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Omnibus User Manual

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OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

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Reactor and Nuclear Systems Division

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ABSTRACT

This manual provides instructions for using the Omnibus front end to the Exnihilo code suite, which contains the Denovo and Shift transport solvers.

1. INTRODUCTION

Exnihilo is a modern radiation transport framework that implements state-of-the-art algorithms, solvers, and solution methodologies, enabling it to solve a wide variety of nuclear engineering and applications problems with the scalability to run on desktop machines and leadership-class supercomputers. The Omnibus code [3] is a powerful, flexible interface to the extensive functionality of Exnihilo. This manual documents the Exnihilo capabilities exposed by Omnibus and demonstrates their use.

Omnibus provides access to the two core Exnihilo transport solvers, the Denovo deterministic solver (page 176) [4] and the Shift Monte Carlo solver (page 167) [5]. In addition, Omnibus allows the two solvers to be coupled using modern hybrid methods (page 224) that accelerate Shift transport solutions using approximate solutions from Denovo. Omnibus also allows time-dependent Shift depletion calculations using the ORIGEN nuclide depletion solver (page 212) [6].

The Exnihilo transport framework is designed to support computational transport using a combination of input models (page 43) (which define a problem's geometry and compositions) and multiple physics implementations (page 85) (which implement approximations to the Boltzmann transport equation). Many classes of particle sources (page 56) and tallies (page 113) can be defined separately from the model's geometry, and custom compositions (page 106) can also be entered by the user.

The Omnibus interface enables other codes such as ADVANTG [7] and SWORD [8] to create, execute, and post-process Denovo problems, but their use is outside the scope of this document. Other radiation transport codes such as VERAShift [9] and SCALE [2] use the Shift and Denovo codes through a lower-level interface via an internal Omnibus-based API. Although these codes are also outside the scope of this manual, the features and some interfaces presented here may inform the use of downstream codes.

1.1 OMNIBUS EXECUTION

At its core, Omnibus is a high-performance, MPI-enabled binary executable, the input of which is a hierarchical problem definition. The Omnibus executable is designed to be launched by a driver, the `omnibus` Python module, which generates a validated input for the executable *before* launching it in parallel.

Pre-execution validation, which can be run using the omnibus-pre (page 16) command, is critically important for high-performance computing (HPC) systems in which tens or hundreds of thousands of CPU hours can potentially be lost if an invalid input causes a single process to fail. It is also a tremendous time saver on other shared computing resources such as institutional clusters, ensuring that the input does not need to be queued and launched before it is validated. If a problem input is rejected, then the Python pre-processor can also construct a descriptive, context-sensitive error message such as:

```
ERROR: From input at ueki-cadis.omn:19:
FATAL ERROR: In /physics/ce, the following unknown inputs were found: 'mood' (did you␣
↪mean 'mode'?)
```

or

```
FATAL ERROR: At ueki-cadis.omn:21: Invalid value 'npe' for keyword 'mode' at /physics/ce/
↪mode:
expected particle transport mode (``n``, ``neutron``, ``np``, ``p``, ``photon``, or␣
↪``pn``), but string is not a particle mode
[mode: Particles to transport]:
    npe
```

Besides validating the user input and providing error messages, the Python input schemas are also used to generate the Omnibus (page 25) and Geometria (page 233) input specifications in this manual.

1.2 PYTHON BINDINGS

Exnihilo uses the SWIG[1] utility to generate Python interfaces to utility classes in Exnihilo. These interfaces power some Omnibus capabilities such as ray tracing, but they may also be used by power users as a high-level interface to many core Exnihilo capabilities, including exploring nuclear data and interacting with problem models.

The following Python modules are installed with Exnihilo[2]:

nemesis: Infrastructure components This collection of utilities includes interfaces to MPI and Silo.

robus: Physics data Robus has containers designed to load and store continuous-energy and multigroup cross sections, nuclides, and compositions.

transcore: Transport core components This package includes cross section storage classes, libraries for reading and writing cross sections, etc. See Multigroup data exploration (page A–91) for an example of creating and visualizing multigroup cross sections.

geometria: Geometry interfaces This module has interfaces to the different geometry models used by Shift. It enables ray tracing of the geometry and extraction of compositions.

physica: Physics packages The physics package includes additional interfaces to the CE data. See CE data (page A–132) for examples.

1.3 POST-PROCESSING TOOLS

Several tools have been developed to support interacting with, processing, and visualizing Exnihilo input and output. Most of the data are read from and written to HDF5 files, so the workflows rely heavily on the Python-based `h5py` module.

1.3.1 OMNIBUS.DATA

The Omnibus data toolset is an `h5py`-based interface to Exnihilo HDF5 input and output files. It allows slices of the data to be taken without loading the entire file into memory, and it includes plotting tools based on `matplotlib`. For examples on how to use this module, see the Denovo (page A–9) and Shift (page A–103) example sections.

Note: The full documentation of the postprocessing tools is outside the scope of this manual. However, if you're using IPython (e.g., through `omnibus-analysis`) or Jupyter notebook to postprocess the data, tab

[1] http://sourceforge.net/projects/swig

[2] SWIG Python bindings will only be available when Exnihilo is built with the SWIG option on and when installing shared libraries.

completion on any of the Omnibus analysis objects will list the available methods for that object. Additionally, adding a question mark symbol after a method or object will provide a help overview showing the arguments that function expects. Finally, the `help` built-in function provides detailed information about available data members and methods of any object.

1.3.2 [POST] BLOCK

When run through omnibus-run (page 15), the post-processing block in the Omnibus input will extract specified data from the HDF5 output in a more human-friendly format. For example, this block will generate an ReST-formatted text file summarizing the run, plot k_{eff} values for Shift eigenvalue problems, and generate `csv`-formatted tables of depletion results. More advanced post-processing blocks such as `[DENOVO][SPECTRUM]`, which will write flux spectra at the given list of points, allow complex extraction of user-specified data.

1.3.3 H5SH

The h5sh tool[3] provides a shell-like interface to browsing HDF5 files. It can be independently downloaded and installed through Python's package manager (`pip install h5sh`).

It can be cumbersome to use the Omnibus python post-processing tools to quickly examine the contents of an Exnihilo output (or input) file. Some developers have gotten into the habit of using `h5ls` and `h5dump` for this, but those tools are impossibly slow for files greater than a few hundred megabytes, and it is inconvenient and slow to use them for multiple consecutive invocations to drill down on a piece of data.

To this end, Exnihilo includes a small but powerful tool that allows the user to browse any HDF5 file as if it were a directory in a shell terminal. HDF5 groups become directories and datasets act as files. It is designed to be intuitive and straightforward. See Using the h5sh tool (page A–152) for an example of its use or the online documentation[4] for more details.

[3] https://pypi.org/project/h5sh/
[4] https://h5sh.readthedocs.io/

2. FRONT END INTERFACE

Your Exnihilo installation contains the `omnibus` executable (which actually drives Denovo and Shift from an XML input file), as well as additional Python scripts that pre-process user input and program output. If using an HPC cluster, then the pre-processing is typically performed on a login node, thus validating and preparing the user input without making it necessary to wait for a job to queue (and without risking the waste of compute hours due to an invalid input being encountered at runtime).

2.1 RUNNING OMNIBUS

The omnibus-run (page 15) script creates an Omnibus XML input file, drives and monitors the omnibus (page 17) executable as it is being run, and post-processes the output.

Unlike most code drivers, omnibus-run is meant to be executed **on the head node** of a cluster rather than on a compute node. Using a machinefile (if the `[RUN=mpi]` option is being used) or pbs submission (for `[RUN=pbs]`), it is able to submit the job to other nodes and monitor the application process. To prevent a terminal disconnect from stopping the monitoring (it will *not* stop the job), it is a good idea to use the screen[5] utility.

Because the pre-processing, execution, and post-processing steps often generate a dozen files or so, it is highly recommended to create a new working directory for every execution step. The Omnibus pre- and post-processors always generate output in the working directory (as opposed to the directory where the input resides), so a good workflow is

```
$ mkdir myrun; cd myrun
$ omnibus-run ../input.omn
```

This makes it easier to delete an entire run without accidentally deleting the input, and it also prevents multiple simultaneous Omnibus runs from clobbering each others' files.

Tip: For systems such as Titan that have special filespaces (Lustre) from which the code is executed, the easiest way to ensure that all Omnibus I/O remains on that system is to leave the `.omn` input file on Lustre and call `omnibus-run` from that directory.

2.1.1 EXAMPLE ON A LOCAL MACHINE

Suppose there is an input file, `batman.omn`, on a local machine:

```
[PROBLEM]
name Batman
description "Dark, brooding."

! -- snip -- !

[RUN=mpi]
np 4
```

If Omnibus is installed with MPI, then one can simply open a terminal and call:

[5] https://kb.iu.edu/d/acuy

```
$ omnibus-run batman.omn
```

This runs the following sequence:

1. The pre-processor will validate the input.
2. After successful validation, the pre-processor will write an `xml` intermediate file read in by the `omnibus` binary executable. If necessary, it will also generate other input files (such as the run tape file used for running on Monte Carlo N-Partcle [MCNP] geometry).
3. The script will launch a local process with arguments such as `mpirun -np 4 omnibus batman.xml` and then will save the output to the current directory and echo it to the screen.
4. When the `omnibus` execution is complete, it will write out tally data and other program output to several different files.
5. A Python post-processor reads the output and converts it to a human-readable format, leaving the original output files for later post-processing.

2.1.2 EXAMPLE ON A CLUSTER USING PBS/TORQUE

In this example, the local machine problem is copied and the run block is changed (see [RUN=pbs] (page 30)):

```
[PROBLEM]
name emmet
description "I'm dark and brooding, too. Oh look guys, a rainbow!!"

! -- snip -- !

[RUN=pbs]
nodes    1
ppn      32
walltime "1:00:00"
```

When `omnibus-run` is executed on the head node, it will launch `qsub`, monitor the job ID until it begins running on the compute node, and will echo output to the screen over an ssh connection. The process on the head node remains almost entirely idle during the problem run, so the user need not worry about incurring the wrath of the system's administrator.

Note: Be aware that some of the pre-processing may be computationally expensive, specifically when using the MCNP model on a large input deck. In that case, it is recommended that one generate the `runtpe` file separately and specify the `runtpe_path` parameter instead of the `input` command so that Omnibus does not run the MCNP pre-processor on the head node. Alternatively, one may be able to run `omnibus-run` or `omnibus-pre` on a compute node.

2.1.3 RUNNING OMNIBUS MANUALLY

Separate scripts are provided for pre- and post-processing an Omnibus input. To generate the Omnibus XML input file from an ASCII input, call:

```
$ omnibus-pre my_problem.omn
```

This will create a Teuchos ParameterList XML input file *`my_problem`*`.inp.xml`. This parameter list is then run with the Omnibus driver:

```
$ mpirun -np 16 omnibus my_problem.inp.xml
```

Post-processing (including plotting keff and Shannon entropy convergence, as well as rendering the XML output into a more human-readable format) is done with the command:

```
$ omnibus-post my_problem.pp.json
```

2.2 OMNIBUS ASCII INPUT FORMAT

The Omnibus ASCII input is a human-readable, minimal input syntax for Omnibus. The underlying Omnibus input data structure is hierarchical, and the ASCII input is designed to flatten the hierarchy. The input consists of (1) "blocks" of input data, each of which represents a database, and (2) cards, which consist of parameters and "commands" which generate parameters or perform other functions.

2.2.1 BLOCKS

Block titles have the following formats

```
[CLASS]
[CLASS name]
[TYPEDCLASS=type]
[TYPEDCLASS=type name]
[TYPEDCLASS][TYPEDSUBCLASS=type name]
[CLASS][SUBCLASS name]
[..][SIBLING]
[.][DAUGHTER]
```

These formats embed the location in the hierarchy, the database class, the database type, and the name of this particular instance of the database class. The "name" (which requires a value with only letters, numbers, and the underscore) is simply a shorthand for declaring the block and adding a "name" parameter. The class type is required for databases with multiple allowed types (e.g., model and physics), but it is disallowed for types that do not. Only the rightmost database can have a type: its parent block types must be omitted.

Relative blocks can be specified using the special `[..]` and `[.]` keywords analogous to POSIX paths. The `[..]` block specifies "belonging to two blocks above the current block location." Similarly, `[.]` means "belonging to one block above the current block location," allowing the easy specification of subdatabases. These specifications simplify deeply nested blocks; in the above example, the full list of blocks is expanded to:

```
[CLASS]
[CLASS name]
[TYPEDCLASS=type]
[TYPEDCLASS=type name]
[TYPEDCLASS][TYPEDSUBCLASS=type name]
[CLASS][SUBCLASS name]
[CLASS][SIBLING]
[CLASS][SIBLING][DAUGHTER]
```

Whitespace in block titles, as well as capitalization for the class and type attributes, is ignored.

2.2.2 CARDS

Cards are started on a new line; an indentation of **four or more spaces** is treated as a continuation of the previous card. Spaces separate values in a parameter list or arguments in a command. For strings, quotation marks can be used to treat whitespace as standard characters. The backslash can be used to escape quotation marks inside a quoted string.

For example, these two parameters demonstrate the correct usage of whitespace:

```
param This is a list of seven parameters
param "This is a single parameter with an \" embedded quotation mark."
```

Tip: One common input error is to mistake a small indentation on the next line for a continuation. This statement declares three parameters inside a block:

```
[WAYNE]
something value value
  business business numbers
  is this working
```

whereas this is one parameter with multiple values:

```
[WAYNE]
something value value
    business business numbers
    is this working
```

Using the syntax highlighting files for Vim and Emacs provided in the Exnihilo environment or using the `omnlexer` Pygments lexer will make such errors very obvious.

2.2.3 OTHER FEATURES

2.2.3.1 Special characters

The following characters are treated as special tokens in the ASCII input:

Table 1: Special characters in Omnibus input.

Token	Name	Use
`!`	Exclamation	Comment: all following characters on the line are ignored
`#`	Hash	Used to include other files
`\`	Backslash	Escapes other special characters
`'`	Single quote	Starts or ends a string
`"`	Quote	Starts or ends a string
`:`	Colon	Separates variable names in column format, or creates separate items in a list
`-`	Dash	A standalone series of dashes is translated to the `None` Python token, used in lists or column format to denote the absence of a value
`->`	Arrow	Creates a two-item tuple indicating a mapping
`$`	Dollar	Encloses a math expression to be evaluated
`|`	Pipe	Encloses units specification

Whitespace is generally ignored. The exception is the line continuation described above in which four leading spaces indicate continuation of the previous line. When embedded in a quoted string, whitespace is preserved.

Any text on a line following an exclamation point is ignored.

2.2.3.2 Math expressions

The Omnibus ASCII input format can evaluate[6]simple math expressions enclosed in a matching pair dollar signs in the input. Like quotations, these signs must be on the same line and separated from other input values by whitespace. An example of a math expression is:

```
x $1/3$ $2**5$
```

2.2.3.3 Unit support

When the Pint[8] python package is installed, Omnibus can automatically convert units to the correct type needed by an input parameter. Units are surrounded by pipes and modify the previously input value. Like quotations and math expressions, units must be defined on a single line and separated from other input values by whitespace. An example of unit conversion is:

```
[DEPLETION]
power       3.14   |Btu / fortnight|
burn_length 1.0e-5 | millenia |
```

Since the [DEPLETION] database (page 212) expects power in units of megawatts and burn length in units of days, the input quantities will be converted to those types when they are exported for the Omnibus binary driver.

The Pint package provides a comprehensive set of available units[9].

Warning: Currently, units are only supported for scalar quantities, not parameters that take lists. Trying to use units in that case will cause an error.

2.2.3.4 Interpolation

Inside numerical lists, the MCNP interpolation/repetition shorthand characters “I,” “ILOG,” “M,” and “R” are implemented. For example,

```
x_coordinates 1 2I 4
```

is interpolated to form

```
x_coordinates 1 2 3 4
```

This feature is tied to the parameter processing itself, so only numeric lists have the ability to interpolate (i.e., the letter `I` is treated just like that letter in normal parameters). This also means that Python or JSON input can use the interpolation/repetition shorthand characters for convenience.

[6] This capability is implemented using the simpleeval[7] library.
[7] https://github.com/danthedeckie/simpleeval
[8] https://pint.readthedocs.io/en/0.9/
[9] https://github.com/hgrecco/pint/blob/master/pint/default_en.txt

Tip: The vacuum-omnibus-input (page 20) script will read the Omnibus input file, reformat it, and rewrite it. If the input and output are not logically the same, then there may be a subtle syntax error in the input file (e.g., not indenting when continuing). This tool only parses the input file; it does no expansion, validation, or defaulting.

Tip: To view a validated and reformatted ASCII version of input, one can explicitly tell the preprocessor to save an `.omn` file:

```
$ omnibus-pre problem.omn -o problem.validated.omn
```

This operation is performed automatically when using the omnibus-run (page 15) command.

2.3 OMNIBUS INPUT AND OUTPUT

Omnibus accepts multiple input formats, prints output to the terminal screen, writes (possibly multiple) intermediate files, and processes the output into more useful formats.

