
serpentTools Documentation

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The serpentTools developer team

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WELCOME!

1.1 serpent-tools

A suite of parsers designed to make interacting with SERPENT¹ 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 montecarlo.vtt.fi

1.1.1 Installation

The `serpentTools` package can be downloaded either as a git repository or as a zipped file. Both can be obtained through the `Clone` or `download` option at the [serpent-tools GitHub](#).

Once the repository has been downloaded or extracted from zip, the package can be installed with:

```
cd serpentTools
python setup.py install
python setup.py test
```

Installing with `setuptools` is preferred over the standard `distutils` module. `setuptools` can be installed with `pip` as:

```
pip install -U setuptools
```

Installing in this manner ensures that the supporting packages, like `numpy` are installed and up to date.

1.1.2 Issues

If you have issues installing the project, find a bug, or want to add a feature, the [GitHub issue page](#) is the best place to do that.

1.1.3 Contributors

Here are all the wonderful people that helped make this project happen

- [Andrew Johnson](#)
- [Dr. Dan Kotlyar](#)
- [Stefano Terlizzi](#)

¹ Leppanen, J. et al. (2015) "The Serpent Monte Carlo code: Status, development and applications in 2013." Ann. Nucl. Energy, 82 (2015) 142-150

- Gavin Ridley

1.1.4 References

The Annals of Nuclear Energy article should be cited for all work using SERPENT. If you wish to cite this project, please cite as:

```
url{@serpentTools
  author = {Andrew Johnson and Dan Kotlyar and Stefano Terlizzi and Gavin Ridley},
  title = {serpentTools: A suite of parsers designed to make
    interacting with SERPENT outputs simple and flawless},
  url = {https://github.com/CORE-GATECH-GROUP/serpent-tools},
  year = {2017}
}
```

1.2 License

MIT License

Copyright (c) 2017-2018 Andrew Johnson, Dan Kotlyar, Stefano Terlizzi, GTRC

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EXAMPLES

2.1 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 `rc` class. This notebook will provide as an intro into using this class.

2.1.1 Basic Usage

```
>>> import serpentTools
INFO      : serpentTools: Using version 0.2.1
>>> from serpentTools.settings import rc, defaultSettings
```

Below are the default values for each setting available

```
>>> for setting in sorted(defaultSettings.keys()):
...     print(setting)
...     for key in defaultSettings[setting]:
...         print('\t', key, '-', defaultSettings[setting][key])
depletion.materialVariables
    default - []
    description - Names of variables to store. Empty list -> all variables.
    type - <class 'list'>
depletion.materials
    default - []
    description - Names of materials to store. Empty list -> all materials.
    type - <class 'list'>
depletion.metadataKeys
    default - ['ZAI', 'NAMES', 'DAYS', 'BU']
    description - Non-material data to store, i.e. zai, isotope names, burnup schedule, etc.
    type - <class 'list'>
    options - default
depletion.processTotal
    default - True
    description - Option to store the depletion data from the TOT block
    type - <class 'bool'>
serpentVersion
    default - 2.1.29
    description - Version of SERPENT
    type - <class 'str'>
    options - ['2.1.29']
verbosity
    default - warning
```

```

type - <class 'str'>
description - Set the level of errors to be shown.
updater - <function updateLevel at 0x000001B7F3DD6598>
options - ['critical', 'error', 'warning', 'info', 'debug']
xs.variableExtras
  default - []
  description - Full SERPENT name of variables to be read
  type - <class 'list'>
xs.variableGroups
  default - []
  description - Name of variable groups from variables.yaml to be expanded into SERPENT variable t
  type - <class 'list'>

```

Settings such as `depletion.metadataKeys` 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. The `rc` class acts as a dictionary, and updating a value is as simple as

```

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

```

The `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:
...     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']"

```

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

```

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

```

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 stored in `serpentTools/variables.yaml` 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', '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', '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.getB1XS`, respectively. By default, `xs.getInfXS` and `xs.getB1XS` default to `True`. This, in conjunction with leaving the `xs.variableGroups` and `xs.variableExtras` 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

As of version 0.1.2, the `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
branching:
  areUncsPresent: False
  floatVariables: [Fhi, Blo]
depletion:
  materials: [fuel*]
  materialVariables:
    [ADENS, MDENS, VOLUME]
```

2.2 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](#)

2.2.1 Basic Operation

The simplest way to read these files is using the `serpentTools.parsers.read()` function

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'
INFO      : serpentTools: Using version 0.2.1
>>> r0 = serpentTools.read(branchFile)
INFO      : serpentTools: Inferred reader for demo.coe: BranchingReader
INFO      : serpentTools: Preparing to read demo.coe
INFO      : serpentTools: Done reading branching file
```

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

```
>>> r0.branches
{('B1000', 'FT1200'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c762438>,
 ('B1000', 'FT600'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c787908>,
 ('B1000', 'nom'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c737ef0>,
 ('B750', 'FT1200'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c752cf8>,
 ('B750', 'FT600'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c77c208>,
 ('B750', 'nom'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c72c860>,
 ('nom', 'FT1200'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c7455f8>,
 ('nom', 'FT600'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c76dac8>,
 ('nom', 'nom'):
  <serpentTools.objects.containers.BranchContainer at 0x2220c7231d0>}
```

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 in the universes dictionary

```
>>> b0.universes
{(0, 0.0, 1): <serpentTools.objects.containers.HomogUniv at 0x2220c781ac8>,
 (0, 1.0, 2): <serpentTools.objects.containers.HomogUniv at 0x2220c78b5f8>,
 (0, 10.0, 3): <serpentTools.objects.containers.HomogUniv at 0x2220c791240>,
 (10, 0.0, 1): <serpentTools.objects.containers.HomogUniv at 0x2220c787a58>,
 (10, 1.0, 2): <serpentTools.objects.containers.HomogUniv at 0x2220c78b6a0>,
 (10, 10.0, 3): <serpentTools.objects.containers.HomogUniv at 0x2220c791320>,
 (20, 0.0, 1): <serpentTools.objects.containers.HomogUniv at 0x2220c787cc0>,
 (20, 1.0, 2): <serpentTools.objects.containers.HomogUniv at 0x2220c78b908>,
 (20, 10.0, 3): <serpentTools.objects.containers.HomogUniv at 0x2220c791588>,
 (30, 0.0, 1): <serpentTools.objects.containers.HomogUniv at 0x2220c78b048>,
 (30, 1.0, 2): <serpentTools.objects.containers.HomogUniv at 0x2220c78bb70>,
 (30, 10.0, 3): <serpentTools.objects.containers.HomogUniv at 0x2220c7917f0>,
 (40, 0.0, 1): <serpentTools.objects.containers.HomogUniv at 0x2220c78b1d0>,
 (40, 1.0, 2): <serpentTools.objects.containers.HomogUniv at 0x2220c78bdd8>,
 (40, 10.0, 3): <serpentTools.objects.containers.HomogUniv at 0x2220c791a58>}
```

The keys here are vectors indicating the universe ID, burnup [MWd/kgU], and burnup index corresponding to the point in the burnup schedule. These universes can be obtained by indexing this dictionary, or by using the *getUniv()* method

```
>>> univ0 = b0.universes[0, 1, 2]
>>> print(univ0)
>>> print(univ0.name)
>>> print(univ0.bu)
>>> print(univ0.step)
>>> print(univ0.day)
<HomogUniv from demo.coe>
0
1.0
2
0
>>> univ1 = b0.getUniv(0, burnup=1)
>>> univ2 = b0.getUniv(0, index=2)
>>> assert univ0 is univ1 is univ2
```

Since the coefficient files do not store the day value of burnup, all *HomogUniv* objects created by the *BranchContainer* default to day zero.

Group constant data is stored in five dictionaries:

1. infExp: Expected values for infinite medium group constants
2. infUnc: Relative uncertainties for infinite medium group constants
3. blExp: Expected values for leakage-corrected group constants
4. blUnc: Relative uncertainties for leakage-corrected group constants
5. metaData: items that do not fit the in the above categories

