any type with string representation*) – Column names for each MT number, if you'd like to change them.

Returns Tabulated representation of the cross section data

Return type `pandas.DataFrame`

Raises

- **ImportError** – If pandas is not installed
- **TypeError** – if MT numbers that don't make sense come up

6.3 Branching Collector

The `xs` module provides classes that condense `HomogUniv` data read in the `serpentTools.BranchingReader`. The goal of these is to arrange the data in a structure that is more beneficial for nodal diffusion codes.

<code>BranchCollector</code>	Main class that collects and arranges branched data
<code>BranchedUniv</code>	Class for storing cross sections for a single universe across branches

6.3.1 serpentTools.xs.BranchCollector

class `serpentTools.xs.BranchCollector` (*source*)

Main class that collects and arranges branched data

New in version 0.7.0.

Parameters **source** (*str or BranchingReader*) – Coefficient file to be read, or a `BranchingReader` that has read the file of interest

filePath

Location of the read file

Type `str`

univIndex

Ordered tuple of universe as they appear in the first dimension of all arrays in `xsTables`

Type `tuple`

universes

Dictionary of universe-specific cross sections. Each entry is a `BranchedUniv` object that stores cross

sections for a single universe.

Type `dict`

xsTables

Dictionary of {k: x} pairs where k corresponds to all cross sections processed and x are large multi-dimensional cross sections. The structure is described with [axis](#)

Type `dict`

property axis

Tuple describing axis of underlying data

Each index contains a description of the changes in group constant data along that axis. Can be set to any iterable, but is converted to a tuple to prevent in-place changes, such as appending to a list or removing one item. Passing an ordered object, `list`, `tuple`, or `numpy.array` is preferred, as the conversion to `tuple` can sort values in un-ordered objects like `set` or `dict` strangely.

Examples

```
>>> col.axis
("Universe", "BOR", "TFU", "Burnup", "Group")
>>> infTot = col.xsTables['infTot']
>>> infTot.shape
(5, 3, 3, 3, 2)
# five universes, three BOR perturbations
# three TFU perturbations, three burnups,
# two energy groups
>>> col.axis = ['u', 'b', 't', 'bu', 'g']
>>> col.axis
('u', 'b', 't', 'bu', 'g')
# pass an unordered set
>>> col.axis = {'u', 'b', 't', 'bu', 'g'}
>>> col.axis
('bu', 'u', 't', 'g', 'b')
# incorrectly set axis
>>> col.axis = [1, 2, 3, 4]
ValueError("Current axis has 5 dimensions, not 4")
```

property burnups

Vector of burnups from coefficient file

Can be set to any iterable that has same number of entries as existing burnup. Automatically converts to `numpy.array`

Examples

```
>>> col.burnups
array([0., 1., 10.])
>>> col.burnups = array([0., 5.6, 56.])
>>> col.burnups
array([0., 5.6, 56.])
>>> col.burnups = [0, 1, 10]
# converted to array of integers
>>> col.burnups
array([0, 1, 10])
```

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```
>>> col.burnups = [0, 1, 2, 3] # not allowed
ValueError("Current burnup vector has 3 items, not 3")
```

collect (*perturbations=None*)

Parse the contents of the file and collect cross sections

Parameters *perturbations* (*tuple or None*) – Tuple where each entry is a state that is perturbed across the analysis, e.g. ("Tfuel", "RhoCool", "CR"). These must appear in the same order as they are ordered in the coefficient file. If *None*, then the number of perturbations will be determined from the coefficient file. This is used to set perturbations and can be adjusted later

classmethod fromFile (*filePath, perturbations=None*)

Create a *BranchCollector* from the contents of the file

Parameters

- **filePath** (*str*) – Location of coefficient file to be read
- **perturbations** (*None or iterable*) – Ordering of perturbation types in coefficient file. If *None*, the number of perturbations will be inferred from file. Otherwise, the number of perturbations must match those in the file. This value can be changed after the fact using *perturbations*, with insight gained from *states*

Returns

- *BranchCollector* object that has processed the contents
- *of the file.*

property perturbations

Iterable indicating the specific perturbation types

Can be set to any iterable, so long as the number of perturbations is preserved. Ordering is important, as changing this does not change the structure of any group constants stored

Example

```
>>> print(col.perturbations)
('BOR', 'TFU')
>>> col.perturbations = ['B', 'T'] # allowed
>>> col.perturbations = [
>>>     'boron conc', 'fuel temp', 'ctrl pos', # not allowed
>>> ]
ValueError("Current number of perturbations is 2, not 3")
```

property states

Iterable describing each perturbation branch.

Length is equal to that of *perturbations*, and the *i*-th index of *states* indicates the values perturbation *perturbations[i]* experiences.

Can be set to any iterable such that the total number of perturbations is preserved

Examples

```
>>> col.states
(('B1000', 'B750', 'nom'), ('FT1200', 'FT600', 'nom'))
# set as numpy array
>>> states = numpy.array([
    [1000., 750., 0.],
    [1200., 600., 900.]
])
>>> col.states = states
>>> col.states
array([[1000., 750., 0],
       [1200., 600., 900]])
# set as individual numpy vectors
>>> col.states = (states[0], states[1])
>>> col.states
(array([1000., 750., 0.]), array([1200., 600., 900.]))
# pass incorrect shape
>>> col.states = (
>>>     (1000, 750, 0), (1200, 600, 900), (0, 1)
>>> )
ValueError("Current number of perturbations is 2, not 3")
# pass incorrect states for one perturbations
>>> cols.states = (
>>>     (1000, 750, 500, 0), (1200, 600, 900)
>>> )
ValueError("Current number of perturbations for state BOR "
           "is 3, not 4")
```

6.3.2 serpentTools.xs.BranchedUniv

class serpentTools.xs.BranchedUniv (univID, collector, ndims=None)

Class for storing cross sections for a single universe across branches

New in version 0.7.0.

Parameters

- **univID** (*str* or *int*) – Unique ID for this universe
- **collector** (*BranchCollector*) – Class that parses and places branched coefficient data
- **ndims** (*int* or *iterable*) – Number of perturbation dimensions

filePath

Location of the file that stores the data on this object

Type *str*

univID

Unique ID for this universe

Type *str* or *int*

collector

Class that parses and places branched coefficient data

Type *BranchCollector*

xsTables

Dictionary with keys representing specific values, e.g. 'infTot' and 'b1Diffcoeff'. Corresponding values are `BranchedDataTable` objects that store cross section and group constant data across perturbation states

Type `dict`

__getitem__ (*key*)

Access the xsTables dictionary

property axis

Tuple describing axis of underlying data

Note: When setting, the universe index of the axis should not be changed. The changes are passed on to `BranchCollector.axis` with an indicator for universe placed in the correct spot

Examples

```
>>> col.axis
('Universe', 'BOR', 'TFU', 'Burnup', 'Group')
>>> u0 = col.universes[0]
>>> u0.axis == col.axis[1:]
True
>>> u0.axis = ['boron conc', 'fuel temp', 'burnup', 'group']
>>> u0.axis
('boron conc', 'fuel temp', 'burnup', 'group')
>>> col.axis
('Universe', 'boron conc', 'fuel temp', 'burnup', 'group')
```

See also:

`BranchCollector.axis`

property burnups

Vector of burnups from coefficient file

See also:

`BranchCollector.burnups`

items()

Iterate over names of cross sections and associated objects

property perturbations

Iterable indicating the specific perturbation types

See also:

`BranchCollector.perturbations`

property states

Iterable describing the names or values of each perturbation branch. Length is equal to that of `perturbations`, and the *i*-th index of states indicates the values perturbation `perturbations[i]` experiences.

See also:

`BranchCollector.states`

SAMPLERS

The `samplers` module contains classes for reading multiple files of the same type, and averaging quantities across all files. This is often used to remove or reduce the stochastic noise associated with a Monte Carlo program. When generating input files for such runs, it is key that each have a unique random seed. This can be facilitated with the `seedFiles()` function, or through the command line with *Random Seed Generation*.

<i>DetectorSampler</i>	Class responsible for reading multiple detector files
<i>SampledDetector</i>	Class to store aggregated detector data
<i>DepletionSampler</i>	Class that reads and stores data from multiple <code>*dep.m</code> files
<i>SampledDepletedMaterial</i>	Class that stores data from a variety of depleted materials

7.1 `serpentTools.samplers.DetectorSampler`

class `serpentTools.samplers.DetectorSampler` (*files*)

Class responsible for reading multiple detector files

The following checks are performed to ensure that all detectors are of similar structure and content

1. Each parser must have the same detectors
2. The reshaped tally data must be of the same size for all detectors

These tests can be skipped by settings `<sampler.skipPrecheck>` to be `False`.

Parameters `files` (*str* or *iterable*) – Single file or iterable (list) of files from which to read. Supports file globs, `*det0.m` expands to all files that end with `det0.m`

detectors

Dictionary of key, values pairs for detector names and corresponding *SampledDetector* instances

Type `dict`

files

Unordered set containing full paths of unique files read

Type `set`

settings

Dictionary of sampler-wide settings

Type `dict`

parsers

Unordered set of all parsers that were successful

Type `set`

map

Dictionary where key, value pairs are files and their corresponding parsers

Type `dict`

__getitem__ (*name*)

Retrieve a detector from *detectors*.

free ()

Remove all parsers and individual containers from memory

process ()

Process the repeated files to obtain true uncertainties

read ()

Read all the files and create parser objects

7.2 serpentTools.samplers.SampledDetector

class `serpentTools.samplers.SampledDetector` (*name*, *allTallies*, *allErrors*, *indexes=None*, *grids=None*)

Class to store aggregated detector data

Parameters

- **name** (*str*) – Name of the detector to be sampled
- **allTallies** (*numpy.ndarray* or *iterable of arrays*) – Array of tally data for each individual detector
- **allErrors** (*numpy.ndarray* or *iterable of arrays*) – Array of absolute tally errors for individual detectors
- **indexes** (*iterable of string*, *optional*) – Iterable naming the bins that correspond to reshaped tally and *errors*.
- **grids** (*dict*, *optional*) – Additional grid information, like spatial or energy-wise grid information.

name

Name of this detector

Type `str`

tallies

Average of tallies from all detectors

Type `numpy.ndarray`

errors

Uncertainty on *tallies* after propagating uncertainty from all individual detectors

Type `numpy.ndarray`

deviation

Deviation across all tallies

Type `numpy.ndarray`

allTallies

Array of tally data from sampled detectors. First dimension is the file index *i*, followed by the tally array for detector *i*.

Type `numpy.ndarray`

allErrors

Array of uncertainties for sampled detectors. Structure is identical to `allTallies`

Type `numpy.ndarray`

grids

Dictionary of additional grid information

Type `dict` or `None`

indexes

Iterable naming the bins that correspond to reshaped `tally` and `errors`. The tuple (`energy`, `ymesh`, `xmesh`) indicates that `tallies` should have three dimensions corresponding to various energy, y-position, and x-position bins. Must be set after `tallies` or `errors` and agree with the shape of each

Type `tuple` or `None`

See also:

`fromDetectors()`

compare (*other*, *lower*=0, *upper*=10, *sigma*=2, *verbosity*=None)

Compare the results of this reader to another.

For values without uncertainties, the `upper` and `lower` arguments control what passes and what messages get raised. If a quantity in `other` is less than `lower` percent different than the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than `upper` percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float* or *int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None* or *str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper` > `lower`, If `sigma`, `lower`, or `upper` are negative

classmethod `fromDetectors` (*name*, *detectors*)

Create a *SampledDetector* from similar detectors

Parameters

- **name** (*str*) – Name of this detector
- **detectors** (iterable of *serpentTools.Detector*) – Iterable that contains detectors to be averaged. These should be structured identically, in shape of the tally data and the underlying grids and indexes.

Returns

Return type *SampledDetector*

Raises

- **TypeError** – If something other than a *serpentTools.Detector* is found
- **ValueError** – If tally data are not shaped consistently
- **KeyError** – If some grid or index information is missing
- **AttributeError** – If one detector is missing grids entirely but grids are present on other grids

classmethod `fromTallyBins` (*name*, *bins*, *grids=None*)

Create a detector instance from 2D detector data

Parameters

- **name** (*str*) – Name of this detector
- **bins** (*numpy.ndarray*) – 2D array taken from Serpent. Expected to have either 12 or 13 columns, where the latter indicates a time bin has been added.
- **grids** (*dict*, *optional*) – Dictionary of underlying energy, space, and/or time data.

Returns

Return type *Detector*

Raises **ValueError** – If the tally data does not appear to be Serpent 2 tally data

meshPlot (*xdim*, *ydim*, *what='tallies'*, *fixed=None*, *ax=None*, *cmap=None*, *cbarLabel=None*, *logColor=False*, *xlabel=None*, *ylabel=None*, *logx=False*, *logy=False*, *loglog=False*, *title=None*, *thresh=None*, ***kwargs*)

Plot tally data as a function of two bin types on a cartesian mesh.

Parameters

- **xdim** (*str*) – Primary dimension - will correspond to x-axis on plot
- **ydim** (*str*) – Secondary dimension - will correspond to y-axis on plot
- **what** (*{'tallies', 'errors'}*) – Color meshes from tally data or uncertainties
- **fixed** (*None* or *dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes*, *optional*) – Ax on which to plot the data. If not provided, create a new plot
- **cmap** (*str*, *optional*) – Valid Matplotlib colormap to apply to the plot.
- **logColor** (*bool*) – If true, apply a logarithmic coloring to the data positive data

- **xlabel** (*str* or *bool*, *optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **ylabel** (*str* or *bool*, *optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **title** (*str*) – Title to apply to the figure.
- **thresh** (*float*) – Do not plot data less than or equal to this value.
- **cbarLabel** (*str*) – Label to apply to colorbar. If not given, infer from what
- **kwargs** (*dict*, *optional*) – Addition keyword arguments to pass to `pcolormesh()`

Returns `Ax` on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **serpentTools.SerpentToolsException** – If data to be plotted, with or without constraints, is not 1D
- **KeyError** – If `fixed` is given and `xdim` or `ydim` are contained in `fixed`
- **AttributeError** – If the data set by `what` not in the allowed selection
- **ValueError** – If the data contains negative quantities and `logColor` is `True`

See also:

- `slice()`
- `matplotlib.pyplot.pcolormesh()`

plot (*xdim=None*, *what='tallies'*, *sigma=None*, *fixed=None*, *ax=None*, *xlabel=None*, *ylabel=None*, *steps=False*, *labels=None*, *logx=False*, *logy=False*, *loglog=False*, *legend=None*, *ncol=1*, *title=None*, ***kwargs*)

Simple plot routine for 1- or 2-D data

Parameters

- **xdim** (*str*, *optional*) – Plot the data corresponding to changing this bin, e.g. "energy". Must exist in *indexes*
- **what** (*{'tallies', 'errors'}*) – Primary data to plot
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **fixed** (*None* or *dict*) – Dictionary controlling the reduction in data down to one dimension
- **ax** (*matplotlib.axes.Axes*, *optional*) – `Ax` on which to plot the data. If not provided, create a new plot

- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label. If `xdim` is given and `xlabel` is `None`, then `xdim` will be applied to the x-axis.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **steps** (*bool*) – If true, plot the data as constant inside the respective bins. Sets `drawstyle` to be `steps-post` unless `drawstyle` given in `kwargs`
- **labels** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: `above`, `right`
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `plot()` or `errorbar()` function.

Returns `Ax` on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises

- **SerpentToolsException** – If data contains more than 2 dimensions
- **AttributeError** – If plot data or `indexes` set up.

See also:

- `slice()`
- `spectrumPlot()` better options for plotting energy spectra

reshapedBins()

Obtain multi-dimensional tally, error, and index data

Returns

- **tallies** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally data along each bin index
- **errors** (*numpy.ndarray*) – Potentially multi-dimensional array corresponding to tally relative error along each bin index
- **indexes** (*list of str*) – Ordering of named bin information, e.g. `"xmesh"`, `"energy"`, corresponding to axis in `tallies` and `errors`

Examples

A detector is created with a single bin with two bins values. These could represent tallying two different reaction rates

```
>>> import numpy
>>> from serpentTools import Detector
>>> bins = numpy.ones((2, 12))
>>> bins[1, 0] = 2
>>> bins[1, 4] = 2
>>> bins[:, -2:] = [
...     [5.0, 0.1],
...     [10.0, 0.2]]
>>> det = Detector("reshape", bins=bins)
>>> tallies, errors, indexes = det.resapedBins()
>>> tallies
array([5.0, 10.0])
>>> errors
array([0.1, 0.2])
>>> indexes
["reaction", ]
```

slice (*fixed*, *data*='tallies')

Return a view of the reshaped array where certain axes are fixed

Parameters

- **fixed** (*dict*) – dictionary to aid in the restriction on the multidimensional array. Keys correspond to the various grids present in *indexes* while the values are used to
- **data** ({'tallies', 'errors'}) – Which data set to slice

Returns View into the respective data where certain dimensions have been removed

Return type `numpy.ndarray`

Raises `AttributeError` – If data is not supported

spectrumPlot (*fixed*=None, *ax*=None, *normalize*=True, *xlabel*=None, *ylabel*=None, *steps*=True, *logx*=True, *logy*=False, *loglog*=False, *sigma*=3, *labels*=None, *legend*=None, *ncol*=1, *title*=None, ***kwargs*)

Quick plot of the detector value as a function of energy.

Parameters

- **fixed** (None or *dict*) – Dictionary controlling the reduction in data
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **normalize** (*bool*) – Normalize quantities per unit lethargy
- **xlabel** (*str* or *bool*, optional) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **ylabel** (*str* or *bool*, optional) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **steps** (*bool*) – Plot tally as constant inside bin
- **logx** (*bool*) – Apply a log scale to x axis.

- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **sigma** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **labels** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **title** (*str*) – Title to apply to the figure.
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()` or `matplotlib.pyplot.errorbar()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises `SerpentToolsException` – if number of rows in data not equal to number of energy groups

See also:

- `slice()`

spreadPlot (*xdim=None, fixed=None, sampleKwargs=None, meanKwargs=None, ax=None, xlabel=None, ylabel=None, logx=False, logy=False, loglog=False, legend=True*)
Plot the mean tally value against all sampled detector data.

Parameters

- **xdim** (*str*) – Bin index to place on the x-axis
- **fixed** (*None or dict*) – Dictionary controlling the reduction in data down to one dimension
- **sampleKwargs** (*dict, optional*) – Additional matplotlib-acceptable arguments to be passed into the plot when plotting data from unique runs, e.g. {"c": k, "alpha": 0.5}.
- **meanKwargs** (*dict, optional*) – Additional matplotlib-acceptable argumentst to be used when plotting the mean value, e.g. {"c": "b", "marker": "o"}
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.

- **loglog** (*bool*) – Apply a log scale to both axes.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

toMatlab (*fileP, reconvert=True, append=True, format='5', longNames=True, compress=True, oned='row'*)

Write a binary MATLAB file from the contents of this object

Parameters

- **fileP** (*str or file-like object*) – Name of the file to write. `.mat` extension is not needed if `append==True`
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{ '5', '4' }*) – Format of file to write. '5' for MATLAB 5 to 7.2, '4' for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{ 'row', 'col' }*) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

Raises `ImportError` – If `scipy` is not installed

See also:

- `scipy.io.savemat()`

7.3 serpentTools.samplers.DepletionSampler

class `serpentTools.samplers.DepletionSampler` (*files*)

Class that reads and stores data from multiple `*dep.m` files

The following checks are performed in order to ensure that depletion files are of similar form:

1. Keys of `materials` dictionary are consistent for all parsers
2. Metadata keys are consistent for all parsers
3. Isotope names and ZZAAA metadata are equal for all parsers

These tests can be skipped by settings `<sampler.skipPrecheck>` to be `False`.

Parameters **files** (*str or iterable*) – Single file or iterable (list) of files from which to read. Supports file globs, `*dep.m` expands to all files that end with `dep.m`

days

Vector of points in time

Type `numpy.ndarray` or `None`

burnup

Nominal burnup in MWd/kgU

Type `numpy.ndarray` or `None`

names

Names of isotopes corresponding to each row in the 2D arrays

Type list of str or `None`

zais

ZZAAAI identifiers for isotopes

Type list of int or `None`

materials

Dictionary with material names as keys and the corresponding `DepletedMaterial` class for that material as values

Type `dict`

metadata

Dictionary with file-wide data names as keys and the corresponding data, e.g. `'zai': [list of zai numbers]`

Deprecated since version 0.9.3: Use attributes like `days` directly

Type `dict`

metadataUncs

Dictionary containing uncertainties in day and burnup vectors

Type `dict`

allMdata

Dictionary where key, value pairs are name of metadata and metadata arrays for all runs. Arrays with be of one greater dimension, as the first index corresponds to the file index.

Type `dict`

files

Unordered set containing full paths of unique files read

Type `set`

settings

Dictionary of sampler-wide settings

Type `dict`

parsers

Unordered set of all parsers that were successful

Type `set`

map

Dictionary where key, value pairs are files and their corresponding parsers

Type `dict`

__getitem__ (*name*)

Retrieve a material from `materials`.

free ()

Remove all parsers and individual containers from memory

iterMaterials()

Yields material names and objects

plot (*xUnits*, *yUnits=None*, *timePoints=None*, *names=None*, *zai=None*, *materials=None*, *ax=None*, *legend=None*, *logx=False*, *logy=False*, *loglog=False*, *labelFmt=None*, *xlabel=None*, *ylabel=None*, *ncol=1*, ***kwargs*)

Plot properties for all materials in this file together.

Parameters

- **xUnits** (*str*) – If *xUnits* is given and *yUnits* is *None*, then the plotted data will be *xUnits* against 'days' name of x value to obtain, e.g. 'days', 'burnup'
- **yUnits** (*str*) – name of y value to return, e.g. 'adens', 'ingTox'
- **timePoints** (*list* or *None*) – If given, select the time points according to those specified here. Otherwise, select all points

Deprecated since version 0.7.0: Will plot against all time points

- **names** (*str* or *list* or *None*) – If given, plot values corresponding to these isotope names. Otherwise, plot values for all isotopes.
- **zai** (*int* or *list* or *None*) – If given, plot values corresponding to these isotope ZZAAAI values. Otherwise, plot for all isotopes

New in version 0.5.1.

- **materials** (*None* or *list*) – Selection of materials from *self.materials* to plot. If *None*, plot all materials, potentially including *tot*
- **ax** (*matplotlib.axes.Axes*, optional) – Ax on which to plot the data. If not provided, create a new plot
- **legend** (*bool* or *str* or *None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **xlabel** (*str* or *bool*, optional) – Label to apply to the x-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label. Otherwise, use *xUnits*
- **ylabel** (*str* or *bool*, optional) – Label to apply to the y-axis. If given as *None*, a label will be determined from other arguments. If not *None* but evaluates to *False*, do not label. Otherwise, use *yUnits*
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **labelFmt** (*str*, optional) – Formattable string for labeling the individual plots. If not given, just label as isotope name, e.g. 'U235'. Will make the following substitutions on the *labelFmt* string, if given:

Keyword	Replacement
'mat '	name of this material
'iso'	specific isotope name
'zai'	specific isotope ZZAAAI

- **ncol** (*int*) – Integer number of columns to apply to the legend.

- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

See also:

- `getValues()`
- `str.format()` - used for formatting labels
- `plot()`

Raises

- **KeyError** – If x axis units are not 'days' nor 'burnup'
- **SerpentToolsException** – If the materials dictionary does not contain any items

process()

Process the repeated files to obtain true uncertainties

read()

Read all the files and create parser objects

7.4 serpentTools.samplers.SampledDepletedMaterial

class `serpentTools.samplers.SampledDepletedMaterial` (*N, name, metadata*)

Class that stores data from a variety of depleted materials

While `adens`, `mdens`, and `burnup` are accessible directly with `material.adens`, all variables read in from the file can be accessed through the `data` dictionary:

```
>>> assert material.adens is material.data['adens']
>>> assert material.adens is material['adens']
# The three methods are equivalent
```

Note: `free()` sets `allData` to an empty dictionary. If `<sampler.freeAll>` is `True`, then `free` will be called after all files have been read and processed.

Parameters

- **N** (*int*) – Number of containers to expect
- **name** (*str*) – Name of this material
- **metadata** (*dict*) – File-wide metadata for this run. Should contain ZAI and names for all isotopes, days, and burnup schedule

data

dictionary that stores all variable data

Type `dict`

zai

Isotopic ZZAAA identifiers, e.g. 93325

Changed in version 0.5.1: Now a list of integers, not strings

Type `list`

names

Names of isotopes, e.g. U235

Type `list`

days

Vector of total, cumulative days of burnup for the run that created this material

Type `numpy.ndarray`

burnup

Vector of total, cumulative burnup [MWd/kgU] for this specific material

Type `numpy.ndarray`

adens

2D array of atomic densities where where row *j* corresponds to isotope *j* and column *i* corresponds to time *i*

Type `numpy.ndarray`

mdens

2D array of mass densities where where row *j* corresponds to isotope *j* and column *i* corresponds to time *i*

Type `numpy.ndarray`

uncertainties

Absolute uncertainties for all variables stored in `data`

Type `dict`

allData

Dictionary where key, value pairs correspond to names of variables stored on this object and arrays of data from all files. The dimensionality will be increased by one, as the first index corresponds to the order in which files were loaded

Type `dict`

__getitem__ (*item*)

Retrieve a value from the data dictionary

compare (*other*, *lower*=0, *upper*=10, *sigma*=2, *verbosity*=None)

Compare the results of this reader to another.

For values without uncertainties, the *upper* and *lower* arguments control what passes and what messages get raised. If a quantity in *other* is less than *lower* percent different that the same quantity on this object, consider this allowable and make no messages. Quantities that are greater than *upper* percent different will have a error messages printed and the comparison will return `False`, but continue. Quantities with difference between these ranges will have warning messages printed.

Parameters

- **other** – Other reader instance against which to compare. Must be a similar class as this one.
- **lower** (*float* or *int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable

- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **verbosity** (*None or str*) – If given, update the verbosity just for this comparison.

Returns `True` if the objects are in agreement with each other according to the parameters specified

Return type `bool`

Raises

- **TypeError** – If `other` is not of the same class as this class nor a subclass of this class
- **ValueError** – If `upper > lower`, If `sigma`, `lower`, or `upper` are negative

finalize()

Produce final uncertainties from all aggregated runs

free()

Clear up data from all sampled parsers

get (*key, default=None*)

Retrieve a value from the dictionary, or default if not found

Parameters

- **key** (*str*) – Name of a quantity that may or may not exist in *data*
- **default** (*object, optional*) – Item to return if `key` is not found

Returns `numpy.ndarray` if `key` was found, otherwise default

Return type `object`

getValues (*xUnits, yUnits, timePoints=None, names=None, zai=None*)

Return material variable data at specified time points and isotopes

If the quantity `yUnits` corresponds to a vector in the `data` dictionary, e.g. `burnup` or `volume`, and not something that varies by isotope, then `names` does not have to be given

Parameters

- **xUnits** (*str*) – name of x value to obtain, e.g. `'days'`, `'burnup'`
- **yUnits** (*str*) – name of y value to return, e.g. `'adens'`, `'burnup'`
- **timePoints** (*list or None*) – If given, select the time points according to those specified here. Otherwise, select all points
- **names** (*str or list or None*) – If given, return y values corresponding to these isotope names. Otherwise, return values for all isotopes.
- **zai** (*str or list or None*) – If given, return y values corresponding to isotopes with these ZZAAAI as would be present in `self.zai`. Otherwise, return values for all isotopes.

New in version 0.5.1.

Returns Array of values.

Return type `numpy.array`

Raises

- **AttributeError** – If the names of the isotopes have not been obtained and specific isotopes have been requested
- **KeyError** – If at least one of the days requested is not present
- **TypeError** – If both `names` and `zai` arguments are passed
- **ValueError** – If one isotope cannot be found

loadFromContainer (*container*)

Copy data from a similar container.

Parameters `container` – Incoming container from which to take data.

Raises

- **`serpentTools.messages.MismatchedContainersError`** – If the incoming container is not the expected type declared at construction
- **`serpentTools.messages.SamplerError`** – If more containers have been loaded than specified at construction

plot (*xUnits*, *yUnits*, *timePoints=None*, *names=None*, *ax=None*, *sigma=3*, *xlabel=None*, *ylabel=None*, *logx=False*, *logy=False*, *loglog=False*, *legend=None*, *ncol=1*, *labelFmt=None*, ***kwargs*)
Plot the average of some data vs. time for some or all isotopes.

Note: `kwargs` will be passed to the errorbar plot for all isotopes. If `c='r'` is passed, to make a plot red, then data for all isotopes plotted will be red and potentially very confusing.

Parameters

- **`xUnits`** (*str*) – name of x value to obtain, e.g. 'days', 'burnup'
- **`yUnits`** (*str*) – name of y value to return, e.g. 'adens', 'burnup'
- **`timePoints`** (*list or None*) – If given, select the time points according to those specified here. Otherwise, select all points
- **`names`** (*list or None*) – If given, return y values corresponding to these isotope names. Otherwise, return values for all isotopes.
- **`ax`** (*matplotlib.axes.Axes*, optional) – Ax on which to plot the data. If not provided, create a new plot
- **`sigma`** (*int*) – Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
- **`xlabel`** (*str or bool*, optional) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **`ylabel`** (*str or bool*, optional) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **`logx`** (*bool*) – Apply a log scale to x axis.
- **`logy`** (*bool*) – Apply a log scale to y axis.
- **`loglog`** (*bool*) – Apply a log scale to both axes.

- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: above, right
- **ncol** (*int*) – Integer number of columns to apply to the legend.
- **labelFmt** (*str, optional*) – Formattable string for labeling the individual plots. If not given, just label as isotope name, e.g. 'U235'. Will make the following substitutions on the labelFmt string, if given:

Keyword	Replacement
'mat'	name of this material
'iso'	specific isotope name
'zai'	specific isotope ZZAAAI

- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.errorbar()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

See also:

- `getValues()`
- `matplotlib.pyplot.errorbar()`

spreadPlot (*xUnits, yUnits, isotope=None, zai=None, sampleKwargs=None, meanKwargs=None, timePoints=None, ax=None, xlabel=None, ylabel=None, logx=False, logy=False, loglog=False, legend=True*)

Plot the mean quantity and data from all sampled files.

Parameters

- **xUnits** (*str*) – name of x value to obtain, e.g. 'days', 'burnup'
- **yUnits** (*str*) – name of y value to return, e.g. 'adens', 'burnup'
- **isotope** (*str, optional*) – Plot data for this isotope
- **zai** (*int, optional*) – Plot data for this isotope. Not allowed if isotope given.
- **sampleKwargs** (*dict, optional*) – Additional matplotlib-acceptable arguments to be passed into the plot when plotting data from unique runs, e.g. {"c": k, "alpha": 0.5}.
- **meanKwargs** (*dict, optional*) – Additional matplotlib-acceptable argumentst to be used when plotting the mean value, e.g. {"c": "b", "marker": "o"}
- **timePoints** (*list or None*) – If given, select the time points according to those specified here. Otherwise, select all points
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as None, a label will be determined from other arguments. If not None but evaluates to False, do not label.

- **ylabel** (*str or bool, optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **legend** (*bool or str or None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: `above`, `right`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

SETTINGS

Presented here are the various settings used by the readers to control what data is stored and how the data is stored. There are specific settings for each reader, and those are of the form `<leader>.<setting>`, so *depletion.materials* is used only by the *DepletionReader*. Without modifying any settings, each reader defaults to storing all of the data present in the output file. Many of the settings instruct the readers to store specific data, such as only materials present in *depletion.materials*.

8.1 Setting Control

Setting control is done using the *rc* global. It acts largely like a dictionary with some validation.

```
class serpentTools.settings.rc
```

```
    __getitem__ ()  
        x.__getitem__(y) <==> x[y]
```

```
    __setitem__ (name, value)  
        Set the value of a specific setting.
```

Parameters

- **name** (*str*) – Full name of the setting
- **value** (*str*) – value to be set

Raises

- **KeyError** – If the value is not one of the allowable options or if the setting does not match an existing setting
- **TypeError** – If the value is not of the correct type

```
    __enter__ ()  
        Use as a context manager to easily reset settings
```

Examples

```
>>> rc["serpentVersion"] = "2.1.30"
>>> rc["serpentVersion"]
"2.1.30"
>>> with rc:
...     rc["serpentVersion"] = "2.1.29"
...     print(rc["serpentVersion"])
"2.1.29"
>>> rc["serpentVersion"]
"2.1.30"
```

The settings are explained below and are used by the readers to control what data are stored when reading from files.

8.2 Shared Settings

There are some settings that are shared between some or all readers. Any setting that does not have a . applies to all readers, such as *verbosity*. Below are a list of setting leaders and the readers impacted by this setting:

Leader	
xs	<i>ResultsReader</i> and <i>BranchingReader</i>

Here are links to locations in the [Examples](#) that display how the settings can be used on the various readers.

Reader	Link to example
<i>BranchingReader</i>	<i>User Control</i>
<i>DepletionReader</i>	<i>Settings</i>

8.3 Default Settings

8.3.1 `branching.floatVariables`

Names of state data variables to convert to floats for each branch:

```
Default: []
Type: list
```

8.3.2 `branching.intVariables`

Name of state data variables to convert to integers for each branch:

```
Default: []
Type: list
```

8.3.3 depletion.materialVariables

Names of variables to store. Empty list -> all variables:

```
Default: []  
Type: list
```

8.3.4 depletion.materials

Names of materials to store. Empty list -> all materials:

```
Default: []  
Type: list
```

8.3.5 depletion.metadataKeys

Non-material data to store, i.e. zai, isotope names, burnup schedule, etc:

```
Default: ['ZAI', 'NAMES', 'DAYS', 'BU']  
Type: list  
Options: [ZAI, NAMES, DAYS, BU]
```

8.3.6 depletion.processTotal

Option to store the depletion data from the TOT block:

```
Default: True  
Type: bool
```

8.3.7 detector.names

List of detectors to store. Empty list -> store all detectors:

```
Default: []  
Type: list
```

8.3.8 microxs.getFY

If true, store the fission yields:

```
Default: True  
Type: bool
```

8.3.9 `microxs.getFlx`

If true, store the group flux ratios:

```
Default: True  
Type: bool
```

8.3.10 `microxs.getXS`

If true, store the micro-group cross sections:

```
Default: True  
Type: bool
```

8.3.11 `sampler.allExist`

True if all the files should exist. Suppresses errors if a file does not exist:

```
Default: True  
Type: bool
```

8.3.12 `sampler.freeAll`

If true, do not retain data from parsers after reading. Limits memory usage after reading:

```
Default: False  
Type: bool
```

8.3.13 `sampler.raiseErrors`

If True, stop at the first error. Otherwise, continue reading but make a note about the error:

```
Default: True  
Type: bool
```

8.3.14 `sampler.skipPrecheck`

If True, no checks are performed prior to preparing data. Set this to be True only if you know all files contain the same data as errors may arise:

```
Default: False  
Type: bool
```

8.3.15 serpentVersion

Version of Serpent:

```
Default: 2.1.31
Type: str
Options: [2.1.29, 2.1.30, 2.1.31]
```

8.3.16 verbosity

Set the level of errors to be shown:

```
Default: warning
Type: str
Options: [critical, error, warning, info, debug]
```

8.3.17 xs.getB1XS

If true, store the critical leakage cross sections:

```
Default: True
Type: bool
```

8.3.18 xs.getInfXS

If true, store the infinite medium cross sections:

```
Default: True
Type: bool
```

8.3.19 xs.reshapeScatter

If true, reshape the scattering matrices to square matrices. By default, these matrices are stored as vectors:

```
Default: False
Type: bool
```

8.3.20 xs.variableExtras

Full SERPENT name of variables to be read:

```
Default: []
Type: list
```

8.3.21 `xs.variableGroups`

Name of variable groups from variables.yaml to be expanded into SERPENT variable to be store:

```
Default: []  
Type: list
```


MISCELLANEOUS

9.1 Data Module

The data module exists to assist with reproducing example problems and the test interface. It should be used sparsely unless following along with an example as it is subject to change.

<code>readDataFile</code>	Return a reader for the data file (test or example) file.
<code>getFile</code>	Retrieve the path to one of the reference or example files

9.1.1 `serpentTools.data.readDataFile`

`serpentTools.data.readDataFile` (*path*, ***kwargs*)

Return a reader for the data file (test or example) file.

All additional keyword arguments will be passed to `serpentTools.read()`.

Parameters *path* (*str*) – The name of the file without any additional directory information

Returns The reader that has processed this file and stored all the data

Return type *object*

Raises **IOError**: – If the file for *path* does not exist

Examples

Obtain a detector file from the examples