The following image describes how files are generated and used while driving Omnibus through the front end:

2.3.1 INPUT FILES

Omnibus ASCII input files (with the '.omn' extension) are described in ASCII input (page 7):

```
[PROBLEM]
name "CE pin cell lava_scempp kcode problem"
mode kcode

[MODEL=mcnp]
input mcnp_godiva.mcnp
```

These are unfolded into hierarchical databases and are then converted to XML for the Omnibus executable. YAML and JSON hierarchical databases are also supported, which may appeal more to power users:

```
{
  "problem": {
    "name": "CE pin cell lava_scempp kcode problem",
    "mode": "kcode",
    },
  "model": {
    "_type": "mcnp",
    "input": "mcnp_godiva.mcnp",
  }
}
```

Python files that can modify an existing (e.g., ASCII-created) input definition are also supported. When pre-processing Python input definitions, a local db variable contains the Omnibus input definition hierarchy and can be modified or extended. This Python method is extremely powerful for automating repetitious tallies, as demonstrated in this example that creates five similar cylindrical mesh tallies sharing an energy grid:

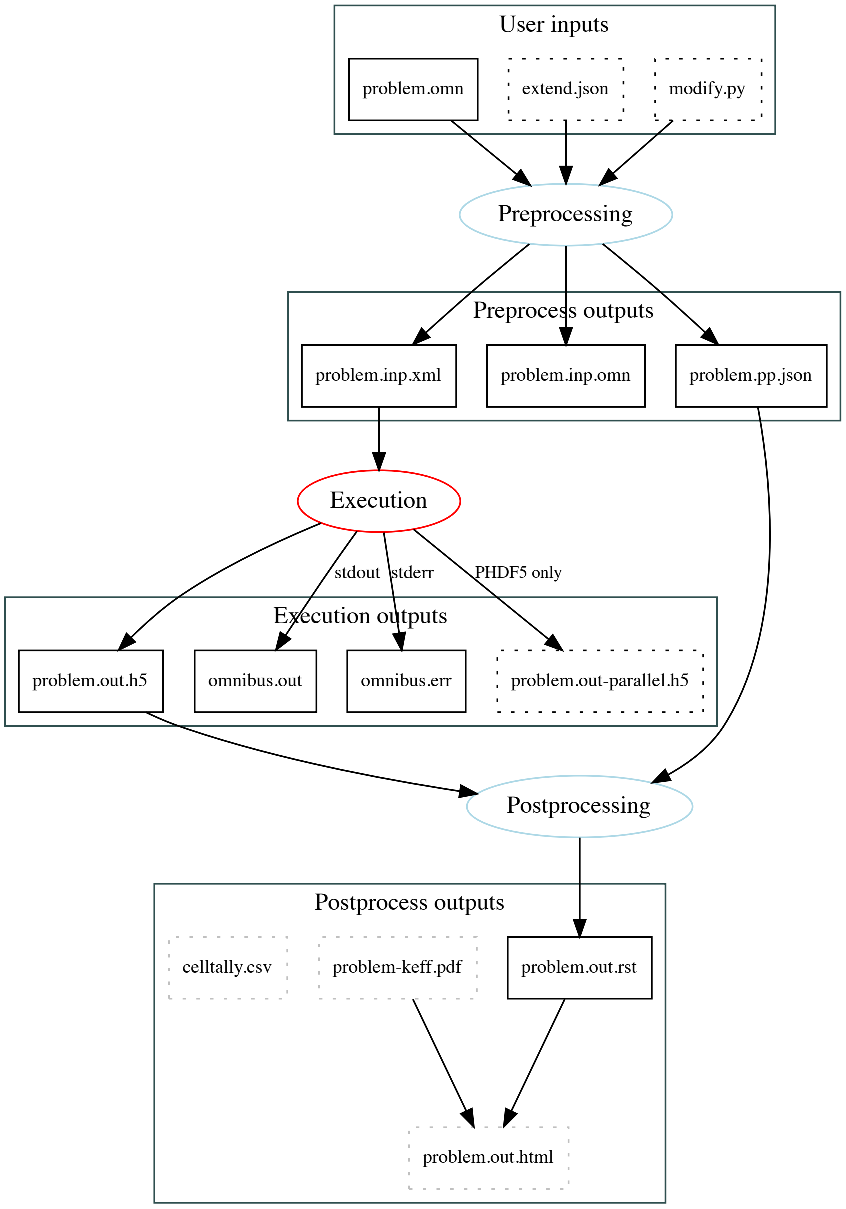

Fig. 1: Execution flow for `omnibus-run`. The small black boxes are the typical input/output files, blue circles are parts of the Python pre-processor run on the head node, the red circle is the Omnibus executable (run on the compute nodes), and dotted lines denote optional files (e.g., multiple input files).

```
import numpy as np

new_tallies = []

neutron_bins = [2e7, 1e5, 1e3, 10, 1, 1e-5]
photon_bins = np.linspace(0, 1e6, 11)[::-1] # 10 linear bins to 1 MeV
reactions   = ["flux"]

targets = [
        # area,      loc,         x,          y,        r
        ( 'PTP', 'FT-A1', -4.66117,  -2.69113, 0.929640,),
        ('SVXF', 'VXF-1',  3.07648,  39.09038, 2.011680,),
        ('SVXF', 'VXF-2', -3.45642,  43.91796, 2.011680,),
        ('SVXF', 'VXF-3', -9.15368,  38.12784, 2.011680,),
        ( 'PTP', 'FT-A1', -4.66117,  -2.69113, 0.929640,),
        ]

# Add each tally to the list
for (area, loc, x, y, r) in targets:
    tal = {
            'name': ":".join((area, loc)),
            'description': "flux in %s target location %s" % (area, loc),
            'reactions': reactions,
            'r': [0.0, r],
            'theta': [0.0, 1.0], # divided by 2pi
            'translate': [x, y, 0],
            'z': [-25.4, 25.4],
            'neutron_bins': neutron_bins,
            'photon_bins': photon_bins,
            }
    new_tallies.append(tal)

# Set all cylindrical tallies
assert 'tally' in db
assert 'cylmesh' not in db['tally']
db['tally']['cylmesh'] = new_tallies
```

This could be integrated into an Omnibus run file by executing:

```
omnibus-run hfir.omn hfir-tallies.py
```

2.3.2 PRE-PROCESSING OUTPUT FILES

The pre-processing step will typically create several files for an input `*problem*.omn`:

`*problem*.pp.json` If using the `omnibus-run` front end, then this will be created: it is a fully processed version of the problem input, with all default parameters explicitly filled.

`*problem*.inp.omn` If using the `omnibus-run` front end, then this will be created: it is a fully processed and reformatted version of the problem input. It also has all parameters filled.

`*problem*.inp.xml` The Teuchos ParameterList XML file is read by the `omnibus` executable.

Additionally, if an MCNP model is being used, then a `runtpe` file will be generated. Finally, if a `[RUN=pbs]` block is present, then a `*problem*.pbs` submission script will be generated.

2.3.3 EXECUTION OUTPUT FILES

Running Omnibus will generate one or more output files:

`*problem*.out.h5` Execution results and data will be written using serial HDF5.

`*problem*.out-parallel.h5` If running on a parallel file system and parallel HDF5 is installed, then some datasets will be written to this file and "externally linked" into the serial HDF5 file. Generally, only data that are decomposed across MPI domains are written to this file.

`omnibus.out` Messages will be written from the executable (and PBS script if applicable) to *stdout*. Generally, only embedded external code (such as Trilinos solvers and SCALE cross section processing routines) write to *stdout*.

`omnibus.err` Messages will be written from the executable (and PBS script if applicable) to *stderr*. These include logging and diagnostic messages during the program run, as described in the next section.

2.4 ERRORS, WARNINGS, AND OTHER MESSAGES

Omnibus can encounter unexpected conditions for a variety of reasons, including:

- problems with the system configuration,
- logic errors in the application code,
- inconsistencies in nuclear data being used, and
- errors in user input.

To the extent possible, Omnibus attempts to detect and gracefully handle these errors to provide feedback to the user that is meant to help in determining the root cause.

2.4.1 LOG MESSAGES

The Exnihilo framework has an internal logging system for writing messages of different levels of severity to the screen. The omnibus-run (page 15) process intercepts these messages, as well as all other output text, and will print formatted logging statements. For some statements that are not very important but that provide the user with an idea of the program status, omnibus-run (page 15) will only display the latest statement. Other higher-level statements will remain on the screen (with levels of color, for terminals that support it, indicating their severity).

The different levels of logging messages are:

DEBUG Very fine-grained diagnostic messages that show a level of detail not typically needed for problem execution.

DIAGNOSTIC Progressive output that shows detailed state information about the problem. Example diagnostics include Denovo iteration count and Shift cycle k-effective estimates.

STATUS Traces the flow of Omnibus showing what part of the program is being executed.

INFO Informational messages unique to the particular problem being run, such as "Loaded 123 cross sections" or "Set default for parameter 'foo' to 123."

WARNING Messages about situations that are unusual, unexpected, or possibly inconsistent: something *might* be wrong. They may indicate the possibility of incorrect solutions, but they may also be totally harmless, depending on the intent of the user. The user should examine these warnings carefully to determine their importance. Examples of warnings are:

- when nuclear data for a requested nuclide is unavailable and a similar nuclide (e.g., ground state or unbound) was substituted;
- when a user requests Silo output, but Silo support is not compiled;
- when volumes are omitted from cells being tallied, so the solutions change from being normalized by volume to being unnormalized; and
- when statistical checks on Shannon entropy fail.

ERROR Messages indicating a definite inconsistency: something *is* wrong. Omnibus is built to attempt to recover gracefully from unexpected program input, cross section data, etc. When a recoverable error occurs, an error message is printed. The user should *very carefully* examine the error to assess its severity. Example error messages include:

- particles being lost while tracking through the geometry;
- CE cross sections not balancing correctly at the particle's energy, suggesting an error in the CE data.

FATAL ERROR This message is the last thing the user will see before the world turns dark: an unrecoverable error (either due to user input or an unexpected program state) has occurred, and the program will shut down. If Omnibus is being monitored inside `omnibus-run`, then it will attempt to kill the process being run (e.g., by signalling `mpiexec` or calling `qdel`).

By default, `DIAGNOSTIC` and higher levels are printed to the screen and echoed to `omnibus.err`, and `INFO` and higher levels are saved to the Omnibus HDF5 output file. There is typically not any output in the `omnibus.out` file; this usually only contains output from third-party libraries.

Tip: The Omnibus input parameter screen_verbosity (page 42) will change the level of message that is written to the screen and the `omnibus.err` file.

Note that the warning labels described above correspond to special prefixes in the program output:

Table 2: Omnibus diagnostic output examples.

Level	Example
DIAGNOSTIC	`Loading nuclide u-235 @ 293K.`
STATUS	`:::  Beginning inactive cycles`
INFO	`>>> Loading CE library ce_v7.0_endf.h5`
WARNING	`*** neutron data for ZAID=1001 is not available for `` ``MT=301 in the splicing AMPX library.`
ERROR	`!!! Geometry error in particle 0:123:  ...`
FATAL ERROR	`!*!*! Couldn't find a CE library for ce_v7.4_endf`

2.4.2 OUT-OF-MEMORY ERRORS

It is very possible for Omnibus to run out of memory in the middle of execution since large data fields are allocated at different points during the run. On some system configurations, Omnibus will be able to correctly detect and report an out-of-memory (OOM) error[10].

[10] The kernel's memory allocation function will correctly return a NULL pointer, indicating a failure to allocate. This will cause the C++ library to throw a `std::bad_alloc` exception, which is then caught by Omnibus.

However, the default behavior[11] on Linux kernels is to *overcommit memory*. Although overcommitment is practical for most real-world applications, its consequence is that an application cannot know exactly when or why it ran out of memory. Rather than printing a useful message about memory allocation, the offending Omnibus process will immediately be terminated (with `SIGKILL`, signal 9) without any opportunity to clean up.

Tip: When launched with [RUN=pbs] (page 30), a problem killed due to an OOM error may produce an `omnibus.err` file that ends with:

```
--------------------------------------------------------------------------
Primary job  terminated normally, but 1 process returned
a non-zero exit code. Per user-direction, the job has been aborted.
--------------------------------------------------------------------------
--------------------------------------------------------------------------
mpiexec noticed that process rank 72 with PID 115153 on node mod-pbs-c62
exited on signal 9 (Killed).
--------------------------------------------------------------------------
```

and an output file that may contain:

```
5 total processes killed (some possibly by mpiexec during cleanup)
!*!*! Omnibus execution failed with error 137
```

To help diagnose OOM errors, Omnibus provides a print_memory (page 41) parameter that will periodically output local and global memory usage. Additionally, the final status or informational update before the error may provide the context for the failure: if the last message is about constructing a Denovo state vector, then it is likely that the Denovo discretization is too fine to fit on the requested number of processors.

Aside from using a machine with more RAM per core, there are two possible actions to take to mitigate OOM errors. If the allocation failure is about *decomposed* data (such as the state vector in Denovo), then it will be necessary to use more processors or nodes to decrease the memory requirement per process. However, if the failure is due to *replicated* data such as material compositions or broadened cross sections in Shift, then the user can reduce the node occupancy (processes per node (page 33)), allowing each process to use more of the available memory on the system.

See Performance considerations (page 178) for a discussion of memory consumption in Denovo.

2.4.3 MISSING CAPABILITIES

Although the Omnibus preprocessing validation *should* encode configuration requirements and feature capabilities through its “applicability” statements and other logic, it is possible that the developers have missed something. If a feature is implemented by SCALE but is not enabled in the installed copy of SCALE (usually due to an unavailable third-party library), then an error message will explain that the build configuration does not support the feature. If a capability is planned for Shift or is only known to work under a limited set of other options, then an error message may explain that the feature is not currently implemented.

2.5 COMMAND LINE TOOLS

2.5.1 OMNIBUS-RUN

Run the Omnibus pre-processor, run Omnibus, and run the post-processor.

[11] https://www.kernel.org/doc/Documentation/vm/overcommit-accounting

Run Omnibus from start to finish.

```
usage: omnibus-run [-h] [--version] [-g] [-c] [-e ENV] [-v] [-q]
                   [--very-quiet] [--silent]
                   [--log {None,DEBUG,STATUS,INFO,WARNING,ERROR,CRITICAL}]
                   [inp [inp ...]]
```

2.5.1.1 Positional Arguments

inp	Input file names (omnibus, yaml, and/or python).

2.5.1.2 Named Arguments

--version	show program's version number and exit
-g, --debug	Enable extended debug assertions
	Default: False
-c, --clobber	Overwrite exiting output files rather than renaming them
	Default: False
-e, --env	Update global environment settings with this JSON file

2.5.1.3 verbosity

-v, --verbose	Print all debug messages
	Default: "STATUS"
-q, --quiet	Only print informational and warning messages
--very-quiet	Only print warning messages
--silent	Print messages only on failure
--log	Possible choices: None, DEBUG, STATUS, INFO, WARNING, ERROR, CRITICAL
	Create a log file with the given verbosity

Exnihilo version (UNKNOWN)

2.5.2 OMNIBUS-PRE

Generate an XML input file for Omnibus, validating input along the way.

Preprocess Omnibus input files.

```
usage: omnibus-pre [-h] [--version] [-g] [-c] [-e ENV] [-v] [-q]
                   [--very-quiet] [--silent]
                   [--log {None,DEBUG,STATUS,INFO,WARNING,ERROR,CRITICAL}]
                   [-o OUTPUT]
                   [inp [inp ...]]
```

2.5.2.1 Positional Arguments

inp	Input file names (omnibus, json, yaml, and/or python).

2.5.2.2 Named Arguments

--version	show program's version number and exit
-g, --debug	Enable extended debug assertions Default: False
-c, --clobber	Overwrite exiting output files rather than renaming them Default: False
-e, --env	Update global environment settings with this JSON file
-o, --output	Output filename (xml, json, omn, yaml)

2.5.2.3 verbosity

-v, --verbose	Print all debug messages Default: "STATUS"
-q, --quiet	Only print informational and warning messages
--very-quiet	Only print warning messages
--silent	Print messages only on failure
--log	Possible choices: None, DEBUG, STATUS, INFO, WARNING, ERROR, CRITICAL Create a log file with the given verbosity

Exnihilo version (UNKNOWN)

2.5.3 OMNIBUS

The actual Omnibus binary executable.

```
usage: omnibus [--version] xml_input
```

Positional arguments:

`xml_input`	Path to the XML parameter input file.

Options:

`--version`	Show usage information and exit.

2.5.4 OMNIBUS-POST

Execute the Omnibus post-processing functions specified in a `[POST]` block. The argument is the "pre-processed" `.pp.json` file produced when running `omnibus-run`.

Post-process Omnibus output.

```
usage: omnibus-post [-h] [--version] [-g] [-c] [-e ENV] [-v] [-q]
                    [--very-quiet] [--silent]
                    [--log {None,DEBUG,STATUS,INFO,WARNING,ERROR,CRITICAL}]
                    pp
```

2.5.4.1 Positional Arguments

pp	Omnibus postprocess file (.pp.json)

2.5.4.2 Named Arguments

--version	show program's version number and exit
-g, --debug	Enable extended debug assertions Default: False
-c, --clobber	Overwrite exiting output files rather than renaming them Default: False
-e, --env	Update global environment settings with this JSON file

2.5.4.3 verbosity

-v, --verbose	Print all debug messages Default: "STATUS"
-q, --quiet	Only print informational and warning messages
--very-quiet	Only print warning messages
--silent	Print messages only on failure
--log	Possible choices: None, DEBUG, STATUS, INFO, WARNING, ERROR, CRITICAL Create a log file with the given verbosity

Exnihilo version (UNKNOWN)

2.5.5 OMNIBUS-ANALYSIS

Load an Omnibus output file into an iPython shell

```
usage: omnibus-analysis [-h] [--version] [-g] [-c] [-e ENV] [-v] [-q]
                        [--very-quiet] [--silent]
                        [--log {None,DEBUG,STATUS,INFO,WARNING,ERROR,CRITICAL}]
                        [--format FORMAT] [--varname VARNAME]
                        [--front-end {ipython,python}]
                        inp
```

2.5.5.1 Positional Arguments

inp	path to Omnibus HDF5 file

2.5.5.2 Named Arguments

--version	show program's version number and exit
-g, --debug	Enable extended debug assertions
	Default: False
-c, --clobber	Overwrite exiting output files rather than renaming them
	Default: False
-e, --env	Update global environment settings with this JSON file
--format	format of the HDF5 file (e.g. 'output','meshmodel')
	Default: "output"
--varname	local variable with loaded file wrapper
	Default: "f"
--front-end	Possible choices: ipython, python
	interactive console type
	Default: "ipython"

2.5.5.3 verbosity

-v, --verbose	Print all debug messages
	Default: "STATUS"
-q, --quiet	Only print informational and warning messages
--very-quiet	Only print warning messages
--silent	Print messages only on failure
--log	Possible choices: None, DEBUG, STATUS, INFO, WARNING, ERROR, CRITICAL
	Create a log file with the given verbosity

Exnihilo version (UNKNOWN)

2.5.6 OMNIBUS-CONF

Print configuration info from an HDF5 output file or the current Omnibus configuration

```
usage: omnibus-conf [-h] [--version] [-g] [-c] [-e ENV] [-v] [-q]
                    [--very-quiet] [--silent]
                    [--log {None,DEBUG,STATUS,INFO,WARNING,ERROR,CRITICAL}]
                    [output]
```

2.5.6.1 Positional Arguments

output	Path to HDF5 file, or blank for current configuration

2.5.6.2 Named Arguments

--version	show program's version number and exit
-g, --debug	Enable extended debug assertions Default: False
-c, --clobber	Overwrite exiting output files rather than renaming them Default: False
-e, --env	Update global environment settings with this JSON file

2.5.6.3 verbosity

-v, --verbose	Print all debug messages Default: "STATUS"
-q, --quiet	Only print informational and warning messages
--very-quiet	Only print warning messages
--silent	Print messages only on failure
--log	Possible choices: None, DEBUG, STATUS, INFO, WARNING, ERROR, CRITICAL Create a log file with the given verbosity

Exnihilo version (UNKNOWN)

2.5.7 VACUUM-OMNIBUS-INPUT

Parse an Omnibus input file and write a clean, consistent copy.

```
usage: vacuum-omnibus-input [-h] [--version] [-g] [-c] [-e ENV] [-v] [-q]
                            [--very-quiet] [--silent]
                            [--log {None,DEBUG,STATUS,INFO,WARNING,ERROR,CRITICAL}]
                            inp [inp ...]
```

2.5.7.1 Positional Arguments

inp	omnibus input file name

2.5.7.2 Named Arguments

--version	show program's version number and exit
-g, --debug	Enable extended debug assertions Default: False
-c, --clobber	Overwrite exiting output files rather than renaming them Default: False
-e, --env	Update global environment settings with this JSON file

2.5.7.3 verbosity

-v, --verbose	Print all debug messages Default: "STATUS"
-q, --quiet	Only print informational and warning messages
--very-quiet	Only print warning messages
--silent	Print messages only on failure
--log	Possible choices: None, DEBUG, STATUS, INFO, WARNING, ERROR, CRITICAL Create a log file with the given verbosity

Exnihilo version (UNKNOWN)

2.5.8 MAKE-DENOVO-MODEL

Create a Denovo mesh model file from a denovo output file

```
usage: make-denovo-model [-h] [--version] [-g] [-c] [-e ENV] [-v] [-q]
                         [--very-quiet] [--silent]
                         [--log {None,DEBUG,STATUS,INFO,WARNING,ERROR,CRITICAL}]
                         [-o OUTP] [--group GROUP] [-z] [-t TOLERANCE]
                         inp
```

2.5.8.1 Positional Arguments

inp	Input file name (.h5).