```
>>> univ0.infExp
{'infDiffcoef': array([ 1.83961 ,  0.682022]),
 'infFiss': array([ 0.00271604,  0.059773  ]),
 'infRem': array([], dtype=float64),
 'infS0': array([ 0.298689 ,  0.00197521,  0.00284247,  0.470054  ]),
 '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 ]),
 'blRem': array([], dtype=float64),
 '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.metaData
{}

```

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

```
>>> univ0.get('infFiss')
array([ 0.00286484,  0.0577559 ])
>>> try:
>>>     univ0.get('infS0', uncertainty=True)
>>> except KeyError as ke: # no uncertainties here
>>>     print(str(ke))
'Variable infS0 absent from uncertainty dictionary'

```

2.2.2 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', 'nom') <BranchContainer for nom, nom from demo.coe>
('B750', 'nom') <BranchContainer for B750, nom from demo.coe>
('B1000', 'nom') <BranchContainer for B1000, nom from demo.coe>
('nom', 'FT1200') <BranchContainer for nom, FT1200 from demo.coe>
('B750', 'FT1200') <BranchContainer for B750, FT1200 from demo.coe>
('B1000', 'FT1200') <BranchContainer for B1000, FT1200 from demo.coe>
('nom', 'FT600') <BranchContainer for nom, FT600 from demo.coe>
('B750', 'FT600') <BranchContainer for B750, FT600 from demo.coe>
('B1000', 'FT600') <BranchContainer for B1000, FT600 from demo.coe>

```

2.2.3 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. Below are the various settings that the *BranchingReader* uses to read and process coefficient files.

```
>>> import six
>>> from serpentTools.settings import rc
>>> from serpentTools.settings import rc, defaultSettings
>>> for setting in defaultSettings:
>>>     if 'xs' in setting or 'branching' in setting:
>>>         print(setting)
>>>         for k, v in six.iteritems(defaultSettings[setting]):
>>>             print('\t', k+':', v)
branching.areUncsPresent
    default: False
    type: <class 'bool'>
    description: True if the values in the .coe file contain uncertainties
branching.intVariables
    default: []
    description: Name of state data variables to convert to integers for
    each branch
    type: <class 'list'>
branching.floatVariables
    default: []
    description: Names of state data variables to convert to floats for
    each branch
    type: <class 'list'>
xs.getInfXS
    default: True
    description: If true, store the infinite medium cross sections.
    type: <class 'bool'>
xs.getB1XS
    default: True
    description: If true, store the critical leakage cross sections.
    type: <class 'bool'>
xs.variableGroups
    default: []
    description: Name of variable groups from variables.yaml to be expanded
    into SERPENT variable to be stored
    type: <class 'list'>
xs.variableExtras
    default: []
    description: Full SERPENT name of variables to be read
    type: <class 'list'>
```

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.variableGroups` and `xs.variableExtras` controls what data is stored on the *HomogUniv* objects. By default, all variables present in the coefficient file are stored.

```
>>> rc['branching.floatVariables'] = ['BOR']
>>> rc['branching.intVariables'] = ['TFU']
>>> rc['xs.getB1XS'] = False
```

```
>>> rc['xs.variableExtras'] = ['INF_TOT', 'INF_SCATT0']
>>> r1 = serpentTools.read(branchFile)
INFO      : serpentTools: Inferred reader for demo.coe: BranchingReader
INFO      : serpentTools: Preparing to read demo.coe
INFO      : serpentTools: Done reading branching file
>>> b1 = r1.branches['B1000', 'FT600']
>>> b1.stateData
{'BOR': 1000.0,
 'DATE': '17/10/18',
 'TFU': 600,
 'TIME': '10:26:48',
 'VERSION': '2.1.29'}
>>> assert isinstance(b1.stateData['BOR'], float)
>>> assert isinstance(b1.stateData['TFU'], int)
```

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

```
>>> univ4 = b1.getUniv(0, 0)
>>> univ4.infExp
{'infTot': array([ 0.313338,  0.54515 ])}
>>> univ4.blExp
{}
```

2.2.4 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.

2.3 DetectorReader

2.3.1 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.

```
>>> from matplotlib import pyplot
>>> import serpentTools
INFO      : serpentTools: Using version 0.2.1
>>> pinFile = 'fuelPin_det0.m'
>>> bwrFile = 'bwr_det0.m'
>>> pin = serpentTools.read(pinFile)
>>> bwr = serpentTools.read(bwrFile)
INFO      : serpentTools: Inferred reader for fuelPin_det0.m: DetectorReader
INFO      : serpentTools: Preparing to read fuelPin_det0.m
INFO      : serpentTools: Done
INFO      : serpentTools: Inferred reader for bwr_det0.m: DetectorReader
INFO      : serpentTools: Preparing to read bwr_det0.m
INFO      : serpentTools: Done
>>> print(pin.detectors)
```

```
>>> print(bwr.detectors)
{'nodeFlx':
  <serpentTools.objects.containers.Detector object at 0x7fb3ae1db978>}
{'spectrum':
  <serpentTools.objects.containers.Detector object at 0x7fb3ae1db9e8>,
 'xymesh':
  <serpentTools.objects.containers.Detector object at 0x7fb3ae1dba20>}
```

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[:, 5, :]
array([[ 1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  2.34759000e-02,  4.53000000e-03],
       [ 2.00000000e+00,  1.00000000e+00,  2.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  5.75300000e-02,  3.38000000e-03],
       [ 3.00000000e+00,  1.00000000e+00,  3.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  8.47000000e-02,  2.95000000e-03],
       [ 4.00000000e+00,  1.00000000e+00,  4.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  1.02034000e-01,  2.63000000e-03],
       [ 5.00000000e+00,  1.00000000e+00,  5.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  1.00000000e+00,  1.00000000e+00,
         1.00000000e+00,  1.10384000e-01,  2.31000000e-03]])
```

Here, only three columns are changing:

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

Note: For SERPENT-1, there would be an additional column 12 that contained the scores for each bin

```
>>> nodeFlx.bins[:, 0]
array([ 1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,  9., 10., 11.,
        12., 13., 14., 15., 16.] )
```

Once each detector is given this binned tally data, the *reshape()* method is called to recast the tallies, errors, and, if applicable, the *scores* columns into individual, multidimensional arrays. For this case, since the only variable

bin quantity is that of the universe, these will all 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])
```

Bin information is retained through the `indexes` attribute. This is an *OrderedDictionary*, as the keys are placed according to their column position. These positions can be found in the SERPENT Manual, and are provided in the `DET_COLS` tuple

```
>>> from serpentTools.objects.containers import DET_COLS
>>> print(DET_COLS)
('value', 'energy', 'universe', 'cell', 'material', 'lattice',
 'reaction', 'zmesh', 'ymesh', 'xmesh', 'tally', 'error', 'scores')
>>> nodeFlx.indexes
OrderedDict([('universe',
              array([ 1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,
                     9., 10., 11., 12., 13., 14., 15., 16.])))])
```

Each item in the `indexes` ordered dictionary corresponds to the unique values of that bin in the original `bins` array. Here, `universe` is the first item and contains an equal number of elements to the size of the first (and only) axis in the `nodeFlx` tally matrix

```
>>> assert nodeFlx.indexes['universe'].size == nodeFlx.tallies.size
```