```
>>> import serpentTools
>>> d = serpentTools.readDataFile('bwr_det0.m')
>>> d.detectors.keys()
dict_keys(['spectrum', 'xymesh'])
```

See also:

- `serpentTools.read()`

9.1.2 serpentTools.data.getFile

`serpentTools.data.getFile(path)`

Retrieve the path to one of the reference or example files

Parameters `path` (*str*) – The name of the file without any additional directory information

Returns Path to a data file that can be read with one of the readers or with `serpentTools.read()`

Return type `str`

Raises `IOError`: – If no match for `path` exists

9.2 Exceptions

`serpentTools` relies on a few custom exceptions, documented below for convenience.

Note: Developers should rely on built-in exceptions whenever possible. These will be fading out over coming versions.

<code>SerpentToolsException</code>	Base-class for all exceptions in this project
<code>SamplerError</code>	Base-class for errors in sampling process
<code>MismatchedContainersError</code>	Attempting to sample from dissimilar containers

9.2.1 serpentTools.messages.SerpentToolsException

exception `serpentTools.messages.SerpentToolsException`

Base-class for all exceptions in this project

with_traceback()

Exception.with_traceback(tb) – set self.__traceback__ to tb and return self.

9.2.2 serpentTools.messages.SamplerError

exception `serpentTools.messages.SamplerError`

Base-class for errors in sampling process

with_traceback()

Exception.with_traceback(tb) – set self.__traceback__ to tb and return self.

9.2.3 serpentTools.messages.MismatchedContainersError

exception `serpentTools.messages.MismatchedContainersError`

Attempting to sample from dissimilar containers

with_traceback()

Exception.with_traceback(tb) – set self.__traceback__ to tb and return self.

9.3 Random Seed Module

Exposed through the `serpentTools.seed` module are functions to assist in generating repeated input files with unique random seeds. These are used to support the command line sub-command *Random Seed Generation*.

<code>seedFiles</code>	Copy input file multiple times with unique seeds.
<code>generateSeed</code>	Generate a random seed with <code>length</code> digits

9.3.1 serpentTools.seed.seedFiles

`serpentTools.seed.seedFiles(inputFile, numSeeds, seed=None, outputDir=None, link=False, length=10)`

Copy input file multiple times with unique seeds.

Parameters

- **inputFile** (*str*) – Path to input file
- **numSeeds** (*int*) – Number of files to create
- **seed** (*int*) – Optional argument to set the seed of the builtin random number generator
- **outputDir** (*str*) – Path to desired output directory. Files will be copied here. If the folder does not exist, try to make the directory. Assumes path relative to directory that contains the input file
- **link** (*bool*) – If True, do not copy the full file. Instead, create a new file with 'include <inputFile>' and the new seed declaration.
- **length** (*int*) – Number of digits for random seeds

Returns List of the names of all files created

Return type *list*

Raises

- **OSError**: – If the requested input file could not be found and `link` does not evaluate to true.
- **ValueError**: – If the number of requested seeds is not a positive integer, nor can be converted to one, or if the length of the random seeds cannot be converted to a positive integer.
- **TypeError**: – Raised if the values passed to `length` or `nseeds` cannot be converted to integers with `int()`

See also:

`generateSeed()` `random.random.seed()` `random.getrandbits()`

9.3.2 serpentTools.seed.generateSeed

`serpentTools.seed.generateSeed (length)`

Generate a random seed with `length` digits

Parameters `length` (*int*) – Positive number of digits in seed

Returns Randomly generated seed with `length` digits

Return type *int*

Raises

- **ValueError**: – If the value of `length` is non-positive
- **TypeError**: – If `length` is not an integer, nor can be coerced into one with `int()`

VARIABLE GROUPS

The *BranchingReader* and *ResultsReader* can also be used to store cross sections and other group constant data on *HomogUniv* objects. The group constants to be stored are controlled by two distinct settings: *xs.variableExtras* and *xs.variableGroups*. The former includes the names of Serpent variables **exactly** how they appear in the specific output file. The latter variables that are commonly grouped together, such as kinetic parameters or general cross sections, without having to exactly specify the names of each variable. Without adjusting these settings, the *BranchingReader* and *ResultsReader* will store all data present in the file.

Below are the various variable groups that can be used in the *xs.variableGroups* setting. These groups follow an inheritance-like pattern. For example, using Serpent 2.1.30, any group not directly placed in the *2.1.30* block, such as *eig*, will be replaced by those variables present in the *base* block.

Below are the variable groups that correspond to each version of Serpent supported by this project. Under each block, such as *six-ff*, are the original SERPENT_STYLE_VARIABLES and their corresponding variable names converted to mixedCaseNames. This conversion is done to fit the style of the project and reduce a few keystrokes for accessing variable names.

10.1 2.1.31

Variable groups for Serpent 2.1.31 are identical to those from Serpent 2.1.30

10.2 2.1.30

10.2.1 n-balance

- BALA_LOSS_NEUTRON_CAPT → balaLossNeutronCapt
- BALA_LOSS_NEUTRON_CUT → balaLossNeutronCut
- BALA_LOSS_NEUTRON_ERR → balaLossNeutronErr
- BALA_LOSS_NEUTRON_FISS → balaLossNeutronFiss
- BALA_LOSS_NEUTRON_LEAK → balaLossNeutronLeak
- BALA_LOSS_NEUTRON_TOT → balaLossNeutronTot
- BALA_NEUTRON_DIFF → balaNeutronDiff
- BALA_SRC_NEUTRON_FISS → balaSrcNeutronFiss
- BALA_SRC_NEUTRON_NXN → balaSrcNeutronNxn
- BALA_SRC_NEUTRON_SRC → balaSrcNeutronSrc

- BALA_SRC_NEUTRON_TOT → balaSrcNeutronTot
- BALA_SRC_NEUTRON_VR → balaSrcNeutronVr

10.2.2 optimization

- DOUBLE_INDEXING → doubleIndexing
- MG_MAJORANT_MODE → mgMajorantMode
- OPTIMIZATION_MODE → optimizationMode
- RECONSTRUCT_MACROXS → reconstructMacroxs
- RECONSTRUCT_MICROXS → reconstructMicroxs
- SPECTRUM_COLLAPSE → spectrumCollapse

10.2.3 rad-data

- ACTINIDE_ACTIVITY → actinideActivity
- ACTINIDE_DECAY_HEAT → actinideDecayHeat
- ACTINIDE_ING_TOX → actinideIngTox
- ACTINIDE_INH_TOX → actinideInhTox
- ALPHA_DECAY_SOURCE → alphaDecaySource
- CS134_ACTIVITY → cs134Activity
- ELECTRON_DECAY_SOURCE → electronDecaySource
- FISSION_PRODUCT_ACTIVITY → fissionProductActivity
- FISSION_PRODUCT_DECAY_HEAT → fissionProductDecayHeat
- FISSION_PRODUCT_ING_TOX → fissionProductIngTox
- FISSION_PRODUCT_INH_TOX → fissionProductInhTox
- INGENSTION_TOXICITY → ingenstionToxicity
- INHALATION_TOXICITY → inhalationToxicity
- NEUTRON_DECAY_SOURCE → neutronDecaySource
- PHOTON_DECAY_SOURCE → photonDecaySource
- SR90_ACTIVITY → sr90Activity
- TE132_ACTIVITY → tel32Activity
- TOT_ACTIVITY → totActivity
- TOT_DECAY_HEAT → totDecayHeat
- TOT_SF_RATE → totSfRate

10.2.4 six-ff

- SIX_FF_EPSILON → sixFfEpsilon
- SIX_FF_ETA → sixFfEta
- SIX_FF_F → sixFfF
- SIX_FF_KEFF → sixFfKeff
- SIX_FF_KINF → sixFfKinf
- SIX_FF_LF → sixFfLf
- SIX_FF_LT → sixFfLt
- SIX_FF_P → sixFfP

10.3 base

10.3.1 adf

- DF_CORN_AREA → dfCornArea
- DF_CORN_DF → dfCornDf
- DF_CORN_IN_CURR → dfCornInCurr
- DF_CORN_NET_CURR → dfCornNetCurr
- DF_CORN_OUT_CURR → dfCornOutCurr
- DF_HET_CORN_FLUX → dfHetCornFlux
- DF_HET_SURF_FLUX → dfHetSurfFlux
- DF_HET_VOL_FLUX → dfHetVolFlux
- DF_HOM_CORN_FLUX → dfHomCornFlux
- DF_HOM_SURF_FLUX → dfHomSurfFlux
- DF_HOM_VOL_FLUX → dfHomVolFlux
- DF_MID_AREA → dfMidArea
- DF_MID_IN_CURR → dfMidInCurr
- DF_MID_NET_CURR → dfMidNetCurr
- DF_MID_OUT_CURR → dfMidOutCurr
- DF_N_CORN → dfNCorn
- DF_N_SURF → dfNSurf
- DF_SURFACE → dfSurface
- DF_SURF_AREA → dfSurfArea
- DF_SURF_DF → dfSurfDf
- DF_SURF_IN_CURR → dfSurfInCurr
- DF_SURF_NET_CURR → dfSurfNetCurr

- `DF_SURF_OUT_CURR` → `dfSurfOutCurr`
- `DF_SYM` → `dfSym`
- `DF_VOLUME` → `dfVolume`

10.3.2 albedos

- `ALB_FLIP_DIR` → `albFlipDir`
- `ALB_IN_CURR` → `albInCurr`
- `ALB_N_SURF` → `albNSurf`
- `ALB_OUT_CURR` → `albOutCurr`
- `ALB_PART_ALB` → `albPartAlb`
- `ALB_SURFACE` → `albSurface`
- `ALB_TOT_ALB` → `albTotAlb`

10.3.3 arr-estimators

- `CONVERSION_RATIO` → `conversionRatio`
- `PU239_CAPT` → `pu239Capt`
- `PU239_FISS` → `pu239Fiss`
- `PU240_CAPT` → `pu240Capt`
- `PU240_FISS` → `pu240Fiss`
- `PU241_CAPT` → `pu241Capt`
- `PU241_FISS` → `pu241Fiss`
- `SM149_CAPT` → `sm149Capt`
- `U235_CAPT` → `u235Capt`
- `U235_FISS` → `u235Fiss`
- `U238_CAPT` → `u238Capt`
- `U238_FISS` → `u238Fiss`
- `XE135_CAPT` → `xe135Capt`

10.3.4 burnup-coeff

- `BURNUP` → `burnup`
- `BURN_DAYS` → `burnDays`
- `BURN_MATERIALS` → `burnMaterials`
- `BURN_MODE` → `burnMode`
- `BURN_STEP` → `burnStep`
- `COEF_BRANCH` → `coefBranch`

- COEF_BU_STEP → coefBuStep
- COEF_IDX → coefIdx

10.3.5 diffusion

- CMM_DIFFCOEF → cmmDiffcoef
- CMM_DIFFCOEF_X → cmmDiffcoefX
- CMM_DIFFCOEF_Y → cmmDiffcoefY
- CMM_DIFFCOEF_Z → cmmDiffcoefZ
- CMM_TRANSPXS → cmmTranspxs
- CMM_TRANSPXS_X → cmmTranspxsX
- CMM_TRANSPXS_Y → cmmTranspxsY
- CMM_TRANSPXS_Z → cmmTranspxsZ

10.3.6 eig

- ABS_KEFF → absKeff
- ABS_KINF → absKinf
- ANA_KEFF → anaKeff
- COL_KEFF → colKeff
- GEOM_ALBEDO → geomAlbedo
- IMP_KEFF → impKeff

10.3.7 files

- BRA_DATA_DILE_PATH → braDataDilePath
- DECAY_DATA_DILE_PATH → decayDataDilePath
- NFY_DATA_DILE_PATH → nfyDataDilePath
- SFY_DATA_DILE_PATH → sfyDataDilePath
- XS_DATA_FILE_PATH → xsDataFilePath

10.3.8 gc-meta

- GC_UNIVERSE_NAME → gcUniverseName
- INF_FISS_FLX → infFissFlx
- INF_FLX → infFlx
- INF_KINF → infKinf
- INF_MICRO_FLX → infMicroFlx
- MACRO_E → macroE

- MACRO_NG → macroNg
- MICRO_E → microE
- MICRO_NG → microNg

10.3.9 kinetics

- ADJ_IFP_ANA_BETA_EFF → adjIfpAnaBetaEff
- ADJ_IFP_ANA_LAMBDA → adjIfpAnaLambda
- ADJ_IFP_GEN_TIME → adjIfpGenTime
- ADJ_IFP_IMP_BETA_EFF → adjIfpImpBetaEff
- ADJ_IFP_IMP_LAMBDA → adjIfpImpLambda
- ADJ_IFP_LIFETIME → adjIfpLifetime
- ADJ_IFP_ROSSI_ALPHA → adjIfpRossiAlpha
- ADJ_INV_SPD → adjInvSpd
- ADJ_MEULEKAMP_BETA_EFF → adjMeulekampBetaEff
- ADJ_MEULEKAMP_LAMBDA → adjMeulekampLambda
- ADJ_NAUCHI_BETA_EFF → adjNauchiBetaEff
- ADJ_NAUCHI_GEN_TIME → adjNauchiGenTime
- ADJ_NAUCHI_LAMBDA → adjNauchiLambda
- ADJ_NAUCHI_LIFETIME → adjNauchiLifetime
- ADJ_PERT_BETA_EFF → adjPertBetaEff
- ADJ_PERT_GEN_TIME → adjPertGenTime
- ADJ_PERT_LIFETIME → adjPertLifetime
- ADJ_PERT_ROSSI_ALPHA → adjPertRossiAlpha
- BETA_EFF → betaEff
- FWD_ANA_BETA_ZERO → fwdAnaBetaZero
- FWD_ANA_LAMBDA → fwdAnaLambda
- LAMBDA → lambda

10.3.10 lifetime

- ANA_DELAYED_EMTIME → anaDelayedEmtime
- ANA_MEAN_NCOL → anaMeanNcol
- ANA_SLOW_TIME → anaSlowTime
- ANA_THERM_FRAC → anaThermFrac
- ANA_THERM_TIME → anaThermTime

10.3.11 memory

- ALLOC_MEMSIZE → allocMemsize
- AVAIL_MEM → availMem
- MAT_MEMSIZE → matMemsize
- MEMSIZE → memsize
- MISC_MEMSIZE → miscMemsize
- RES_MEMSIZE → resMemsize
- UNKNOWN_MEMSIZE → unknownMemsize
- UNUSED_MEMSIZE → unusedMemsize
- XS_MEMSIZE → xsMemsize

10.3.12 misc

- ANA_AFGE → anaAfge
- ANA_ALF → anaAlf
- ANA_EALF → anaEalf
- FISSE → fisse
- IMP_AFGE → impAfge
- IMP_ALF → impAlf
- IMP_EALF → impEalf
- NUBAR → nubar

10.3.13 n-balance

- BALA_LOSS_NEUTRON_CAPT → balaLossNeutronCapt
- BALA_LOSS_NEUTRON_CUT → balaLossNeutronCut
- BALA_LOSS_NEUTRON_FISS → balaLossNeutronFiss
- BALA_LOSS_NEUTRON_LEAK → balaLossNeutronLeak
- BALA_LOSS_NEUTRON_TOT → balaLossNeutronTot
- BALA_NEUTRON_DIFF → balaNeutronDiff
- BALA_SRC_NEUTRON_FISS → balaSrcNeutronFiss
- BALA_SRC_NEUTRON_NXN → balaSrcNeutronNxn
- BALA_SRC_NEUTRON_SRC → balaSrcNeutronSrc
- BALA_SRC_NEUTRON_TOT → balaSrcNeutronTot
- BALA_SRC_NEUTRON_VR → balaSrcNeutronVr

10.3.14 neutron-physics

- DOPPLER_PREPROCESSOR → dopplerPreprocessor
- IMPL_CAPT → implCapt
- IMPL_FISS → implFiss
- IMPL_NXN → implNxn
- NEUTORN_ERG_NE → neutornErgNe
- NEUTRON_EMAX → neutronEmax
- NEUTRON_EMIN → neutronEmin
- NEUTRON_ERG_TOL → neutronErgTol
- SAMPLE_CAPT → sampleCapt
- SAMPLE_FISS → sampleFiss
- SAMPLE_SCATT → sampleScatt
- TMS_MODE → tmsMode
- USE_DBRC → useDbrc
- USE_DELNU → useDelnu
- USE_URES → useUres

10.3.15 nuclides

- TOT_DECAY_NUCLIDES → totDecayNuclides
- TOT_DOSIMETRY_NUCLIDES → totDosimetryNuclides
- TOT_NUCLIDES → totNuclides
- TOT_PHOTON_NUCLIDES → totPhotonNuclides
- TOT_REA_CHANNELS → totReaChannels
- TOT_TRANSMU_REA → totTransmuRea
- TOT_TRANSPORT_NUCLIDES → totTransportNuclides

10.3.16 optimization

- MG_MAJORANT_MODE → mgMajorantMode
- OPTIMIZATION_MODE → optimizationMode
- RECONSTRUCT_MACROXS → reconstructMacroxs
- RECONSTRUCT_MICROXS → reconstructMicroxs
- SPECTRUM_COLLAPSE → spectrumCollapse

10.3.17 parallel

- `MPI_REPRODUCIBILITY` → `mpiReproducibility`
- `MPI_TASKS` → `mpiTasks`
- `OMP_HISTORY_PROFILE` → `ompHistoryProfile`
- `OMP_REPRODUCIBILITY` → `ompReproducibility`
- `OMP_THREADS` → `ompThreads`
- `SHARE_BUF_ARRAY` → `shareBufArray`
- `SHARE_RES2_ARRAY` → `shareRes2Array`

10.3.18 parameters

- `B1_BURNUP_CORRECTION` → `b1BurnupCorrection`
- `B1_CALCULATION` → `b1Calculation`
- `BATCH_INTERVAL` → `batchInterval`
- `CYCLES` → `cycles`
- `GROUP_CONSTANT_GENERATION` → `groupConstantGeneration`
- `IMPLICIT_REACTION_RATES` → `implicitReactionRates`
- `NEUTRON_TRANSPORT_MODE` → `neutronTransportMode`
- `PHOTON_TRANSPORT_MODE` → `photonTransportMode`
- `POP` → `pop`
- `SEED` → `seed`
- `SKIP` → `skip`
- `SRC_NORM_MODE` → `srcNormMode`
- `UFS_MODE` → `ufsMode`
- `UFS_ORDER` → `ufsOrder`

10.3.19 pin-power

- `PPW_FF` → `ppwFf`
- `PPW_HOM_FLUX` → `ppwHomFlux`
- `PPW_LATTICE` → `ppwLattice`
- `PPW_LATTICE_TYPE` → `ppwLatticeType`
- `PPW_PINS` → `ppwPins`
- `PPW_POW` → `ppwPow`

10.3.20 poisons

- I135_MICRO_ABS → i135MicroAbs
- I135_YIELD → i135Yield
- PM147_MICRO_ABS → pm147MicroAbs
- PM147_YIELD → pm147Yield
- PM148M_MICRO_ABS → pm148mMicroAbs
- PM148M_YIELD → pm148mYield
- PM148_MICRO_ABS → pm148MicroAbs
- PM148_YIELD → pm148Yield
- PM149_MICRO_ABS → pm149MicroAbs
- PM149_YIELD → pm149Yield
- SM149_MACRO_ABS → sm149MacroAbs
- SM149_MICRO_ABS → sm149MicroAbs
- SM149_YIELD → sm149Yield
- XE135_MACRO_ABS → xe135MacroAbs
- XE135_MICRO_ABS → xe135MicroAbs
- XE135_YIELD → xe135Yield

10.3.21 rad-data

- ACTINIDE_ACTIVITY → actinideActivity
- ACTINIDE_DECAY_HEAT → actinideDecayHeat
- ACTINIDE_ING_TOX → actinideIngTox
- ACTINIDE_INH_TOX → actinideInhTox
- ALPHA_DECAY_SOURCE → alphaDecaySource
- BETA_DECAY_SOURCE → betaDecaySource
- CS134_ACTIVITY → cs134Activity
- FISSION_PRODUCT_ACTIVITY → fissionProductActivity
- FISSION_PRODUCT_DECAY_HEAT → fissionProductDecayHeat
- FISSION_PRODUCT_ING_TOX → fissionProductIngTox
- FISSION_PRODUCT_INH_TOX → fissionProductInhTox
- INGENSTION_TOXICITY → ingenstionToxicity
- INHALATION_TOXICITY → inhalationToxicity
- NEUTRON_DECAY_SOURCE → neutronDecaySource
- PHOTON_DECAY_SOURCE → photonDecaySource
- SR90_ACTIVITY → sr90Activity

- TE132_ACTIVITY → tel32Activity
- TOT_ACTIVITY → totActivity
- TOT_DECAY_HEAT → totDecayHeat
- TOT_SF_RATE → totSfRate

10.3.22 sampling

- AVG_REAL_COL → avgRealCol
- AVG_SURF_CROSS → avgSurfCross
- AVG_TRACKING_LOOPS → avgTrackingLoops
- AVG_TRACKS → avgTracks
- AVG_VIRT_COL → avgVirtCol
- DT_EFF → dtEff
- DT_FRAC → dtFrac
- DT_THRESH → dtThresh
- LOST_PARTICLES → lostParticles
- MIN_MACROXS → minMacroxs
- REA_SAMPLING_EFF → reaSamplingEff
- REA_SAMPLING_FAIL → reaSamplingFail
- ST_FRAC → stFrac
- TOT_COL_EFF → totColEff

10.3.23 stats

- CYCLE_IDX → cycleIdx
- MEAN_POP_SIZE → meanPopSize
- MEAN_POP_WGT → meanPopWgt
- SIMULATION_COMPLETED → simulationCompleted
- SOURCE_POPULATION → sourcePopulation

10.3.24 times

- BATEMAN_SOLUTION_TIME → batemanSolutionTime
- BURNUP_CYCLE_TIME → burnupCycleTime
- CPU_USAGE → cpuUsage
- ESTIMATED_RUNNING_TIME → estimatedRunningTime
- INIT_TIME → initTime
- MPI_OVERHEAD_TIME → mpiOverheadTime

- OMP_PARALLEL_FRAC → ompParallelFrac
- PROCESS_TIME → processTime
- RUNNING_TIME → runningTime
- TOT_CPU_TIME → totCpuTime
- TRANSPORT_CPU_USAGE → transportCpuUsage
- TRANSPORT_CYCLE_TIME → transportCycleTime

10.3.25 total-rr

- ALBEDO_LEAKRATE → albedoLeakrate
- INI_BURN_FMASS → iniBurnFmass
- INI_FMASS → iniFmass
- TOT_ABSRATE → totAbsrate
- TOT_BURN_FMASS → totBurnFmass
- TOT_CAPTRATE → totCaptrate
- TOT_CUTRATE → totCutrate
- TOT_FISSRATE → totFissrate
- TOT_FLUX → totFlux
- TOT_FMASS → totFmass
- TOT_GENRATE → totGenrate
- TOT_LOSSRATE → totLossrate
- TOT_PHOTON_PRODRATE → totPhotonProdrate
- TOT_POWDENS → totPowdens
- TOT_POWRER → totPowrer
- TOT_RR → totRr
- TOT_SRCRATE → totSrcrate

10.3.26 ures

- URES_AVAIL → uresAvail
- URES_DILU_CUT → uresDiluCut
- URES_EMAX → uresEmax
- URES_EMIN → uresEmin
- URES_SEED → uresSeed

10.3.27 versions

- `COMPILE_DATE` → `compileDate`
- `COMPLETE_DATE` → `completeDate`
- `CONFIDENTIAL_DATA` → `confidentialData`
- `CPU_MHZ` → `cpuMhz`
- `CPU_TYPE` → `cpuType`
- `DEBUG` → `debug`
- `HOSTNAME` → `hostname`
- `INPUT_FILE_NAME` → `inputFileName`
- `START_DATE` → `startDate`
- `TITLE` → `title`
- `VERSION` → `version`
- `WORKING_DIRECTORY` → `workingDirectory`

10.3.28 xs

- `ABS` → `abs`
- `CAPT` → `capt`
- `CHID` → `chid`
- `CHIP` → `chip`
- `CHIT` → `chit`
- `DIFFCOEF` → `diffcoef`
- `FISS` → `fiss`
- `INVV` → `invv`
- `KAPPA` → `kappa`
- `NSF` → `nsf`
- `NUBAR` → `nubar`
- `RABSXS` → `rabsxs`
- `REMXS` → `remxs`
- `S0` → `s0`
- `S1` → `s1`
- `S2` → `s2`
- `S3` → `s3`
- `S4` → `s4`
- `S5` → `s5`
- `S6` → `s6`

- $S7 \rightarrow s7$
- $SCATT0 \rightarrow scatt0$
- $SCATT1 \rightarrow scatt1$
- $SCATT2 \rightarrow scatt2$
- $SCATT3 \rightarrow scatt3$
- $SCATT4 \rightarrow scatt4$
- $SCATT5 \rightarrow scatt5$
- $SCATT6 \rightarrow scatt6$
- $SCATT7 \rightarrow scatt7$
- $TOT \rightarrow tot$
- $TRANSPXS \rightarrow transpxs$

10.3.29 xs-prod

- $SCATT2 \rightarrow scatt2$
- $SCATTP0 \rightarrow scattp0$
- $SCATTP1 \rightarrow scattp1$
- $SCATTP3 \rightarrow scattp3$
- $SCATTP4 \rightarrow scattp4$
- $SCATTP5 \rightarrow scattp5$
- $SCATTP6 \rightarrow scattp6$
- $SCATTP7 \rightarrow scattp7$
- $SP0 \rightarrow sp0$
- $SP1 \rightarrow sp1$
- $SP2 \rightarrow sp2$
- $SP3 \rightarrow sp3$
- $SP4 \rightarrow sp4$
- $SP5 \rightarrow sp5$
- $SP6 \rightarrow sp6$
- $SP7 \rightarrow sp7$

COMMAND LINE INTERFACE

`serpentTools` includes minor command line functionality. Provided you have installed according to [Installation](#), you can access this interface with:

```
$ python -m serpentTools
```

Where the above command is executed from the terminal, neglecting the `$`. More information can be found in [Terminal terminology](#).

Note: Outputs here are accurate up to version 0.6.1+12 Please alert the developers if any major differences are found, or a method to automatically update this can be found

Display the available options by passing the `-h` flag:

```
$ python -m serpentTools -h
usage: serpentTools [-h] [--version] [-v | -q] [-c CONFIG_FILE]
                  {seed,list,to-matlab} ...

optional arguments:
  -h, --help            show this help message and exit
  --version             show program's version number and exit
  -v                   increase verbosity v: info, vv: debug
  -q                   suppress warnings and errors q: error, qq: critical
  -c CONFIG_FILE, --config-file CONFIG_FILE
                        path to settings file

sub-commands:
  {seed,list,to-matlab}
                        sub-command help
  seed                 copy an input file with unique random number seeds
  list                 show the default settings
  to-matlab             convert output file to .mat file
```

11.1 Random Seed Generation

The seed subcommand utilizes the `serpentTools.seed` module to produce repeated input files with unique random seeds. This is helpful for running repeated analyses to reduce the stochastic nature of Monte Carlo calculations. Options for forcing the number of digits, utilizing the SERPENT `include` command rather than fully copying the file, and new output directories are afforded to the user.