2.5.8.2 Named Arguments

--version	show program's version number and exit
-g, --debug	Enable extended debug assertions Default: False
-c, --clobber	Overwrite exiting output files rather than renaming them Default: False
-e, --env	Update global environment settings with this JSON file
-o, --output	Mesh model output filename (.h5)
--group	HDF5 group that contains the matids Default: "denovo"
-z, --disable-compression	Disable compression of the source term Default: True
-t, --mix-tolerance	Change the threshold for combining similar mixtures Default: 0.0

2.5.8.3 verbosity

-v, --verbose	Print all debug messages Default: “STATUS”
-q, --quiet	Only print informational and warning messages
--very-quiet	Only print warning messages
--silent	Print messages only on failure
--log	Possible choices: None, DEBUG, STATUS, INFO, WARNING, ERROR, CRITICAL Create a log file with the given verbosity

Exnihilo version (UNKNOWN)

2.5.9 DENOVO-POINT-OUTPUT

Save spectra from a Denovo output file

```
usage: denovo-point-output [-h] [--version] [-g] [-c] [-e ENV] [-v] [-q]
                           [--very-quiet] [--silent]
                           [--log {None,DEBUG,STATUS,INFO,WARNING,ERROR,CRITICAL}]
                           [--block BLOCK] [--field FIELD]
                           [--strength STRENGTH] [--on-disk]
                           output locfile
```

2.5.9.1 Positional Arguments

output	Path to Denovo .out.h5 file
locfile	Path to point locations, or - for stdin

2.5.9.2 Named Arguments

--version	show program’s version number and exit
-g, --debug	Enable extended debug assertions Default: False
-c, --clobber	Overwrite exiting output files rather than renaming them Default: False
-e, --env	Update global environment settings with this JSON file
--block	Name of the Denovo run block to extract Default: “denovo”
--field	Name of the energy-dependent output field (default: flux) Default: “flux”
--strength, -s	Source strength normalization Default: 1.0
--on-disk, -k	Read point data without loading entire file into memory Default: False

2.5.9.3 verbosity

-v, --verbose	Print all debug messages Default: “STATUS”
-q, --quiet	Only print informational and warning messages
--very-quiet	Only print warning messages
--silent	Print messages only on failure
--log	Possible choices: None, DEBUG, STATUS, INFO, WARNING, ERROR, CRITICAL Create a log file with the given verbosity

Exnihilo version (UNKNOWN)

3. OMNIBUS INPUT DESCRIPTION

The Omnibus input is split into a hierarchy of blocks comprised of databases, sublists, and parameters. The front end also supports “commands” for creating or modifying input parameters, as well as additional pre-processing and post-processing for validation.

Databases, sublists, and parameters all have the following properties:

Name The name of the parameter as it appears in the input. Some parameters have shorter aliases (e.g., `nemin` for `n_energy_min`) that appear in the documentation just below the full parameter name.

Description The text immediately below the name should describe what it means and how it is used.

Applicable when A series of rules describing when the parameter may or may not be used. These rules take into account other parameters as well as the build configuration. Bulleted “applicability” items indicate that all the conditions must be met.

Default If present, a default value for the parameter or database. The default may be a fixed value (e.g., `3.0`), or it may be a procedure based on the other input parameters, in which case a rough description of the default is given. For databases and sublists, the default may appear as a Python expression (e.g., `{'_type': "none"}` for a database with type “none”). If no default is given, then the parameter or database is *required* in the given context. However, a few parameters and databases are optional and are marked accordingly.

Export The parameter will be renamed when writing to the `.inp.xml` file for historical reasons.

Note: This documentation was generated automatically with the following version of Exnihilo:

version 6.3.pre-b13 (branch ‘master’ on ‘upstream’, r729: #9809b44f on 2020JUL16)

date 2020-07-16 22:02:43

3.1 OMNIBUS INPUT FILE CONTENTS

Each of the top-level blocks (and the overall problem input file) are described here.

database **`[COMP]`**

Composition options and definitions. See [COMP] (page 106).

Default (empty database)

database **`[DENOVO]`**

Denovo solver options. See [DENOVO] (page 176).

Applicable when

- ‘Denovo’ is enabled in this build; and
- solver is ‘denovo’

database **`[DEPLETION]`**

ORIGEN nuclide depletion options. See [DEPLETION] (page 212).

Applicable when

- 'depletion' is enabled in this build; and
- solver is 'depletion'

deprecated `geometry`
: Deprecated entry `geometry` has been renamed to `model`.

Update to model

database `[HYBRID]`
: Monte Carlo acceleration method. See [HYBRID] (page 224).

Applicable when problem mode is `hybrid`

database `[MODEL]`
: Representation of geometry and compositions. See [MODEL] (page 43).

database `[OUTPUT]`
: Output options. See [OUTPUT] (page 39).

Default (empty database)

sublist `[PHYSICS]`
: Physics treatment. See [PHYSICS] (page 85).

Default void physics when in mode `raytrace`

database `[POST]`
: Post-processing options. See [POST] (page 229).

Default (empty database)

database `[PRE]`
: Pre-processing options. See [PRE] (page 227).

Default (empty database)

database `[PROBLEM]`
: Problem identifiers and mode. See [PROBLEM] (page 27).

sublist `[RESPONSE]`
: Tally responses. See [RESPONSE] (page 111).

Applicable when

- using Shift, or in adjoint mode with `adjoint_source tally`; and
- solver is 'shift'

Default (empty sublist)

database `[RUN]`
: Execution parameter. See [RUN] (page 29).

Default (empty `none` database)

database `[SHIFT]`
: Shift Monte Carlo solver options. See [SHIFT] (page 167).

Applicable when

- 'Shift' is enabled in this build; and
- solver is 'shift'

parameter **`solvers`***(advanced)*

List of solvers being used.

Default based on presence of Shift/Denovo

Type list in which each element is a string

sublist **`[SOURCE]`**

Particle source definition. See [SOURCE] (page 56).

Default model-defined source if applicable, or global fission for kcode

Applicable when using Shift, in forward mode, or in adjoint mode with `adjoint_source source`

postprocessor

Only a single 'sourcerer' source may be present.

Applicability solver is 'shift'

Applicability solver is 'denovo'

Applicability problem mode is `kcode`

database **`[TALLY]`**

Tallies and Monte Carlo diagnostics. See [TALLY] (page 113).

Default (empty database)

Applicable when using Shift, or in adjoint mode with `adjoint_source tally`

3.2 PROBLEM ATTRIBUTES: [PROBLEM]

The problem database specifies top-level information about the problem being run. It includes the output file name, a unique problem identifier, and the overall solution technique.

parameter **`adjoint_source`**

Which block to use to construct adjoint source.

Choose whether a cell or mesh tally from the [TALLY] block or a manually defined source from the [SOURCE] block is used as an adjoint source. Currently there are a number of limitations on using tallies as adjoint sources.

Warning: Creating an adjoint source from tallies is experimental: the adjoint source strength and spectrum may unexpected, or the particular type of selected tally might not be implemented. Contact the developers to find out if the latest capabilities meet your needs.

Default `source`

Type `source` or `tally`

Applicable when `mode` is `adjoint`

parameter **`mode`**

Problem mode.

Valid modes are:

kcode Solve the *k*-eigenvalue problem for criticality safety or reactor physics analysis.

forward Solve a fixed-source problem for shielding calculations, etc.

adjoint Solve an adjoint fixed-source problem with the [SOURCE] or [TALLY] block interpreted as adjoint source (see adjoint_source (page 27)). Only Denovo can run adjoint problems.

raytrace Use the Denovo ray tracer to generate discretized materials for the problem. No transport will be performed.

hybrid Run a forward transport problem in Shift using deterministic acceleration.

Type `adjoint`, `forward`, `hybrid`, `kcode`, or `raytrace`

parameter **`name`**

Descriptive problem name.

Default `Untitled`

Type string

parameter **`num_threads`**

Number of OpenMP threads per process.

Currently, only Shift transport supports multithreading. Denovo solution time will not be affected by increasing the number of threads.

Default `1`

Type positive integer

Applicable when ‘OpenMP’ is enabled in this build

preprocessor (advanced)

Ignore manual input of pid, rev.

parameter **`pid`***(advanced)*

Unique identifier automatically set for this problem run.

The problem identifier (pid) is a unique string generated by the Omnibus pre-processor to ensure that input and output files are properly correlated. The problem ID value added to the XML input file is copied to all HDF5 output files. It is comprised of the problem execution date and a randomly generated unique identifier string (UUID).

Default unique problem identifier

Type string

parameter **`scale_rev`***(advanced)*

SCALE source revision used to generate this file.

Default current Exnihilo revision

Type integer

parameter `seed`

Random number generator seed.

The random number generator seed is used for multiple parts of both Denovo and Shift runs:

- Shift particle sourcing and transport
- Denovo uncollided flux (if the MC option is enabled)
- Denovo material ray tracing (if not using the `rays_deterministic` option)
- Denovo source point sampling

Default `2272013`

Type non-negative integer

3.3 EXECUTION: [RUN]

The [RUN] database enables support for running the Omnibus executable with the omnibus-run (page 15) command. The auto-run feature will format and echo program output to the screen, and it automatically saves the output and error streams to disk.

If the `SCALE` and `DATA` environment variables are not set, `omnibus-run` will use the values determined at configuration time.

Table 3: Available types for the [RUN] database

Type	Description	Applicability
none (page 29)	Do not run; only perform pre-processing	
serial (page 29)	Run on a single CPU core	
mpi (page 30)	Run on multiple cores by directly calling MPI	'MPI' is enabled in this build
pbs (page 30)	Run by submitting a PBS job	'MPI' is enabled in this build
cray (page 34)	Run on Cray supercomputers	'MPI' is enabled in this build
titan	Alias to `cray` type	—

3.3.1 [RUN=NONE]

Do not run; only perform pre-processing.

3.3.2 [RUN=SERIAL]

Run as a serial process on the local machine, echoing output to the user. If the `omnibus-run` process is aborted, the `omnibus` command will also abort.

parameter `hostname`*(advanced)*

Cluster name for automatically determining processor options.

Default based on hostname or PBS_O_HOST environment

Type `__unknown__`, `apollo`, `cades`, `eos`, `excalibur`, `falcon`, `falcon2`, `oic`, `poseidon2`, `remus`, `romulus`, or `titan`

parameter `omnibus`*(advanced)*

Path to the Omnibus executable.

Default `'/.../omnibus'`

Type file path for reading

3.3.3 [RUN=MPI]

Run as an MPI process on the local machine, echoing output to the user. If the `omnibus-run` process is aborted, the `mpirun omnibus` command will also abort.

parameter **`hostname`***(advanced)*

Cluster name for automatically determining processor options.

Default based on hostname or PBS_O_HOST environment

Type `__unknown__`, `apollo`, `cades`, `eos`, `excalibur`, `falcon`, `falcon2`, `oic`, `poseidon2`, `remus`, `romulus`, or `titan`

parameter **`mpiexec`***(advanced)*

Path to the MPI run command.

Default `'/.../mpiexec'`

Type file path for reading

parameter **`mpiexec_args`**

MPI execution arguments passed to mpiexec.

Default Based on CMake configuration and value for `np`

Type list in which each element is a string

parameter **`np`**

Number of processors to run.

Default `PBS_NP` if inside a PBS session

Type positive integer

parameter **`omnibus`***(advanced)*

Path to the Omnibus executable.

Default `'/.../omnibus'`

Type file path for reading

3.3.4 [RUN=PBS]

Create a PBS run file for this job. An example of a typical PBS run block is

```
[RUN=pbs]
nodes    1
ppn      16
pmem     7900mb
walltime "24:00:00"
```

If the `omnibus-run` command is aborted while the job is run, the job **will not** be automatically aborted. The `qdel` command must be invoked independently to abort the job.

The `cpp` option specifies the number of cores to be used by each MPI task: `cpp 2` will use half the cores available on the node. Alternatively, the number of processors per node can be set using the `ppn` parameter. The product of these two parameters cannot exceed the number of cores available on a compute node.

Additionally, the number of total MPI tasks used to run Exnihilo can be reduced below the requested number of nodes and cores with the `np` option, which has a default based on the number of requested nodes and cores. Adjusting this parameter may be necessary if, for example, Shift is to be decomposed into a non-power-of-2 number of blocks.

parameter **`account`**
: Account number to charge for time (e.g., NFI000, NSED).

  Default based on hostname

  Type string

parameter **`attributes`**
parameter **`attr`**
: key=value pairs for PBS attributes (`-W` argument).

  Default based on hostname

  Type list in which each element is a string

parameter **`bind`**
: Bind processes to hardware tasks.

  Type boolean

postprocessor
: Ensure that the layout is consistent with the host cluster.

  Applicability Host cluster has been detected or specified

parameter **`cpp`**
: Number of cores to assign to each process.

  Type positive integer

parameter **`detach`**
: Simply submit the job and to not follow it.

  Default `False`

  Type boolean

parameter **`email`**
: Email address of recipient.

  Default result of `git config author.email` (optional)

  Type string

parameter **`environ`**
: Environment variables to export in the PBS script.

  Default `---`

  Type list of variables (each element is a string without special characters)

parameter **`extra_cmds`**
: Extra commands to run at the beginning of the PBS script.

  Default `---`

  Type list in which each element is a string

parameter **`hold`**
: Set jobs to 'hold' status when submitting.

Default `False`

Type boolean

Applicable when `detach` is `True`

parameter **`hostname`***(advanced)*
Cluster name for automatically determining processor options.

Default based on hostname or PBS_O_HOST environment

Type `__unknown__`, `apollo`, `cades`, `eos`, `excalibur`, `falcon`, `falcon2`, `oic`, `poseidon2`, `remus`, `romulus`, or `titan`

parameter **`join`**
Output joining flags.

Default `oe`

Type string

parameter **`modules`**
Modules to load at the beginning of the script execution.

Default based on hostname

Type list in which each element is a string

parameter **`mpiexec`***(advanced)*
Path to the MPI run command.

Default `'/.../mpiexec'`

Type file path for reading

parameter **`mpiexec_args`**
MPI execution arguments passed to mpiexec.

Default Based on host layout

Type list in which each element is a string

parameter **`name`**
Job name.

Default base name of problem input file

Type string without special characters

parameter **`node_kw`***(advanced)*
PBS keyword to specify the number of nodes.

Default usually ‘nodes_ppn,’ but ‘nodes’ on Titan and ‘select’ on others

Type `nodes_ppn`, `nodes`, or `select`

preprocessor (advanced)
Automatically determine the layout from the host and the given arguments.

parameter **`nodes`**
Number of compute nodes to use.

Type positive integer

parameter **`np`**

Total number of MPI processes.

Type positive integer

parameter **`omnibus`***(advanced)*

Path to the Omnibus executable.

Default `'/.../omnibus'`

Type file path for reading

parameter **`pmem`**

Amount of memory per reserved processor (e.g., '7900mb').

Optional

Type string

parameter **`ppn`**

Number of processes to execute on each node.

Type positive integer

parameter **`project`**

Project name used in the -*P* flag.

Default based on hostname

Type string

parameter **`qdel`**

PBS deletion command or path.

Default `qdel`

Type string

parameter **`qos`**

PBS job classification option.

Default based on hostname and job specs

Type string

parameter **`qstat`**

PBS status command or path.

Default `qstat`

Type string

parameter **`qsub`**

PBS submission command or path.

Tip: To generate a PBS file but not actually submit or hold it, set qsub to "echo", and set `detach true`. With these two options, no PBS commands will be invoked.

Default `qsub`

Type string

parameter **`queue`**
parameter **`q`**
Queue to use.

Optional

Type string

parameter **`walltime`**
Wall time limit.

Note: It is common to have colons as part of the wall time. Since colons must be escaped in Omnibus ASCII input, the `walltime` input parameter will typically need escaping:

```
[RUN=pbs]
walltime "24:00:00"
```

Type `hh:mm:ss` or `mm:ss` or number of seconds

parameter **`when_email`**
When to email.

Default `ea`

Type string

Applicable when Email is present

3.3.5 [RUN=CRAY]

Create a PBS file for this job to run on Cray machines. An example PBS run block is:

```
[RUN=cray]
nodes    1024
ppn      16
account  nfi000
walltime "12:00:00"
```

Just like with PBS, if the `omnibus-run` command is aborted while the job is run, the job **will not** be automatically aborted. The `qdel` command must be invoked independently to abort the job.

If the number of cores is less than or equal to 8 (the number of “shared core units”), the `-j 2` option will automatically be appended to stride the cores by 1.

parameter **`account`**
Account number to charge for time (e.g., NFI000, NSED).

Default based on hostname

Type string

parameter **`aprun`***(advanced)*

Path to the aprun command.

> **Default** `'/.../mpiexec'`
>
> **Type** file path for reading

parameter **`attributes`**
parameter **`attr`**

key=value pairs for PBS attributes (`-W` argument).

> **Default** based on hostname
>
> **Type** list in which each element is a string

parameter **`bind`**

Bind processes to hardware tasks.

> **Type** boolean

postprocessor

Ensure that the layout is consistent with the host cluster.

> **Applicability** Host cluster has been detected or specified

parameter **`cpp`**

Number of cores to assign to each process.

> **Type** positive integer

parameter **`debug`**

Show the aprun layout.

> **Default** `False`
>
> **Type** boolean

parameter **`detach`**

Simply submit the job and to not follow it.

> **Default** `False`
>
> **Type** boolean

parameter **`email`**

Email address of recipient.

> **Default** result of `git config author.email` (optional)
>
> **Type** string

parameter **`environ`**

Environment variables to export in the PBS script.

> **Default** `---`
>
> **Type** list of variables (each element is a string without special characters)

parameter **`extra_cmds`**

Extra commands to run at the beginning of the script.

Default `'ulimit -c unlimited' 'export ATP_ENABLED=1'`

Type list in which each element is a string

parameter **`hold`**

Set jobs to 'hold' status when submitting.

Default `False`

Type boolean

Applicable when `detach` is `True`

parameter **`hostname`***(advanced)*

Cluster name for automatically determining processor options.

Default based on hostname or PBS_O_HOST environment

Type `__unknown__`, `apollo`, `cades`, `eos`, `excalibur`, `falcon`, `falcon2`, `oic`, `poseidon2`, `remus`, `romulus`, or `titan`

parameter **`join`**

Output joining flags.

Default `oe`

Type string

parameter **`mem`**

Memory required per MPI task (with G/M/K extension).

Default `''`

Type string

parameter **`modules`**

Modules to load at the beginning of the script execution.

Default based on hostname

Type list in which each element is a string

parameter **`name`**

Job name.

Default base name of problem input file

Type string without special characters

parameter **`node_kw`***(advanced)*

PBS keyword to specify the number of nodes.

Default usually 'nodes_ppn,' but 'nodes' on Titan and 'select' on others

Type `nodes_ppn`, `nodes`, or `select`

preprocessor (advanced)

Automatically determine the layout from the host and the given arguments.

parameter **`nodes`**

Number of compute nodes to use.

Type positive integer

parameter `np`

Total number of MPI processes.

Type positive integer

parameter `omnibus`*(advanced)*

Path to the Omnibus executable.

Default `'/.../omnibus'`

Type file path for reading

parameter `pin_system`

Pin system tasks to a single CPU core.

Default True if not using all cores on a node

Type boolean

Applicable when `hostname` is `titan` or `eos`

parameter `place`

How to distribute jobs on the node.

Default `'scatter:excl'`

Type string

Applicable when `hostname` is `excalibur`

parameter `ppn`

Number of processes to execute on each node.

Type positive integer

parameter `project`

Project name used in the *-P* flag.

Default based on hostname

Type string

parameter `qdel`

PBS deletion command or path.

Default `qdel`

Type string

parameter `qos`

PBS job classification option.

Default based on hostname and job specs

Type string

parameter `qstat`

PBS status command or path.

Default `qstat`

Type string

parameter **`qsub`**
PBS submission command or path.

Default `qsub`

Type string

parameter **`queue`**
parameter **`q`**
Queue to use.

Optional

Type string

parameter **`shared_gpu`**
Allow all processes to access GPU.