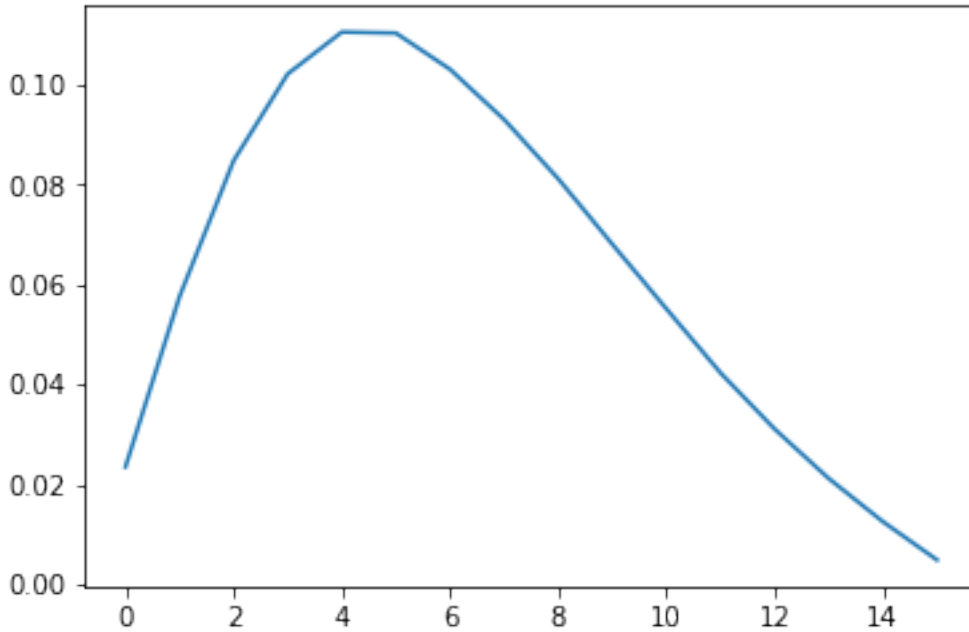
2.3.2 Plotting Routines

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.

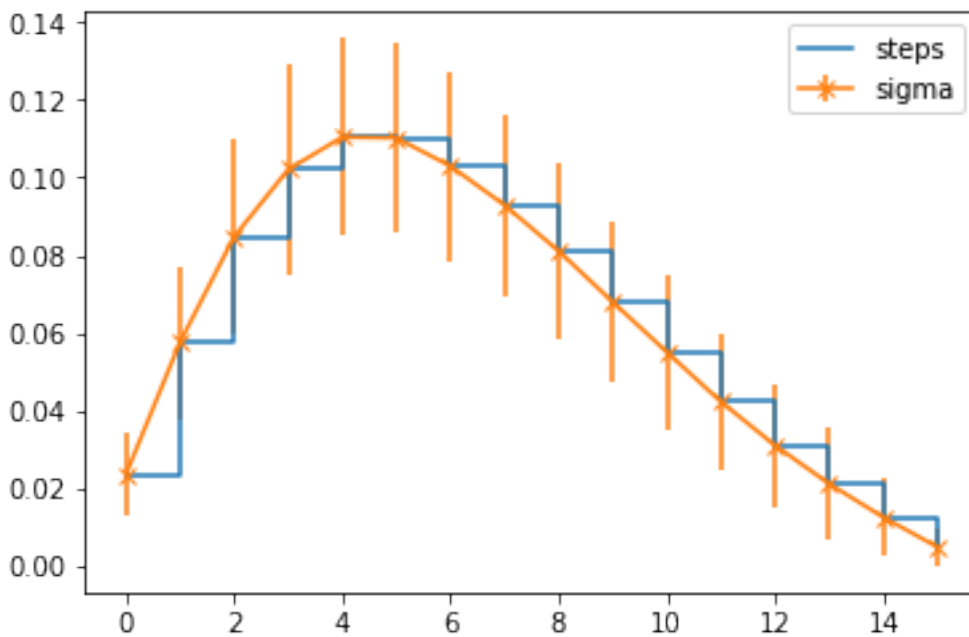
Option	Description
<code>what</code>	What data to plot
<code>ax</code>	Pre-prepared figure on which to add this plot
<code>xdim</code>	Quantity from <code>indexes</code> to use as x-axis
<code>sigma</code>	Confidence interval to place on errors
<code>steps</code>	Draw tally values as constant inside bin

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

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

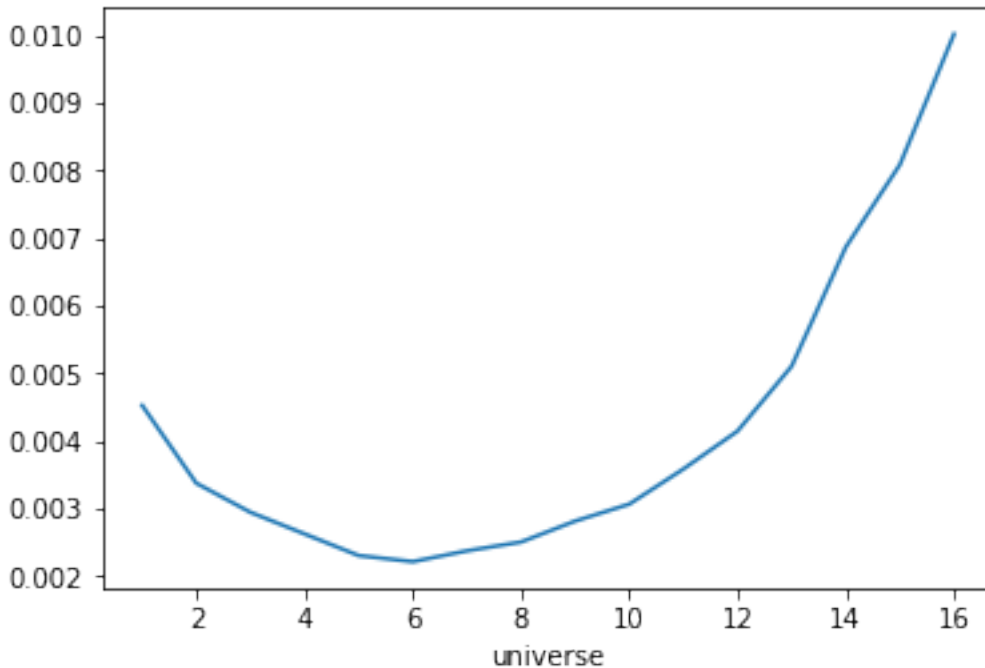



```
>>> ax = nodeFlx.plot(steps=True, label='steps')
>>> nodeFlx.plot(sigma=100, ax=ax, marker='x', label='sigma')
>>> ax.legend()
```



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');
```



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

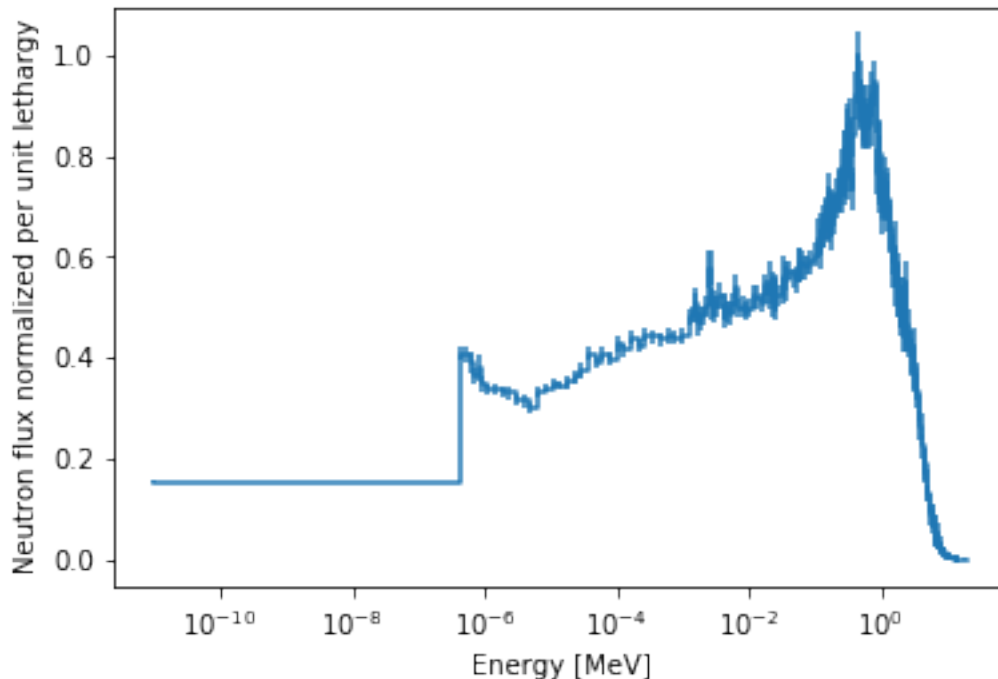
```
>>> spectrum = bwr.detectors['spectrum']
>>> print(spectrum.grids['E'][:5, :])
[[ 1.00002000e-11  4.13994000e-07  2.07002000e-07]
 [ 4.13994000e-07  5.31579000e-07  4.72786000e-07]
 [ 5.31579000e-07  6.25062000e-07  5.78320000e-07]
 [ 6.25062000e-07  6.82560000e-07  6.53811000e-07]
 [ 6.82560000e-07  8.33681000e-07  7.58121000e-07]]
```

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

Option	Default	Description
normalize	True	Normalize tallies per unit lethargy
sigma	3	Level of confidence for statistical errors
xscale	'log'	Set the x scale to be log or linear
yscale	'linear'	Set the y scale to be log or linear

Since our detector has energy bins and reaction bins, we need to reduce down to one-dimension with the `fixed` command. More on this in the next section. Here, the spectrum is plotted for the first reaction type, total flux for this detector.