```
$ python -m serpentTools seed -h
usage: serpentTools seed [-h] [--seed SEED] [-l LENGTH]
                        [--output-dir OUTPUT_DIR] [--link]
                        file N

positional arguments:
  file                input file to copy
  N                  integer number of files to create

optional arguments:
  -h, --help          show this help message and exit
  --seed SEED         Seed to start with the builtin random generator
  -l LENGTH, --length LENGTH
                        Number of digits in random seeds
  --output-dir OUTPUT_DIR
                        Copy files into this directory
  --link              Reference input file with include statement, rather
                        than copying the whole file
```

11.2 Conversion to Binary .mat files

Starting in version 0.6.2, `serpentTools` can convert text SERPENT output files and convert them to binary .mat files. This relies upon *scipy*, and can be called from the command line as follows:

```
$ python -m serpentTools to-matlab -h
usage: serpentTools to-matlab [-h] [-o OUTPUT] [-a] [--format {4,5}] [-l]
                             [--large] [--oned {col,row}]
                             file

positional arguments:
  file                output file to read and convert

optional arguments:
  -h, --help          show this help message and exit
  -o OUTPUT, --output OUTPUT
                        Name of output file to write. If not given, replace
                        extension with .mat
  -a, --append        Append to existing file if found. Otherwise overwrite.
                        Default: False
  --format {4,5}      Format of file to write. 4 for MATLAB 4, 5 for MATLAB
                        5+. Default: 5
  -l, --longNames     Allow variable names up to 63 characters. Otherwise,
                        enforce 31 character names. Default: False
  --large             Don't compress arrays when writing.
  --oned {col,row}    Write 1D arrays as row or column vectors
```

Conversion will exit with no errors if the file is able to be converted, or with the following exit codes:

- 1: *scipy* not found
- 3: That file type is not supported at this time.

If you desperately need a file type to be converted, please reach out to the developers on the [GH Issue board](#). Alternatively, if you're feeling ambitious, follow through the [Developer's Guide](#) for guidelines on adding the feature and submitting a pull request.

DEVELOPER'S GUIDE

This section serves as a guide for people who would like to add functionality to this project. If that is not your desire, this chapter can be skipped without any loss of comprehension.

Note: Developers are encouraged to read and follow new guiding principles in *Updated Data Model* leading up to version 0.10.0

12.1 Contributing

First, thanks for your interest in contributing to this project! This document should help us expedite the process of reviewing issues and pull requests. For a quick look at all the issues that are up for grabs, take a look at the current [unclaimed issues](#). If you claim an issue, use the `Assignees` setting to let us know that you've got it!

12.1.1 Scope

The scope of this project is to simplify and expedite analysis stemming from `SERPENT` outputs. In the future we may expand this project to expand to interacting heavily with input files, but that is currently beyond the scope of this project. Any and all issues, features and pull requests will be examined through this scope.

12.1.2 Issues

The goal for this project is to become the de facto method for processing `SERPENT` outputs and, if you're looking at this, there is some way we can improve. The [GitHub issue tracker](#) is the preferred way to post bug reports and feature requests.

Bug Reports

The more information given, the quicker we can reproduce and hopefully resolve the issue. Please see [issue-template](#) for a template that should be used for reporting bugs. One of the developers will add a [bug label](#) and start moving to resolve the issue posthaste.

Feature Requests

We are very interested in adding functionality from the SERPENT community! Requests can be done through the issue tracker as well. You can create an issue on the issue tracker with `[Feature]` or `[Request]` in the title. Describe what you would like to add, some expected results, and the purpose behind the feature. The development team will apply an `enhancement` label and proceed accordingly.

12.1.3 Pull Requests

Pull requests are how we review, approve, and incorporate changes into the `master` branch. If you have code you want to contribute, please look at the content in the *Developer's Guide* for things like *Pull Request Checklist*, *Coding Style*, and more.

When your content is ready for the pull request, follow the `pull-request-template` and make a request! Someone of the core development team will review the changes according to the criteria above and make changes and/or approve for merging!

The `develop` branch is the primary branch for this project. All pull requests, except for bugs on public releases, should be compared against this branch. When a pull request is approved and has passed the required checks, it should be `squashed and merged` into the `develop` branch. Squashing a branch converts a series of commits into a single commit onto the main branch, creating a tidy git history.

For pull requests into `master`, as in releases, these should simply be merged without squashing. When viewing the `git log` on the `master` or `develop` branches, one is presented only with approved and closed pull requests, not incremental commits that led to a PR being closed.

12.2 Updated Data Model

The goal of this document is to describe developer-specific changes that should drive the next phase of development. The contents reflect changes that will be introduced between release `0.9.3` and the next major release of `0.10.0`.

12.2.1 Goals and non-goals

The new data model and developer guide is provided to help the next release of `serpentTools` have:

1. Little to no high-level API breaks
2. Less superfluous code like the settings interface
3. Generic, library-like readers and containers
4. Inherited methods only when they make sense and are implemented
5. Standard base classes like `collections.abc.Mapping` when appropriate

These items should be accomplished without:

1. Breaking the ease of `serpentTools.read()`
2. Removing plotting capabilities
3. Removing filtering capabilities

12.2.2 Data Model

Separation of readers and containers

Objects that store information from Serpent files should be separated from objects that read Serpent files. Much of this is inspired by #335, and will help 1) reduce left-over code and methods related to reading files, and 2) support integration with other file formats. Classes that store the file data will be designated as `<X>File` like `ResultFile`, while classes that read file data will be designated as `<X>Reader`, e.g. `ResultReader`.

These file classes will emulate the previous behavior of creating a reader and then reading the file through `classmethod()`, like below:

```
class DemoFile:

    @classmethod
    def fromSerpent(cls, fp, *args, **kwargs):
        # process
        # return an instance of DemoFile or cls()
```

Here, a user or a new read function can call `DemoFile.fromSerpent` to parse the file and store its contents. This helps reduce the likelihood of partially instantiated readers running around, like creating a `ResultsReader` and trying to plot before calling `read`.

This has an additional benefit of allowing additional class methods for creating files from alternative data types. A `fromHdf` method would be extra wonderful. But, new file formats are not the intended goal of version 0.10.0.

Reusable readers

Readers should be reusable and configurable. Users should be able to pass settings either through the `__init__` method and/or as attributes to control what data is read. This is how the settings module will be deprecated and removed. Settings can be controlled through `property` decorators.

The primary task of a reader will be to read a file, or incoming stream of data, and produced a corresponding `<X>File` instance. Readers should also be capable of reading multiple files or streams, clearing caches or temporary variables as necessary. The implementation should support the following:

```
>>> r = DemoReader()
>>> f0 = r.read(examplefile0)
>>> f1 = r.read(examplefile1)
```

This should save time when reading multiple files of the same type, especially if filtering is used in all cases.

Supported file inputs

When possible, readers should support:

- string file names
- `pathlib.Path`
- Generic `io.TextIOBase`
- Classes fulfilling the `file object` API (`read`, `readline`, etc.)

This will improve integration with the python ecosystem, but also support reading in-memory streams like `io.StringIO` for testing or `zipfile.ZipFile` for reading compressed files.

Generic Containers

Containers like detectors and homogeneous universes should be introduced into the main API, with a sufficiently generic interface. Some of this work has already been implemented on the `serpentTools.Detector` and its related subclasses. The main change to the current implementations would be things like

1. Making `serpentTools.objects.HomogUniv.addData()` accept arrays rather than string data to be converted and split
2. Making `serpentTools.objects.DepletedMaterial` accept name, day, zai, and/or burnup vectors directly, rather than a metadata argument.
3. Providing adequate setters, like `__setitem__` when applicable, that allow data to be provided from a generic source.

These routines will also help the file objects create these auxiliary containers when reading additional file formats.

Math methods

Some classes may benefit from implementing methods like `__add__` or `__mul__` to scale and modify stored data. Converting a power profile stored on a detector from W to MW with:

```
>>> det /= 1E6
```

or compute the difference between two detectors with:

```
>>> diff = det0 - det1
```

Sufficient checks should be made that the `other` object has a compatible data layout (two detectors have similar indexes, grids etc).

Additional information on methods like this can be found in the [Python data model](#) documentation.

12.2.3 Proposed integration

This is not going to be easy, as there will undoubtedly be some backwards incompatible changes introduced. However, the end product will be a python package that will be more friendly to users and developers, and, hopefully, easier to extend and maintain.

The following changes are proposed:

1. A new module be introduced under the name `serpentTools.next` (name up for discussion). This should reside inside the main source directly in `serpentTools/next/`
2. This new module will remain detached from the main API, meaning that all features must be utilized with:

```
>>> import serpentTools.next
>>> r0 = serpentTools.next.read(filep)
```

3. Parsers, file-objects, and containers should be implemented inside this new module. These need not inherit from the current `BaseObject`. When it makes sense, the use of the `collections.abc` should be used to provide maximum features for minimal work
4. Tests should be written using `pytest` that ensure the new parsers store identical data as the previous parsers. These will become the foundation for the next round of regression tests.
5. A dedicated changelog will be added to track features that are removed, modified, or deprecated in this process. Keeping this up to date is of tantamount importance to alert developers and users on the eventual release.

12.2.4 Release Targets

The following release targets are proposed. No dates are enforced.

Except for critical bug fixes, all work should pause on the master branch. This will hopefully reduce the amount of features to be back-ported into the new library.

When the `next` module is complete and ready for release, a beta release of the form `0.10.0b0` should be made and pushed to the Python package index. Users should be alerted through appropriate channels.

After this point, a new main release on the `0.9.x` tree should be made. Users should be alerted to changes, primarily in `serpentTools.read()` and the settings interface. These are likely to have the largest changes to non-developer end-users.

The beta version should be live and un-touched for a sufficient amount of time. How long is difficult to say, but two weeks seems like a good low end target.

If/when sufficient bugs are found and fixed, a new beta release should be made and pushed.

Once the beta period is complete, a release candidate, `0.10.0rc0` or similar, should be made and pushed. Users should be alerted through appropriate channels. This release candidate should be live for a reasonable amount of time.

If/when sufficient bugs are found and fixed, a new release candidate should be made and pushed.

Work should be done to merge the `next` module as the main parsing and analysis library. This is the primary goal of the following major release `0.11.0`, following a similar beta and release candidate period. The new features should still exist inside `0.11.0` in the `serpentTools.next` module, but users and developers should be alerted that these features will be removed, favoring importing from the main `serpentTools` API.

Version `0.12.0` will fully remove the `serpentTools.next` module.

12.3 Documentation

All public functions, methods, and classes should have adequate documentation through docstrings, examples, or inclusion in the appropriate file in the `docs` directory. Good forethought into documenting the code helps resolve issues and, in the case of docstrings, helps produce a full manual.

12.3.1 Docstrings

Docstrings are defined in [PEP 257](#) and are characterized by `"""triple double quotes"""`. These can be used to reduce the effort in creating a full manual, and can be viewed through python consoles to give the user insight into what is done, what is required, and what is returned from a particular object. This project uses [numpydoc style docstrings](#):

```
def foo(a, b=None):
    """Simple one line docstring

    Parameters
    -----
    a : float
        Some value
    b : bool, optional
        A flag

    Returns
    -----
```

(continues on next page)

(continued from previous page)

```
returnType
    Description of the return type

"""
```

Deprecation

If an object is deprecated or will be modified in future versions, then the `deprecated()` and `willChange()` decorators should be applied to the object, and a note should be added to the docstring indicating as much. This can be done with the sphinx `deprecated` directive.

12.3.2 Examples

When possible, features should be demonstrated, either through Jupyter notebooks in the `examples/` directory, or with an `Examples` section in the docstring. Specifically, all readers should be demonstrated as Jupyter notebooks that detail the typical usage, user control settings, and examples of how the data is stored and accessed.

Converting

These Jupyter notebooks can be converted to `.rst` files for inclusion in the manual with the command `jupyter nbconvert --to=rst <file>`, with:

```
$ jupyter nbconvert --to=rst Notebook.ipynb
```

However, there are some tweaks that should be made so that the documentation renders properly and has helpful links to objects in the project.

The `nbconvert` command will place the following blocks around python code:

```
.. code:: ipython3

    print('hello world!')

.. parsed-literal::

    hello world!
```

When building this documentation on `readthedocs`, the `ipython3` statement can cause the code not to be rendered. This is summarized [here](#), but it appears that the `ipython3` lexer is [not trivially installed](#) and is not found on `readthedocs`. For now, all these instances of `ipython3` should be removed from the `.rst` version of the notebook so that the wonderful code examples are proudly displayed in our documentation. The above code block should be replaced with:

```
.. code::

    print('hello world!')

.. parsed-literal::

    hello world!
```

It is recommended to use the template in `examples/rstTemplate.tpl` to ease this conversion process. This can be passed to with

```
$ jupyter nbconvert --to=rst --template=rstTemplate.tpl Notebook.ipynb
```

Upon conversion, move the file into the `docs/examples` directory and include the file name in `docs/examples/index.rst`.

Images

Executing `nbconvert` will create a directory containing the images contained in the notebook. When moving the `.rst` version of the notebook into the `docs/examples` folder, make sure that all links to images are correct.

Linking to the API

When referring to python classes, attributes, functions, or methods, it is strongly recommended to utilize [python object references](#). This creates direct links from your text to the object declaration in our [api section](#) that allows people to get more detail on whatever you are referencing, powered by the `docstrings` on that object. Two such examples are given below:

- `:class:`serpentTools.DepletionReader`` becomes [serpentTools.DepletionReader](#)
- `:meth:`~serpentTools.objects.DepletedMaterial.plot`` is shortened to [plot\(\)](#)

12.3.3 Verifying

You worked hard on this documentation, and we want your great work to be properly displayed once completed. In order to reduce the chances of some errors, try running the following from inside the `docs` directory:

```
$ make clean html
```

Navigate to the files created in `_build/html` to ensure that images are loaded properly, code is rendered properly, and the converted notebook looks exactly how you expect it to look.

Warning: If there is an issue with rendering your example, we will likely call upon you to fix these issues.

Note: Building the documentation locally requires `sphinx` and a handful of other packages. Installing these is outside the scope of this guide, partially because [the sphinx team has a great guide already](#). Check this out if you are having issues running the `make clean install` commands from the `docs` directory.

12.3.4 Adding Objects to API

New reader or container objects should be included in the [api section of the documentation](#), as with any function that the end user may utilize. For documenting these, we utilize the `sphinx autodoc` features to use the `docstrings` to automatically document new features. This is most simply done by calling `.. autoclass::` or `.. autofunction::` like:

```
.. autofunction:: serpentTools.plot.plot
.. autoclass:: serpentTools.ResultsReader
```

For new readers, those should be included in their own file, such as `docs/api/myNewReader.rst`, which can be as bare as:

```
My New Reader
=====

.. autoclass:: serpentTools.parsers.new.MyNewReader
```

Be sure to include your new file in `docs/api/index.rst`, or else your file will be left out of the documentation. Proper documentation of the class or function requires thorough and concise documentation of all attributes, class methods, and construction arguments. Follow the above guides, such as *Docstrings*, and this process *should* go smoothly.

12.4 Pull Request Checklist

Below is the criteria that will be used in the process of reviewing pull requests (PR):

1. The content of the PR fits within the scope of the project - *Scope*
2. The code included in the PR is written in good *pythonic* fashion, and follows the style of the project - *Coding Style*
3. The code directly resolves a previously raised issue - *Issues*
4. PR does not cause unit tests and builds to fail
5. Changes are reflected in documentation - *Documentation*

12.4.1 CI Testing

We utilize *Travis* to perform our continuous integration, or *CI*. Two types of tests are run: unit tests and tests on the example notebooks. The former are used to perform more granular testing over the project, while the latter ensure our example notebooks are runnable.

Unit Tests

Unit tests should cover all public methods and a sufficient set of use cases to reduce the amount of bugs that make it into releases. Unit tests are run using *pytest* from the project directory:

```
$ ls
examples/ LICENSE serpentTools/ tests/ ...
$ pytest
```

If the `pytest-cov` package is installed, you can view the coverage, or how much of the project is touched by tests, with:

```
$ pytest --cov=serpentTools
```

It is always preferable to increase coverage to decreasing coverage, but minor deviations are acceptable. The coverage is not a factor in passing or failing CI, but substantial changes to the test suite should serve a valid purpose if the coverage does decrease.

Notebook Tests

We try to provide a *Jupyter notebook* for each of the main readers in the package. These are converted to be used in our main documentation, and serve as a handy way for new users to discover the features provided with `serpentTools`. In order to ensure that these are valid notebooks as changes are introduced, our *CI* converts these to python scripts and runs them using the `test notebooks` script. It is beneficial to run this script during major changes to the API, as well as correcting any errors or deprecated/removed features.

12.4.2 Lint

We also recommend using a *linter* to analyze the project for code that might induce errors and does not conform to our style guide - *Coding Style*. This is applied on proposed changes using `flake8`. Code to be merged into this project should not cause any unit tests to break, nor introduce lint. If you are working on a feature/bug-fix branch, you can compare the lint that would be introduced with

```
$ git diff --unified=0 develop | flake8 --diff
```

Here, `develop` is the intended target branch into which these changes will be merged.

12.5 Version Control

`serpentTools` uses *git* for version control. All the source code can be found at <https://github.com/CORE-GATECH-GROUP/serpent-tools>. Two main branches are provided: `master` and `develop`, and the *git* flow branching model is followed. The `master` branch should be considered stable and updated coincident with each release. The `develop` branch is updated with more frequency as features are introduced. This is the main branch of the project, and features should be introduced off of this branch.

`serpentTools` follows the *semantic versioning* system, where the version number as found in `setup.py`, `serpentTools/__init__.py`, and `docs/conf.py` has the following form: `major.minor.patch`, e.g. `0.8.0` or `1.1.20`. Each of the numbers should be incremented prior to new releases with the following designation:

1. Changes that are not backwards compatible should be denoted by incrementing the major number.
2. Changes that are backwards compatible and introduce sufficient new features to the API should be denoted by incrementing the minor number.
3. Changes that are largely internal and not recognizable by end-users should be denoted by incrementing the patch number

Note: Until a stable 1.0.0 release, the positions are essentially shifted, e.g. the version is `0.major.minor`

12.5.1 Releases

Following a release, the following actions should be performed:

1. Archived and installable python files should be created
2. Archived and installable python files should be uploaded to the python package index, *PyPI*
3. The tag should be pushed to GitHub and marked as a release, including information on the changes introduced in this release

This section details changes and procedures that, if followed, will increase chances of a painless release.

Updating the package version

Before and after a release, the project version number should be updated in the following places:

1. `setup.py`
2. `serpentTools/__init__.py`
3. `docs/conf.py`

The new version should be indicative of the changes introduced between this release and the previous release.

Generating distributions

The new distribution, that can be uploaded to *PyPI*, can be generated with

```
python setup.py sdist bdist_wheel
```

This will produce a source distribution and binary python wheel in the `dist` directory, each of the form `dist/serpentTools-<version>.<extension>`. Before tagging and pushing releases to *PyPI*, the distribution should be checked with

```
twine check dist/serpentTools-<version>*
```

twine will check that the package is compatible with the standards set by *PyPI* prior to uploading. Following a successful check, the distribution can be pushed to the package index using

```
..code:: sh
```

```
twine upload dist/serpentTools-<version>*
```

Tagging

Releases should be done with *git tags* from the master branch and then pushed to GitHub. Annotated tags should be used and can be created with

```
git tag -s <version>
```

Pushing these tags to GitHub creates a new *release*. If a message is used, the messages should be a brief message describing the changes on this tag. On the release page, a more detail list of changes, such as pull requests and issues closed, should be listed.

12.5.2 Commit Messages

When possible, please provide commit messages that:

- have a initial single summary line (~<50 characters),
- followed by a blank line,
- followed by as detailed of a description as possible wrapped to ~70 characters wide

Helpful and detailed commit messages can make searching for changes easier and accelerate the review process. As an added benefit, if your pull request is a single commit, GitHub will automatically populate the request summary with your commit message!

Other references:

- [git documentation on commit messages](#)
- [Good example commit message - Tim Pope](#)

12.6 Logging and Reporting

The primary internal logging is performed with a logger named `serpentTools`, that can be obtained using:

```
>>> import logging
>>> logging.getLogger("serpentTools")
```

If you want to see the messages produced by this logger, you have a few options. First, the Python logging system must be configured. This can be done simply with:

```
>>> import logging
>>> logging.basicConfig(format="%(levelname)-s: %(message)-s")
# Display a basic warning
>>> logging.warning("This is a warning")
WARNING: This is a warning
```

To show the internal messages, one can modify the verbosity through the *Settings* interface with:

```
>>> serpentTools.settings.rc["verbosity"] = "debug"
```

where "debug" can be one of "debug", "info", "warning", "error" or "critical".

Alternatively, the level can be adjusting using the python `logging` module:

```
>>> logging.getLogger("serpentTools").setLevel(logging.DEBUG)
```

12.6.1 Developer Reference

Note: The use of built-in python warning support through the `warnings` module should be preferred. These functions will be phased out in future versions

This chapter describes the various functions used to convey progress updates or issues to the user. Functions in this module should be used over a general `print` statement, as this module can be extended to log messages to a file in the future. In order of increasing severity:

<i>debug</i>	Log a debug message.
<i>info</i>	Log an info message
<i>warning</i>	Log a warning that something could go wrong or should be avoided.
<i>error</i>	Log that something caused an exception but was suppressed.
<i>critical</i>	Log that something has gone horribly wrong.

serpentTools.messages.debug

`serpentTools.messages.debug(message)`
Log a debug message.

serpentTools.messages.info

`serpentTools.messages.info(message)`
Log an info message

serpentTools.messages.warning

`serpentTools.messages.warning(message)`
Log a warning that something could go wrong or should be avoided.

serpentTools.messages.error

`serpentTools.messages.error(message)`
Log that something caused an exception but was suppressed.

serpentTools.messages.critical

`serpentTools.messages.critical(message)`
Log that something has gone horribly wrong.

12.6.2 Decorators

Two decorators are provided in the `messages` module that are used to indicate functions or methods who's behavior will be changing or removed in the future.

<i>deprecated</i>	Decorator that warns that different function should be used instead.
<i>willChange</i>	Decorator that warns that some functionality may change.

serpentTools.messages.deprecated

`serpentTools.messages.deprecated(useInstead)`
Decorator that warns that different function should be used instead.

serpentTools.messages.willChange

`serpentTools.messages.willChange` (*changeMsg*)
 Decorator that warns that some functionality may change.

12.6.3 Custom Handlers

class `serpentTools.messages.DictHandler` (*level=0*)
 Bases: `logging.Handler`

Handler that stores log messages in a dictionary

logMessages

Dictionary of lists where each key is a log level such as 'DEBUG' or 'WARNING'. The list associated with each key contains all messages called under that logging level

Type `dict`

close ()

Tidy up before removing from list of handlers

emit (*record*)

Store the message in the log messages by level.

Does no formatting to the record, simply stores the message in *logMessages* dictionary according to the records *levelname*

Anticipates a `logging.LogRecord` object

flush ()

Clear the log messages dictionary

12.7 Coding Style

For the most part, this project follows the **PEP 8** standard with a few differences. Some points are included here

- 79 characters per line
- Four spaces per indentation level
- Avoiding extraneous whitespace:

```
Yes: spam(ham[1], {eggs: 2})
No:  spam( ham[ 1 ], { eggs: 2 } )
```

Some of the specific style points for this project are included below

- `mixedCase` for variables, methods, and functions
- `CamelCase` for classes:

```
class DemoClass(object):

    def doSomething(self, arg0, longerArgumentName):
        pass
```

- Directly call the `__init__` method from a parent class, e.g.:

```
class MyQueue(list):  
  
    def __init__(self, items):  
        list.__init__(self)  
        self.extend(items)
```

- Arrange imports in the following order:
 1. imports from the standard library: os, sys, etc.
 2. imports from third party code: numpy, matplotlib, etc.
 3. imports from the serpentTools package
- Longer import paths are preferred to shorter:

```
# yes  
from really.long.path.to.a import function  
function()  
# not preferred  
import really  
really.long.path.to.a.function()
```

12.8 Plotting

Many of the readers and containers in this project have plot routines to quickly visualize relevant data. The goal for these plots is to quickly provide presentation-worthy plots by default, with options for formatting via additional arguments. This document serves as a guide for writing plot functions that have a cohesive syntax across the project and require little to no knowledge of *matplotlib* to make a fantastic plot.

Note: Plot functions should contain sufficient formatting such that, with minimal user input, processional and publishable plots are produced.

This cohesion is accomplished by decorating plot routines with the `magicPlotDocDecorator()` and by supporting a collection of additional arguments used for formatting the plot. These magic strings are detailed in [Magic Plot Decorator Options](#) and can be included in any function decorated by `magicPlotDocDecorator()` as `{legend}`.

When appropriate, plot functions should accept a `matplotlib.axes.Axes` argument on which to plot the data. This is useful for subplotting, or for creating a plot and then continuing the plotting inside this function. If not given, the function should create a new `matplotlib.axes.Axes` object. All plotting should be done on this axes object, such as:

```
def plot(ax=None):  
    ax = ax or pyplot.axes()  
    ax.plot([1,2,3])  
    return ax
```

By returning the axes object, users can further apply labels, place the plot into subplots, or more.

Axes for all plots should be labeled without user intervention, but should support user-defined labels. This process can be expedited by utilizing `formatPlot()` as the last stage of the plotting process. This function accepts a variety of keyword arguments that are used to set axis labels or scaling, even placing the legend outside the plot. Taking the simple plot method from above, we can modify this method to accept user arguments for labels, but also have default labels should the user not provide them:

```
def plot(ax=None, xlabel=None, ylabel=None):
    ax = ax or pyplot.axes()
    ax.plot([1, 2, 3])
    xlabel = xlabel or "Default x label"
    ax = formatPlot(ax, xlabel=xlabel,
                    ylabel=ylabel or "Y axis")
    return ax
```

12.8.1 Plotting Utilities

Plot Functions

The `serpentTools.plot` module contains some functions to assist in plotting and for describing plot functions. These are not required for use, but their behavior, and the advice given in [Plotting](#), should be followed. This will yield a consistent and flexible plotting environment to the user without having to dive deep into the `matplotlib` framework.

<code>cartMeshPlot</code>	Create a cartesian mesh plot of the data
<code>plot</code>	Shortcut plot for plotting series of labeled data onto a plot

`serpentTools.plot.cartMeshPlot`

`serpentTools.plot.cartMeshPlot` (*data*, *xticks=None*, *yticks=None*, *ax=None*, *cmap=None*, *logColor=False*, *normalizer=None*, *cbarLabel=None*, *thresh=None*, ***kwargs*)

Create a cartesian mesh plot of the data

Parameters

- **data** (*numpy.array*) – 2D array of data to be plotted
- **xticks** (*iterable or None*) –
- **yticks** (*iterable or None*) – Values corresponding to lower x/y boundary of meshes. If not given, treat this as a matrix plot like `matplotlib.pyplot.imshow()`. If given, they should contain one more item than number of elements in their dimension to give dimensions for all meshes.
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **cmap** (*str*, optional) – Valid Matplotlib colormap to apply to the plot.
- **logColor** (*bool*) – If true, apply a logarithmic coloring
- **normalizer** (callable or `matplotlib.colors.Normalize`) – Custom normalizer for this plot. If an instance of `matplotlib.colors.Normalize`,
- **normalizer** – Custom normalizer for this plot. If an instance of `matplotlib.colors.Normalize`, use directly. Otherwise, assume a callable object and call as `norm = normalizer(data, xticks, yticks)`
- **cbarLabel** (*None or str*) – Label to apply to colorbar
- **{thresh}** –

- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.pcolormesh()` or `matplotlib.pyplot.imshow()` if `xticks` and `yticks` are `None`

Returns `Ax` on which the data was plotted.

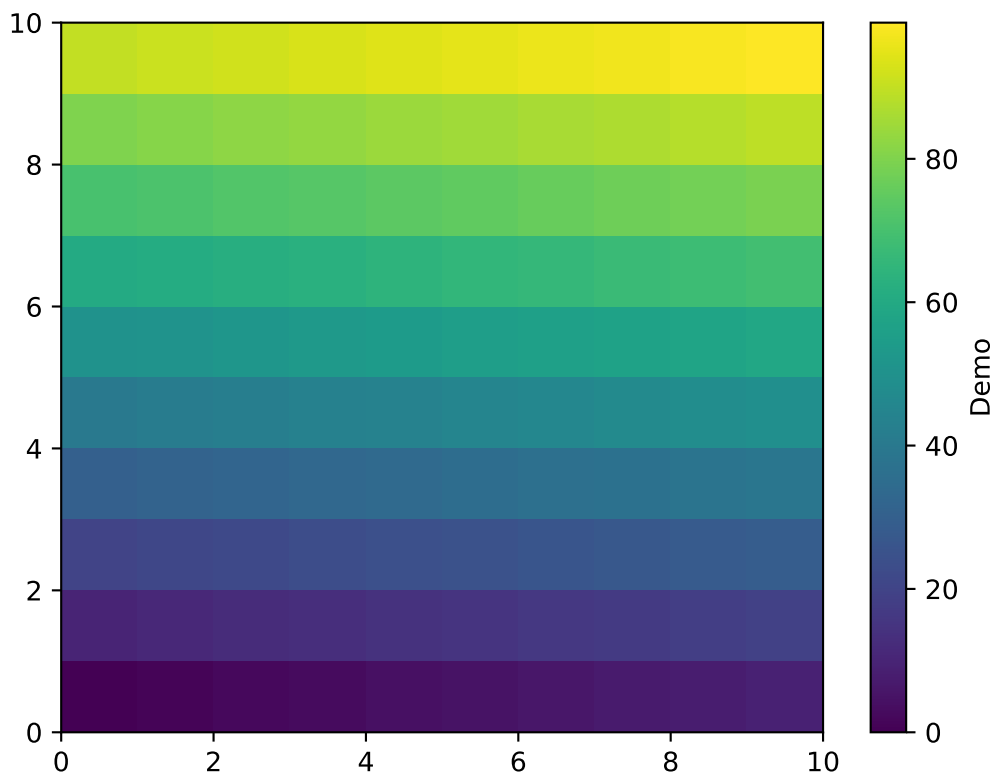
Return type `matplotlib.axes.Axes`

Raises

- **ValueError** – If `logColor` and data contains negative quantities
- **TypeError** – If only one of `xticks` or `yticks` is `None`.

Examples

```
>>> from serpentTools.plot import cartMeshPlot
>>> from numpy import arange
>>> data = arange(100).reshape(10, 10)
>>> x = y = arange(11)
>>> cartMeshPlot(data, x, y, cbarLabel='Demo')
```

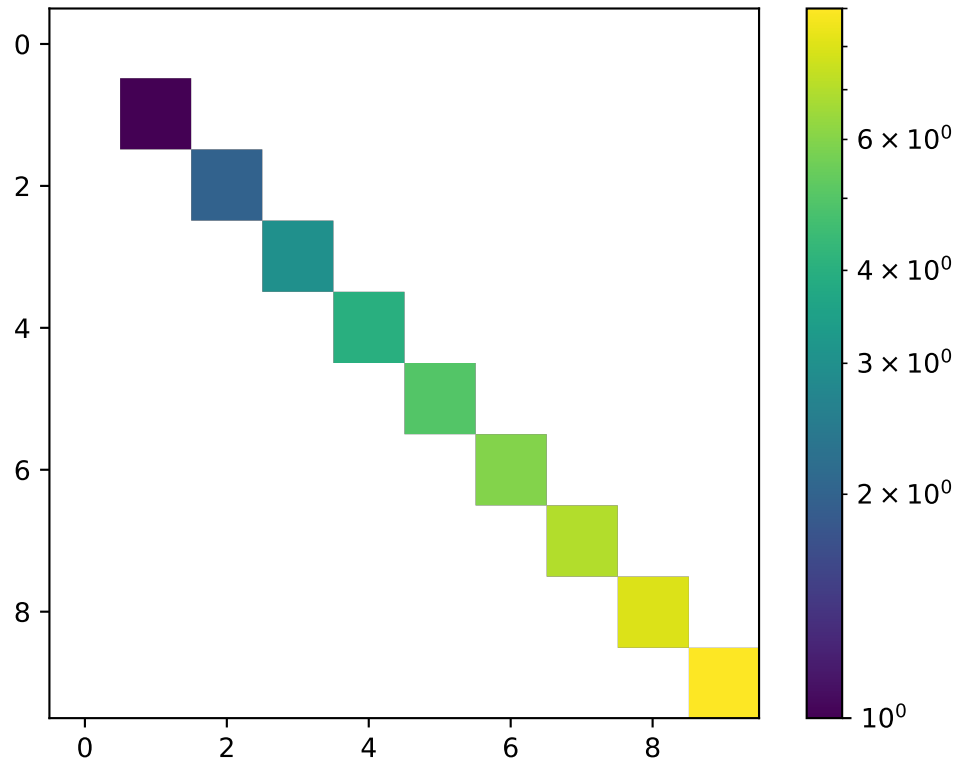


```
>>> from serpentTools.plot import cartMeshPlot
>>> from numpy import eye
>>> data = eye(10)
```

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```
>>> for indx in range(10):
...     data[indx] *= indx
>>> cartMeshPlot(data, logColor=True)
```



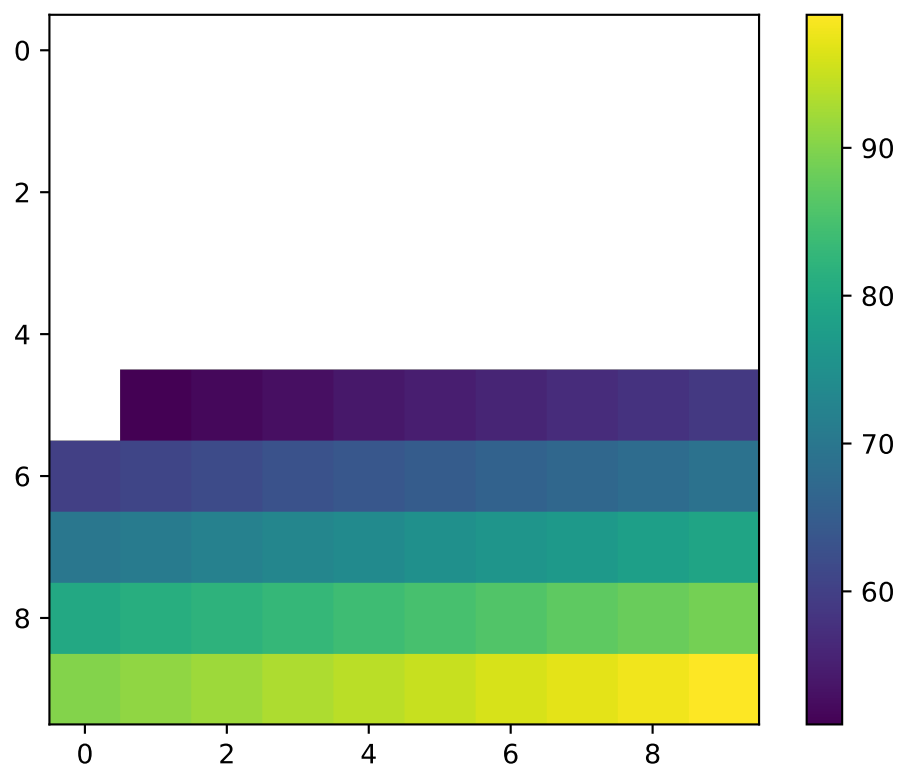
All values less than or equal to zero are excluded from the color normalization. The `logColor` argument works well for plotting sparse matrices, as the zero-valued indices can be identified without obscuring the trends presented in the non-zero data.

Alternatively, one can use the `thresh` argument to set a threshold for plotted data. Any value less than or equal to `thresh` will not be colored, and the colorbar will be updated to reflect this.

```
>>> from serpentTools.plot import cartMeshPlot
>>> from numpy import arange
>>> data = arange(100).reshape(10, 10)
>>> cartMeshPlot(data, thresh=50)
```

See also:

- `matplotlib.pyplot.pcolormesh()`
- `matplotlib.pyplot.imshow()`
- `matplotlib.colors.Normalize`



serpentTools.plot.plot

`serpentTools.plot.plot(xdata, plotData, ax=None, labels=None, yerr=None, **kwargs)`

Shortcut plot for plotting series of labeled data onto a plot

If `plotData` is an array, it is assumed that each column represents one set of data to be plotted against `xdata`. The same assumption is made for `yerr` if given.

Parameters

- **xdata** (*numpy.array or iterable*) – Points along the x axis to plot
- **plotData** (*numpy.array or iterable*) – Data to be plotted
- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **labels** (*None or iterable*) – Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
- **yerr** (*None or numpy.array or iterable*) – Absolute error for each data point in `plotData`
- **kwargs** (*dict, optional*) – Addition keyword arguments to pass to `matplotlib.pyplot.plot()` or `matplotlib.pyplot.errorbar()`

Returns Ax on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises `IndexError` – If `yerr` is not `None` and does not match the shape of `plotData`

Plot Formatters

The following functions can be used to tidy up a plot given our wide-range of supported arguments.

<code>formatPlot</code>	Apply a range of formatting options to the plot.
<code>placeLegend</code>	Add a legend to the axes instance.
<code>setAx_xlims</code>	Set the x limits on an Axes object
<code>setAx_ylims</code>	Set the y limits on an Axes object
<code>addColorbar</code>	Quick utility to add a colorbar to an axes object
<code>normalizerFactory</code>	Construct and return a <code>Normalize</code> for this data

serpentTools.utils.plot.formatPlot

`serpentTools.utils.plot.formatPlot(ax, xlabel=None, ylabel=None, logx=False, logy=False, loglog=False, title=None, legend=True, legendcols=1, axkwargs=None, legendkwargs=None)`

Apply a range of formatting options to the plot.

Parameters

- **ax** (`matplotlib.axes.Axes`, optional) – Ax on which to plot the data. If not provided, create a new plot
- **xlabel** (*str or bool, optional*) – Label to apply to the x-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.

- **ylabel** (*str* or *bool*, *optional*) – Label to apply to the y-axis. If given as `None`, a label will be determined from other arguments. If not `None` but evaluates to `False`, do not label.
- **loglog** (*bool*) – Apply a log scale to both axes.
- **logx** (*bool*) – Apply a log scale to x axis.
- **logy** (*bool*) – Apply a log scale to y axis.
- **title** (*str*, *optional*) – Title to apply to this axes object
- **legend** (*bool* or *str* or *None*) – Automatically label the plot. No legend will be made if a single item is plotted. Pass one of the following values to place the legend outside the plot: `above`, `right`
- **legendcols** (*int*, *optional*) – Number of columns to apply to the legend, if applicable
- **axkwargs** (*dict*, *optional*) – Additional keyword arguments to be passed to `matplotlib.axes.Axes.set()`. Values like `xlabel`, `ylabel`, `xscale`, `yscale`, and `title` will be respected, even though they are also arguments to this function
- **legendkwargs** (*dict*, *optional*) – Additional keyword arguments to be passed to `matplotlib.axes.Axes.legend()`. Values like `title` and `ncol` will be respected.

Returns `Ax` on which the data was plotted.

Return type `matplotlib.axes.Axes`

Raises **`TypeError`** – If the `ax` argument is not an instance of `matplotlib.pyplot.axes.Axes`

serpentTools.utils.plot.placeLegend

`serpentTools.utils.plot.placeLegend(ax, legend, handlesAndLabels=None, **kwargs)`

Add a legend to the axes instance.

A legend will be drawn if at least one of the following criteria are met:

1. `legend` is not one of the supported string legend control arguments that dictate where the legend should be placed
2. More than one item has been plotted

Parameters

- **ax** (`matplotlib.axes.Axes`, *optional*) –
- **on which to plot the data. If not provided, create a new (`Ax`) –**
- **plot** –
- **legend** (*bool* or *str* or *None*) –
- **label the plot. No legend will be made if a (`Automatically`) –**
- **item is plotted. Pass one of the following values (`single`) –**
- **place the legend outside the plot (`to`) –**

- **handlesAndLabels** (*tuple (legend handles, labels), optional*) – Exact legend handles (graphical element) and labels (string element) to be used in making the legend. If not provided, will be fetched from `matplotlib.axes.Axes.get_legend_handles_labels()`
- **kwargs** (*dict, optional*) – Additional keyword arguments to be passed to `matplotlib.axes.Axes.legend()`, if applicable

Returns

- `matplotlib.axes.Axes`
- *Ax on which the data was plotted.*

serpentTools.utils.plot.setAx_xlims

`serpentTools.utils.plot.setAx_xlims(ax, xmin, xmax, pad=10)`

Set the x limits on an Axes object

Parameters

- **ax** (`matplotlib.axes.Axes`) – Ax to be updated
- **xmin** (*float*) – Current minimum extent of x axis
- **xmax** (*float*) – Current maximum extent of x axis
- **pad** (*float, optional*) – Padding, in percent, to apply to each side of the current min and max

serpentTools.utils.plot.setAx_ylims

`serpentTools.utils.plot.setAx_ylims(ax, ymin, ymax, pad=10)`

Set the y limits on an Axes object

Parameters

- **ax** (`matplotlib.axes.Axes`) – Ax to be updated
- **ymin** (*float*) – Current minimum extent of y axis
- **ymax** (*float*) – Current maximum extent of y axis
- **pad** (*float, optional*) – Padding, in percent, to apply to each side of the current min and max

serpentTools.utils.plot.addColorbar

`serpentTools.utils.plot.addColorbar(ax, mappable, norm=None, cbarLabel=None)`

Quick utility to add a colorbar to an axes object

The color bar is placed adjacent to the provided axes argument, rather than in the provided space.

Parameters

- **mappable** (*iterable*) – Collection of meshes, patches, or values that are used to construct the colorbar.
- **norm** (`matplotlib.colors.Normalize`, *optional*) – Normalizer for this plot. Can be a subclass like `matplotlib.colors.LogNorm`

- **cbarLabel** (*str*, *optional*) – If given, place this as the y-label for the colorbar

Returns The colorbar that was added

Return type `matplotlib.colorbar.Colorbar`

serpentTools.utils.plot.normalizerFactory

`serpentTools.utils.plot.normalizerFactory` (*data*, *norm*, *logScale*, *xticks*, *yticks*)

Construct and return a `Normalize` for this data

Parameters

- **data** (`numpy.ndarray`) – Data to be plotted and normalized
- **norm** (None or callable or `matplotlib.colors.Normalize`) – If a `Normalize` object, then use this as the normalizer. If callable, set the normalizer with `norm(data, xticks, yticks)`. If not None, set the normalizer to be based on the min and max of the data
- **logScale** (*bool*) – If this evaluates to true, construct a `matplotlib.colors.LogNorm` with the minimum set to be the minimum of the positive values.
- **xticks** (`numpy.ndarray`) –
- **yticks** (`numpy.ndarray`) – Arrays ideally corresponding to the data. Used with callable *norm* function.

Returns

- `matplotlib.colors.Normalize`
- or `matplotlib.colors.LogNorm`
- or *object* – Object used to normalize colormaps against these data

Docstring Formatters for Plots

Many of the plot routines accept common parameters, such as `logx` for applying a log scale to the x-axis. To reduce the amount of repeated code, the following formatting functions operate on the docstrings of a plot function/method and save a lot of extra code.

See [Magic Plot Decorator Options](#) for a listing of what is replaced by what when calling `serpentTools.plot.magicPlotDocDecorator()`.

`serpentTools.utils.docstrings.magicPlotDocDecorator` (*f*)

Decorator that replaces a lot magic strings used in plot functions.

Allows docstrings to contain keyword that will be replaced with a valid and proper explanation of the keyword. Keywords must be wrapped in single brackets, i.e. {x}

Magic Plot Decorator Options

Note: These keyword arguments should only be used when they are appropriate for the specific plot method. Colormaps don't really make sense for line plots, but can be very useful for 2D contour and mesh plots. `cmap` should be a supported argument for most of these plot types, but not for line plots, unless it makes sense to do such.

1. **ax:** `ax: matplotlib.axes.Axes` or `None` Ax on which to plot the data.
2. **cmap:** `cmap: str` or `None` Valid Matplotlib colormap to apply to the plot.
3. **kwargs:** `kwargs:` Addition keyword arguments to pass to
4. **labels:** `labels: None` or `iterable` Labels to apply to each line drawn. This can be used to identify which bin is plotted as what line.
5. **legend:** `legend: bool` or `str` Automatically label the plot. Pass one of the following values to place the legend outside the plot: above, right
6. **loglog:** `loglog: bool` Apply a log scale to both axes.
7. **logx:** `logx: bool` Apply a log scale to x axis.
8. **logy:** `logy: bool` Apply a log scale to y axis.
9. **matLabelFmt:** `labelFmt: str` or `None` Formattable string for labeling the individual plots. If not given, just label as isotope name, e.g. 'U235'. Will make the following substitutions on the `labelFmt` string, if given:

Keyword	Replacement
'mat '	name of this material
'iso '	specific isotope name
'zai '	specific isotope ZZAAAI

10. **ncol:** `ncol: int` Integer number of columns to apply to the legend.
11. **rax:** `matplotlib.axes.Axes` Ax on which the data was plotted.
12. **sigma:** `sigma: int` Confidence interval to apply to errors. If not given or 0, no errors will be drawn.
13. **title:** `title: str` Title to apply to the figure.
14. **xlabel:** `xlabel: str` or `None` Label for x-axis.
15. **ylabel:** `ylabel: str` or `None` Label for y-axis.

12.9 Converter Utilites

One goal for this project is to allow users to use `serpentTools` as a pipeline for taking *SERPENT* data to other programs. The first demonstration of this is creating binary `.mat` files that can be read into MATLAB, when a large text file would cause issues, done with the *MatlabConverter*.

Classes intending do first look for specific methods for gathering data on each object. These are obscured from the public API as they don't serve a direct purpose besides a simple method by which to translate data from one place to the next. This collection is called inside the primary `convert` method, which is responsible for gathering and writing the data into the new form.

Keeping with the *MatlabConverter* as an example, it looks for `_gather_matlab` method. This method simply places data into a dictionary, but do to the layout of each object, must be reimplemented as a unique

method. Due to the simplicity of `scipy.io.savemat()`, the main writing function, `serpentTools.io.base.MatlabConverter.convert()`, is rather light. However, some data forms may require more depth to ensure fidelity in the converted data.

There may be some cases where a conversion does not make sense for all data types. Detector objects are the few pieces of data that can have a spatial grid attached, yet this grid varies across detectors. It may be advantageous to implement converters directly as instance methods. The decision will be up to the developer and the review process in that case.