Default True when running Denovo on Titan

Type boolean

parameter **`tasks_per_unit`**
Number of processors/hwthreads to use per core unit.

Controls either the number of integer cores used per compute unit or hyperthreading.

Default based on CPUs per node

Type non-negative integer

deprecated **`threads_per_task`**
Deprecated entry `threads_per_task` has been renamed to `cpp`.

Update to cpp

parameter **`walltime`**
Wall time limit.

Type `hh:mm:ss` or `mm:ss` or number of seconds

parameter **`when_email`**
When to email.

Default `ea`

Type string

Applicable when Email is present

3.4 OUTPUT OPTIONS: [OUTPUT]

Omnibus, Denovo, and Shift are used on a multitude of platforms and system configurations and are run at many scales, ranging from single-CPU jobs that produce very little output to 300k-core jobs with hundreds of gigabytes of output. When large amounts of data are written to disk, the I/O performance of HDF5 (the output format used by Omnibus) can make a dramatic difference in write time.

Like Exnihilo, HDF5 supports both desktop and supercomputer platforms. HDF5 also supports a feature found on many larger computational clusters: a parallel file system (PFS). Unlike a networked file system (NFS), in which a file is mirrored or mounted over a network, and updates on one computer will be seen on the remainder of the network, a PFS actually supports writing to and reading from a file concurrently from multiple compute nodes. An example of a PFS is Lustre, on which files are decomposed across multiple separate hard disks. The more disks that a file is stored on, the higher the peak theoretical I/O bandwidth.

Warning: HDF5 will perform *extremely* poorly when writing in parallel to an NFS drive. (Factor-of-100 slowdowns have been seen.) Install the psutil[12] python package to allow Omnibus to detect and warn about the file system being written to.

HDF5 can be compiled using MPI to enable "collective" operations, in which each application process can write a subset of the data (e.g., the locally KBA-decomposed Denovo mesh) to a file, and HDF5 will combine the data into a single file automatically. If the HDF5 implementation being used is compiled correctly (for example, configured with `--with-io-romio-flags="--with-file-system=nfs+ufs+lustre"`), it will be able to interface with the parallel file system and change the file layout when a new HDF5 file is created.

The file layout (number of aggregators and chunk size) is system- and output-dependent; its performance[13] is tightly coupled to low-level HDF5 parameters, as well. Omnibus attempts to choose the output parameters for some known systems; a lustre (page 42) command is available to change the stripe and aggregator size and to update the HDF5 chunk size to match.

Since parallel HDF5 is not installed on (or performant on) all systems, Exnihilo implements its own collective operations for domain-decomposed data. With this "pseudo-parallel" mode, data from each domain are sent sequentially to processor 0 and then are written out using serial HDF5 calls. The disable_parallel_hdf5 (page 39) option forces this alternative implementation to be enabled, even if HDF5 is available.

When parallel HDF5 is enabled (and the problem is being run on more than one process), a second output file with the extension `-parallel.h5` will be created for collective operations. The created fields (such as Denovo flux and depletion number densities) will be linked into the main HDF5 file using the "external link" feature of HDF5, so *only* the main *.h5* file should ever need to be opened, although both files will need to be retained.

parameter **`disable_parallel_hdf5`***(advanced)*

Disable MPI-I/O and write only from a single process.

Default True unless the file system is parallel

Type boolean

Applicable when 'PARALLEL_HDF5' is enabled in this build

[12] http://pythonhosted.org/psutil/

[13] https://support.hdfgroup.org/pubs/papers/howison_hdf5_lustre_iasds2010.pdf

postprocessor
Disallow parallel HDF5 compatibility with non-PFS.

Applicability 'PARALLEL_HDF5' is enabled in this build; `disable_parallel_hdf5` is `False`; and the problem run is parallel

Applicability `file_system` is `__unknown__`, `nfs`, `nfs3`, `nfs4`, `hfs`, `ntfs`, `ext3`, `ext4`, `tmpfs`, `sysfs`, `btrfs`, `hugetlbfs`, `apfs`, or `xfs`

parameter **`display_counter`***(advanced)*
Write terminal commands for an interactive counter.

Default True if `stderr` is a terminal display

Type boolean

Applicable when The 'tqdm' python package is installed

parameter **`file_system`***(advanced)*
parameter **`fs`***(advanced)*
File system type where output is being written.

Default Based on output of the `mount` command

Type `__unknown__`, `__parallel__`, `lustre`, `panasys`, `nfs`, `nfs3`, `nfs4`, `hfs`, `ntfs`, `ext3`, `ext4`, `tmpfs`, `sysfs`, `btrfs`, `hugetlbfs`, `apfs`, or `xfs`

postprocessor
Disallow NFS output if a PFS is available.

Applicability 'PARALLEL_HDF5' is enabled in this build

Applicability the problem run is parallel

Applicability `file_system` is `__unknown__`, `nfs`, `nfs3`, `nfs4`, `hfs`, `ntfs`, `ext3`, `ext4`, `tmpfs`, `sysfs`, `btrfs`, `hugetlbfs`, `apfs`, or `xfs`

parameter **`hdf5_alignment`***(advanced)*
Alignment threshold and alignment value for HDF5.

Default `0 0`

Units B

Type list in which each element is a non-negative integer

Applicable when

- 'PARALLEL_HDF5' is enabled in this build; and
- `disable_parallel_hdf5` is `False`; and
- the problem run is parallel

parameter **`hdf5_chunk`***(advanced)*
Target size of HDF5 chunks; chunks will be this size or smaller.

Default `65536`

Units B

Type positive integer

preprocessor (advanced)

Set default Lustre striping based on `hostname`.

Applicability 'PARALLEL_HDF5' is enabled in this build

Applicability `disable_parallel_hdf5` is `False`

Applicability the problem run is parallel

parameter **`hdf5_mpiinfo_key`***(advanced)*

`MPI_Info` keys for parallel HDF5 file creation.

Default `---`

Type list in which each element is a string

Applicable when

- 'PARALLEL_HDF5' is enabled in this build; and
- `disable_parallel_hdf5` is `False`; and
- the problem run is parallel

parameter **`hdf5_mpiinfo_value`***(advanced)*

`MPI_Info` values for parallel HDF5 file creation.

Default `---`

Type list in which each element is a string

Applicable when

- 'PARALLEL_HDF5' is enabled in this build; and
- `disable_parallel_hdf5` is `False`; and
- the problem run is parallel

postprocessor

The parameters `hdf5_mpiinfo_key` and `hdf5_mpiinfo_value` must have the same length.

Applicability 'PARALLEL_HDF5' is enabled in this build

Applicability `disable_parallel_hdf5` is `False`

Applicability the problem run is parallel

parameter **`log_memory`***(advanced)*

Periodically print memory usage to screen.

Default True if using Denovo

Type boolean

parameter **`log_timestamp`**

Prepend a timestamp with this format to each log message.

The formatting for a time stamp is the standard strftime[14] formatting. For example, a value of `[%H:%M:%S]` may produce a log message that looks like:

[14] https://en.cppreference.com/w/cpp/chrono/c/strftime

```
>>> [11:29:43] Time-stamped message
```

Optional

Type string

parameter **`log_verbosity`**
Minimum level of output to save to log file.

Default `info`

Type `debug`, `diagnostic`, `status`, `info`, `warning`, `error`, or `critical`

command **`lustre`**
Set stripe size, aggregator, and HDF5 chunk size [kB, #].

Creates hdf5_mpiinfo_key

Creates hdf5_mpiinfo_value

Creates hdf5_alignment

Creates hdf5_chunk

Applicable when `file_system` is `__unknown__`, `__parallel__`, `lustre`, or `panasys`

parameter **`output`***(advanced)*
Destination path for the HDF5 output file.

Default *`input`*`.out.h5`

Type file path to write (extension '.h5')

parameter **`output_parallel`***(advanced)*
Destination path for parallel HDF5 output.

Default *`input`*`.out-parallel.h5`

Type file path to write (extension '.h5')

Applicable when

- 'PARALLEL_HDF5' is enabled in this build; and
- `disable_parallel_hdf5` is `False`; and
- the problem run is parallel

deprecated **`print_memory`**
Deprecated entry `print_memory` has been renamed to `log_memory`.

Update to log_memory

parameter **`screen_verbosity`**
Minimum level of output to print to screen.

Default `diagnostic`

Type `debug`, `diagnostic`, `status`, `info`, `warning`, `error`, or `critical`

3.5 MODEL DEFINITION: [MODEL]

We define a *model* as the answer to the question: "What is where?" A model can include compositions, spatial geometry, and even sources and tallies. As a radiation transport *framework*, Exnihilo supports model definitions in several formats.

Every model contains a geometry that can be discretized and solved using Denovo with the built-in ray tracer, and most models can also be used by the Shift Monte Carlo code. Furthermore, material definitions can be converted to multigroup cross sections through the SCALE cross section processing libraries or mixed into multigroup cross sections input in ANISN formats.

Table 4: Feature matrix for the supported models.

Model	Denovo	Shift	Compositions	Sources	Tallies
DAGMC	Yes	Yes	—	—	—
Geant4	Yes	*No*	Yes	—	—
Geometria	Yes	Yes	—	—	—
MCNP	Yes	Yes	Yes	Yes	*No*
Mesh	Yes	Yes	—	Yes	—
RTK	Yes	Yes	—	—	—
SCALE	Yes	Yes	Yes	*No*	*No*
SWORD	Yes	*No*	Yes	Yes	Yes
VERA	Yes	Yes	—	—	—

If using Shift to obtain volume-averaged reaction rates in geometric cells, the volume of the cells must be obtained *a priori*. Some models support automatic calculation a subset of cells; only Reactor ToolKit input: [MODEL=rtk] (page 53) supports automatic calculation of all cell volumes due to the restricted simple nature of the geometry. For all other models, the cell volumes can be manually specified with the "volumes" and "volume_cells" keywords:

```
volumes       1.0 2.34  0.5
volume_cells  1   200   15
```

Here, the cells are the "cell labels" (e.g., the cell card IDs in MCNP) and the volumes are the corresponding volumes in cm^3. The volumes are used only in the normalization of tallies, including depletion tallies.

3.5.1 MATERIAL AND CELL IDS

The model internally defines vectors of "matids" and "cellids" that correspond to user-defined material names and cell labels. Although Omnibus attempts to make these internal identifiers invisible to the user, an occasional advanced option or low-level error message may include references to these.

The material ID is simply the index into the list of compositions (page 106) in the problem; these are written to the `comp/compositions` dataset in the Omnibus output file. Note that for the MCNP model (page 44), these are *usually not* the user-assigned `m` label.

Cell IDs correspond to identifiable user-created spatial regions in the problem. If arrays or universes are used, a single cell ID might correspond to multiple regions in space. Cell IDs are not written to the output file because

- cells are typically much more numerous than materials;

- some models such as RTK do not have user-provided identifiers for cells; and
- some models such as Geometria reserve cell IDs as implementation details, so some cell IDs correspond to no physical point in space.

User-provided labels corresponding to cell and material IDs can both be obtained without having to run the Omnibus executable. The following snippet uses the Python bindings (page 2) to print the meanings of all matids and cellids in the model:

```python
from omnibus.raytrace.load import load_mcnp
model = load_mcnp('ueki.runtpe')
print("Materials:")
print("\n".join("  {:3d} -> {:s}".format(c.compid, c.name)
                for c in model.compositions))
print("Cells:")
print("\n".join("  {:3d} -> {:s}".format(i, geo.cell_to_label(i))
                for i in range(geo.num_cells)))
```

Table 5: Available types for the [MODEL] database

Type	Description	Applicability
mcnp (page 44)	MCNP model definition	'Lava' is enabled in this build
scale (page 50)	SCALE KENO input file	'SCALE_GEO' is enabled in this build
geometria (page 52)	Geometria input definition	'GG' is enabled in this build
gg	Alias to `geometria` type	—
rtk (page 53)	RTK input specification	
mesh (page 53)	Explicit meshed problem in HDF5 format	'HDF5' is enabled in this build
geant (page 54)	Geant4 GDML model input	'Geant' is enabled in this build
sword (page 54)	SWORD model description	'SWORD' is enabled in this build
dagmc (page 55)	DAGMC CAD geometry definition	'DAGMC' is enabled in this build
vera (page 56)	VERA input specification	'VERA' is enabled in this build

3.6 MCNP INPUT: [MODEL=MCNP]

Exnihilo supports reading MCNP [18] input files through ORNL's Lava library [7]. The user's MCNP input file must be processed through MCNP using the `mcnp5 ix inp={inp}` command in order to generate the `runtpe` file that Lava requires. The Omnibus pre-processor does this automatically.

Note: If using Shift cell tallies with an MCNP model, the user must include a cell tally or input volumes for desired cells *in the MCNP input* to ensure that volumes to automatically be propagated into Shift.

3.6.1 FEATURES

- Any MCNP5-compatible geometry is supported.
- MT cards for the materials are automatically converted to their equivalent SCALE IDs, so for example `6000` with a corresponding `grph` card will be converted to the SCALE ID for graphite, `3006000`.
- In depletion calculations, groups of axis-aligned planes can be moved at each time step without restarting (see [MODEL][MOVABLE=surfaces] (page 50))
- SDEF sources can be transported with Shift using the [SOURCE=mcnp] (page 61) source definition.

3.6.2 LIMITATIONS

- MCNP6 is not supported; MCNPX will not be supported.
- Library suffixes for nuclides in the material block are *ignored*: only the `TMP` (temperature) card on each cell is used to determine the composition temperature. The composition temperature is then used when loading CE nuclides.
- Tally definitions are ignored.
- MCNP sources cannot be automatically biased in hybrid modes.
- Only MT cards natively supported by MCNP5 will be interpreted as chemically bound elements.

3.6.3 NAMING

Geometry cell names are the same as the numerical cell "names" given in the cell block of the MCNP input. Unlike MCNP, which can tally a single *instance* of a cell that is present in different arrays or universes with a special input such as *2>4>1*, Shift will lump all instances of a cell into the same tally.

Most material compositions processed from MCNP have the form `mNNN`, where `NNN` is the material name specified on the `m` card. However, if the material is present in the cell definition block at multiple densities and/or temperatures, multiple copies of the composition will be present. Lower-density compositions will have the form `mNNN (FF.F%)`, where `FF.F` is the percentage mass density compared to the highest-density instance of the material.

3.6.4 NUCLIDE MAPPING

Exnihilo implements a number of hard-coded mappings to convert both bound and unbound MCNP nuclides to their equivalent IDs in SCALE. The following translations are performed for unbound nuclides:

Table 6: Mappings between unusual nuclide IDs.

MCNP ID	SCALE ID
1001	8001001
1002	8001002
27458	1027058
47510	1047110
48515	1048115
52527	1052127
52529	1052129
61548	1061148
67566	1067166
95642	95242
95242	1095242
95644	1095244

The MT cards in MCNP input mark that atoms in the material are chemically bound, so a $S(\alpha,\beta)$ collision kernel for thermal energies is to be applied. In SCALE, individual nuclides are marked as having bound collision data, so the following nuclides in bound materials in MCNP are translated to special SCALE IDs:

Table 7: Mappings between MCNP MT cards and SCALE IDs.

MTn	ZAID	SCALE ID
al27	13027	1013027
be	4009	3004009
be/o	4009	5004009
benz	1001	6001001
	6000	5006000
	6012	5006000
beo	4009	3004009
	8016	8016
dortho	1002	4001002
dpara	1002	5001002
fe56	26056	1026000
grph	6000	3006000
	6012	3006000
h/zr	1001	7001001
hortho	1001	4001001
hpara	1001	5001001
hwtr	1002	1002
lmeth	1001	1001001
lwtr	1001	1001
o/be	8016	5008016
	8017	8017
	8018	8018
o2/u	8016	1008016
	8017	8017
	8018	8018
poly	1001	9001001
sio2	14028	1014028
	14029	1014029
	14030	1014030
smeth	1001	2001001
u/o2	92238	92238
zr/h	40000	1040090
	40090	1040090
	40091	1040091
	40092	1040092
	40094	1040094
	40096	1040096

command **`autoname`**

Attempt to provide MCNP material names using their compositions.

The `autoname` command is an experimental tool that loads the MCNP runtpe file into memory using the Exnihilo Python bindings (page 2) and uses the MCNP-defined compositions to construct a "best guess" of their name based on their most abundant elements.

Tip: After `autoname` has been run once, a user can extract the created names from the `*PROBLEM*.inp.omn` file created in the run directory, replace the `autoname` command with those names, and modify them as desired.

Creates mat_names

Creates mat_name_mno

parameter **`cell_raytrace`**

Transform cell labels into material IDs for raytracing.

Default `False`

Type boolean

Applicable when problem mode is `raytrace`

parameter **`extents`**

Bounding box for the active region of the geometry.

Setting the model boundary enables certain Exnihilo features that require "global" boundaries. These include:

- Global mesh tallies
- Global initial fission source
- Automatic Shannon entropy mesh
- MCNP source discretization for Denovo

Default `-1e+100 1e+100 -1e+100 1e+100 -1e+100 1e+100`

Type locations for -X,+X,-Y,+Y,-Z,+Z (each element is a real number)

command **`input`**

Generate an MCNP runtpe file and set `runtpe_path`.

This command uses the version of MCNP configured with Exnihilo to generate a run tape. To change the cross section lookup directory `xsdir`, set the environment variable `DATAPATH` before running the Omnibus pre-processor. An informational message will acknowledge that the environment variable is being used in the particular MCNP run.

Tip: The MCNP executable path can be overridden by modifying the execution environment with the `-e env.json` argument to omnibus-run (page 15). Use a JSON environment file that looks like

```
{"cmake": {"MCNP_EXECUTABLE": "/path/to/mcnp5"}}
```

Creates runtpe_path

command **m**

Map 'mat_name_mno' to 'mat_names' from pairs or arrow-separated items.

Creates mat_name_mno

Creates mat_names

parameter **mat_name_mno**

MCNP material 'names' corresponding to the given mat_name override.

Default `---`

Type Integer material numbers in MCNP (each element is a positive integer (optional leading 'm'))

postprocessor

The parameters `mat_names` and `mat_name_mno` must have the same length.

parameter **mat_names**

parameter **mat_name**

Override names for materials in the geometry.

Custom names can be added to the model that will be reflected in material plots inside VisIT and inside post-processing data elements. MCNP material card numbers are specified alongside new names to use:

```
mat_name_mno :mat_names
    1   "sodium iodide"
    2   "carbon steel"
    13  polyethylene
    14  iron
    105 air
    106 concrete
```

Default `---`

Type list in which each element is a non-empty string

sublist **[MOVABLE]**

Geometry elements that can be modified during the simulation. See [MODEL][MOVABLE] (page 49).

Default (empty sublist)

database **[RAYTRACE]**

Volume calculation. See [MODEL][RAYTRACE] (page 49).

Optional

Applicable when problem mode is `raytrace`

parameter **runtpe_path** *(advanced)*

Path to the MCNP runtpe file.

Type file path for reading

parameter **volume_cells**

Cell labels corresponding to the given volume overrides.

Default `---`

Type list of cell labels (each element is a string)

postprocessor

The parameters `volumes` and `volume_cells` must have the same length.

parameter **`volumes`**

Provide or override volumes for cells in the geometry.

Default `---`

Units cm^3

Type list in which each element is a positive real number

3.6.5 [MODEL][MOVABLE]

Table 8: Available types for the [MOVABLE] database

Type	Description	Applicability
surfaces (page 50)	Movable surface group	

3.6.6 [MODEL][RAYTRACE]

Volume calculation.

parameter **`axes`**

Axis/axes along which to fire rays for ray trace.

Default `xyz`

Type axis or axes ('x','zy','xyz')

parameter **`error_tolerance`**

Fraction of lost rays to tolerate before aborting.