```
>>> spectrum.spectrumPlot(fixed={'reaction': 1})
```



2.3.3 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']
>>> for key in xy.indexes:
>>>     print(key, xy.indexes[key])
energy [1 2]
ymesh [ 1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20]
xmesh [ 1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20]
```

Traversing the first axis in the `tallies` array corresponds to changing the value of the reaction. 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])
[ 0.0401505  0.0352695  0.0330053  0.0292071  0.0267413]
>>> print(xy.tallies[0, 0, :5])
[ 0.0401505  0.0352695  0.0330053  0.0292071  0.0267413]
```

Slicing

As the detectors produced by SERPENT can contain multiple bin types, as seen in `DET_COLS`, 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 2 along the axis that corresponds to the reaction bin

```
>>> print(spectrum.indexes['reaction'])
[1 2]
>>> spectrum.slice({'reaction': 2})[:20]
array([[ 1.84253000e+03,   3.27275000e+01,   1.65728000e+01,
         7.78628000e+00,   1.56444000e+01,   3.88358000e+00,
         2.43967000e+01,   1.42860000e+01,   5.06925000e+00,
         5.08734000e+00,   4.62725000e+00,   1.03671000e+01,
         1.76183000e+00,   7.40425000e+00,   3.71261000e+00,
         3.10994000e+01,   1.45352000e+01,   1.13481000e+01,
         1.80058000e+01,   1.57873000e+01])
```

As the fission reaction corresponded to reaction tally 1 in the original matrix.

This method also works for slicing the error and score matrices by using `what='errors'` or `'scores'`, respectively.

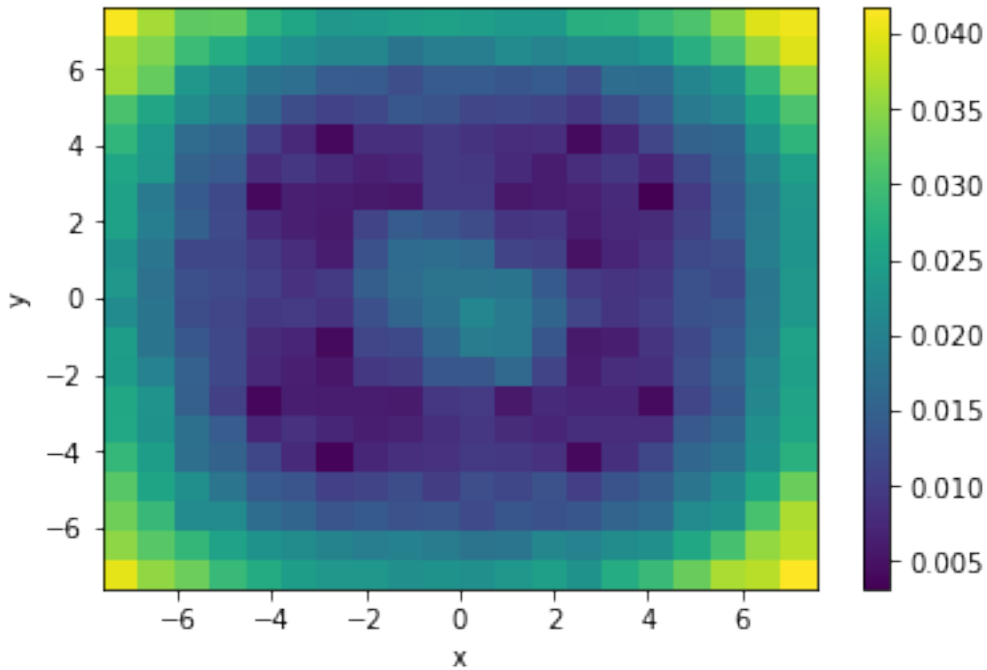
```
>>> spectrum.slice({'reaction': 2}, 'errors')[:20]
array([[ 0.0061 ,   0.01354,   0.01527,   0.01992,   0.01574,   0.02734,
         0.01549,   0.01713,   0.01376,   0.01549,   0.01491,   0.01391,
         0.01632,   0.01631,   0.02035,   0.02192,   0.01766,   0.01279,
         0.02488,   0.01606])
```

This call returns the relative error in the fission rate, reaction 2.

Plotting

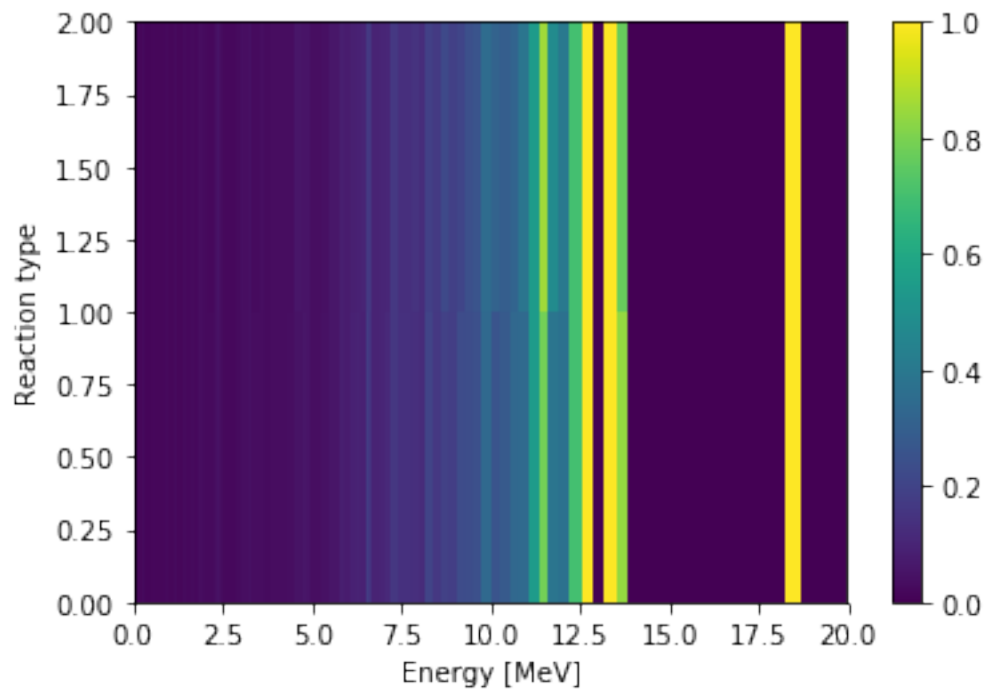
For data with dimensionality greater than one, the `meshPlot()` method can be used to plot some 2D slice of the data. Passing a dictionary as the `fixed` argument restricts the tally data down to two dimensions. Since the `xymesh` detector is three dimensions, (energy, x, and y), we must pick an energy group to plot.