Converters should also make sure, prior to potentially expensive collection steps are taken, that the user is in the best position to execute this operation. As of this writing and 0.6.1, `scipy` is not a requirement for this package, yet it is required for MATLAB conversion. Therefore, the `MatlabConverter` implements a check for `scipy` in `checkImports()`. The other check method, `checkContainerReq()`, is responsible for checking the container has the required data gathering routines, e.g. `_gather_matlab`. These checks are called at creation of the converter object.

class `serpentTools.io.base.MatlabConverter` (*container, output*)

Class for assisting in writing container data to MATLAB

Parameters

- **obj** (`serpentTools` container) – Parser or container to be written to file
- **fileP** (*str or file-like object*) – Name of the file to write

See also:

- `serpentTools.io.toMatlab()` - high level function for writing to MATLAB that uses this class

checkContainerReq (*container*)

Ensure that data from the container can be collected.

checkImports ()

Ensure that `scipy` ≥ 1.0 is installed.

convert (*reconvert, append=True, format='5', longNames=True, compress=True, oned='row'*)

Save contents of object to `.mat` file

Parameters

- **fileP** (*str or file-like object*) – Name of the file to write
- **reconvert** (*bool*) – If this evaluates to true, convert values back into their original form as they appear in the output file, e.g. `MAT_TOTAL_ING_TOX`. Otherwise, maintain the `mixedCase` style, `total_ingTox`.
- **append** (*bool*) – If true and a file exists under `output`, append to that file. Otherwise the file will be overwritten
- **format** (*{ '5', '4' }*) – Format of file to write. '5' for MATLAB 5 to 7.2, '4' for MATLAB 4
- **longNames** (*bool*) – If true, allow variable names to reach 63 characters, which works with MATLAB 7.6+. Otherwise, maximum length is 31 characters
- **compress** (*bool*) – If true, compress matrices on write
- **oned** (*{ 'row', 'col' }*;) – Write one-dimensional arrays as row vectors if `oned=='row'` (default), or column vectors

See also:

`scipy.io.savemat()`

12.10 Parsing Engines

The *KeywordParser* and *PatternReader* contained in `serpentTools/engines.py` are part of the `drewtils v0.1.9` package and are provided under the following license

```
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```

These are designed to facilitate the parsing of files with a regular structure. For example, the depletion files all contain “chunks” of data that are separated by empty lines. Each chunk leads off with either the name of the material and associated variable, or the metadata, e.g. `ZAI`, `DAYS`. These parsers help break up these files into more digestible pieces.

Note: For developers, it is not required that these classes be used. These are bundled with this project to eliminate the need to install extra packages. Some of the readers, like the *BranchingReader* are not well suited for this type of parsing.

<i>KeywordParser</i>	Class for parsing a file for chunks separated by various keywords.
<i>PatternReader</i>	Class that can read over a file looking for patterns.

12.10.1 serpentTools.engines.KeywordParser

class serpentTools.engines.**KeywordParser** (*filePath*, *keys*, *separators=None*, *eof=""*)

Class for parsing a file for chunks separated by various keywords.

Parameters

- **filePath** (*str*) – Object to be read. Any object with `read` and `close` methods
- **keys** (*Iterable*) – List of keywords/phrases that will indicate the start of a chunk
- **separators** (*Iterable or None*) – List of additional phrases that can separate two chunks. If not given, will default to empty line `'\n'`.
- **eof** (*str*) – String to indicate the end of the file

line

Most recently read line

Type *str*

parse()

Parse the file and return a list of keyword blocks.

Returns List of key word argument chunks.

Return type *list*

seekToTop()

Reset the file pointer to the start of the file.

yieldChunks()

Return each chunk of text as a generator.

Yields *list* – The next chunk in the file.

12.10.2 serpentTools.engines.PatternReader

class serpentTools.engines.**PatternReader** (*filePath*)

Class that can read over a file looking for patterns.

Parameters **filePath** (*str*) – path to the file that is to be read

line

Most recently read line

Type *str*

match

Match from the most recently read line

Type regular expression match or *None*

searchFor (*pattern*)

Return true if the pattern is found.

Parameters **pattern** (*str or compiled regular expression*) –

Returns *bool*

Return type True if the pattern was found

seekToTop()

Reset the file pointer to the start of the file.

yieldMatches (*pattern*)

Generator that returns all match groups that match pattern.

Parameters **pattern** (*str or compiled regular expression*) – Seek through the file and yield all match groups for lines that contain this pattern.

Yields *sequential match groups*

The *CSCStreamProcessor* is provided to help with reading sparse matrices provided by Serpent. These are currently found in the depletion and fission matrix files.

class serpentTools.parsers.base.**CSCStreamProcessor** (*stream, regex, dtype=<class 'float'>*)

Read through a block of text and produce sparse matrices

Note: Rows and columns matched by *regex* will be reduced by one prior to storage. Since we primarily interact with one-indexed MATLAB arrays, we need to convert the indices to something *numpy* can properly understand

Parameters

- **stream** (*IO stream from an opened file*) – Object with a `readline` function that returns the next line of text to be read
- **regex** (*str or compiled regular expression*) – Regular expression that matches the following:
 0. Row of matrix
 1. Column of matrix
 2. Values to be added into resulting matrix.

All values in `match.groups()[2:]` will be converted to `datatype` and appended into *data*. The rows and columns are used to populate *indices* and *indptr* vectors
- **datatype** (*object*) – Data type of the numeric values of this matrix.

data

Column matrix of all values matched by *regex* after first two positions. Each column can be used to build a sparse matrix with *indices* and *indptr*

Type `numpy.ndarray`

indices

CSC-format indices pointer array

Type `numpy.ndarray`

indptr

CSC-format index pointer array. Row indices for column *i* are stored in `indices[indptr[i]:indptr[i + 1]]`. Values for column *i* are stored in `data[indptr[i]:indptr[i + 1]]`.

Type `numpy.ndarray`

line

Last line read after calling `process()`. Will be the first non-empty line that does not match the passed regular expression

Type `str`

See also:

- `scipy.sparse.csc_matrix`

12.11 Adding Support for Serpent Versions

One of the main goals for this project is to include support for more SERPENT versions. The goal of this document is to detail what steps are required in order to include support for additional SERPENT versions.

Note: Supporting additional versions is an ongoing task. See [#117](#) and linked issues for updates

12.11.1 Checklist

1. Include the version as an option in the *serpentVersion* setting - [serpentVersion](#)
2. Update the *Default Settings*
3. Update `serpentTools/variables.yaml` to include the version and any new variable groups present in the results files - [New Variables](#)
4. If `serpentTools/variables.yaml` is updated, update [Variable Groups](#) using the script `docs/rstVariableGroups.py`

12.11.2 New Variables

As detailed in [Variable Groups](#), `serpentTools` utilizes a collection of variable groups to expedite what data is extracted from results and branching files. Some versions of SERPENT may have different data, as more features are added to the code, while some may have the same data with different names. Variables and variable groups can be added to `serpentTools/variables.yaml` as sets. Since the order of the variables present in the file is not important, and we are simply interested in *if* a variable found in a file is in a group, the `set` provides a good framework for this inspection.

The basic structure of `serpentTools/variables.yaml` is given below for a single version:

```
version
  |- group_0
    | - variable_0
    | - variable_1
    ...
  |- group_1
    | - variable_0
    | - variable_1
    ...
  ...
```

There is also a base version that serves as a catch-all, as detailed in [Variable Lookup Procedure](#).

Variables are loaded from `serpentTools/variables.yaml` as nested dictionaries:

```
variables = {
  version0: {group_0: {variable_0, variable_1, ...},
             group_1: {variable_0, variable_1, ...},
```

(continues on next page)

(continued from previous page)

```

        ...
    },
    version1: {group_0: {variable_0, variable_1, ...},
               group_1: {variable_0, variable_1, ...},
               ...
    },
    ...
}

```

Variable Lookup Procedure

The lookup procedure for variable groups is as follows. For a specific SERPENT version V and variable group g ,

- If the variable group is explicitly declared under **variables** [V], then take the variables from `variables[V][g]`
- If the group is declared under **variables** ['base'], then take the variables from `variables['base'][g]`
- Otherwise, raise an error

The 'base' serves to store variables that are invariant across all SERPENT versions. As the development of SERPENT progresses, it is not unlikely that the 'base' group may dwindle, as each version listed in `serpentTools/variables.yaml` expands.

Shared Variable Groups

For variable groups that are similar between two versions but not contained in 'base', one can take advantage of [YAML anchors and aliases](#), implemented in PyYAML as `&` and `*` characters. An example of sharing a group between two versions this way is given below:

```

parentV:
  parentG: !!set &parentG
            {vx0, vx1, ...}
childV:
  childG: *parentG

```

Loading such a file would return a dictionary like:

```

{parentV: {parentG: {vx0, vx1, ...}},
 childV: {childV:{vx0, vx1, ...}}}

```

12.11.3 Versions with New File Formats

In the event that a future version of SERPENT causes substantial changes to the layout of output files, such that present readers will not work, then version-specific read methods will have to be written. If/when this happens, a procedure will be developed and added here.

MapStrVersions

This is a mapping variable located in the ResultsReader parser. The variable is a nested dictionary, where the keys describe the version and the nested dictionary describes the various data blocks within the results file (`_res.m`).

In general the results file is divided into three main blocks: - metadata: general description of the simulation - resdata: time-dependent values, e.g. k-eff - universes: universe dependent values, such as cross-sections. The mapping through the variable MapStrVersions should reflect this.

The basic mapping definition relies on the following structure:

```
MapStrVersions = {'2.1.29':                                     # serpent version
{'meta': 'VERSION',                                           # The starting keyword of the
↪ metadata block
'rslt': 'MIN_MACROXS',                                       # The starting keyword of the resdata block
'univ': 'GC_UNIVERSE_NAME',                                   # The starting keyword of the universes block
'days': 'BURN_DAYS',                                         # A keyword used in Serpent to describe time,
↪ days
'burn': 'BURNUP',                                             # A keyword used in Serpent to describe burnup, MWd/
↪ kgU
'infxs': 'INF_',                                             # A prefix in Serpent used to describe infinite cross-
↪ sections
'blxs': 'B1_',                                               # A prefix in Serpent used to
↪ describe b1 cross-sections
'varsUnc': ['MICRO_NG', 'MICRO_E', 'MACRO_NG', 'MACRO_E']}] # Only the variables that
↪ have no uncertainties in the universe block
```

In order to support different serpent versions, these keywords would need to be updated.

12.12 Comparison Methods

We are currently developing methods for our readers and containers to be able for comparing between like objects. This could be used to compare the effect of changing fuel enrichment on pin powers or criticality, or used to compare the effect of different SERPENT settings. The BaseObject that every object **should** inherit from contains the bulk of the input checking, so each reader and object needs to implement a private `_compare` method with the following structure:

```
def _compare(self, other, lower, upper, sigma):
    return <boolean output of comparison>
```

Note: While these methods will iterate over many quantities, and some quantities may fail early on in the test, the comparison method should continue until all quantities have been tested.

The value `sigma` should be used to compare quantities with uncertainties by constructing intervals bounded by $x \pm S\sigma$, where `sigma` = S . Quantities that do not have overlapping confidence windows will be considered too different and should result in a `False` value being returned from the method.

The `lower` and `upper` arguments should be used to compare values that do not have uncertainties. Both will be float values, with `lower` less than or equal to `upper`. This functionality is implemented with the `serpentTools.utils.directCompare()` function, while the result is reported with `serpentTools.utils.logDirectCompare()`.

12.12.1 Use of messaging module

Below is a non-definitive nor comprehensive list of possible comparison cases and the corresponding message that should be printed. Using a range of message types allows the user to be able to easily focus on things that are really bad by using our *verbosity* setting.

- Two objects contain different data sets, e.g. different dictionary values - *warning()* displaying the missing items, and then apply test to items in both objects
- Two items are identically zero, or arrays of zeros - *debug()*
- Two items are outside of the *sigma* confidence intervals - *error()*
- Two items without uncertainties have relative difference
 - less than *lower* - *debug()*
 - greater than or equal to *upper* - *error()*
 - otherwise - *warning()*
- Two items are identical - *debug()*
- Two arrays are not of similar size - *error()*

12.12.2 High-level Logging and Comparison Utilities

The *utils* module contains a collection of functions that can be used to compare quantities and automatically log results. When possible, these routines should be favored over hand-writing comparison routines. If the situation calls for custom comparison functions, utilize or extend logging routines from *Low-level Logging Utilities* appropriately.

```
serpentTools.utils.compare.compareDictOfArrays(d0, d1, desc, lower=0, upper=10,
                                                sigma=2, u0={}, u1={}, relative=True)
```

High-level routine for evaluating the similarities of two dictionaries

The following tests are performed

1. Find a set of keys that both exist in *d0* and *d1* and point to arrays with identical shapes using *getKeyMatchingShapes()*
2. For each key in this common set, compare the values with *logDirectCompare()* or *getLogOverlaps()*. The latter is used if the key exists in *u0* and *u1*, provided uncertainty arrays are of identical shapes.

Parameters

- **d0** (*dict*) – Reference dictionary
- **d1** (*dict*) – Dictionarie to be compared to the reference
- **desc** (*str*) – Descption of the two dictionaries. Should describe what data they represent.
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **u0** (*dict*) –

- **u1** (*dict*) – If `uncKeys` is not `None`, then find the uncertainties for data in `d0` and `d1` under the same keys.
- **relative** (*bool*) – If this evaluates to `true`, then uncertainties in `u0` and `u1` are relative.

Returns `True` If all comparisons pass

Return type `bool`

`serpentTools.utils.compare.getCommonKeys` (*d0, d1, quantity, desc0='first', desc1='second', herald=<function error>*)

Return a set of common keys from two dictionaries

Also supports printing warning messages for keys not found on one collection.

If `d0` and `d1` are *dict*, then the keys will be obtained with `d1.keys()`. Otherwise, assume we have an iterable of keys and convert to *set*.

Parameters

- **d0** (*dict or iterable*) –
- **d1** (*dict or iterable*) – Dictionary of keys or iterable of keys to be compared
- **quantity** (*str*) – Indicator as to what is being compared, e.g. `'metadata'`
- **desc0** (*dict or None*) –
- **desc1** (*dict or None*) – Description of the origin of each value set. Only needed if `quiet` evaluates to `True`.
- **herald** (*callable*) – Function that accepts a single string argument used to notify that differences were found. If the function is not a callable object, a `serpentTools.messages.critical()` message will be printed and `serpentTools.messages.error()` will be used.

Returns Keys found in both `d[{0, 1}]`

Return type *set*

`serpentTools.utils.compare.directCompare` (*obj0, obj1, lower, upper*)

Return `True` if values are close enough to each other.

Wrapper around various comparison tests for strings, numeric, and arrays.

Parameters

- **obj0** (*str or float or int or numpy.ndarray*) –
- **obj1** (*str or float or int or numpy.ndarray*) – Objects to compare
- **lower** (*float or int*) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (*float or int*) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **quantity** (*str*) – Description of the value being compared. Will be used to notify the user about any differences

Returns

Status code of the comparison.

- 0 - Values are identical to floating point precision or, for strings/booleans, are identical with the `==` operator

- 1 - Values are not identical, but the max difference is less than `lower`.
- 10 - Values differ, with the max difference greater than `lower` but less than `upper`
- 100 - Values differ by greater than or equal to `upper`
- 200 - Values should be identical (strings, booleans), but are not
- 250 - Numeric data has different shapes
- 255 - Values are of different types
- -1 - Type comparison is not supported. This means that developers should either implement a test for this data type, or use a different function

Return type `int`

See also:

- `logDirectCompare()` - Function that utilizes this and logs the results using the `serpentTools.messages` module

`serpentTools.utils.compare.logDirectCompare(obj0, obj1, lower, upper, quantity)`
Compare objects using `directCompare()` and log the result

Parameters

- **obj0** (`str` or `float` or `int` or `numpy.ndarray`) –
- **obj1** (`str` or `float` or `int` or `numpy.ndarray`) – Objects to compare
- **lower** (`float` or `int`) – Lower limit for relative tolerances in percent Differences below this will be considered allowable
- **upper** (`float` or `int`) – Upper limit for relative tolerances in percent. Differences above this will be considered failure and errors messages will be raised
- **quantity** (`str`) – Description of the value being compared. Will be used to notify the user about any differences

Returns `True` if the objects agree according to tolerances, or numerics differ less than `upper`.
`False` otherwise

Return type `bool`

Raises **TypeError**: – If the objects being compared are not supported by `directCompare()`.
Developers should either extend the function or utilize a different comparison function

See also:

- `directCompare()` - function that does the comparison
- `getOverlaps()` - function for evaluating values with uncertainties
- `getLogOverlaps()` - function that logs the result of statistical comparisons

`serpentTools.utils.compare.splitDictByKeys(map0, map1, keySet=None)`
Return various sub-sets and dictionaries from two maps.

Used to test the internal workings on `getKeyMatchingShapes()`

Parameters

- **map0** (`dict`) –
- **map1** (`dict`) – Dictionaries to compare

- **keySet** (*set or None*) – Iterable collection of keys found in `map0` and `map1`. Missing keys will be returned from this function under the `missing0` and `missing1` sets. If `None`, take to be the set of keys that exist in both maps

Returns

- **missing0** (*set*) – Keys that exist in `keySet` but not in `map0`
- **missing1** (*set*) – Keys that exist in `keySet` but not in `map1`
- **differentTypes** (*dict*) – Dictionary with tuples `{key: (t0, t1)}` indicating the values `map0[key]` and `map1[key]` are of different types
- **badShapes** (*dict*) – Dictionary with tuples `{key: (t0, t1)}` indicating the values `map0[key]` and `map1[key]` are arrays of different shapes
- **goodKeys** (*set*) – Keys found in both `map0` and `map1` that are of the same type or point to arrays of the same shape

`serpentTools.utils.compare.getKeyMatchingShapes` (*map0, map1, quantity, keySet=None, desc0='first', desc1='second'*)

Return a set of keys in `map0/1` that point to arrays with identical shapes.

Parameters

- **keySet** (*set or list or tuple or iterable or None*) – Iterable container with keys that exist in `map0` and `map1`. The contents of `map0/1` under these keys will be compared. If `None`, will be determined by `splitDictByKeys()`
- **map0** (*dict*) –
- **map1** (*dict*) – Two dictionaries containing at least all the keys in `keySet`. Objects under keys in `keySet` will have their sizes compared if they are `numpy.ndarray`. Non-arrays will be included only if their types are identical
- **quantity** (*str*) – Indicator as to what is being compared, e.g. 'metadata'
- **desc0** (*str*) –
- **desc1** (*str*) – Descriptions of the two dictionaries being compared. Used to alert the user to the shortcomings of the two dictionaries

Returns Set of all keys that exist in both dictionaries and are either identical types, or are arrays of identical shapes

Return type `set`

See also:

- `splitDictByKeys()`

`serpentTools.utils.compare.getOverlaps` (*arr0, arr1, unc0, unc1, sigma, relative=True*)

Return the indicies of overlapping confidence intervals

Parameters

- **arr0** (`numpy.ndarray`) –
- **arr1** (`numpy.ndarray`) – Arrays containing the expected values to be compared
- **unc0** (`numpy.ndarray`) –
- **unc1** (`numpy.ndarray`) – Associated absolute uncertainties, 1σ , corresponding to the values in `arr0` and `arr1`

- **sigma** (*int*) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **relative** (*bool*) – True if uncertainties are relative and should be multiplied by their respective values. Otherwise, assume values are absolute

Returns Boolean array of equal shape to incoming arrays. Every index with True as the value indicates that the confidence intervals for the arrays overlap at those indices.

Return type `numpy.ndarray`

Examples

Using absolute uncertainties:

```
>>> from numpy import ones, zeros, array
>>> a0 = ones(4)
>>> a1 = ones(4) * 0.5
>>> u0 = array([0, 0.2, 0.1, 0.2])
>>> u1 = array([1, 0.55, 0.25, 0.4])
```

Here, the first point in the confidence interval for a0 is completely contained within that of a1. The upper limit of a1[1] is contained within the confidence interval for a0. The confidence intervals for the third point do not overlap, while the lower bound of a0[3] is within the confidence interval of a1[3].

```
>>> getOverlaps(a0, a1, u0, u1, 1, relative=False)
array([True, True, False, True])
```

This function also works for multi-dimensional arrays as well.