Default `1e-05`

Type real number inside (0, 1)

parameter **`max_local_warnings`**

Max number of lost ray warnings to print per domain.

Default `10`

Type non-negative integer

parameter **`num_batches`**

Number of batches to use for estimating variance.

Default `8`

Type positive integer

parameter **`ray_spacing`**

Average spacing between rays in each batch.

Units cm^3

Type positive real number

parameter **`rays_deterministic`**
Use face midpoints rather than stratified sampling.

Default `False`

Type boolean

parameter **`trace`**
Whether to trace materials or cell volumes.

Default `cell`

Type `mat` or `cell`

3.6.7 [MODEL][MOVABLE=SURFACES]

The "movable" surface option allows the translation of multiple surfaces simultaneously in the MCNP model. Currently this works only for simple axis-aligned planes.

Warning: Because translations and surface deduplication are applied while generating the runtpe file, moving one surface label may end up affecting other coincident surfaces. Exnihilo will raise an error during setup if this happens: the input deck will need to be modified to remove coincident planes or include all equivalent (coincident) surfaces in the surface group specification.

parameter **`initial`**
Movement to apply before the first transport.

Default `0.0`

Units cm

Type real number

parameter **`name`**
Name of the surface group.

Type string without special characters

parameter **`surfaces`**
List of MCNP surface labels to move over time.

Type list in which each element is a positive integer

3.7 SCALE INPUT: [MODEL=SCALE]

As an alternative to SCALE's CSAS-Shift sequence, the geometry and composition definitions from a SCALE input file can be processed and run through Omnibus. Any valid SCALE sequence inputs with a single GEOMETRY and COMPOSITION blocks can be transported on automatically.

Details on defining SCALE geometry inputs may be found in the SCALE manual [2].

3.7.1 FEATURES

- Supports KENO-V.a and KENO-VI geometry definitions, including geometries defined as part of a sequence (such as MAVRIC or CSAS-Shift).
- Supports all standard composition definitions.

3.7.2 LIMITATIONS

- Only the **GEOMETRY** and **COMP** data blocks from the SCALE input will be used. The sequence itself is ignored, as are all other blocks (such as parameters and plotting inputs). This *includes* cross section processing blocks: see Multigroup physics: [PHYSICS=mg] (page 96) for specifying the physics treatment through Omnibus.
- Only the *first* one of each of those blocks will be used. If multiple sequences are chained together in the input, all but the first will be ignored.

If no composition block is present, then the user must specify compositions separately; this advanced use case is outside the scope of the manual.

3.7.3 NAMING

For KENO-VI geometries, cell names take the form *`unit.instance`*, where "unit" is the integer unit number, and "instance" is the index of the media instance in the list of media for that unit.

Composition names are saved as `media N`, where `N` is the media number specified in the composition block.

3.7.4 GEOMETRY CONVENTIONS

The legacy geometry implementation in KENO differs from the new Geometria-powered implementation, which leads to confusingly different conventions that will hopefully be resolved. Until then, some of the differences are sketched out here.

- A *universe* in Geometria generally corresponds to a *unit* in SCALE. However, each instance of an array placed as a hole (in KENO-VI) is *also* a universe.
- Numbering in Geometria generally uses zero-based indexing, so the lower-left element in an array has coordinates `[0 0 0]` in the output.
- The "sense" of a surface or shape in Geometria generally takes the opposite sign of an input in a KENO region definition vector. See the [UNIVERSE][CELL] (page 244) section for more details.

parameter **`input`**

Path to the KENO VI input file.

Type file path for reading (extension '.inp')

database **`[RAYTRACE]`**

Volume calculation. See [MODEL][RAYTRACE] (page 49).

Optional

Applicable when problem mode is `raytrace`

parameter **`volume_cells`**

Cell labels corresponding to the given volume overrides.

Default `---`

Type list of cell labels (each element is a string)

postprocessor

The parameters `volumes` and `volume_cells` must have the same length.

parameter **`volumes`**

Provide or override volumes for cells in the geometry.

Default `---`

Units cm^3

Type list in which each element is a positive real number

3.8 GEOMETRIA INPUT: [MODEL=GEOMETRIA]

The Geometria (internally designated “GG”) geometry engine underpins the new SCALE geometry implementation. Geometria supports a less automatic but more rigorous geometry definition than KENO. Its input is an Omnibus-style problem definition (see Geometria Input Description (page 233)) that is translated to an XML file.

This input model only supports geometry definitions; compositions must be input either via an HDF5 input file or in a [COMP] block (page 106).

command `input`

Generate a Geometria XML representation from an `.gg.omn` input.

Creates xml_path

database `[RAYTRACE]`

Volume calculation. See [MODEL][RAYTRACE] (page 49).

Optional

Applicable when problem mode is `raytrace`

parameter `simplify_max_surfaces`*(advanced)*

Threshold for making a “complex” cell “simple.”

In the GG implementation, a “simple” cell is a cell in which crossing a boundary always causes a particle to leave a cell. (An example of a simple cell is the moderator region inside a square and outside a circle.) Some cells, however, have internal surface boundaries that can be crossed while remaining inside the cell. (An example of a “complex” cell is a square region with two non-overlapping squares excluded. Crossing one of the inner planes that comprise the squares does not necessarily put the particle inside the inner squares.) The bookkeeping for a particle inside these cells is more complicated than the simple cell, because all the distances along the particle’s path must be calculated and tracked, and every surface crossing requires the cell’s logic expression to be reevaluated to determine whether the particle is inside.

If a complex cell is erroneously treated as simple, tracking errors will result; so it is necessary to be conservative in initially calling a cell complex. In GG, a cell is assumed complex if it contains a “positive” shape in its definition (i.e., it is the “outside” of a shape). This has the unfortunate consequence of forcing the assumption that common simple shapes, such as a pin inside a pin cell, are in fact complex. The solution is a piece of code that checks a cell at construction time. It loops over all combinations of the surface IDs connected to the cell to determine if any surface crossing will allow a particle inside the cell to remain inside the cell:

- Fill the “surface sense” vector with the next combination of bits
- If the logic expression evaluates to “false,” skip this iteration
- Loop over every surface sense
  - Flip this surface’s sense
  - If the cell logic expression still evaluates to “true,” the cell is definitely complex. Return early.
  - Restore the flipped sense

The performance of the above loop scales exponentially with the number of surfaces connected to a cell. (If the cell only has two surfaces, 4 outer logic evaluations must be made; for four surfaces, 16 must be made; for ten surfaces, 1024 must be made.) Therefore, this parameter defaults to checking only cells composed of at most 10 surfaces. Testing results show that this has a negligible build-time penalty but can improve tracking time by almost a factor of two, as in the case of the C5G7 benchmark, in which each pin cell would be marked "complex" without this code.

Default `10`

Type integer in the range [0,16)

parameter **`volume_cells`**

Cell labels corresponding to the given volume overrides.

Default `---`

Type list of cell labels (each element is a string)

postprocessor

The parameters `volumes` and `volume_cells` must have the same length.

parameter **`volumes`**

Provide or override volumes for cells in the geometry.

Default `---`

Units cm^3

Type list in which each element is a positive real number

parameter **`xml_path`***(advanced)*

Path to the GG geometry XML input file.

Type file path for reading (extension '.xml')

3.9 REACTOR TOOLKIT INPUT: [MODEL=RTK]

RTK is an internal geometry engine used for PWR geometry under the VERA framework produced by CASL. The RTK model implemented by Omnibus reads a geometry from an XML input file. In general, the Insilico front-end should be used for creating reactors with RTK geometries.

parameter **`input`**

Path to the RTK geometry XML or HDF5 file.

Type file path for reading (extension '.xml' or '.h5')

3.10 BRICK MESH INPUT: [MODEL=MESH]

The "mesh" model type allows a discretized problem to be transported on in Denovo and Shift. It is defined by an external HDF5 file with a field of materials, mixtures, and (optionally) a source description. The file format's specification is described in HDF5 Mesh Model Specification (page B–4)

This file format is primarily intended for Denovo problems, both for analytical benchmarks and allowing the user to "restart" from a previously discretized geometry using the make-denovo-model (page 21) utility. Shift does not support mix tables or the source description.

parameter **`input`**

Path to the mesh geometry hdf5 file.

Type file path for reading (extension '.h5')

postprocessor

Check that the mesh model is in the correct format.

3.11 GEANT4 INPUT: [MODEL=GEANT]

Exnihilo supports Geant4 [15] inputs stored as GDML files. The materials and geometry are both read through Exnihilo.

Caution: Because Geant4 defines a number of nuclides that may be important to high-energy physics but that are not important to neutronics calculations, it may be necessary to use the `omit_zaid` and `orig_zaid`/`subs_zaid` options in the physics if those nuclides are not present on the cross section libraries.

3.11.1 LIMITATIONS

- Tracking particles in Shift is not supported. Currently, Geant4 can only be discretized in Denovo or ray-traced in Python.

parameter **`input`**
Path to the Geant4 GDML input file.

Type file path for reading (extension '.gdml')

database **`[RAYTRACE]`**
Volume calculation. See [MODEL][RAYTRACE] (page 49).

Optional

Applicable when problem mode is `raytrace`

parameter **`volume_cells`**
Cell labels corresponding to the given volume overrides.

Default `---`

Type list of cell labels (each element is a string)

postprocessor
The parameters `volumes` and `volume_cells` must have the same length.

parameter **`volumes`**
Provide or override volumes for cells in the geometry.

Default `---`

Units cm^3

Type list in which each element is a positive real number

3.12 SWORD INPUT: [MODEL=SWORD]

The SoftWare for Optimization of Radiation Detectors [8] interface requires files generated by the release (non-beta) version of SWORD 6.0 or higher, as only new versions write the problem's geometry and material definitions as Geant4 GDML files.

In addition to the geometry and material definitions, the SWORD model supports source definitions using [SOURCE=sword] (page 62) and can construct adjoint sources (tallies) using [TALLY][SWORD] (page 141).

3.12.1 LIMITATIONS

- Since SWORD's tracking engine is based on that of Geant (page 54), tracking particles in Shift is not supported. Only Denovo discretization and raytracing are supported.

command **`input`**

Generate a binary SWORD representation from a .sword input.

Creates xdr_path

parameter **`xdr_path`***(advanced)*

Path to the SWORD binary input file.

Type file path for reading (extension '.xdr')

3.13 DAGMC INPUT: [MODEL=DAGMC]

Direct Accelerated Geometry Monte Carlo (DAGMC) is a package in MOAB that has been integrated into Exnihilo to support CAD-based models. This package allows for Monte Carlo transport on complex 3D geometries that have been created by traditional solid modeling software. The model must be pre-processed so that the geometry is a faceted HDF5 file, and volumes must be tagged with specific properties.

Table 9: MOAB volume properties used in the DAGMC model.

Name	Description
mat	Material ID (must be an integer), or the value "graveyard".
label	Cell label, ignored for the graveyard volume.
implicit_mat	Specified only in the graveyard cell, the matid that will be given to cells marked as implicit complements.

There can only be a single graveyard cell, which will be given the cell label "EXTERIOR," and there can be multiple implicit complements, which all share the label "IMPLICIT_COMPLEMENT".

3.13.1 FEATURES

- Any faceted CAD geometry of varying complexity can be used.
- Reflecting boundaries are supported.

3.13.2 LIMITATIONS

- Labeling materials by name is not supported. Volumes in the geometry must be tagged with the corresponding material ID.
- Volumes without material labels will be given a matid of 0.
- The extents of the geometry must be an axis-aligned rectangular prism.

parameter **`input`**

Path to the MOAB facet file.

Type file path for reading (extension '.h5m')

parameter **`mat_input`**

Path to the material composition file.

Optional

Type file path for reading (extension '.h5')

database **[RAYTRACE]**
Volume calculation. See [MODEL][RAYTRACE] (page 49).

Optional

Applicable when problem mode is `raytrace`

parameter **`volume_cells`**
Cell labels corresponding to the given volume overrides.

Default `---`

Type list of cell labels (each element is a string)

postprocessor
The parameters `volumes` and `volume_cells` must have the same length.

parameter **`volumes`**
Provide or override volumes for cells in the geometry.

Default `---`

Units cm^3

Type list in which each element is a positive real number

3.14 VERA INPUT: [MODEL=VERA]

The model for a Virtual Environment for Reactor Applications (VERA) [9] XML input can be run through the Omnibus front end. The material compositions will be built from the model. Since the VERA geometry can only describe the geometry from the core out through the reactor vessel, the VERA input allows for an Omnibus input file defining the ex-core geometry to be specified. If this ex-core file is given, it will be included in the built geometry.

The [TALLY][VERA] (page 134) can be used to create a tally for the outermost region of the vessel. This tally can then be optimized for when running in hybrid mode.

parameter **`input`**
Path to the VERA XML input file.

Type file path for reading (extension '.xml')

3.15 PARTICLE SOURCE DEFINITIONS: [SOURCE]

The source database specifies the source particle distribution for a fixed-source problem, as well as the starting source for an eigenvalue problem. Any combination of types is allowed.

The total strength of all sources is used as a global multiplier for all tallies in fixed-source mode. (The total strength is ignored for the starting source in kcode mode; only the relative strengths of the sources are used.) An alternative to modifying the total source strength is to modify the `normalization` property of the tallies.

If using Shift with mode kcode, and no source is provided, the default source is a uniform source with global extents isotropically emitting neutrons with a U-235 watt spectrum. Since some geometry types cannot determine global extents by default (e.g., MCNP requires an `extents` keyword), be warned that this default may fail to sample enough particles in fissionable regions.

Table 10: Available types for the [SOURCE] database

Type	Description	Applicability
separable (page 57)	Source separable in space, energy, angle	
fissionmesh (page 59)	Fixed fission source from a Shift tally or mesh source	
mesh (page 61)	Discretized source from the mesh model HDF5 file	model is ‘mesh’ and solver is ‘denovo’
mcnp (page 61)	Source from MCNP SDEF cards	model is ‘mcnp’
sword (page 62)	SWORD source/spectra definitions	model is ‘sword’
material (page 63)	Volumetric material composition emission	
surface_census (page 64)	Emit particles from a pre-computed surface source	
sourcerer (page 65)	Use a Denovo solution as a fission source	solver is ‘shift’; solver is ‘denovo’; and problem mode is `kcode`

3.15.1 [SOURCE=SEPARABLE]

Exnihilo views the source particle type as being an extension of the energy phase space. This facilitates hybrid methods, since in deterministic solvers the neutron and photon groups are adjacent and treated identically, and it makes some source definitions (such as naturally emitting materials) more straightforward.

parameter `allow_biasing`
Enable source biasing for hybrid problem modes.

Default `False`

Type boolean

database `[ANGLE]`
Particle angular distribution. See [SOURCE][ANGLE] (page 66).

Default (empty `isotropic` database)

parameter `biased_distribution_sample_attempts`*(advanced)*
Number of distribution sampling attempts before abandoning the current cell/group phase space.

Default `1000000`

Type positive integer

parameter `biased_src_sample_attempts`*(advanced)*
Number of sampling attempts of a biased source before declaring a particle lost.

Default `10`

Type positive integer

parameter `cell_only`

parameter **`cell`**

Emit particles only in the given cells.

The `cell_only` criteria can be used in conjunction with `fissionable_only` and `material_only`, where it is combined using an **and** operation (i.e., emit particles in the given cells **and** in the given materials).

Optional

Type list in which each element is a string

parameter **`description`**
parameter **`desc`**

Optional longer descriptive string.

Default `''`

Type string

database **`[ENERGY]`**

Energy spectrum. See [SOURCE][ENERGY] (page 66).

Default Watt spectrum when in 'kcode' mode

parameter **`fissionable_only`**
parameter **`fis`**

Emit particles only in fissionable regions.

The `fissionable_only` criteria can be used in conjunction with `material_only` and `cell_only`, where it is combined using an **and** operation (i.e., emit particles in fissionable materials **and** in the given cells).

Default True if 'kcode' mode

Type boolean

parameter **`l2_error`**

Maximum requested source discretization L2 error.

Default `0.01`

Type real number inside (0, 1)

Applicable when using Denovo or hybrid

parameter **`material_only`**
parameter **`mat`**

Emit particles only in the given materials.

The `material_only` criteria can be used in conjunction with `fissionable_only` and `cell_only`, where it is combined using an **and** operation (i.e., emit particles in the given materials **and** in the given cells).

Optional

Type list in which each element is a non-empty string

parameter **`max_samples`**

Maximum number of point samples to use for discretization.

Default `10000000000.0`

Type positive integer

Applicable when using Denovo or hybrid

parameter **`name`**

Short title or label for the source.

Default type of the source database

Type string without special characters

parameter **`num_rejection_samples`**
parameter **`rej`**

How many samples to try before declaring a particle 'lost.'

Default `50000`

Type positive integer

parameter **`samples_per_batch`**
parameter **`batch_samples`**

Number of point samples per discretization batch.

Default `100000.0`

Type positive integer

Applicable when using Denovo or hybrid

database **`[SHAPE]`**

Spatial distribution type. See [SOURCE][SHAPE] (page 66).

parameter **`strength`**
parameter **`q`**

Source strength.

Default `1.0`

Units $\frac{\text{particle}}{\text{s}}$

Type positive real number

3.15.2 [SOURCE=FISSIONMESH]

The fission mesh source allows a fission neutron production mesh tally from a prior run (kcode or fixed source) to be used as a source. This source could either be a starting source in a kcode calculation (to reduce the number of inactive cycles needed) or a fixed source (so that a coupled neutron-gamma problem can be run separately from the kcode calculation). The `input` parameter points to the name of the `tallies.h5` file; and the `mesh_tally_name` parameter should be the name of the fission mesh tally.

By default, this source uses a U-235 energy spectrum.

parameter **`allow_biasing`**

Enable source biasing for hybrid problem modes.

Default `False`

Type boolean

parameter **`biased_distribution_sample_attempts`***(advanced)*
Number of distribution sampling attempts before abandoning the current cell/group phase space.

Default `1000000`

Type positive integer

parameter **`biased_src_sample_attempts`***(advanced)*
Number of sampling attempts of a biased source before declaring a particle lost.

Default `10`

Type positive integer

parameter **`cell_averaged`**
parameter **`avg`**
Whether the field values are volume-averaged strengths.

Type boolean

Applicable when `format` is `source`

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

preprocessor (advanced)
Default energy spectrum is U-235 Watt spectrum.

database **`[ENERGY]`**
Energy spectrum. See [SOURCE][ENERGY] (page 66).

Default Watt spectrum when in 'kcode' mode

parameter **`field`**
Path to the source definition in the input file.

Default 'strength' if cell-averaged, else 'pdf'

Type string

Applicable when `format` is `source`

parameter **`format`**
Format of hdf5 file.

Default `tally`

Type `source` or `tally`

parameter **`input`**
Name of file containing source distribution.

Type file path for reading (extension '.h5')

parameter **`name`**
Short title or label for the source.

Default type of the source database

Type string without special characters

parameter `num_rejection_samples`
parameter `rej`
How many samples to try before declaring a particle ‘lost.’

Default `50000`

Type positive integer

parameter `strength`
parameter `q`
Source strength.

Default `1.0`

Units $\frac{\text{particle}}{\text{s}}$

Type positive real number

parameter `tally_name`
Name of the fission source rate mesh tally.

Type string without special characters

Applicable when `format` is `tally`

3.15.3 [SOURCE=MESH]

This “mesh” source is specifically for manually constructed Denovo source strengths and multigroup spectra. To use a field of source strengths in Shift, use the mesh shape (page 76) as part of a separable source.

parameter `description`
parameter `desc`
Optional longer descriptive string.

Default `''`

Type string

parameter `name`
Short title or label for the source.