```
>>> xy.meshPlot('x', 'y', fixed={'energy': 1});
# plot the fast spectrum flux
```



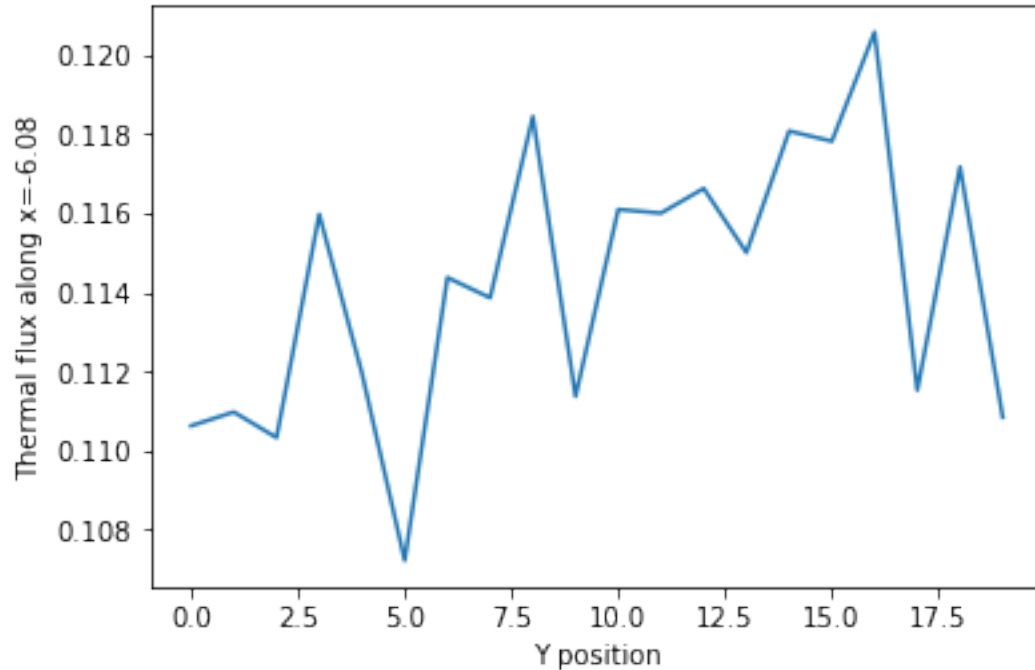
The `meshPlot()` also supports a range of labeling options

```
>>> spectrum.meshPlot('e', 'reaction', what='errors',
...                   ylabel='Reaction type',
...                   xlabel='Energy [MeV]');
```



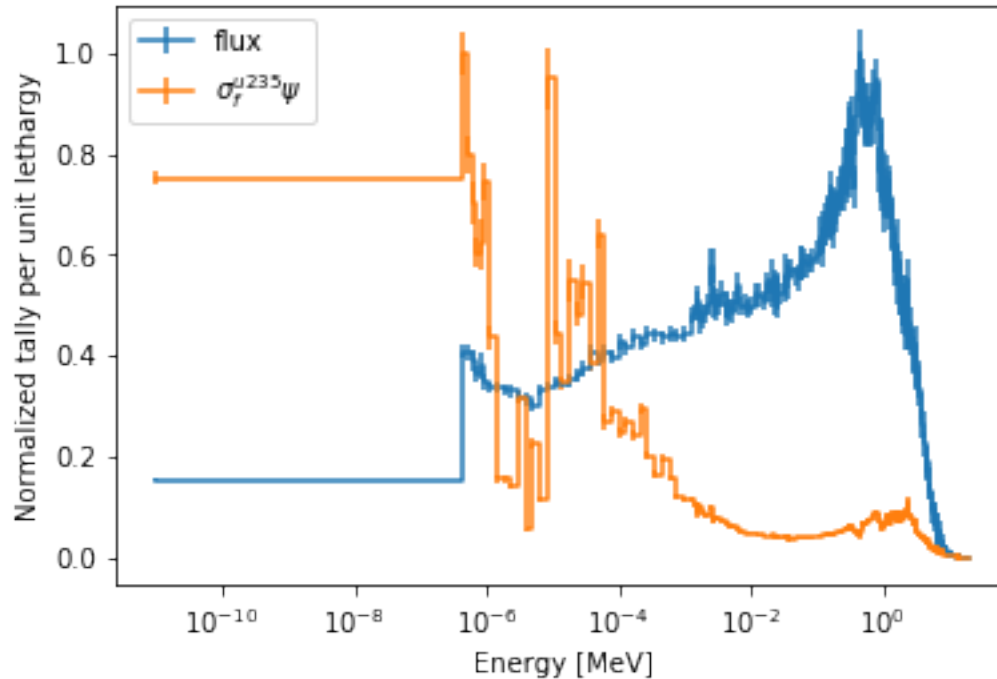
Using the `slicing` arguments allows access to the 1D plot methods from before

```
>>> xy.plot(fixed={'energy': 2, 'xmesh': 2},
...         xlabel='Y position',
...         ylabel='Thermal flux along x={}'
...         .format(xy.grids['X'][2, 0]));
```



The underlying matplotlib plot routines can be used to plot multiple data sets on the same plot.

```
>>> ax = pyplot.axes()
>>> labels = (
...     'flux',
...     r'$\sigma_f^{\psi}$') # render as mathtype
>>> reactions = spectrum.indexes['reaction']
>>> for reac, label in zip(reactions, labels):
...     spectrum.spectrumPlot({'reaction': reac}, steps=True, sigma=3,
...                             ax=ax, label=label)
>>> ax.set_ylabel('Normalized tally per unit lethargy')
>>> ax.legend()
```



2.3.4 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.

2.3.5 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

2.4 DepletionReader

2.4.1 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 six
>>> import serpentTools
>>> from serpentTools.settings import rc
INFO      : serpentTools: Using version 0.2.1
>>> depFile = 'demo_dep.m'
>>> dep = serpentTools.read(depFile)
INFO      : serpentTools: Inferred reader for demo_dep.m: DepletionReader
```

```
INFO      : serpentTools: Preparing to read demo_dep.m
INFO      : serpentTools: Done reading depletion file
```

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
{'bglass0': <serpentTools.objects.materials.DepletedMaterial at 0x23905154668>,
 'fuel0': <serpentTools.objects.materials.DepletedMaterial at 0x2390578eeb8>,
 'total': <serpentTools.objects.materials.DepletedMaterial at 0x2390579e978>}
```

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

```
>>> dep.metadata.keys()
dict_keys(['zai', 'burnup', 'names', 'days'])
>>> dep.metadata['burnup']
array([ 0. ,  0.02,  0.04, ...,  1.36,  1.38,  1.4 ,  1.42])
>>> dep.metadata['names']
['Xe135', 'I135', 'U234', 'U235', 'U236', 'U238', 'Pu238',
 'Pu239', ..., 'lost', 'total']
```

2.4.2 DepletedMaterial

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. ,  0.02,  0.04, ...,  1.36,  1.38,  1.4 ,  1.42])
>>> fuel.days is dep.metadata['days']
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(['a', 'adens', 'burnup', 'gsrc', ..., 'volume'])
>>> fuel.adens
array([[ 0.00000000e+00,  2.43591000e-09,  4.03796000e-09, ...,
         4.70133000e-09,  4.70023000e-09,  4.88855000e-09],
       [ 0.00000000e+00,  6.06880000e-09,  8.11783000e-09, ...,
         8.05991000e-09,  8.96359000e-09,  9.28554000e-09],
       [ 4.48538000e-06,  4.48486000e-06,  4.48432000e-06, ...,
         4.44726000e-06,  4.44668000e-06,  4.44611000e-06],
       ...,
       [ 0.00000000e+00,  3.03589000e-11,  7.38022000e-11, ...,
         1.62829000e-09,  1.63566000e-09,  1.64477000e-09],
       [ 0.00000000e+00,  1.15541000e-14,  2.38378000e-14, ...,
         8.60736000e-13,  8.73669000e-13,  8.86782000e-13],
       [ 6.88332000e-02,  6.88334000e-02,  6.88336000e-02, ...,
         6.88455000e-02,  6.88457000e-02,  6.88459000e-02]])
```