```
>>> a2 = a0.reshape(2, 2)
>>> a3 = a1.reshape(2, 2)
>>> u2 = u0.reshape(2, 2)
>>> u3 = u1.reshape(2, 2)
>>> getOverlaps(a2, a3, u2, u3, 1, relative=False)
array([[ True,  True],
       [False, False]])
```

Raises `IndexError` – If the shapes of incoming arrays do not agree

See also:

- `getLogOverlaps()` - High-level function that uses this to report if two values have overlapping confidence intervals

`serpentTools.utils.compare.getLogOverlaps(quantity, arr0, arr1, unc0, unc1, sigma, relative=True)`

Wrapper around `getOverlaps()` that logs the result

Parameters

- **quantity** (*str*) – Name of the value being compared
- **arr0** (`numpy.ndarray`) –
- **arr1** (`numpy.ndarray`) –
- **unc0** (`numpy.ndarray`) –

- **unc1** (`numpy.ndarray`) – Arrays and their uncertainties to evaluate
- **sigma** (`int`) – Size of confidence interval to apply to quantities with uncertainties. Quantities that do not have overlapping confidence intervals will fail
- **relative** (`bool`) – If uncertainties are relative. Otherwise, assume absolute uncertainties.

Returns True if all locations `arr0` and `arr1` are either identical or within allowable statistical variations.

Return type `bool`

See also:

- `getOverlaps()` - This function performs all the comparisons while this function simply reports the output using `serpentTools.messages`

`serpentTools.utils.docstrings.compareDocDecorator(f)`

Decorator that updates doc strings for comparison methods.

Similar to `serpentTools.plot.magicPlotDocDecorator()` but for comparison functions

12.12.3 Low-level Logging Utilities

The `messages` module contains a collection of functions that can be used to notify the user about the results of a comparison routine.

`serpentTools.messages.logIdentical(obj0, obj1, quantity)`

Two objects are identical.

`serpentTools.messages.logNotIdentical(obj0, obj1, quantity)`

Values should be identical but aren't.

`serpentTools.messages.logAcceptableLow(obj0, obj1, quantity)`

Two values differ, but inside nominal and acceptable ranges.

`serpentTools.messages.logAcceptableHigh(obj0, obj1, quantity)`

Two values differ, enough to merit a warning but not an error.

`serpentTools.messages.logOutsideTols(obj0, obj1, quantity)`

Two values differ outside acceptable tolerances.

`serpentTools.messages.logIdenticalWithUncs(value, unc0, unc1, quantity)`

Notify that two values have identical expected values.

`serpentTools.messages.logInsideConfInt(value0, unc0, value1, unc1, quantity)`

Two values are within acceptable statistical limits.

`serpentTools.messages.logOutsideConfInt(value0, unc0, value1, unc1, quantity)`

Two values are outside acceptable statistical limits.

`serpentTools.messages.logDifferentTypes(type0, type1, quantity)`

Two values are of different types.

`serpentTools.messages.logMissingKeys(quantity, desc0, desc1, in0, in1, herald=<function error>)`

Log a warning message that two objects contain different items

Parameters

- **quantity** (`str`) – Indicator as to what is being compared, e.g. 'metadata'

- **desc0** (*str*) –
- **desc1** (*str*) – Descriptions of the two originators
- **in0** (*set or iterable*) –
- **in1** (*set or iterable*) – Items that are unique to originators 0 and 1, respectively
- **herald** (*callable*) – Callable function that accepts a single string. This will be called with the error message. If not given, defaults to `error()`

`serpentTools.messages.logBadTypes` (*quantity, desc0, desc1, types*)

Log an error message for containers with mismatched types

Parameters

- **quantity** (*str*) – Indicator as to what is being compared, e.g. 'metadata'
- **desc0** (*str*) –
- **desc1** (*str*) – Descriptions of the two originators
- **types** (*dict*) – Dictionary where the keys represent the locations of items with mismatched types. Corresponding keys should be a list or tuple of the types for objects from desc0 and desc1 stored under key

`serpentTools.messages.logBadShapes` (*obj0, obj1, quantity*)

Log an error message that two arrays are of different shapes.

Parameters

- **obj0** (`numpy.ndarray`) –
- **obj1** (`numpy.ndarray`) – Arrays that have been compared and found to have different shapes
- **quantity** (*str*) – Descriptor of the quantity being compared, e.g. what these objects represent

12.13 Data Model

This project has two key offerings to the SERPENT community.

1. Scripting tools that are capable of interpreting the output files
2. Purpose-built containers for storing, accessing, and utilizing the data in the output files

12.13.1 Readers

The readers are the core of this package, and should have a logical and consistent method for structuring data. Each reader contained in this project should:

1. Be capable of reading the intended output file
2. Yield to the user the data in a logical manner
3. Default to storing all the data without user input
4. Receive input from the user regarding what data to restrict/include
5. Report activity at varying levels, including failure, to the user

The third and fourth points refer to use of the `serpentTools.settings` module to receive user input. The final point refers to use of the logging and messaging functions included in `serpentTools.messages`.

For example, the `DepletionReader` stores data in the following manner:

```
Reader
| - filePath
| - fileMetadata
|   - isotope names
|   - isotope ZAIs
|   - depletion schedule in days and burnup
| - materials
# for each material:
| - DepletedMaterial-n
|   - name
|   - atomic density
|   - mass density
|   - volume
|   etc
```

Here, the reader primarily creates and stores material objects, and the useful data is stored on these objects. Some files, like the fission matrix and depletion matrix files may not have a structure that naturally favors this object-oriented approach.

12.13.2 Containers

The readers are primarily responsible for creating and populating containers, that are responsible for storing and retrieving data. Just like the `DepletedMaterial` has shortcuts for analysis like `getValues()` and `plot()`, each such container should easily and naturally provide access to the data, and also perform some common analysis on the data.

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DEVELOPER TEAM

Here are all the wonderful people that helped make this project happen

- [Andrew Johnson](#)
- [Dan Kotlyar](#)
- [Stefano Terlizzi](#)
- [Gavin Ridley](#)
- [Paul Romano](#)
- [Anton Travleev](#)
- [@nicolaborate](#)

PUBLICATIONS

The following is a non-exhaustive list of publications using `serpentTools`. Please reach out if you wish to add a publication to this list.

15.1 Overview

Andrew Johnson, Dan Kotlyar, Stefano Terlizzi, and Gavin Ridley, “*serpentTools: A Python Package for Expediting Analysis with Serpent.*” *Nuclear Science and Engineering* (in press) (2020)

15.2 Journal

M. Krecicki and D. Kotlyar, “*Low enriched nuclear thermal propulsion neutronic, thermal hydraulic, and system design space analysis.*” *Nuclear Engineering and Design* (2020)

A. Johnson and D. Kotlyar, “*A Transport-Free Method for Predicting the Post-Depletion Spatial Neutron Flux Distribution.*” *Nuclear Science and Engineering* (2019)

G. Pereira, A. Johnson, Y. Bilodid, E. Fridman, and D. Kotlyar, “*Applying the Serpent-DYN3D code sequence for the decay heat analysis of metallic fuel sodium fast reactor.*” *Annals of Nuclear Energy* (2019)

15.3 Conference

A. Johnson and D. Kotlyar, “*Application of a Custom Depletion Framework to the Prediction of Neutron Flux Distribution Through Depletion.*” in proceedings of PHYSOR 2020: Transition to a Scalable Nuclear Future, Cambridge, UK, 2020

C. Kazaroff and A. Johnson and D. Kotlyar and J. Parker, “*Economic Benefits of Higher Enriched Assays for 24-month Cycle Length.*” in proceedings of Global/Top Fuel 2019, Seattle, WA, 2019

A. Johnson and D. Kotlyar, “*Prediction of Spatial Flux Through Depletion.*” in proceedings of ANS M&C 2019: Bridging Theory and Applications, Portland, OR, 2019

A. Johnson and D. Kotlyar, “*serpent-tools: A Python Package for Expediting Analysis with Serpent Data.*” in proceedings of ANS M&C 2019: Bridging Theory and Applications, Portland, OR, 2019

M. Krecicki, and D. Kotlyar, “*Sensitivity Studies of the Tungsten Vector on the Performance of a LEU NTP Engine.*” in proceedings of Nuclear and Emerging Technologies for Space, Richland, WA, 2019.

A. Johnson and D. Kotlyar, “*Comparative Study of Monte Carlo Burnup Schemes for Full Core Calculations.*” in proceedings of PHYSOR 2018: Reactor Physics paving the way towards more efficient systems, Cancun, Mexico, 2018.

GLOSSARY

Anaconda Python distribution that makes installing packages like *numpy* easier for Windows. Includes over 700 packages. For a smaller, more minimal approach, see *Miniconda*. For more information, see <https://www.anaconda.com/>.

Anaconda Prompt Modified Windows prompt to be used with the *Anaconda* python distribution. Reconfigures python paths to point to packages installed via *conda*

conda From <https://www.conda.io/docs/>:

Conda is an open source package management system and environment management system that runs on Windows, macOS, and Linux. Conda quickly installs, runs, and updates packages and their dependencies

CI Continuous integration. Software we utilize to check that pull requests don't break the code.

git Distributed version control system. Allows us to test and implement new features with ease. For more information, see <https://git-scm.com>.

Jupyter notebook Powerful web application used in this project, for examples and tutorials containing real python code. From <https://jupyter.org>:

The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text.

lint Bits of potentially erroneous code. Can be identified by a *linter*

linter Program that analyzes source code to check for errors, bugs, stylistic issues, and other potential hangups.

matplotlib Primary python package for plotting data. Highly customizable and extensible. More information at <https://matplotlib.org>

Miniconda Minimal installer for *conda*. From <https://conda.io>:

Miniconda is a small, bootstrap version of Anaconda that only includes conda, Python, the packages they depend on, and a small number of useful packages

numpy Widely-used python package that allows multidimensional arrays and linear algebra routines. More information at <https://www.numpy.org>

pip Recommended tool for installing Python packages. More at <https://pypi.org/project/pip/>

PyPI Python package index. Where packages that can easily be fetched and installed via *pip* can be found. <https://pypi.org>

pytest Fully featured python test runner. More at <https://pytest.org/en/latest/>

scipy Widely-used python package that contains more mathematical support and data structures, such as sparse matrices. Not required for this package, but allows the sparsity of some matrices to be exploited. More information at <https://docs.scipy.org/doc/scipy/reference/>

SERPENT Monte Carlo particle transport code developed at VTT Technical Research Centre of Finland, Ltd [[serpent](#)]. Produces output files that can be parsed by this project. More information, including distribution and licensing of SERPENT can be found at <http://montecarlo.vtt.fi>.

twine Python package for interacting with and uploading packages to *PyPI*

yaml Human-readable format used for configuration files in this project. For more information, see <https://pyyaml.org/wiki/PyYAMLDocumentation>

INDICES AND TABLES

- `genindex`
- `modindex`
- `search`

BIBLIOGRAPHY

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Symbols

<code>__contains__()</code>	(<i>serpentTools.BranchingReader</i> method), 84	<code>__getitem__()</code>	(<i>serpentTools.samplers.DepletionSampler</i> method), 174
<code>__contains__()</code>	(<i>serpentTools.DepletionReader</i> method), 86	<code>__getitem__()</code>	(<i>serpentTools.samplers.DetectorSampler</i> method), 166
<code>__contains__()</code>	(<i>serpentTools.DetectorReader</i> method), 93	<code>__getitem__()</code>	(<i>serpentTools.samplers.SampledDepletedMaterial</i> method), 177
<code>__contains__()</code>	(<i>serpentTools.HistoryReader</i> method), 95	<code>__getitem__()</code>	(<i>serpentTools.settings.rc</i> method), 183
<code>__contains__()</code>	(<i>serpentTools.XSPlotReader</i> method), 108	<code>__getitem__()</code>	(<i>serpentTools.xs.BranchedUniv</i> method), 164
<code>__contains__()</code>	(<i>serpentTools.objects.BranchContainer</i> method), 145	<code>__iter__()</code>	(<i>serpentTools.BranchingReader</i> method), 84
<code>__contains__()</code>	(<i>serpentTools.objects.UnivTuple</i> method), 156	<code>__iter__()</code>	(<i>serpentTools.DepletionReader</i> method), 86
<code>__enter__()</code>	(<i>serpentTools.settings.rc</i> method), 183	<code>__iter__()</code>	(<i>serpentTools.DetectorReader</i> method), 93
<code>__getitem__()</code>	(<i>serpentTools.BranchingReader</i> method), 84	<code>__iter__()</code>	(<i>serpentTools.HistoryReader</i> method), 95
<code>__getitem__()</code>	(<i>serpentTools.BumatReader</i> method), 83	<code>__iter__()</code>	(<i>serpentTools.XSPlotReader</i> method), 108
<code>__getitem__()</code>	(<i>serpentTools.DepletionReader</i> method), 86	<code>__iter__()</code>	(<i>serpentTools.objects.BranchContainer</i> method), 145
<code>__getitem__()</code>	(<i>serpentTools.DetectorReader</i> method), 93	<code>__iter__()</code>	(<i>serpentTools.objects.UnivTuple</i> method), 156
<code>__getitem__()</code>	(<i>serpentTools.HistoryReader</i> method), 95	<code>__len__()</code>	(<i>serpentTools.BranchingReader</i> method), 84
<code>__getitem__()</code>	(<i>serpentTools.ResultsReader</i> method), 100	<code>__len__()</code>	(<i>serpentTools.DetectorReader</i> method), 93
<code>__getitem__()</code>	(<i>serpentTools.XSPlotReader</i> method), 108	<code>__len__()</code>	(<i>serpentTools.HistoryReader</i> method), 95
<code>__getitem__()</code>	(<i>serpentTools.objects.BranchContainer</i> method), 145	<code>__len__()</code>	(<i>serpentTools.XSPlotReader</i> method), 108
<code>__getitem__()</code>	(<i>serpentTools.objects.DepletedMaterial</i> method), 147	<code>__len__()</code>	(<i>serpentTools.objects.BranchContainer</i> method), 145
<code>__getitem__()</code>	(<i>serpentTools.objects.HomogUniv</i> method), 152	<code>__len__()</code>	(<i>serpentTools.objects.UnivTuple</i> method), 156
<code>__getitem__()</code>	(<i>serpentTools.objects.UnivTuple</i> method), 156	<code>__len__()</code>	(<i>serpentTools.objects.XSData</i> method), 157
<code>__getitem__()</code>	(<i>serpentTools.objects.XSData</i> method), 157	<code>__setitem__()</code>	(<i>serpentTools.objects.BranchContainer</i> method), 145
		<code>__setitem__()</code>	(<i>serpentTools.objects.HomogUniv</i> method), 152
		<code>__setitem__()</code>	(<i>serpentTools.settings.rc</i> method),

183

A

activity (*serpentTools.objects.DepletedMaterial* attribute), 147
 addColorbar() (in module *serpentTools.utils.plot*), 231
 addData() (*serpentTools.objects.DepletedMaterial* method), 147
 addData() (*serpentTools.objects.HomogUniv* method), 152
 adens (*serpentTools.objects.DepletedMaterial* attribute), 147
 adens (*serpentTools.samplers.SampledDepletedMaterial* attribute), 177
 allData (*serpentTools.samplers.SampledDepletedMaterial* attribute), 177
 allErrors (*serpentTools.samplers.SampledDetector* attribute), 167
 allMdata (*serpentTools.samplers.DepletionSampler* attribute), 174
 allTallies (*serpentTools.samplers.SampledDetector* attribute), 166
 Anaconda, 255
 Anaconda Prompt, 255
 arrays (*serpentTools.HistoryReader* attribute), 95
 axis() (*serpentTools.xs.BranchCollector* property), 161
 axis() (*serpentTools.xs.BranchedUniv* property), 164

B

b1Exp (*serpentTools.objects.HomogUniv* attribute), 151
 b1Unc (*serpentTools.objects.HomogUniv* attribute), 151
 bins (*serpentTools.CartesianDetector* attribute), 119
 bins (*serpentTools.CylindricalDetector* attribute), 132
 bins (*serpentTools.Detector* attribute), 112
 bins (*serpentTools.HexagonalDetector* attribute), 125
 bins (*serpentTools.SphericalDetector* attribute), 139
 BranchCollector (class in *serpentTools.xs*), 160
 BranchContainer (class in *serpentTools.objects*), 144
 BranchedUniv (class in *serpentTools.xs*), 163
 branches (*serpentTools.BranchingReader* attribute), 84
 BranchingReader (class in *serpentTools*), 84
 bu (*serpentTools.objects.HomogUniv* attribute), 151
 BumatReader (class in *serpentTools*), 83
 burnup (*serpentTools.BumatReader* attribute), 83
 burnup (*serpentTools.DepletionReader* attribute), 86
 burnup (*serpentTools.objects.DepletedMaterial* attribute), 146
 burnup (*serpentTools.samplers.DepletionSampler* attribute), 174

burnup (*serpentTools.samplers.SampledDepletedMaterial* attribute), 177
 burnup() (*serpentTools.objects.UnivTuple* property), 156
 burnups() (*serpentTools.xs.BranchCollector* property), 161
 burnups() (*serpentTools.xs.BranchedUniv* property), 164

C

CartesianDetector (class in *serpentTools*), 118
 cartMeshPlot() (in module *serpentTools.plot*), 225
 checkContainerReq() (*serpentTools.io.base.MatlabConverter* method), 234
 checkImports() (*serpentTools.io.base.MatlabConverter* method), 234
 checkSparse() (*serpentTools.DepmtxReader* method), 91
 CI, 255
 clear() (*serpentTools.objects.BranchContainer* method), 145
 close() (*serpentTools.messages.DictHandler* method), 223
 collect() (*serpentTools.xs.BranchCollector* method), 162
 collector (*serpentTools.xs.BranchedUniv* attribute), 163
 compare() (*serpentTools.BranchingReader* method), 84
 compare() (*serpentTools.BumatReader* method), 83
 compare() (*serpentTools.CartesianDetector* method), 119
 compare() (*serpentTools.CylindricalDetector* method), 133
 compare() (*serpentTools.DepletionReader* method), 86
 compare() (*serpentTools.DepmtxReader* method), 91
 compare() (*serpentTools.Detector* method), 113
 compare() (*serpentTools.DetectorReader* method), 93
 compare() (*serpentTools.HexagonalDetector* method), 126
 compare() (*serpentTools.HistoryReader* method), 95
 compare() (*serpentTools.MicroXSReader* method), 97
 compare() (*serpentTools.objects.DepletedMaterial* method), 147
 compare() (*serpentTools.objects.HomogUniv* method), 152
 compare() (*serpentTools.objects.XSDData* method), 157
 compare() (*serpentTools.ResultsReader* method), 100
 compare() (*serpentTools.samplers.SampledDepletedMaterial* method), 177

- [compare\(\)](#) (*serpentTools.samplers.SampledDetector method*), 167
[compare\(\)](#) (*serpentTools.SensitivityReader method*), 105
[compare\(\)](#) (*serpentTools.SphericalDetector method*), 139
[compare\(\)](#) (*serpentTools.XSPlotReader method*), 108
[compareAttributes\(\)](#) (*serpentTools.objects.HomogUniv method*), 153
[compareB1Data\(\)](#) (*serpentTools.objects.HomogUniv method*), 153
[compareDictOfArrays\(\)](#) (*in module serpentTools.utils.compare*), 241
[compareDocDecorator\(\)](#) (*in module serpentTools.utils.docstrings*), 246
[compareGCDData\(\)](#) (*serpentTools.objects.HomogUniv method*), 154
[compareInfData\(\)](#) (*serpentTools.objects.HomogUniv method*), 154
[compareMaterials\(\)](#) (*serpentTools.DepletionReader method*), 87
[compareMetadata\(\)](#) (*serpentTools.DepletionReader method*), 87
[compareMetadata\(\)](#) (*serpentTools.ResultsReader method*), 100
[compareResults\(\)](#) (*serpentTools.ResultsReader method*), 100
[compareUniverses\(\)](#) (*serpentTools.ResultsReader method*), 101
[conda](#), 255
[convert\(\)](#) (*serpentTools.io.base.MatlabConverter method*), 234
[coords](#) (*serpentTools.HexagonalDetector attribute*), 126
[copy\(\)](#) (*serpentTools.objects.BranchContainer method*), 145
[count\(\)](#) (*serpentTools.objects.UnivTuple method*), 156
[critical\(\)](#) (*in module serpentTools.messages*), 222
[CSCStreamProcessor](#) (*class in serpentTools.parsers.base*), 237
[CylindricalDetector](#) (*class in serpentTools*), 132
- ## D
- [data](#) (*serpentTools.objects.DepletedMaterial attribute*), 146
[data](#) (*serpentTools.parsers.base.CSCStreamProcessor attribute*), 237
[data](#) (*serpentTools.samplers.SampledDepletedMaterial attribute*), 176
[day](#) (*serpentTools.objects.HomogUniv attribute*), 151
[days](#) (*serpentTools.BumatReader attribute*), 83
[days](#) (*serpentTools.DepletionReader attribute*), 86
[days](#) (*serpentTools.objects.DepletedMaterial attribute*), 146
[days](#) (*serpentTools.samplers.DepletionSampler attribute*), 173
[days](#) (*serpentTools.samplers.SampledDepletedMaterial attribute*), 177
[days\(\)](#) (*serpentTools.objects.UnivTuple property*), 156
[debug\(\)](#) (*in module serpentTools.messages*), 222
[decayHeat](#) (*serpentTools.objects.DepletedMaterial attribute*), 147
[deltaT](#) (*serpentTools.DepmtxReader attribute*), 91
[DepletedMaterial](#) (*class in serpentTools.objects*), 146
[DepletionReader](#) (*class in serpentTools*), 86
[DepletionSampler](#) (*class in serpentTools.samplers*), 173
[depmtx](#) (*serpentTools.DepmtxReader attribute*), 91
[DepmtxReader](#) (*class in serpentTools*), 91
[deprecated\(\)](#) (*in module serpentTools.messages*), 222
[describe\(\)](#) (*serpentTools.objects.XSData method*), 158
[Detector](#) (*class in serpentTools*), 111
[DetectorReader](#) (*class in serpentTools*), 93
[detectors](#) (*serpentTools.DetectorReader attribute*), 93
[detectors](#) (*serpentTools.samplers.DetectorSampler attribute*), 165
[DetectorSampler](#) (*class in serpentTools.samplers*), 165
[deviation](#) (*serpentTools.samplers.SampledDetector attribute*), 166
[DictHandler](#) (*class in serpentTools.messages*), 223
[directCompare\(\)](#) (*in module serpentTools.utils.compare*), 242
- ## E
- [emit\(\)](#) (*serpentTools.messages.DictHandler method*), 223
[energies](#) (*serpentTools.objects.XSData attribute*), 157
[energies](#) (*serpentTools.SensitivityReader attribute*), 105
[energies](#) (*serpentTools.XSPlotReader attribute*), 108
[energy](#) (*serpentTools.CartesianDetector attribute*), 119
[energy](#) (*serpentTools.CylindricalDetector attribute*), 133
[energy](#) (*serpentTools.Detector attribute*), 112
[energy](#) (*serpentTools.HexagonalDetector attribute*), 126
[energy](#) (*serpentTools.SphericalDetector attribute*), 139
[energyIntegratedSens](#) (*serpentTools.SensitivityReader attribute*), 105
[error\(\)](#) (*in module serpentTools.messages*), 222
[errors](#) (*serpentTools.CartesianDetector attribute*), 119
[errors](#) (*serpentTools.CylindricalDetector attribute*), 133

errors (*serpentTools.Detector* attribute), 112
errors (*serpentTools.HexagonalDetector* attribute), 126
errors (*serpentTools.samplers.SampledDetector* attribute), 166
errors (*serpentTools.SphericalDetector* attribute), 139

F

filePath (*serpentTools.xs.BranchCollector* attribute), 160
filePath (*serpentTools.xs.BranchedUniv* attribute), 163
files (*serpentTools.samplers.DepletionSampler* attribute), 174
files (*serpentTools.samplers.DetectorSampler* attribute), 165
finalize() (*serpentTools.samplers.SampledDepletedMaterial* method), 178
flush() (*serpentTools.messages.DictHandler* method), 223
fluxRatio (*serpentTools.MicroXSReader* attribute), 97
fluxUnc (*serpentTools.MicroXSReader* attribute), 97
formatPlot() (in module *serpentTools.utils.plot*), 229
free() (*serpentTools.samplers.DepletionSampler* method), 174
free() (*serpentTools.samplers.DetectorSampler* method), 166
free() (*serpentTools.samplers.SampledDepletedMaterial* method), 178
fromDetectors() (*serpentTools.samplers.SampledDetector* class method), 167
fromFile() (*serpentTools.xs.BranchCollector* class method), 162
fromkeys() (*serpentTools.objects.BranchContainer* method), 145
fromTallyBins() (*serpentTools.CartesianDetector* class method), 120
fromTallyBins() (*serpentTools.CylindricalDetector* class method), 133
fromTallyBins() (*serpentTools.Detector* class method), 113
fromTallyBins() (*serpentTools.HexagonalDetector* class method), 127
fromTallyBins() (*serpentTools.samplers.SampledDetector* class method), 168
fromTallyBins() (*serpentTools.SphericalDetector* class method), 140

G

gc (*serpentTools.objects.HomogUniv* attribute), 151

gcUnc (*serpentTools.objects.HomogUniv* attribute), 151
generateSeed() (in module *serpentTools.seed*), 192
get() (*serpentTools.BranchingReader* method), 85
get() (*serpentTools.DepletionReader* method), 88
get() (*serpentTools.DetectorReader* method), 94
get() (*serpentTools.HistoryReader* method), 96
get() (*serpentTools.objects.BranchContainer* method), 145
get() (*serpentTools.objects.DepletedMaterial* method), 148
get() (*serpentTools.objects.HomogUniv* method), 154
get() (*serpentTools.objects.XSData* method), 158
get() (*serpentTools.ResultsReader* method), 101
get() (*serpentTools.samplers.SampledDepletedMaterial* method), 178
get() (*serpentTools.XSPlotReader* method), 109
getCommonKeys() (in module *serpentTools.utils.compare*), 242
getFile() (in module *serpentTools.data*), 190
getFY() (*serpentTools.MicroXSReader* method), 98
getKeyMatchingShapes() (in module *serpentTools.utils.compare*), 244
getLogOverlaps() (in module *serpentTools.utils.compare*), 245
getOverlaps() (in module *serpentTools.utils.compare*), 244
getUniv() (*serpentTools.objects.BranchContainer* method), 145
getUniv() (*serpentTools.ResultsReader* method), 101
getValues() (*serpentTools.objects.DepletedMaterial* method), 148
getValues() (*serpentTools.samplers.SampledDepletedMaterial* method), 178
getXS() (*serpentTools.MicroXSReader* method), 98
git, 255
grids (*serpentTools.Detector* attribute), 112
grids (*serpentTools.samplers.SampledDetector* attribute), 167
groups (*serpentTools.objects.HomogUniv* attribute), 152

H

hasData() (*serpentTools.objects.HomogUniv* method), 155
hasExpectedData() (*serpentTools.objects.XSData* method), 158
hasNuData (*serpentTools.objects.XSData* attribute), 157
hasUncs() (*serpentTools.BranchingReader* property), 85
HexagonalDetector (class in *serpentTools*), 125
hexPlot() (*serpentTools.HexagonalDetector* method), 127

hexType (*serpentTools.HexagonalDetector* attribute), 126
 HistoryReader (class in *serpentTools*), 95
 HomogUniv (class in *serpentTools.objects*), 151

I

index() (*serpentTools.objects.UnivTuple* method), 156
 indexes (*serpentTools.CartesianDetector* attribute), 119
 indexes (*serpentTools.CylindricalDetector* attribute), 133
 indexes (*serpentTools.Detector* attribute), 112
 indexes (*serpentTools.HexagonalDetector* attribute), 126
 indexes (*serpentTools.samplers.SampledDetector* attribute), 167
 indexes (*serpentTools.SphericalDetector* attribute), 139
 indices (*serpentTools.parsers.base.CSCStreamProcessor* attribute), 237
 indptr (*serpentTools.parsers.base.CSCStreamProcessor* attribute), 237
 infExp (*serpentTools.objects.HomogUniv* attribute), 151
 info() (in module *serpentTools.messages*), 222
 infUnc (*serpentTools.objects.HomogUniv* attribute), 151
 ingTox (*serpentTools.objects.DepletedMaterial* attribute), 147
 inhTox (*serpentTools.objects.DepletedMaterial* attribute), 147
 ioConvertName() (*serpentTools.HistoryReader* static method), 96
 ioReconvertName() (*serpentTools.HistoryReader* static method), 96
 isIso (*serpentTools.objects.XSData* attribute), 157
 items() (*serpentTools.BranchingReader* method), 85
 items() (*serpentTools.DepletionReader* method), 88
 items() (*serpentTools.DetectorReader* method), 94
 items() (*serpentTools.HistoryReader* method), 96
 items() (*serpentTools.objects.BranchContainer* method), 145
 items() (*serpentTools.xs.BranchedUniv* method), 164
 items() (*serpentTools.XSPlotReader* method), 109
 iterBranches() (*serpentTools.BranchingReader* method), 85
 iterDets() (*serpentTools.DetectorReader* method), 94
 iterMaterials() (*serpentTools.samplers.DepletionSampler* method), 174

J

Jupyter notebook, 255

K

keys() (*serpentTools.DepletionReader* method), 88
 keys() (*serpentTools.objects.BranchContainer* method), 145
 keys() (*serpentTools.XSPlotReader* method), 109
 KeywordParser (class in *serpentTools.engines*), 236

L

latGen (*serpentTools.SensitivityReader* attribute), 105
 lethargyWidths (*serpentTools.SensitivityReader* attribute), 105
 line (*serpentTools.engines.KeywordParser* attribute), 236
 line (*serpentTools.engines.PatternReader* attribute), 236
 line (*serpentTools.parsers.base.CSCStreamProcessor* attribute), 237
 lint, 255
 linter, 255
 loadFromContainer() (*serpentTools.samplers.SampledDepletedMaterial* method), 179
 logAcceptableHigh() (in module *serpentTools.messages*), 246
 logAcceptableLow() (in module *serpentTools.messages*), 246
 logBadShapes() (in module *serpentTools.messages*), 247
 logBadTypes() (in module *serpentTools.messages*), 247
 logDifferentTypes() (in module *serpentTools.messages*), 246
 logDirectCompare() (in module *serpentTools.utils.compare*), 243
 logIdentical() (in module *serpentTools.messages*), 246
 logIdenticalWithUncs() (in module *serpentTools.messages*), 246
 logInsideConfInt() (in module *serpentTools.messages*), 246
 logMessages (*serpentTools.messages.DictHandler* attribute), 223
 logMissingKeys() (in module *serpentTools.messages*), 246
 logNotIdentical() (in module *serpentTools.messages*), 246
 logOutsideConfInt() (in module *serpentTools.messages*), 246
 logOutsideTols() (in module *serpentTools.messages*), 246

M

magicPlotDocDecorator() (in module *serpentTools.utils.docstrings*), 232

- ul style="list-style-type: none; padding-left: 0;">
- majorant (*serpentTools.XSPlotReader* attribute), 108
- map (*serpentTools.samplers.DepletionSampler* attribute), 174
- map (*serpentTools.samplers.DetectorSampler* attribute), 166
- match (*serpentTools.engines.PatternReader* attribute), 236
- materials (*serpentTools.BumatReader* attribute), 83
- materials (*serpentTools.DepletionReader* attribute), 86
- materials (*serpentTools.samplers.DepletionSampler* attribute), 174
- materials (*serpentTools.SensitivityReader* attribute), 105
- MatlabConverter (class in *serpentTools.io.base*), 234
- matplotlib, 255
- mdens (*serpentTools.objects.DepletedMaterial* attribute), 147
- mdens (*serpentTools.samplers.SampledDepletedMaterial* attribute), 177
- meshPlot() (*serpentTools.CartesianDetector* method), 120
- meshPlot() (*serpentTools.CylindricalDetector* method), 134
- meshPlot() (*serpentTools.Detector* method), 113
- meshPlot() (*serpentTools.HexagonalDetector* method), 128
- meshPlot() (*serpentTools.samplers.SampledDetector* method), 168
- meshPlot() (*serpentTools.SphericalDetector* method), 140
- metadata (*serpentTools.DepletionReader* attribute), 86
- metadata (*serpentTools.objects.XSData* attribute), 157
- metadata (*serpentTools.ResultsReader* attribute), 99
- metadata (*serpentTools.samplers.DepletionSampler* attribute), 174
- metadata (*serpentTools.XSPlotReader* attribute), 108
- metadataUncs (*serpentTools.samplers.DepletionSampler* attribute), 174
- microGroups (*serpentTools.objects.HomogUniv* attribute), 152
- MicroXSReader (class in *serpentTools*), 97
- Miniconda, 255
- MismatchedContainersError, 191
- MT (*serpentTools.objects.XSData* attribute), 157
- MTdescip (*serpentTools.objects.XSData* attribute), 157
- ## N
- n0 (*serpentTools.DepmtxReader* attribute), 91
 - n1 (*serpentTools.DepmtxReader* attribute), 91
 - name (*serpentTools.CartesianDetector* attribute), 118
 - name (*serpentTools.CylindricalDetector* attribute), 132
 - name (*serpentTools.Detector* attribute), 112
 - name (*serpentTools.HexagonalDetector* attribute), 125
 - name (*serpentTools.objects.HomogUniv* attribute), 151
 - name (*serpentTools.samplers.SampledDetector* attribute), 166
 - name (*serpentTools.SphericalDetector* attribute), 138
 - names (*serpentTools.DepletionReader* attribute), 86
 - names (*serpentTools.objects.DepletedMaterial* attribute), 146
 - names (*serpentTools.samplers.DepletionSampler* attribute), 174
 - names (*serpentTools.samplers.SampledDepletedMaterial* attribute), 177
 - negativeMTDescription() (*serpentTools.objects.XSData* static method), 158
 - nEne (*serpentTools.SensitivityReader* attribute), 105
 - nfy (*serpentTools.MicroXSReader* attribute), 97
 - nMat (*serpentTools.SensitivityReader* attribute), 104
 - nMu (*serpentTools.SensitivityReader* attribute), 105
 - normalizerFactory() (in module *serpentTools.utils.plot*), 232
 - nPert (*serpentTools.SensitivityReader* attribute), 105
 - numGroups (*serpentTools.objects.HomogUniv* attribute), 152
 - numInactive (*serpentTools.HistoryReader* attribute), 95
 - numpy, 255
 - nZai (*serpentTools.SensitivityReader* attribute), 105
- ## O
- orderedUniv() (*serpentTools.objects.BranchContainer* property), 145
- ## P
- parse() (*serpentTools.engines.KeywordParser* method), 236
 - parsers (*serpentTools.samplers.DepletionSampler* attribute), 174
 - parsers (*serpentTools.samplers.DetectorSampler* attribute), 165
 - PatternReader (class in *serpentTools.engines*), 236
 - perts (*serpentTools.SensitivityReader* attribute), 105
 - perturbations() (*serpentTools.xs.BranchCollector* property), 162
 - perturbations() (*serpentTools.xs.BranchedUniv* property), 164
 - photonProdRate (*serpentTools.objects.DepletedMaterial* attribute), 147
 - pip, 255
 - pitch (*serpentTools.HexagonalDetector* attribute), 125
 - placeLegend() (in module *serpentTools.utils.plot*), 230

- [plot\(\)](#) (in module *serpentTools.plot*), 229
[plot\(\)](#) (*serpentTools.CartesianDetector* method), 121
[plot\(\)](#) (*serpentTools.CylindricalDetector* method), 135
[plot\(\)](#) (*serpentTools.DepletionReader* method), 88
[plot\(\)](#) (*serpentTools.Detector* method), 114
[plot\(\)](#) (*serpentTools.HexagonalDetector* method), 129
[plot\(\)](#) (*serpentTools.objects.DepletedMaterial* method), 149
[plot\(\)](#) (*serpentTools.objects.HomogUniv* method), 155
[plot\(\)](#) (*serpentTools.objects.XSData* method), 159
[plot\(\)](#) (*serpentTools.ResultsReader* method), 102
[plot\(\)](#) (*serpentTools.samplers.DepletionSampler* method), 175
[plot\(\)](#) (*serpentTools.samplers.SampledDepletedMaterial* method), 179
[plot\(\)](#) (*serpentTools.samplers.SampledDetector* method), 169
[plot\(\)](#) (*serpentTools.SensitivityReader* method), 106
[plot\(\)](#) (*serpentTools.SphericalDetector* method), 141
[plotDensity\(\)](#) (*serpentTools.DepmtxReader* method), 92
[pop\(\)](#) (*serpentTools.objects.BranchContainer* method), 146
[popitem\(\)](#) (*serpentTools.objects.BranchContainer* method), 146
[process\(\)](#) (*serpentTools.samplers.DepletionSampler* method), 176
[process\(\)](#) (*serpentTools.samplers.DetectorSampler* method), 166
[PyPI](#), 255
[pytest](#), 255
[Python Enhancement Proposals](#)
 [PEP 257](#), 215
 [PEP 8](#), 223
- ## R
- [rc](#) (class in *serpentTools.settings*), 183
[read\(\)](#) (in module *serpentTools*), 81
[read\(\)](#) (*serpentTools.BranchingReader* method), 85
[read\(\)](#) (*serpentTools.BumatReader* method), 84
[read\(\)](#) (*serpentTools.DepletionReader* method), 89
[read\(\)](#) (*serpentTools.DepmtxReader* method), 92
[read\(\)](#) (*serpentTools.DetectorReader* method), 94
[read\(\)](#) (*serpentTools.HistoryReader* method), 96
[read\(\)](#) (*serpentTools.MicroXSReader* method), 99
[read\(\)](#) (*serpentTools.ResultsReader* method), 103
[read\(\)](#) (*serpentTools.samplers.DepletionSampler* method), 176
[read\(\)](#) (*serpentTools.samplers.DetectorSampler* method), 166
[read\(\)](#) (*serpentTools.SensitivityReader* method), 107
[read\(\)](#) (*serpentTools.XSPlotReader* method), 109
[readDataFile\(\)](#) (in module *serpentTools.data*), 189
[readDepmtx\(\)](#) (in module *serpentTools*), 82
[resdata](#) (*serpentTools.ResultsReader* attribute), 99
[reshaped](#) (*serpentTools.objects.HomogUniv* attribute), 151
[reshapedBins\(\)](#) (*serpentTools.CartesianDetector* method), 122
[reshapedBins\(\)](#) (*serpentTools.CylindricalDetector* method), 136
[reshapedBins\(\)](#) (*serpentTools.Detector* method), 115
[reshapedBins\(\)](#) (*serpentTools.HexagonalDetector* method), 130
[reshapedBins\(\)](#) (*serpentTools.samplers.SampledDetector* method), 170
[reshapedBins\(\)](#) (*serpentTools.SphericalDetector* method), 142
[ResultsReader](#) (class in *serpentTools*), 99
- ## S
- [SampledDepletedMaterial](#) (class in *serpentTools.samplers*), 176
[SampledDetector](#) (class in *serpentTools.samplers*), 166
[SamplerError](#), 190
[saveAsMatlab\(\)](#) (*serpentTools.DepletionReader* method), 89
[scipy](#), 255
[searchFor\(\)](#) (*serpentTools.engines.PatternReader* method), 236
[seedFiles\(\)](#) (in module *serpentTools.seed*), 191
[seekToTop\(\)](#) (*serpentTools.engines.KeywordParser* method), 236
[seekToTop\(\)](#) (*serpentTools.engines.PatternReader* method), 236
[sensitivities](#) (*serpentTools.SensitivityReader* attribute), 105
[SensitivityReader](#) (class in *serpentTools*), 104
[SERPENT](#), 256
[SerpentToolsException](#), 190
[setAx_xlims\(\)](#) (in module *serpentTools.utils.plot*), 231
[setAx_ylims\(\)](#) (in module *serpentTools.utils.plot*), 231
[setData\(\)](#) (*serpentTools.objects.XSData* method), 159
[setDefault\(\)](#) (*serpentTools.objects.BranchContainer* method), 146
[setMTs\(\)](#) (*serpentTools.objects.XSData* method), 159
[setNuData\(\)](#) (*serpentTools.objects.XSData* method), 159
[settings](#) (*serpentTools.DepletionReader* attribute), 86
[settings](#) (*serpentTools.samplers.DepletionSampler* attribute), 174

settings (*serpentTools.samplers.DetectorSampler* attribute), 165
 showMT() (*serpentTools.objects.XSData* method), 160
 slice() (*serpentTools.CartesianDetector* method), 123
 slice() (*serpentTools.CylindricalDetector* method), 136
 slice() (*serpentTools.Detector* method), 116
 slice() (*serpentTools.HexagonalDetector* method), 130
 slice() (*serpentTools.samplers.SampledDetector* method), 171
 slice() (*serpentTools.SphericalDetector* method), 142
 spectrumPlot() (*serpentTools.CartesianDetector* method), 123
 spectrumPlot() (*serpentTools.CylindricalDetector* method), 137
 spectrumPlot() (*serpentTools.Detector* method), 116
 spectrumPlot() (*serpentTools.HexagonalDetector* method), 130
 spectrumPlot() (*serpentTools.samplers.SampledDetector* method), 171
 spectrumPlot() (*serpentTools.SphericalDetector* method), 143
 SphericalDetector (class in *serpentTools*), 138
 splitDictByKey() (in module *serpentTools.utils.compare*), 243
 spontaneousFissionRate (*serpentTools.objects.DepletedMaterial* attribute), 147
 spreadPlot() (*serpentTools.samplers.SampledDepletedMaterial* method), 180
 spreadPlot() (*serpentTools.samplers.SampledDetector* method), 172
 stateData (*serpentTools.objects.BranchContainer* attribute), 145
 states() (*serpentTools.xs.BranchCollector* property), 162
 states() (*serpentTools.xs.BranchedUniv* property), 164
 step (*serpentTools.objects.HomogUniv* attribute), 151
 step() (*serpentTools.objects.UnivTuple* property), 156

T

tabulate() (*serpentTools.objects.XSData* method), 160
 tallies (*serpentTools.CartesianDetector* attribute), 119
 tallies (*serpentTools.CylindricalDetector* attribute), 133
 tallies (*serpentTools.Detector* attribute), 112

tallies (*serpentTools.HexagonalDetector* attribute), 125
 tallies (*serpentTools.samplers.SampledDetector* attribute), 166
 tallies (*serpentTools.SphericalDetector* attribute), 139
 toDataFrame() (*serpentTools.objects.DepletedMaterial* method), 150
 toMatlab() (*serpentTools.CartesianDetector* method), 124
 toMatlab() (*serpentTools.CylindricalDetector* method), 137
 toMatlab() (*serpentTools.DepletionReader* method), 90
 toMatlab() (*serpentTools.DepmtxReader* method), 93
 toMatlab() (*serpentTools.Detector* method), 117
 toMatlab() (*serpentTools.DetectorReader* method), 94
 toMatlab() (*serpentTools.HexagonalDetector* method), 131
 toMatlab() (*serpentTools.HistoryReader* method), 96
 toMatlab() (*serpentTools.ResultsReader* method), 103
 toMatlab() (*serpentTools.samplers.SampledDetector* method), 173
 toMatlab() (*serpentTools.SensitivityReader* method), 107
 toMatlab() (*serpentTools.SphericalDetector* method), 144
 twine, 256

U

uncertainties (*serpentTools.samplers.SampledDepletedMaterial* attribute), 177
 universe() (*serpentTools.objects.UnivTuple* property), 156
 universes (*serpentTools.objects.BranchContainer* attribute), 145
 universes (*serpentTools.ResultsReader* attribute), 99
 universes (*serpentTools.xs.BranchCollector* attribute), 160
 univID (*serpentTools.xs.BranchedUniv* attribute), 163
 univIndex (*serpentTools.xs.BranchCollector* attribute), 160
 UnivTuple (class in *serpentTools.objects*), 156
 update() (*serpentTools.objects.BranchContainer* method), 146

V

values() (*serpentTools.DepletionReader* method), 90
 values() (*serpentTools.objects.BranchContainer* method), 146

`values()` (*serpentTools.XSPlotReader* method), 109
`volume` (*serpentTools.objects.DepletedMaterial* attribute), 146

W

`warning()` (in module *serpentTools.messages*), 222
`willChange()` (in module *serpentTools.messages*), 223
`with_traceback()` (*serpentTools.messages.MismatchedContainersError* method), 191
`with_traceback()` (*serpentTools.messages.SamplerError* method), 190
`with_traceback()` (*serpentTools.messages.SerpentToolsException* method), 190

X

`x` (*serpentTools.CartesianDetector* attribute), 119
`XSData` (class in *serpentTools.objects*), 157
`xsdata` (*serpentTools.objects.XSData* attribute), 157
`xsections` (*serpentTools.XSPlotReader* attribute), 108
`XSPlotReader` (class in *serpentTools*), 108
`xsTables` (*serpentTools.xs.BranchCollector* attribute), 161
`xsTables` (*serpentTools.xs.BranchedUniv* attribute), 163
`xsUnc` (*serpentTools.MicroXSReader* attribute), 97
`xsVal` (*serpentTools.MicroXSReader* attribute), 97

Y

`y` (*serpentTools.CartesianDetector* attribute), 119
`yaml`, 256
`yieldChunks()` (*serpentTools.engines.KeywordParser* method), 236
`yieldMatches()` (*serpentTools.engines.PatternReader* method), 236

Z

`z` (*serpentTools.CartesianDetector* attribute), 119
`z` (*serpentTools.HexagonalDetector* attribute), 126
`zai` (*serpentTools.DepmtxReader* attribute), 91
`zai` (*serpentTools.objects.DepletedMaterial* attribute), 146
`zai` (*serpentTools.samplers.SampledDepletedMaterial* attribute), 176
`zais` (*serpentTools.DepletionReader* attribute), 86
`zais` (*serpentTools.samplers.DepletionSampler* attribute), 174
`zais` (*serpentTools.SensitivityReader* attribute), 105