Default type of the source database

Type string without special characters

3.15.4 [SOURCE=MCNP]

The MCNP source uses the Lava library to extract and use the source definition from an `SDEF` card. It supports automatic interpretation of the particle type (defaulting to the problem mode) and the strength (from the `WGT` parameter) as well as the actual distributions themselves.

The MCNP biasing parameters will be respected when sampling this source. This also applies to creating a discrete Denovo source from an MCNP source: regions where the source is biased to emit more frequently will have better statistical estimates of the source. The weight is accounted for during discretization to ensure that the total source strength is correct as the number of source samples approaches infinity.

It is important to note that currently the MCNP source is *replicated* across processors when discretizing. This means that MCNP sources that encompass many cells, especially with a fine-group energy structure, may require more memory than an individual CPU core can allocate.

Note: Currently, the MCNP source is only available if the MCNP geometry is being used.

---

parameter **`description`**
parameter **`desc`**

Optional longer descriptive string.

Default `''`

Type string

parameter **`extents`**

Optional bounding box for MCNP source.

To allow for an MCNP source to be discretized in parallel, it is necessary to replicate the spatial mesh that overlaps the source. By default, this option replicates the entire spatial mesh. On large problems, fully replicating the entire mesh may cause the program to abort for lack of memory.

The solution is to manually define an axis-aligned bounding box that encloses the source region. Thus only the part of the mesh containing the source is replicated.

Tip: When the source discretization takes place, an informational message will print the 'actual' extents (based on sample particles) of the source bounding box. If the source boundaries are not readily available, it may be sufficient to discretize the source on a few-cell mesh problem and use the sampled extents (expanded by some fraction) as the bounding box for the full problem run.

Default `-1e+100 1e+100 -1e+100 1e+100 -1e+100 1e+100`

Type locations for -X,+X,-Y,+Y,-Z,+Z (each element is a real number)

parameter **`name`**

Short title or label for the source.

Default type of the source database

Type string without special characters

3.15.5 [SOURCE=SWORD]

This source option imports source descriptions from the SWORD input model. Currently, it only works with Denovo and is incompatible with other source definitions.

parameter **`allow_biasing`**

Enable source biasing for hybrid problem modes.

Default `False`

Type boolean

parameter **`biased_distribution_sample_attempts`***(advanced)*

Number of distribution sampling attempts before abandoning the current cell/group phase space.

Default `1000000`

Type positive integer

parameter **`biased_src_sample_attempts`***(advanced)*
Number of sampling attempts of a biased source before declaring a particle lost.

Default `10`

Type positive integer

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

parameter **`name`**
Short title or label for the source.

Default type of the source database

Type string without special characters

3.15.6 [SOURCE=MATERIAL]

Volumetric material composition emission.

parameter **`allow_biasing`**
Enable source biasing for hybrid problem modes.

Default `False`

Type boolean

parameter **`biased_distribution_sample_attempts`***(advanced)*
Number of distribution sampling attempts before abandoning the current cell/group phase space.

Default `1000000`

Type positive integer

parameter **`biased_src_sample_attempts`***(advanced)*
Number of sampling attempts of a biased source before declaring a particle lost.

Default `10`

Type positive integer

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

sublist **`[MATERIAL]`**
Definition for a single source material. See [SOURCE][MATERIAL] (page 67).

parameter **`name`**
Short title or label for the source.

Default type of the source database

Type string without special characters

parameter **`num_rejection_samples`**
parameter **`rej`**
How many samples to try before declaring a particle 'lost.'

Default `50000`

Type positive integer

database **`[RAYTRACE]`**
Material raytrace options. See [SOURCE][RAYTRACE] (page 67).

sublist **`[SPECTRUM]`**
Material source spectrum. See [SOURCE][SPECTRUM] (page 66).

3.15.7 [SOURCE=SURFACE_CENSUS]

Emit particles from a pre-computed surface source.

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

parameter **`input`**
Surface particle input file.

Type file path for reading (extension '.h5')

parameter **`name`**
Short title or label for the source.

Default type of the source database

Type string without special characters

parameter **`surfaces`**
Surfaces in input to read.

Type list in which each element is a string

parameter **`translation`**
Translates the particle by the given transform.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

3.15.8 [SOURCE=SOURCERER]

Use a Denovo solution as a fission source.

parameter `a`

Value for the ‘a’ constant in Watt equation.

Units MeV

Type positive real number

Applicable when `use_watt_spectrum` is `True`

parameter `b`

Value for the ‘b’ constant in Watt equation.

Units $\frac{1}{\mathrm{MeV}}$

Type positive real number

Applicable when `use_watt_spectrum` is `True`

parameter `description`
parameter `desc`

Optional longer descriptive string.

Default `''`

Type string

parameter `name`

Short title or label for the source.

Default type of the source database

Type string without special characters

preprocessor (advanced)

Default Watt spectrum to U-235.

Applicability `use_watt_spectrum` is `True`

command `nuclide`

Produce a Watt spectrum corresponding to the given nuclide.

Creates a

Creates b

parameter `num_rejection_samples`
parameter `rej`

How many samples to try before declaring a particle ‘lost.’

Default `50000`

Type positive integer

parameter `use_watt_spectrum`
parameter `use_watt`

Forces the energy spectrum to be a Watt spectrum.

Default `True`

Type boolean

3.15.9 [SOURCE][SHAPE]

Table 11: Available types for the [SHAPE] database

Type	Description	Applicability
box (page 68)	Axis-aligned cuboid shape	
cos_box (page 69)	Box, cosine distribution in multiple dimensions	
flattened_cos_box (page 70)	Box, $1 - (1 - cos)^2$ distribution in multiple dimensions	
squared_cos_box (page 71)	Box, $(1 - cos)^2$ distribution in multiple dimensions	
cyl (page 72)	Axis-aligned cylinder shape	
cylinder	Alias to `cyl` type	—
cylshell (page 73)	Cylindrical shell shape	
cylindershell	Alias to `cylshell` type	—
sphere (page 74)	Sphere shape	
sphereshell (page 74)	Spherical shell shape	
point (page 75)	Single point	
multipoint (page 75)	Multiple points	
global (page 76)	Box covering the geometry extents	
mesh (page 76)	Discretized mesh source	

3.15.10 [SOURCE][ENERGY]

Table 12: Available types for the [ENERGY] database

Type	Description	Applicability
histogram (page 77)	Histogram energy distribution	
mono (page 78)	Monoenergetic line energy distribution	
lines (page 78)	Multiple line energy distribution	
watt (page 79)	Watt fission energy spectrum	
origen (page 79)	ORIGEN decay source spectrum input	

3.15.11 [SOURCE][ANGLE]

Table 13: Available types for the [ANGLE] database

Type	Description	Applicability
isotropic (page 80)	Isotopic in angle	
mono (page 81)	Monodirectional	

3.15.12 [SOURCE][SPECTRUM]

The `[SPECTRUM]` energy distributions have exactly the same options as the [ENERGY] (page 66) entries with the same name, *except* that spectra also have a required `per_decay` entry and a name for each. This allows a single material source to emit multiple particles with different spectra at different rate per unit of activity.

Table 14: Available types for the [SPECTRUM] database

Type	Description	Applicability
histogram (page 81)	Histogram energy distribution	
mono (page 81)	Monoenergetic line energy distribution	
lines (page 82)	Multiple line energy distribution	
watt (page 82)	Watt fission energy spectrum	
origen (page 83)	ORIGEN decay source spectrum input	

3.15.13 [SOURCE][MATERIAL]

Definition for a single source material.

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

parameter **`name`**
Name of the material with this source.

Type string

parameter **`specific_activity`**
parameter **`activity`**
List of specific activity for each spectra.

Units $\frac{\text{becquerel}}{\text{kg}}$

Type list in which each element is a positive real number

postprocessor
The parameters `spectra` and `specific_activity` must have the same length.

parameter **`spectra`**
List of source spectra names for this material.

Type list in which each element is a string

3.15.14 [SOURCE][RAYTRACE]

Material raytrace options.

parameter **`axes`**
Axis/axes along which to fire rays for ray trace.

Default `xyz`

Type axis or axes (‘x’,’zy’,’xyz’)

parameter **`error_tolerance`**
Fraction of lost rays to tolerate before aborting.

Default `1e-05`

Type real number inside (0, 1)

parameter **`max_local_warnings`**
Max number of lost ray warnings to print per domain.

Default `10`

Type non-negative integer

parameter **`rays_deterministic`**
Use face midpoints rather than stratified sampling.

Default `False`

Type boolean

parameter **`rays_per_face`**
Number of ray trace rays to be fired per mesh face.

Default `4`

Type positive square integer

parameter **`x`**
Raytrace mesh edges along the X axis.

Type monotonically increasing list with at least two values (each element is a real number)

parameter **`y`**
Raytrace mesh edges along the Y axis.

Type monotonically increasing list with at least two values (each element is a real number)

parameter **`z`**
Raytrace mesh edges along the Z axis.

Type monotonically increasing list with at least two values (each element is a real number)

3.15.15 [SOURCE][SHAPE=BOX]

Axis-aligned cuboid shape.

command **`box`**
Expand into parameters `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax`.

Creates xmin

Creates xmax

Creates ymin

Creates ymax

Creates zmin

Creates zmax

parameter **`xmax`**
Maximum x coordinate of box.

Type real number

parameter **xmin**
Minimum x coordinate of box.

Type real number

parameter **ymax**
Maximum y coordinate of box.

Type real number

parameter **ymin**
Minimum y coordinate of box.

Type real number

parameter **zmax**
Maximum z coordinate of box.

Type real number

parameter **zmin**
Minimum z coordinate of box.

Type real number

3.15.16 [SOURCE][SHAPE=COS_BOX]

Box, cosine distribution in multiple dimensions.

command **box**
Expand into parameters `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax`.

Creates xmin

Creates xmax

Creates ymin

Creates ymax

Creates zmin

Creates zmax

parameter **cos_dir**
Directions for which the source has a cosine distribution.

Default `z`

Type axis or axes (‘x’,’zy’,’xyz’)

deleted **num_cdf_bins**
Entry `num_cdf_bins` has been deleted: The cosine CDF is integrated analytically.

parameter **xmax**
Maximum x coordinate of box.

Type real number

parameter **xmin**
Minimum x coordinate of box.

Type real number

parameter **ymax**

Maximum y coordinate of box.

Type real number

parameter **ymin**

Minimum y coordinate of box.

Type real number

parameter **zmax**

Maximum z coordinate of box.

Type real number

parameter **zmin**

Minimum z coordinate of box.

Type real number

3.15.17 [SOURCE][SHAPE=FLATTENED_COS_BOX]

Box, $1 - (1 - cos)^2$ distribution in multiple dimensions.

command **box**

Expand into parameters `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax`.

Creates xmin

Creates xmax

Creates ymin

Creates ymax

Creates zmin

Creates zmax

parameter **cos_dir**

Directions for which the source has a flattened cosine distribution.

Default `z`

Type axis or axes ('x','zy','xyz')

deleted **num_cdf_bins**

Entry `num_cdf_bins` has been deleted: The cosine CDF is integrated analytically.

parameter **xmax**

Maximum x coordinate of box.

Type real number

parameter **xmin**

Minimum x coordinate of box.

Type real number

parameter **`ymax`**
Maximum y coordinate of box.

Type real number

parameter **`ymin`**
Minimum y coordinate of box.

Type real number

parameter **`zmax`**
Maximum z coordinate of box.

Type real number

parameter **`zmin`**
Minimum z coordinate of box.

Type real number

3.15.18 [SOURCE][SHAPE=SQUARED_COS_BOX]

Box, $(1 - cos)^2$ distribution in multiple dimensions.

command **`box`**
Expand into parameters `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax`.

Creates xmin

Creates xmax

Creates ymin

Creates ymax

Creates zmin

Creates zmax

parameter **`cos_dir`**
Directions for which the source has a squared cosine distribution.

Default `z`

Type axis or axes (‘x’,’zy’,’xyz’)

parameter **`xmax`**
Maximum x coordinate of box.

Type real number

parameter **`xmin`**
Minimum x coordinate of box.

Type real number

parameter **`ymax`**
Maximum y coordinate of box.

Type real number

parameter **`ymin`**

Minimum y coordinate of box.

Type real number

parameter **`zmax`**

Maximum z coordinate of box.

Type real number

parameter **`zmin`**

Minimum z coordinate of box.

Type real number

3.15.19 [SOURCE][SHAPE=CYL]

The cylinder shape is defined along one of the three cartesian axes. Its origin (base) is defined as the center point of the lower circular face. The `height` extends in the positive direction from the origin along the given `axis`.

parameter **`axis`**

Axis of the cylinder.

Type axis (‘x’,’y’,’z’)

parameter **`height`**

parameter **`h`**

Height of cylinder from the base.

Type real number

command **`origin`**

Expand into parameters `origin_x`, `origin_y`, and `origin_z`.

Creates origin_x

Creates origin_y

Creates origin_z

parameter **`origin_x`**

parameter **`xo`**

X coordinate of the center of the cylinder’s base.

Type real number

parameter **`origin_y`**

parameter **`yo`**

Y coordinate of the center of the cylinder’s base.

Type real number

parameter **`origin_z`**

parameter **`zo`**

Z coordinate of the center of the cylinder’s base.

Type real number

parameter **`radius`**

parameter **`r`**

Radius of the cylinder.

Type real number

3.15.20 [SOURCE][SHAPE=CYLSHELL]

Cylindrical shell shape.

parameter **`axis`**
: Axis of the cylinder.

  Type axis ('x','y','z')

parameter **`height`**
parameter **`h`**
: Height of cylinder from the base.

  Type real number

parameter **`inner_radius`**
parameter **`ir`**
: Inner radius of the cylindrical shell.

  Type real number

command **`origin`**
: Expand into parameters `origin_x`, `origin_y`, and `origin_z`.

  Creates origin_x

  Creates origin_y

  Creates origin_z

parameter **`origin_x`**
parameter **`xo`**
: X coordinate of the center of the cylinder's base.

  Type real number

parameter **`origin_y`**
parameter **`yo`**
: Y coordinate of the center of the cylinder's base.

  Type real number

parameter **`origin_z`**
parameter **`zo`**
: Z coordinate of the center of the cylinder's base.

  Type real number

parameter **`outer_radius`**
parameter **`or`**
: Outer radius of the cylindrical shell.

  Type real number

3.15.21 [SOURCE][SHAPE=SPHERE]

Sphere shape.

command **`origin`**
Expand into parameters `origin_x`, `origin_y`, and `origin_z`.

Creates origin_x

Creates origin_y

Creates origin_z

parameter **`origin_x`**
parameter **`xo`**
X coordinate of sphere source origin.

Type real number

parameter **`origin_y`**
parameter **`yo`**
Y coordinate of sphere source origin.

Type real number

parameter **`origin_z`**
parameter **`zo`**
Z coordinate of sphere source origin.

Type real number

parameter **`radius`**
parameter **`r`**
Radius of sphere source.

Type real number

3.15.22 [SOURCE][SHAPE=SPHERESHELL]

Spherical shell shape.

parameter **`inner_radius`**
parameter **`ir`**
Inner radius of spherical shell.

Type real number

command **`origin`**
Expand into parameters `origin_x`, `origin_y`, and `origin_z`.

Creates origin_x

Creates origin_y

Creates origin_z

parameter **`origin_x`**
parameter **`xo`**
X coordinate of sphere source origin.

Type real number

parameter **`origin_y`**
parameter **`yo`**
Y coordinate of sphere source origin.

Type real number

parameter **`origin_z`**
parameter **`zo`**
Z coordinate of sphere source origin.

Type real number

parameter **`outer_radius`**
parameter **`or`**
Outer radius of spherical shell.

Type real number

3.15.23 [SOURCE][SHAPE=POINT]

Single point.

command **`point`**
Expand into parameters `x`, `y`, and `z`.

Creates x

Creates y

Creates z

parameter **`x`**
X position of point source.

Type real number

parameter **`y`**
Y position of point source.

Type real number

parameter **`z`**
Z position of point source.

Type real number

3.15.24 [SOURCE][SHAPE=MULTIPOINT]

Multiple points.

parameter **`probability`**
Probability of each point being selected.

Type list of non-negative floats (each element is a non-negative real number)

postprocessor
The parameters `x`, `y`, `z`, and `probability` must have the same length.

parameter **`x`**
X positions of point sources.

Type list in which each element is a real number

parameter **`y`**
Y positions of point sources.

Type list in which each element is a real number

parameter **`z`**
Z positions of point sources.

Type list in which each element is a real number

3.15.25 [SOURCE][SHAPE=GLOBAL]

The "global" source is a labor-saving way to attempt to sample particles inside the geometry. It works by querying the geometry for a bounding box (currently, only RTK and SCALE geometries are supported), and then sampling points uniformly inside that box. Any point outside the geometry will be rejected. The `sample_attempts` parameter determines how many samples inside the bounding box to attempt before a warning is emitted.

Warning: If the bounding box of the geometry is much different than the underlying geometry, the rejection fraction may be high, and the source sampling may be very slow. This is especially true in the case of fissionable-only sources, for which an additional rejection step is overlaid.

parameter **`sample_attempts`**
Number of geometry positions to sample per source particle.

Default `1000`

Type positive integer

3.15.26 [SOURCE][SHAPE=MESH]

Discretized mesh source.

parameter **`cell_averaged`**
parameter **`avg`**

Whether the field values are volume-averaged strengths. See cell_averaged (page 60) in [SOURCE=fissionmesh].

parameter **`field`**
Path to the source definition in the input file.

Default 'strength' if cell-averaged, else 'pdf'

Type string

Applicable when `format` is `source`

parameter **`format`**
Format of hdf5 file.

Default `tally`

Type `source` or `tally`

parameter **`input`**

Name of file containing source distribution.

Type file path for reading (extension '.h5')

parameter **`tally_name`**

Name of the fission source rate mesh tally.

Type string without special characters

Applicable when `format` is `tally`

3.15.27 [SOURCE][ENERGY=HISTOGRAM]

Histogram energy distribution.

parameter **`energy`**
parameter **`e`**

Histogram energy bin bounds.

Units eV

Type list of non-negative monotonically increasing floats (each element is a non-negative real number)

parameter **`particle_type`**
parameter **`pt`**

Particle type to emit.

Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter **`probability`**
parameter **`p`**

Probability of an energy bin being selected.

For a discrete source distribution with the following spectrum:

```
strength (p / eV / s)
  5.0                       +--------+
                            |        |
  4.0                       |        |
                            |        |
  3.0              +--------|        |
                   |        |        |
  2.0  +--+        |        |        |
       |  |  +-----|        |        |
  1.0  |  |--|     |        |        |
       |  |  |     |        |        |
  0.0  |--|--|-----|--------|--------|
       0  1  2     4        7       10 eV
```

the source strength (page 59) should be set to

$$q_{\mathrm{tot}} = \int q(E)\,\mathrm{d}E = 30\ \mathrm{p/s}$$

and the input for the integrated probability for each bin will be:

```
energy:probability   ! strength spectrum
     0  0.067        ! p * 30 / 1  = 2
     1  0.033        ! p * 30 / 1  = 1
     2  0.1          ! p * 30 / 2  = 1.5
     4  0.3          ! p * 30 / 3  = 3.
     7  0.5          ! p * 30 / 3  = 5.
    10  ---
```

Type list of non-negative floats (each element is a non-negative real number)

3.15.28 [SOURCE][ENERGY=MONO]

Monoenergetic line energy distribution.

parameter **energy**
parameter **e**

Source energy.

Units eV

Type positive real number

parameter **particle_type**
parameter **pt**

Particle type to emit.