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

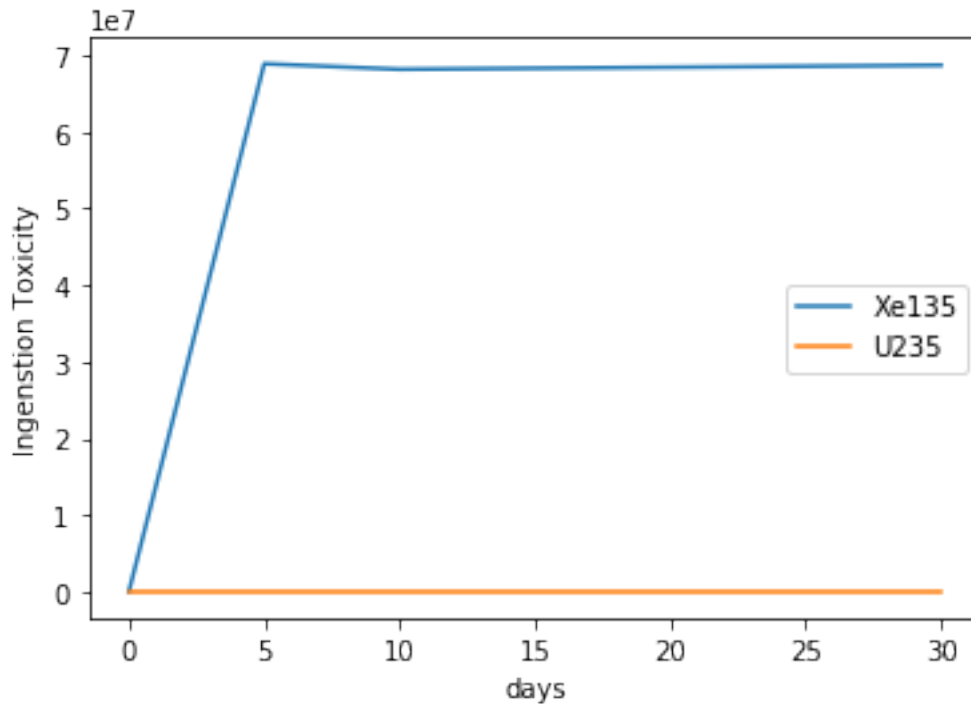
2.4.3 Data Retrieval

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.

```
>>> dayPoints = [0, 5, 10, 30]
>>> iso = ['Xe135', 'U235']
>>> vals = fuel.getValues('days', 'a', dayPoints, iso)
>>> print(vals.shape)
(2, 4)
>>> print(vals)
[[ 0.00000000e+00  3.28067000e+14  3.24606000e+14  3.27144000e+14]
 [ 5.36447000e+07  5.34519000e+07  5.32499000e+07  5.24766000e+07]]
```

The *DepletedMaterial* uses this slicing for the built-in `plot()` method

```
>>> fuel.plot('days', 'ingTox', dayPoints, iso,
              ylabel='Ingenstion Toxicity');
```



2.4.4 Limitations

Currently, the *DepletionReader* cannot catch materials with underscore in the name, due to variables like `ING_TOX` also containing an underscore. Issue [#58](#)

2.4.5 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.

```
>>> from serpentTools.settings import rc, defaultSettings
>>> for setting in defaultSettings:
>>>     if 'depletion' in setting:
>>>         print(setting)
>>>         for k, v in six.iteritems(defaultSettings[setting]):
>>>             print('\t', k, v)
depletion.materials
  type <class 'list'>
  description Names of materials to store. Empty list -> all materials.
  default []
depletion.processTotal
  type <class 'bool'>
  description Option to store the depletion data from the TOT block
  default True
depletion.materialVariables
  type <class 'list'>
  description Names of variables to store. Empty list -> all variables.
  default []
depletion.metadataKeys
  type <class 'list'>
  description Non-material data to store, i.e. zai, isotope names, burnup schedule, etc.
  options default
  default ['ZAI', 'NAMES', 'DAYS', 'BU']
```

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.

Note: Creating the DepletionReader in this manner is functionally equivalent to `serpentTools.read(depFile)`

```
>>> rc['depletion.processTotal'] = False
>>> rc['depletion.metadataKeys'] = ['BU']
>>> rc['depletion.materialVariables'] = ['ADENS']
>>> rc['depletion.materials'] = [r'bglass\d+']
>>>
>>> bgReader = serpentTools.parsers.DepletionReader(depFile)
>>> bgReader.read()
INFO      : serpentTools: Preparing to read demo_dep.m
INFO      : serpentTools: Done reading depletion file
>>> bgReader.materials
{'bglass0': <serpentTools.objects.materials.DepletedMaterial at 0x239057dcb00>}
>>> bglass = bgReader.materials['bglass0']
>>> bglass.data
{'adens': array([[ 0.          ,  0.          ,  0.          , ...,  0.          ,  0.          ,
                  0.          ],
                 [ 0.          ,  0.          ,  0.          , ...,  0.          ,  0.          ,
                  0.          ],
                 [ 0.          ,  0.          ,  0.          , ...,  0.          ,  0.          ,
                  0.          ],
                 ...,
                 [ 0.          ,  0.          ,  0.          , ...,  0.          ,  0.          ,
                  0.          ],
                 [ 0.          ,  0.          ,  0.          , ...,  0.          ,  0.          ,
                  0.          ]])
```

```
[ 0.      , 0.      , 0.      , ..., 0.      , 0.      ,  
  0.      ],  
[ 0.0715841, 0.0715843, 0.0715845, ..., 0.0715968, 0.0715969,  
  0.0715971]]})  
>>> bglass.data.keys()  
dict_keys(['adens'])
```

2.4.6 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.

2.4.7 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](#)

3.1 Settings

class `serpentTools.settings.UserSettingsLoader`

Class that stores the active user settings.

expandVariables ()

Extend the keyword groups into lists of serpent variables.

Returns Names of all variables to be scraped

Return type set

getReaderSettings (*settingsPrefix*)

Get all module-wide and reader-specific settings.

Parameters **settingsPrefix** (*str or list*) – Name of the specific reader. Will look for settings that lead with readerName, e.g. `depletion.metadataKeys` or `xs.variables`

Returns Single level dictionary with `settingName: settingValue` pairs

Return type dict

Raises `KeyError` – If the reader name is not located in the readers settings dictionary

loadYaml (*filePath, strict=True*)

Update the settings based on the contents of the yaml file

New in version 0.2.0.

Parameters

- **filePath** (*str, or FileType*) – Path to config file
- **strict** (*bool*) – Fail at the first incorrect setting. If false, failed settings will not be loaded and alerts will be raised

Raises

- `KeyError` or `TypeError` – If settings found in the config file are not valid
- `FileNotFound` or `OSError` – If the file does not exist

setValue (*name, value*)

Set the value of a specific setting.

Parameters

- **name** (*str*) – Full name of the setting

- **value** (*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

3.2 Messages

System-wide methods for producing status update and errors.

See also:

- <https://docs.python.org/2/library/logging.html>
- <https://www.python.org/dev/peps/pep-0391/>

exception `serpentTools.messages.MismatchedContainersError`
Attempting to sample from dissimilar containers

exception `serpentTools.messages.SamplerError`
Base-class for errors in sampling process

exception `serpentTools.messages.SerpentToolsException`
Base-class for all exceptions in this project

`serpentTools.messages.critical` (*message*)
Log that something has gone horribly wrong.

`serpentTools.messages.debug` (*message*)
Log a debug message.