Type particle type (`n`, `neutron`, `p`, or `photon`)

3.15.29 [SOURCE][ENERGY=LINES]

Multiple line energy distribution.

parameter **energy**
parameter **e**

Individual line energies.

Units eV

Type monotonically increasing list (each element is a positive real number)

parameter **particle_type**
parameter **pt**

Particle type to emit.

Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter **probability**
parameter **p**

Probability of each line being selected.

Type list of non-negative floats (each element is a non-negative real number)

3.15.30 [SOURCE][ENERGY=WATT]

The Watt distribution samples a fission spectrum:

$$f(E) = c \exp(-E/a) \sinh(\sqrt{bE})$$

where c is a normalization constant.

parameter **`a`**

Value for the 'a' constant in Watt equation.

Units MeV

Type positive real number

parameter **`b`**

Value for the 'b' constant in Watt equation.

Units $\frac{1}{\text{MeV}}$

Type positive real number

preprocessor (advanced)

Default Watt spectrum to U-235.

command **`nuclide`**

Produce a Watt spectrum corresponding to the given nuclide.

Creates a

Creates b

3.15.31 [SOURCE][ENERGY=ORIGEN]

Reads photon spectra out of an ORIGEN master library.

command **`activities`**

Map 'zaid' to 'activity' from pairs or arrow-separated items.

Creates zaid

Creates activity

parameter **`activity`**

Activities of each nuclide.

Default (empty sublist)

Type list in which each element is a positive real number

Applicable when

- `particle_type` is `p`; and
- using an ORIGEN gamma library

postprocessor

The parameters `zaid` and `activity` must have the same length.

Applicability `particle_type` is `p`

Applicability using an ORIGEN gamma library

postprocessor
ORIGEN file type and source definition must be consistent.

parameter `apply_origen_strength`
Multiply the source strength by the strength of the ORIGEN distribution.

Default `True`

Type boolean

parameter `input`
parameter `filename`
File (f71/mpdkxgam) containing the ORIGEN-generated spectrum.

Default `'/.../origen.rev04.mpdkxgam.data'`

Type file path for reading

parameter `particle_type`
parameter `pt`
Particle type to emit.

Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter `source_type`
parameter `st`
Indicates origin of the source.

Default based on source type

Type source type (`a`, `alpha`, `alpha_neutron`, `an`, `d`, `delayed`, `delayed_neutron`, `dn`, `g`, `gamma`, `n`, `neutron`, `p`, `photon`, `sf`, `sfn`, `spontaneous_fission`, `spontaneous_fission_neutron`, `tn`, `total_gamma`, `total_neutron`, or `total_photon`)

parameter `statepoint`
Statepoint in the file from which to read the source.

Type non-negative integer

Applicable when using an ORIGEN concentration file

parameter `zaid`
Element/nuclide IDs (MZZZAAA).

Default (empty sublist)

Type list in which each element is a positive integer

Applicable when

- `particle_type` is `p`; and
- using an ORIGEN gamma library

3.15.32 [SOURCE][ANGLE=ISOTROPIC]

Note that when defining a source for Denovo calculations, the only allowable angular discretization is isotropic.

3.15.33 [SOURCE][ANGLE=MONO]

Monodirectional.

parameter **`direction`**
parameter **`dir`**
Direction source particles are emitted.

Type length-3 float vector (each element is a real number)

3.15.34 [SOURCE][SPECTRUM=HISTOGRAM]

Histogram energy distribution.

parameter **`energy`**
parameter **`e`**
Histogram energy bin bounds.

Units eV

Type list of non-negative monotonically increasing floats (each element is a non-negative real number)

parameter **`name`**
Name of the spectrum.

Type string without special characters

parameter **`particle_type`**
parameter **`pt`**
Particle type to emit.

Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter **`per_decay`**
Particles emitted per decay.

Type positive real number

parameter **`probability`**
parameter **`p`**
Probability of an energy bin being selected.

Type list of non-negative floats (each element is a non-negative real number)

3.15.35 [SOURCE][SPECTRUM=MONO]

Monoenergetic line energy distribution.

parameter **`energy`**
parameter **`e`**
Source energy.

Units eV

Type positive real number

parameter **`name`**
Name of the spectrum.

Type string without special characters

parameter `particle_type`
parameter `pt`
Particle type to emit.

Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter `per_decay`
Particles emitted per decay.

Type positive real number

3.15.36 [SOURCE][SPECTRUM=LINES]

Multiple line energy distribution.

parameter `energy`
parameter `e`
Individual line energies.

Units eV

Type monotonically increasing list (each element is a positive real number)

parameter `name`
Name of the spectrum.

Type string without special characters

parameter `particle_type`
parameter `pt`
Particle type to emit.

Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter `per_decay`
Particles emitted per decay.

Type positive real number

parameter `probability`
parameter `p`
Probability of each line being selected.

Type list of non-negative floats (each element is a non-negative real number)

3.15.37 [SOURCE][SPECTRUM=WATT]

Watt fission energy spectrum.

parameter `a`
Value for the ‘a’ constant in Watt equation.

Units MeV

Type positive real number

parameter `b`
Value for the ‘b’ constant in Watt equation.

Units $\frac{1}{\text{MeV}}$

Type positive real number

parameter `name`
Name of the spectrum.

Type string without special characters

preprocessor (advanced)
Default Watt spectrum to U-235.

command `nuclide`
Produce a Watt spectrum corresponding to the given nuclide.

Creates a

Creates b

parameter `per_decay`
Particles emitted per decay.

Type positive real number

3.15.38 [SOURCE][SPECTRUM=ORIGEN]

ORIGEN decay source spectrum input.

command `activities`
Map ‘zaid’ to ‘activity’ from pairs or arrow-separated items.

Creates zaid

Creates activity

parameter `activity`
Activities of each nuclide.

Default (empty sublist)

Type list in which each element is a positive real number

Applicable when

- `particle_type` is `p`; and
- using an ORIGEN gamma library

postprocessor
The parameters `zaid` and `activity` must have the same length.

Applicability `particle_type` is `p`

Applicability using an ORIGEN gamma library

postprocessor
ORIGEN file type and source definition must be consistent.

parameter `apply_origen_strength`
Multiply the source strength by the strength of the ORIGEN distribution.

Default `True`

Type boolean

parameter **`input`**
parameter **`filename`**
File (f71/mpdkxgam) containing the ORIGEN-generated spectrum.

Default `'/.../origen.rev04.mpdkxgam.data'`

Type file path for reading

parameter **`name`**
Name of the spectrum.

Type string without special characters

parameter **`particle_type`**
parameter **`pt`**
Particle type to emit.

Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter **`per_decay`**
Particles emitted per decay.

Type positive real number

parameter **`source_type`**
parameter **`st`**
Indicates origin of the source.

Default based on source type

Type source type (`a`, `alpha`, `alpha_neutron`, `an`, `d`, `delayed`, `delayed_neutron`, `dn`, `g`, `gamma`, `n`, `neutron`, `p`, `photon`, `sf`, `sfn`, `spontaneous_fission`, `spontaneous_fission_neutron`, `tn`, `total_gamma`, `total_neutron`, or `total_photon`)

parameter **`statepoint`**
Statepoint in the file from which to read the source.

Type non-negative integer

Applicable when using an ORIGEN concentration file

parameter **`zaid`**
Element/nuclide IDs (MZZZAAA).

Default (empty sublist)

Type list in which each element is a positive integer

Applicable when

- `particle_type` is `p`; and
- using an ORIGEN gamma library

3.16 PHYSICS ENGINES: [PHYSICS]

Omnibus currently supports two coupled-physics packages: multigroup (MG) and continuous energy (CE). Continuous-energy physics is restricted to Shift; multigroup physics is usable by both Shift and Denovo.

Table 15: Available types for the [PHYSICS] database

Type	Description	Applicability
ce (page 85)	SCALE continuous energy physics	'SCALE_CE' is enabled in this build and solver is 'shift'
mg (page 96)	SCALE multigroup physics	'SCALE_MG' is enabled in this build
void (page 85)	All materials are replaced with void	`/problem/mode` is `forward`, `adjoint`, or `raytrace`
sce	Alias to `ce` type	—
smg	Alias to `mg` type	—

3.16.1 VOID PHYSICS: [PHYSICS=VOID]

The special `void` physics type creates a one-group transport problem with void cross sections for all materials. It is used primarily in conjunction with the `raytrace` visualization mode, but it can also be used for preliminary model verification.

parameter **`mode`**

Particles to transport.

Default Default mode to 'n' for kcode, or based on sources if present

Type particle transport mode (`n`, `neutron`, `np`, `p`, `photon`, or `pn`)

parameter **`name`**

Label for the physics.

Default `void`

Type string without special characters

parameter **`num_groups`***(advanced)*

Number of energy groups.

Default one for each particle type

Type positive integer

3.17 CONTINUOUS-ENERGY PHYSICS: [PHYSICS=CE]

The CE physics implementation in Shift is driven by AMPX-processed cross sections and tabulated physics data. The methodology behind the AMPX cross section processing is documented in the AMPX manual [10], and the physics processes are documented in the KENO section of the SCALE manual [2].

3.17.1 FEATURES

- Neutron only, photon only, and coupled neutron-photon problems
- Optional Doppler broadening interpolation between library temperatures at load time
- Optional Doppler-broadened resonance correction (DBRC) enables upscattering for high-Z nuclides

3.17.2 LIMITATIONS

- Photon cross sections do not include Bremsstrahlung reactions, so low-energy photon physics will not perform as expected.
- Data inconsistencies in ENDF are propagated through AMPX and may result in errors or warnings during transport.
- Photonuclear reactions are not supported.

command `ampx_kerma`

Load KERMA factors from an AMPX library.

Creates splice

parameter `balance_tol`*(advanced)*

Tolerance for printing a diagnostic about xs balance errors.

Default `0.005`

Type real number inside (0, 1)

database `[BROADEN]`

Temperature-corrected cross section Doppler broadening. See [PHYSICS][BROADEN] (page 93).

Optional

Applicable when

- `mode` is `n` or `np`; and
- not using the pole method

command `ce_lib`

Set the CE library path using SCALE file resolution.

The `FileNameAliases.txt` file installed to the prefix directory (usually the same as `$SCALE`) is used to resolve the data location. The possible values as of SCALE 6.2.3 follow.

Table 16: SCALE CE library path aliases in SCALE 6.2.

Path	Description
ce	ENDF/B-VII.1
ce_v7	ENDF/B-VII.0
ce_v7.0	ENDF/B-VII.0
ce_v7.1	ENDF/B-VII.1
ce_v7_endf	ENDF/B-VII.0
ce_v7.0_endf	ENDF/B-VII.0
ce_v7.1_endf	ENDF/B-VII.1

If the Omnibus build in use has the CMake variable `SCALE_HPC_DATA_DIR` defined, Shift will preferentially load HDF5 data from that instead of the XML files.

Creates ce_lib_path

parameter `ce_lib_path`

Path to SCALE CE Library XML or HDF5 file.

Type file path for reading (extension '.xml' or '.h5')

postprocessor
The SCALE `CELibrary` package must be enabled to use legacy XML CE data files.

Applicability CE library is the `xml` legacy format

parameter **`ce_pole_lib_path`**
Path to the HDF5 file containing pole and residue data.

Optional

Type file path for reading (extension '.h5')

Applicable when

- `mode` is `n` or `np`; and
- CE library is in `HDF5` format

parameter **`dbrc`**
Enable Doppler broadened rejection correction.

DBRC adjusts the free-gas sampling of elastic scattering. In particular, it adjusts the sampling of the target nuclide speed when the target is a heavy nuclide.

This correction improves the accuracy of epithermal neutron scatter off of heavy nuclides. However, because it increases the rejection fraction when sampling the elastic scattering kernel, it may incur a performance penalty.

Default `True`

Type boolean

Applicable when `mode` is `n` or `np`

parameter **`dbrc_energy_max`**
Maximum incident neutron energy for DBRC.

Default `210.0`

Units eV

Type positive real number

Applicable when `dbrc` is `True`

postprocessor
Parameter `dbrc_energy_min` must be less than `dbrc_energy_max`.

Applicability `dbrc` is `True`

parameter **`dbrc_energy_min`**
Minimum incident neutron energy for DBRC.

Default `0.4`

Units eV

Type positive real number

Applicable when `dbrc` is `True`

parameter **`dbrc_lib_path`**

Absolute path to the DBRC data directory.

This option can be used to override the default path to the SCALE CE DBRC data. It can only be used with the legacy (xml) format cross sections; HDF5 cross section libraries include the DBRC data as a new temperature-independent reaction type.

Table 17: Default DBRC data paths in SCALE 6.2.

XML CE library path	DBRC library path
`$DATA/ce_v7.0_endf.xml`	`$DATA/cekenolib_7.0/dbrc/`
`$DATA/ce_v7.1_endf.xml`	`$DATA/cekenolib_7.1/dbrc/`

Default `$DATA/cekenolib_7.X/dbrc/`

Type directory path for reading

Applicable when

- CE library is the `xml` legacy format; and
- `dbrc` is `True`

parameter **`disable_collision_yields`**

Disables banking photons from all neutron collision reactions, but not from fission.

Default `False`

Type boolean

Applicable when `mode` is `np`

command **`energy_limits`**

Expand into parameters `n_energy_min` and `n_energy_max`.

Creates n_energy_min

Creates n_energy_max

database **`[FISSION]`**

Fission-kinetics parameters. See [PHYSICS][FISSION] (page 94).

Default (empty database)

Applicable when neutrons are being transported

parameter **`kappa_library`**

Read neutron fission and capture heating from the provided libary.

Optional

Type file path for reading (extension '.h5')

Applicable when `mode` is `n` or `np`

parameter **`mixture_ordering`***(advanced)*

Internal sorting criterion for nuclides in the mix table.

Default `legacy`

Type `legacy`, `ascending_density`, `descending_density`, `ascending_zaid`, or `descending_zaid`

parameter **`mode`**
Particles to transport.

Default Default mode to 'n' for kcode, or based on sources if present

Type particle transport mode (`n`, `neutron`, `np`, `p`, `photon`, or `pn`)

postprocessor
Kcode problems must be run in mode 'n' or 'np.'

parameter **`n_energy_max`**
parameter **`nemax`**
Maximum global neutron_energy cutoff for cross sections.

Default `20000000.0`

Units eV

Type positive real number

Applicable when `mode` is `n` or `np`

postprocessor
Parameter `n_energy_min` must be less than `n_energy_max`.

Applicability `mode` is `n` or `np`

parameter **`n_energy_min`**
parameter **`nemin`**
Minimum global neutron energy cutoff for cross sections.

Default `1e-05`

Units eV

Type positive real number

Applicable when `mode` is `n` or `np`

parameter **`name`**
Label for the physics.

Default `ce`

Type string without special characters

parameter **`num_xsgrid_points`**
Number of points used in the xs lookup acceleration grid.

Default `16384`

Type positive integer

Applicable when `xs_accel` is `True`

parameter **omit_zaid_n**
Set the neutron cross section to zero for these nuclides.

Default `8018`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `mode` is `n` or `np`

parameter **omit_zaid_p**
Set the photon cross section to zero for these nuclides.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `mode` is `p` or `np`

parameter **orig_zaid_n**
Replace CE data for these nuclides in problem materials.

The ZAID remapping options allow a ZAID (or SCALE ID) present in the problem input to be replaced with a different ZAID. These options are most useful when entered in column input form:

```
orig_zaid_n :subs_zaid_n
       1001       8001001
      11022          11023
```

This is usually necessary when the selected library is missing cross sections for a nuclide in the model's compositions.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `mode` is `n` or `np`

parameter **orig_zaid_p**
Replace photon CE data for these nuclides in problem materials.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `mode` is `p` or `np`

parameter **otf_elastic_scattering**
Use on-the-fly elastic scattering rather than table lookups.

Default `False`

Type boolean

Applicable when `mode` is `n` or `np`

parameter **p_energy_max**
parameter **pemax**
Maximum global photon energy cutoff for cross sections.

Default `25000000.0`

Units eV

Type positive real number

Applicable when `mode` is `p` or `np`

postprocessor
Parameter `p_energy_min` must be less than `p_energy_max`.

Applicability `mode` is `p` or `np`

parameter **`p_energy_min`**
parameter **`pemin`**
Minimum global photon energy cutoff for cross sections.

Default `10000.0`

Units eV

Type positive real number

Applicable when `mode` is `p` or `np`

parameter **`probability_tables`**
parameter **`ptab`**
Use the probability table method for the unresolved resonance region (URR).

Default `True`

Type boolean

Applicable when `mode` is `n` or `np`

parameter **`reactions`***(advanced)*
Reactions to load (AMPX_MT values).

Default `---`

Type list in which each element is a MT number or name (e.g., N_GAMMA, 102)

sublist **`[SPLICE]`**
Inject cross sections from a source other than the library. See [PHYSICS][SPLICE] (page 93).

Default (empty sublist)

parameter **`subs_zaid_n`**
Substitute ZAID corresponding to 'orig_zaid_n.'

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `mode` is `n` or `np`

postprocessor
The parameters `orig_zaid_n` and `subs_zaid_n` must have the same length.

Applicability `mode` is `n` or `np`

parameter **`subs_zaid_p`**
Substitute ZAID corresponding to 'orig_zaid_p.'

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `mode` is `p` or `np`

postprocessor

The parameters `orig_zaid_p` and `subs_zaid_p` must have the same length.

Applicability `mode` is `p` or `np`

parameter **`thermal_energy_cutoff`**

Thermalization energy cutoff for scattering kernels.

Default `10.0`

Units eV

Type positive real number

Applicable when `mode` is `n` or `np`

parameter **`xs_accel`**

Accelerate cross section calculation.

Accelerate total and fission cross section lookup in a material using a log-spaced energy grid. For improved performance, this should always be enabled when neutron transport is enabled.

Default *True* when neutron transport is enabled

Type boolean

Applicable when `xs_cache` is `tot` or `totfisnu`

parameter **`xs_cache`**

Preserve cross sections between collisions.

This option enables microscopic cross sections to be cached as a particle streams between materials. This is primarily a performance optimization (in many problems it should have no effect on the results), but it subtly changes the physics of streaming through multiple materials when a neutron is in the unresolved resonance regions of the energy spectrum.

In some codes, streaming from one material to another resets the probability band values. As a consequence, if a particle streams through two instances of the same material by traveling through a void, its probability table band will be resampled in the second material.

Unless the `xs_cache` value is set to `none`, the physics constructs a hash table of nuclide IDs with probability table data (and in which the particle's energy is inside the URR) encountered since the last collision. When streaming through the same nuclide at different temperatures, the cross section band [CDF] is preserved, but the cross sections will be updated for the correct temperature. This is more physical than resetting the band at material boundaries and can affect, for example, k_{eff} of highly voided BWRs.

When `xs_cache` is set to `tot`, the total cross sections of all encountered nuclides will be cached. When the option is set to `totfisnu`, the total, fission, and nu values are all pre-calculated (when a particle enters a nuclide) and cached.

Default *totfisnu* when problem mode is kcode else *tot*

Type `none`, `ptab`, `tot`, or `totfisnu`

postprocessor

Cannot set `xs_cache` to `ptab` unless `probability_tables` is `True`.

3.17.3 [PHYSICS][BROADEN]

Temperature-corrected cross section Doppler broadening.

parameter `delta_t`
: Finite difference grid spacing for Leal-Hwang temperature interpolation.

  Default `1.0`

  Units K

  Type positive real number

  Applicable when not using legacy broadener

parameter `energy_tol`
: Relative difference for considering two energy points equal.

  Default `1e-10`

  Type real number inside (0, 1)

  Applicable when not using legacy broadener

parameter `kinematics`
: Interpolate collision data.