`serpentTools.messages.deprecated` (*useInstead*)
Decorator that warns that different function should be used instead.

`serpentTools.messages.error` (*message*)
Log that something caused an exception but was suppressed.

`serpentTools.messages.info` (*message*)
Log an info message, e.g. status update.

`serpentTools.messages.updateLevel` (*level*)
Set the level of the logger.

`serpentTools.messages.warning` (*message*)
Log a warning that something could go wrong or should be avoided.

`serpentTools.messages.willChange` (*changeMsg*)
Decorator that warns that some functionality may change.

3.3 Parser Module

The main module associated with reading SERPENT files. For information on each individual reader, please see the dedicated file listed below

Reader	Hyperlink
Branching	Branching Reader
Bumat	Bumat Reader
Depletion	Depletion Reader
Detector	Detector Reader
FissionMatrix	Fission Matrix Reader
Results	Results Reader

`serpentTools.parsers.inferReader(filePath)`

Attempt to infer the correct reader type.

Parameters `filePath` (*str*) – File to be read.

Raises `SerpentToolsException` – If a reader cannot be inferred

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

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

Note: If you know the type of reader you will be using, it is best to either pass in the string argument, or directly use the appropriate reader class

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
dep	DepletionReader
branch	BranchingReader
det	DetectorReader
results	ResultsReader
bumat	BumatReader
fission	FissionMatrixReader

Returns Correct subclass corresponding to the file type

Return type `serpentTools.objects.readers.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.

`serpentTools.parsers.depmtx(filePath)`

Read the contents of the `depmtx` file and return contents

Note: If `scipy` is not installed, matrix `A` will be full. This can cause some warnings or errors if sparse or non-sparse solvers are used.

Parameters `fileP` (*str*) – Path to depletion matrix file

Returns

- `t` (*float*) – Length of time
- `n0` (*numpy.ndarray*) – Initial isotopic vector
- `zai` (*numpy.array*) – String identifiers for each isotope in `n0` and `n1`
- `a` (*numpy.array or scipy.sparse.csc_matrix*) – Decay matrix. Will be sparse if `scipy` is installed
- `n1` (*numpy.array*) – Final isotopic vector

3.4 Parsing Engines

The classes contained in `serpentTools/engines.py` are part of the [drewtils v0.1.9](#) package and are provided under the following license:

The MIT License (MIT)

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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.

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
str

Most recently read line

parse ()
Parse the file and return a list of keyword blocks.

Returns List of key word argument chunks.

Return type list

yieldChunks ()
Return each chunk of text as a generator.

Yields *list* – The next chunk in the file.

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
str

Most recently read line

match
regular expression match or None

Match from the most recently read line

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

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 patten.

Yields *sequential match groups*

3.5 Containers

Many of the readers utilize custom built objects for storing data in a logical and accessible format. These containers are detailed here.

Note: Variables taken from SERPENT will be converted to mixedCase and stored under those names. for example, INF_TOT would be stored as infTot

class `serpentTools.objects.containers.BranchContainer` (*filePath*, *branchID*, *branchNames*, *stateData*)

Class that stores data for a single branch.

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

dict

Name: value pairs for the variables defined on each branch card

universes

dict

Dictionary storing the homogenized universe objects. Keys are tuples of (universeID, burnup, burnIndex)

addUniverse (*univID*, *burnup=0*, *burnIndex=0*, *burnDays=0*)

Add a universe to this branch.

Data for the universes are produced at specific points in time. The additional arguments help track when the data for this universe were created.

Warning: This method will overwrite data for universes that already exist

Parameters

- **univID** (*int or str*) – Identifier for this universe
- **burnup** (*float or int*) – Value of burnup [MWd/kgU]
- **burnIndex** (*int*) – Point in the depletion schedule
- **burnDays** (*int or float*) – Point in time

Returns **newUniv**

Return type *serpentTools.objects.containers.HomogUniv*

getUniv (*univID*, *burnup=None*, *index=None*)

Return a specific universe given the ID and time of interest

If burnup and index are given, burnup is used to search

Parameters

- **univID** (*int*) – Unique ID for the desired universe
- **burnup** (*float or int*) – Burnup [MWd/kgU] of the desired universe
- **index** (*int*) – Point of interest in the burnup index

Returns `univ` – Requested Universe

Return type `serpentTools.objects.containers.HomogUniv`

Raises

- `KeyError`: – If the requested universe could not be found
- `SerpentToolsException`: – If neither burnup nor index are given

orderedUniv

Universe keys sorted by ID and by burnup

class `serpentTools.objects.materials.DepletedMaterial` (*name, metadata*)

Base class for storing material data from a depleted material file

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
```

Parameters

- **name** (*str*) – Name of this material
- **metadata** (*dict*) – Dictionary with file metadata

data

dict

dictionary that stores all variable data

zai

list

Isotopic ZZAAA identifiers, e.g. 93325

names

list

Names of isotopes, e.g. U235

days

numpy.ndarray

Vector of total, cumulative days of burnup for the run that created this material

burnup

numpy.ndarray

Vector of total, cumulative burnup [MWd/kgU] for this specific material

adens

numpy.ndarray

2D array of atomic densities where where row *j* corresponds to isotope *j* and column *i* corresponds to time *i*

mdens

numpy.ndarray

2D array of mass densities where where row *j* corresponds to isotope *j* and column *i* corresponds to time *i*

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

plot (*xUnits*, *yUnits*, *timePoints=None*, *names=None*, *ax=None*, *autolabel=True*, *legend=True*, *xlabel=None*, *ylabel=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'
- **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** (*None or matplotlib.pyplot.axes*) – If given, add the data to this plot. Otherwise, create a new plot
- **legend** (*bool*) – Automatically add the legend
- **autolabel** (*bool*) – Automatically label the axis
- **xlabel** (*None or str*) – If given, use this as the label for the x-axis. Otherwise, use *xUnits*
- **ylabel** (*None or str*) – If given, use this as the label for the y-axis. Otherwise, use *yUnits*
- **kwargs** – Optional keyword arguments to pass to *matplotlib.pyplot.plot*

Returns Axes corresponding to the figure that was plotted

Return type *matplotlib.pyplot.axes*

See also:

- *getValues()*
- *matplotlib.pyplot.plot()*

class *serpentTools.objects.containers.Detector* (*name*)

Class that stores detector data from a single detector file

Parameters

- **name** (*str*) – Name of this detector
- **Attributes** –
- **bins** (*numpy.ndarray*) – Tally data directly from SERPENT file

- **grids** (*dict*) – Dictionary with additional data describing energy grids or mesh points
- **tallies** (*None or numpy.array*) – Reshaped tally data to correspond to the bins used
- **errors** (*None or numpy.array*) – Reshaped relative error data corresponding to bins used
- **scores** (*None or numpy.array*) – Reshaped array of tally scores. SERPENT 1 only
- **indexes** (*None or OrderedDict*) – Collection of unique indexes for each requested bin

addTallyData (*bins*)

Add tally data to this detector

reshape ()

Reshape the tally data into a multidimensional array

This method reshapes the tally and uncertainty data into arrays where the array axes correspond to specific bin types. If a detector was set up to tally two group flux in a 5 x 5 xy mesh, then the resulting tally data would be in a 50 x 12/13 matrix in the original `detN.m` file. The tally data and relative error would be rebroadcasted into 2 x 5 x 5 arrays, and the indexing information is stored in `self.indexes`

Returns *shape* – Dimensionality of the resulting array

Return type *list*

Raises `SerpentToolsException`: – If the bin data has not been loaded

class `serpentTools.objects.containers.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

str

name of the universe

bu

float

burnup value

step

float

temporal step

day

float

depletion day

infExp

dict

Expected values for infinite medium group constants

infUnc

dict

Relative uncertainties for infinite medium group constants

b1Exp

dict

Expected values for leakage corrected group constants

b1Unc

dict

Relative uncertainties for leakage-corrected group constants

metadata

dict

Other values that do not conform to inf/b1 dictionaries

addData (*variableName*, *variableValue*, *uncertainty=False*)

Sets the value of the variable and, optionally, the associate s.d.

Warning: This method will overwrite data for variables that already exist

Parameters

- **variableName** (*str*) – Variable Name
- **variableValue** – Variable Value
- **uncertainty** (*bool*) – Set to `True` in order to retrieve the uncertainty associated to the expected values

Raises `TypeError` – If the uncertainty flag is not boolean

get (*variableName*, *uncertainty=False*)

Gets the value of the variable `VariableName` from the dictionaries

Parameters

- **variableName** (*str*) – Variable Name
- **uncertainty** (*bool*) – Boolean Variable- set to `True` in order to retrieve the uncertainty associated to the expected values

Returns

- *x* – Variable Value
- *dx* – Associated uncertainty

Raises

- `TypeError` – If the uncertainty flag is not boolean
- `KeyError` – If the variable requested is not stored on the object

3.6 Branching Reader

The [*BranchingReader*](#) is designed to read the files generated by the [automated burnup sequence](#). The output format is described at the [SERPENT Wiki](#).

The reader stores homogenized universe data for each universe at each point in time for each branch in *HomogUniv* objects.

class `serpentTools.parsers.branching.BranchingReader` (*filePath*)

Parser responsible for reading and working with automated branching files.

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

iterBranches ()

Iterate over branches yielding paired branch IDs and containers

read ()

Read the branching file and store the coefficients.

3.7 Bumat Reader

Warning: This reader is not implemented yet. This merely serves as a placeholder

class `serpentTools.parsers.bumat.BumatReader` (*filePath*, *readerSettingsLevel*)

Parser responsible for reading and working with burned material files.

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

3.8 Depletion Reader

Warning: Does not support depleted materials with underscores, i.e. `fuel_1` will not be matched with the current methods

class `serpentTools.parsers.depletion.DepletionReader` (*filePath*)

Parser responsible for reading and working with depletion files.

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

materials

dict

Dictionary with material names as keys and the corresponding `DepletedMaterial` class for that material as values

metadata

dict

Dictionary with file-wide data names as keys and the corresponding data, e.g. `'zai': [list of zai numbers]`

settings

dict

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

__delattr__

`x.__delattr__('name') <==> del x.name`

__format__ ()

default object formatter

```

__getattr__
    x.__getattr__('name') <==> x.name

__hash__

__reduce__()
    helper for pickle

__reduce_ex__()
    helper for pickle

__repr__

__setattr__
    x.__setattr__('name', value) <==> x.name = value

__sizeof__() → int
    size of object in memory, in bytes

read()
    Read through the depletion file and store requested data.

```

3.9 Detector Reader

```

class serpentTools.parsers.detector.DetectorReader(filePath)
    Parser responsible for reading and working with detector files.

    Parameters filePath (str) – path to the depletion file

    detectors
        dict

        Dictionary where key, value pairs correspond to detector names and their respective DetectorObject

    read()
        Read the file and store the detectors.

```

3.10 Fission Matrix Reader

Warning: This reader is not implemented yet. This merely serves as a placeholder

```

class serpentTools.parsers.fissionMatrix.FissionMatrixReader(filePath, readerSettingsLevel)
    Parser responsible for reading and working with fission matrix files.

    Parameters filePath (str) – path to the depletion file

```

3.11 Results Reader

Warning: This reader is not implemented yet. This merely serves as a placeholder

```

class serpentTools.parsers.results.ResultsReader(filePath, readerSettingsLevel)
    Parser responsible for reading and working with result files.

```


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

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.

4.1 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!

4.1.1 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.

4.1.2 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.

4.1.3 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.

4.2 Version Control

This project utilizes [versioneer](#) to update the project version based on release and commit history. Using this tool allows the project version to match [PEP 440](#) style versions, with minor exceptions for developer (non-public release) versions. For public releases, where sufficient changes have been made through added features, bug fixes, or wholesale changes, the version will be of the form `major.release.patch`. Changes in `major` indicate vast user-facing changes to the core functionality and/or API, while changes to `release` indicate a new feature added or substantial improvement that does not alter the user-facing API. In the event of bug fixes or minor tweaks, the `patch` number should be incremented.

For non-public releases, e.g. the `develop` branch, [versioneer](#) includes some additional information in the project version. Here, the version is of the form `major.minor.patch[+/-]N.commit[.dirty]`. `[+/-]N` indicates that this version is `N` commits ahead of or behind the latest public release, and `commit` is the short version of the latest commit on the branch for this version. `dirty` will be present if the current version has uncommitted changes. This level of precision with respect to versioning allows for easy identification if people are working on multiple branches and/or having issues.

4.2.1 Releases

Releases should be done with [git tags](#) from the `master` branch and then pushed to GitHub. [versioneer](#) works by locating these tags in the git history, and works best with annotated tags, which can be created with:

```
git tag -a <version>
git tag -s <version>
git tag -m <msg> <version>
```

Pushing these tags to GitHub creates a new [release](#), and shares the tag with all who have cloned the repository. 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.

In the future, python installers such as [python wheels](#) can be built by running `python setup.py bdist_wheel`. These can be manually uploaded to the release page, or the [python package index](#) for users who only want the python files without examples or documentation.

4.3 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()
```

4.4 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.

4.4.1 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 [numpy style docstrings](#), examples of which are given below

Functions and Methods

Below is the `depmtx()` function annotated using short and longer docstrings:

```
def depmtx(filePath):  
    """Return t, no, zai, a, and nl values from the depmtx file."""
```

or:

```
def depmtx(filePath):  
    """  
    Read the contents of the ``depmtx`` file and return contents  
  
    .. note::  
  
        If ``scipy`` is not installed, matrix ``A`` will be full.  
        This can cause some warnings or errors if sparse or  
        non-sparse solvers are used.  
  
    Parameters  
    -----  
    fileP: str  
        Path to depletion matrix file  
  
    Returns  
    -----  
    t: float  
        Length of time  
    n0: numpy.ndarray  
        Initial isotopic vector  
    zai: numpy.array  
        String identifiers for each isotope in ``n0`` and ``n1``  
    a: numpy.array or scipy.sparse.csc_matrix  
        Decay matrix. Will be sparse if scipy is installed  
    nl: numpy.array  
        Final isotopic vector  
    """
```

Both docstrings indicate what the function does, and what is returned. The latter, while more verbose, is preferred in most cases, for the following reasons. First, far more information is yielded to the reader. Second, the types of the inputs and outputs are given and clear. Some IDEs can obtain the expected types from the docstrings and inform the user if they are using an incorrect type.

More content can be added to the docstring, including

- Raises - Errors/warnings raised by this object
- See Also - follow up information that may be useful
- Yields - If this object is a generator. Similar to Returns

Classes

Classes can have a more lengthy docstring, as they often include attributes to which the class has access. Below is an example of the docstring for the `DepletionReader`:

```

"""
Parser responsible for reading and working with depletion files.

Parameters
-----
filePath: str
    path to the depletion file

Attributes
-----
materials: dict
    Dictionary with material names as keys and the corresponding
    :py:class:`~serpentTools.objects.DepletedMaterial` class
    for that material as values
metadata: dict
    Dictionary with file-wide data names as keys and the
    corresponding dataas values, e.g. 'zai': [list of zai numbers]
settings: dict
    names and values of the settings used to control operations
    of this reader

"""

```

Class docstrings can be added to the class signature, or to the `__init__` method, as:

```

class Demo(object):
    """
    Demonstration class

    Parameters
    -----
    x: str
        Just a string

    Attributes
    -----
    capX: str
        Capitalized x

    """

```

or:

```

def __init__(self, x):
    """
    Demonstration class

    Parameters
    -----
    x: str
        Just a string

    Attributes
    -----
    capX: str
        Capitalized x

    """

```

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.

4.4.2 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.

4.5 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

4.5.1 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.

4.5.2 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.

4.6 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*

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