  Default `False`

  Type boolean

parameter `legacy`
: Use legacy CE Resource interpolation.

  Default `False`

  Type boolean

  Applicable when CE library is the `xml` legacy format

parameter `temperature_tol`
: Tolerance for reusing existing broadened cross sections.

  Default `4.0`

  Units K

  Type positive real number

parameter `union_energy`
: Unionize lower and upper library temperature energy grids.

  Default `True`

  Type boolean

  Applicable when not using legacy broadener

3.17.4 [PHYSICS][SPLICE]

Table 18: Available types for the [SPLICE] database

Type	Description	Applicability
ampx (page 94)	Splice multigroup data from an AMPX library	

3.17.5 [PHYSICS][FISSION]

Fission-kinetics parameters.

command **`fission_cells`**

Generate 'union_fission_cells' and 'union_fission_lengths' from colon-separated unions.

Creates union_fission_cells

Creates union_fission_lengths

parameter **`fission_gammas`**
parameter **`fiss_gam`**

Generate fission gammas.

Default True if and only if `mode` is `np`

Type boolean

Applicable when neutrons and photons are being transported

postprocessor

check fission particle production options.

parameter **`fission_neutrons`**
parameter **`fiss_neut`**

Generate fission neutrons.

Default True if and only if `mode` is not `kcode`

Type boolean

parameter **`union_fission_cells`***(advanced)*

Flattened list of cells in each union.

Default (empty sublist)

Type list of cell names (each element is a string)

parameter **`union_fission_lengths`***(advanced)*

Number of cells per union in the above list.

Default (empty sublist)

Type list in which each element is a integer

3.17.6 [PHYSICS][SPLICE=AMPX]

The AMPX data splicing option allows multigroup data from an AMPX library to be spliced into the CE transport. This feature allows specialized reactions to be calculated during transport (e.g., KERMA tallies).

Currently, only multigroup reaction rates can be inserted. No probability tables or collision data can be inserted.

If a CE reaction is already present, the AMPX splicer will not override it. To get around this, the user can manually specify the list of reactions to load in the Continuous-energy physics: [PHYSICS=ce] (page 85) block, omitting the reactions to be loaded as multigroup data.

command **`mg_lib`**

Set `mg_lib` to the given value using SCALE DATA resolution.

Creates xs_library

parameter **`name`**
Descriptive name for the data being spliced in.

Type string without special characters

parameter **`orig_zaid_n`**
Replace MG data for these nuclides in problem materials.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

parameter **`orig_zaid_p`**
Replace photon MG data for these nuclides in problem materials.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

parameter **`reactions`***(advanced)*
Multigroup reactions to splice into the CE data (AMPX_MT values).

Default (empty sublist)

Type list in which each element is a MT number or name (e.g., N_GAMMA, 102)

parameter **`subs_zaid_n`**
Substitute ZAID corresponding to ‘orig_zaid_n.’

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

postprocessor
The parameters `orig_zaid_n` and `subs_zaid_n` must have the same length.

parameter **`subs_zaid_p`**
Substitute ZAID corresponding to ‘orig_zaid_p.’

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

postprocessor
The parameters `orig_zaid_p` and `subs_zaid_p` must have the same length.

parameter **`xs_library`**
Path to AMPX library to load data.

Type file path for reading

3.18 MULTIGROUP PHYSICS: [PHYSICS=MG]

The SCALE multigroup physics package as implemented in Exnihilo can use various multigroup cross section library formats, including:

- AMPX-processed cross sections [10],
- User-defined macroscopic cross sections,
- GIP format macroscopic cross sections, and
- ANISN-formatted multigroup libraries [19].

When compositions (as opposed to user-specified multigroup cross sections) are provided, Omnibus uses SCALE to calculate infinite homogeneous medium cross sections for all materials. No self-shielding is performed. The default cross section processing is primarily intended for generating deterministic solutions for hybrid calculations.

Warning: The default multigroup cross sections generated by Omnibus are only recommended for qualitative transport behavior. Obtaining accurate multigroup cross sections for general problems requires a great deal of experience using SCALE cross section processing that incorporates self-shielding.

The Monte Carlo implementation of MG physics uses the same methods as KENO multigroup physics. Depending on the scattering order of the overall problem and of each particular material, the scattering model takes three forms.

- Isotropic scattering has the standard physical formulation.
- P_1 scattering forces the particle to scatter with an exiting cosine *equal to the mean cosine*. That is, instead of sampling the exiting cosine from a linear distribution, the cosine is sampled from a delta function equal to $\mu_0 = \int_{-1}^{1} \mu\sigma_s(\mu)\,\mathrm{d}\mu$. Thus, in an isotropically scattering medium in a P_1 problem, the particle's exiting direction will be exactly perpendicular to the particle's incident direction (since isotropic scattering has $\mu_0 = 0$). This is not physical, but it is the physics behavior in MG KENO.
- Higher order P_N scattering selects exiting angles from a quadrature.

3.18.1 FEATURES

- Neutron only, photon only, and coupled neutron-photon problems

3.18.2 LIMITATIONS

- Anisotropic Monte Carlo particle scattering uses the same angular approximations as the multigroup KENO package in SCALE.

parameter **`ampx_path`**

Path to an AMPX working library input file.

This input requires a *working* library with at least the number of materials present in the model. For a library with N materials, the cross sections for matids (page 43) $[0, N)$ are assigned based on the ids of materials in the AMPX file *after being sorted in ascending order*. For example, if a working library has materials with IDs $[1, 21, 12]$ (intentionally unsorted); the mapping of material IDs to AMPX library IDs is

```
0 -> 1
1 -> 12
2 -> 21
```

There is an additional option implicit_void (page 99) that assigns void cross sections to matid 0. Thus if the AMPX library has media IDs 1, 3, 5, and if `implicit_void` is true, then the mapping will be

```
0 -> 0
1 -> 1
2 -> 3
3 -> 5
```

Type file path for reading (extension '.ampx')

Applicable when `xsgen` is `ampx`

parameter **`anisn_info_path`**

Path to an ADVANTG-format ANISN metadata file.

Type file path for reading (extension '.info')

Applicable when `xsgen` is `anisncomp`

command **`anisn_lib`**

Set ANISN library and metadata paths using a search path.

Creates anisn_path

Creates anisn_zaid_path

Creates anisn_info_path

parameter **`anisn_path`**

Path to an ANISN cross section input.

Type file path for reading (extension '.bin')

Applicable when `xsgen` is `anisncomp`

parameter **`anisn_table`**

ANISN table IDs corresponding to `anisn_zaid`.

Default `---`

Type list in which each element is a positive integer

Applicable when `xsgen` is `anisncomp`

postprocessor

The parameters `anisn_zaid` and `anisn_table` must have the same length.

Applicability `xsgen` is `anisncomp`

parameter **`anisn_zaid`**

Replace the given ZAIDs with corresponding ANISN table IDs.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `xsgen` is `anisncomp`

parameter **`anisn_zaid_path`**
Path to an ADVANTG-format ANISN zaid map.

Type file path for reading (extension '.zaid')

Applicable when `xsgen` is `anisncomp`

parameter **`disable_upscattering`**
parameter **`noup`**
Remove upscattering by altering cross sections.

For shielding calculations, thermal neutrons may contribute little to the detector response. However, converging the distribution of thermal neutrons through upscatter iterations can be expensive.

This option adjusts all material cross sections so that their scattering matrix is strictly lower triangular. The default behavior is to lump upscattering cross sections into within-group scattering, adjusting the outscatter cross sections so that:

$$\sigma_{s,g,g} \leftarrow \sum_{g'=1}^{g} \sigma_{s,g,g'}$$

$$\sigma_{s,g,g'} \leftarrow 0,\ g' = [1,\dots,g-1]$$

where the outscatter cross section is

$$\sigma_s(E^g \to E^{g'}) \equiv \sigma_{s,g,g'}$$

Default True if only transporting photons or using hybrid solve

Type boolean

command **`energy_limits`**
Expand into parameters `n_energy_min` and `n_energy_max`.

Creates n_energy_min

Creates n_energy_max

database **`[GIP]`**
GIP input file metadata. See [PHYSICS][GIP] (page 104).

Applicable when `xsgen` is `gip`

parameter **`gip_path`**
Path to a GIP working library file.

Type file path for reading (extension '.gip')

Applicable when `xsgen` is `gip`

parameter **`implicit_capture`**
Enable implicit capture for Monte Carlo transport.

Default `True`

Type boolean

Applicable when solver is ‘shift’

parameter **`implicit_void`***(advanced)*

Insert ‘void’ material of matid=0 before AMPX-specified mats.

Default `False`

Type boolean

Applicable when `xsgen` is `ampx`

parameter **`mc_pn_scattering`***(advanced)*

Enable high-order scattering for MC transport.

Default True when Shift is enabled

Type boolean

Applicable when PN order is greater than 1

postprocessor

Multigroup Monte Carlo transport requires `pn_order` to be zero or odd.

Applicability `mc_pn_scattering` is `True`

command **`mg_lib`**

Set `mg_lib` to the given value using SCALE DATA resolution.

The aliases for the SCALE multigroup libraries can be found at *`INSTALL`*`/etc/LibraryAliases.txt`. The SCALE `FileNameAliases.txt` file is used to resolve the data files. The current options for multigroup libraries are:

Table 19: Multigroup physics library aliases and filenames in SCALE 6.2.

Alias for mg_lib	Filename
broad_n	xn56v7.1
broad_ng	xn28g19v7.1
fine_n	xn252v7.1
fine_ng	xn200g47v7.1
ultra_fine_n	xn999v7.1
v7-238	xn238v7.0
v7-238n	xn238v7.0
v7.0-238n	xn238v7.0
xn238v7	xn238v7.0
v7-252n	xn252v7.1
v7.1-252	xn252v7.1
v7.1-252n	xn252v7.1
v7-200n47g	xn200g47v7.1
v7.1-200n47g	xn200g47v7.1
v7.0-200n47g	xn200g47v7.0
v7-27n19g	xn27g19v7.0
v7.0-27n19g	xn27g19v7.0
v7-28n19g	xn28g19v7.1
v7.1-28n19g	xn28g19v7.1
v7-56	xn56v7.1
v7-56n	xn56v7.1
v7.1-56	xn56v7.1
v7.1-56n	xn56v7.1
v7-999	xn999v7.0
v7-999n	xn999v7.0
v7.1-999	xn999v7.1
v7.1-999n	xn999v7.1
test_n	test8g_v7.1
test-8grp	test8g_v7.1

Creates xs_library

parameter **`mode`**

Particles to transport.

Default Default mode to ‘n’ for kcode, or based on sources if present

Type particle transport mode (`n`, `neutron`, `np`, `p`, `photon`, or `pn`)

postprocessor

Kcode problems must be run in mode ‘n’ or ‘np.’

parameter **`n_energy_max`**

parameter **`nemax`**

Maximum global neutron_energy cutoff for cross sections.

Default `20000000.0`

Units eV

Type positive real number

Applicable when `mode` is `n` or `np`

postprocessor
Parameter `n_energy_min` must be less than `n_energy_max`.

Applicability `mode` is `n` or `np`

parameter **`n_energy_min`**
parameter **`nemin`**
Minimum global neutron energy cutoff for cross sections.

Default `1e-05`

Units eV

Type positive real number

Applicable when `mode` is `n` or `np`

parameter **`name`**
Label for the physics.

Default `mg`

Type string without special characters

parameter **`neutron_bounds`**
parameter **`nbounds`**
Neutron group boundaries.

Default `---`

Type positive floats in decreasing order (each element is a positive real number)

Applicable when `xsgen` is `ampx`, `gip`, `inline`, or `xml`

parameter **`num_groups`***(advanced)*
Number of energy groups.

Default based on given user input

Type positive integer

postprocessor
Inline and GIP cross section definitions require group boundaries.

Applicability `xsgen` is `gip` or `inline`

parameter **`omit_zaid`**
Omit the provided nuclides from the XS processing.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `xsgen` is `scalecomp` or `anisncomp`

parameter **`orig_zaid`**
Replace MG data for these nuclides in problem materials.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `xsgen` is `scalecomp` or `anisncomp`

parameter **`p_energy_max`**
parameter **`pemax`**
Maximum global photon energy cutoff for cross sections.

Default `25000000.0`

Units eV

Type positive real number

Applicable when `mode` is `p` or `np`

postprocessor
Parameter `p_energy_min` must be less than `p_energy_max`.

Applicability `mode` is `p` or `np`

parameter **`p_energy_min`**
parameter **`pemin`**
Minimum global photon energy cutoff for cross sections.

Default `10000.0`

Units eV

Type positive real number

Applicable when `mode` is `p` or `np`

parameter **`photon_bounds`**
parameter **`pbounds`**
Photon group boundaries.

Default `---`

Type positive floats in decreasing order (each element is a positive real number)

Applicable when `xsgen` is `ampx`, `gip`, `inline`, or `xml`

parameter **`pn_order`**
Scattering order of problem.

Type non-negative integer

parameter **`processing`**
Type of cross section processing to apply.

Default `fulcrum`

Type `fulcrum` or `none`

Applicable when `xsgen` is `scalecomp`

parameter **`subs_zaid`**
Substitute ZAID corresponding to 'orig_zaid.'

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when `xsgen` is `scalecomp` or `anisncomp`

postprocessor
The parameters `orig_zaid` and `subs_zaid` must have the same length.

Applicability `xsgen` is `scalecomp` or `anisncomp`

parameter **`subtract_upscattering`**
parameter **`subup`**
Remove upscattering by subtracting from the total cross section.

Instead of lumping upscatter cross sections into the self-scattering cross section, delete the upscatter cross sections and reduce the total cross section accordingly.

$$\sigma_{\mathrm{t},g} \leftarrow \sigma_{\mathrm{t},g} - \sum_{g'=1}^{g-1} \sigma_{\mathrm{s},g,g'}$$
$$\sigma_{\mathrm{s},g,g'} \leftarrow 0,\ g' = [1, \ldots, g-1]$$

where the outscatter cross section is

$$\sigma_{\mathrm{s}}(E^g \to E^{g'}) \equiv \sigma_{\mathrm{s},g,g'}$$

Default `False`

Type boolean

Applicable when `disable_upscattering` is `True`

parameter **`transport_correction`**
Modify the anisotropy of the scattering cross sections to help preserve solution positivity.

Default `none`

Type `diagonal`, `cesaro`, or `none`

postprocessor
The `cesaro` transport correction requires `pn_order` >= 2.

Applicability `transport_correction` is `cesaro`

parameter **`xml_path`**
Path to an XML cross section input file.

Type file path for reading (extension ‘.xml’)

Applicable when `xsgen` is `xml`

sublist **`[XS]`**
Manual isotropic cross section input. See [PHYSICS][XS] (page 105).

Applicable when `xsgen` is `inline`

parameter **`xs_library`**
SCALE multigroup library name or master library path.

Type file path for reading

Applicable when `xsgen` is `scalecomp`

parameter **`xsgen`***(advanced)*

Type of cross section data input.

The `xsgen` parameter specifies in what format the cross sections are defined for multigroup physics. It is defined automatically by the front end (based on what input the user provides) and should not ever have to be set manually.

Table 20: Possible cross section input formats.

Option	Description
`inline`	The [XS] (page 105) subdatabase is used to define cross sections for every material.
`ampx`	The cross sections for every material are defined in AMPX format. This file is specified using the `ampx_path` parameter.
`gip`	The cross sections for every material are defined in GIP format. This file is specified using the `gip_path` parameter. Other required parameters describing the file must be in the [GIP] sub-database.
`scalecomp`	SCALE multigroup cross sections will be built from composition information pulled from the model.
`anisncomp`	Mixed cross sections will be calculated from ANISN/ADVANTG multigroup libraries using compositions pulled from the model.
`xml`	The cross sections for every material are defined in a separate XML file format. This file is specified using the `xml_path` parameter.

Default based on the user-given input types

Type `scalecomp`, `anisncomp`, `ampx`, `gip`, `inline`, or `xml`

3.18.3 [PHYSICS][GIP]

The GIP file format is supported only for legacy applications. It is essentially a Fortran data dump. Each group of data is written as a single Fortran record comprised of a `(num_reactions, num_moments, num_materials)` array. The number of reactions here is equal to `ihm` plus an extra value if upscattering is present.

parameter **`ihm`**

Cross section table length in GIP file.

Type non-negative integer

parameter **`ihs`**

Position of within-group scattering in GIP file.

Type non-negative integer

parameter **`iht`**
Postition of total cross section in GIP file.

Type non-negative integer

parameter **`isct`**
PN scattering order in GIP file.

Type non-negative integer

parameter **`iups`**
Number of thermal (upscatter) groups in GIP file.

Type non-negative integer

parameter **`nmat`**
Number of materials in GIP file.

Type non-negative integer

parameter **`strict`**
Whether edit cross sections correspond to the GIP standard.

With the `strict` option, the "edit" reactions on the GIP file are assumed to have the following interpretation:

Table 21: GIP reaction tables.

Table	Reaction
iht - 4	χ
iht - 3	Σ_f
iht - 2	Σ_a
iht - 1	$\nu\Sigma_f$

Default `False`

Type boolean

3.18.4 [PHYSICS][XS]

This sub-database specifies all cross sections for a single material. If the material is fissionable, all of `fission`, `nu`, and `chi` must be present. If it is not fissionable, then none of them can be present.

parameter **`chi`**
Fission spectrum.

Default `---`

Type list of non-negative floats (each element is a non-negative real number)

postprocessor
The parameters `total`, `fission`, `nu`, and `chi` must have the same length. Empty lists are ignored.

parameter **`fission`**
Fission cross section.

Default `---`

Type list of non-negative floats (each element is a non-negative real number)

parameter **`matid`**
Material ID.

Type non-negative integer

parameter **`name`**
Label for the material.

Default given matid

Type string without special characters

parameter **`nu`**
Neutron production.

Default `---`

Type list of non-negative floats (each element is a non-negative real number)

parameter **`s0`**
Isotropic scattering cross section.

Type list of non-negative floats (each element is a non-negative real number)

parameter **`total`**
Total cross section by group.

Type list of non-negative floats (each element is a non-negative real number)

3.19 COMPOSITIONS: [COMP]

The *[COMP]* block controls output and management of compositions and enables defining them manually. The matids in each block must correspond to the matids in the problem geometry.

command **`autocolor`**
Attempt to provide color values using their compositions.

Creates color_key

Creates color_val

Applicable when

- 'ENABLE_PYTHON_WRAPPERS' is enabled in this CMake build; and
- The 'matplotlib' python package is installed

parameter **`color_key`***(advanced)*
Name of compositions for which colors are being set.

Default `---`

Type list in which each element is a string

parameter **`color_val`***(advanced)*
Compositions color to be set.

Default `---`

Type list in which each element is a X11 color, HTML color like #FF00ee, tuple, or empty

postprocessor
The parameters `color_key` and `color_val` must have the same length.

command **`colors`**
Map 'color_key' to 'color_val' from pairs or arrow-separated items.

VisIT supports custom colors to be associated with each material in its plotting routines. Materials not specified in this list will be filled with grey. Incorrect material names will generate an error:

```
colors
    m1       "light blue"
    "void"   "dark grey"
    m13      "#aaeeff"
    m14      "DarkSlateGray"
    m105     "#5555FF"
    m106     "pale goldenrod"
```

Valid color names are either HTML-style hexadecimal RGB tuples or *X11 colors*.

For complicated inputs with variable materials, the Python raytracer and coloring modules can be used to automatically assign colors based on materials compositions. (See the `omnibus.raytracer.colors` module.)

Creates color_key

Creates color_val

parameter **`compgen`***(advanced)*
Type of composition input.

Default based on the user-given comp types

Type `model`, `hdf5`, or `inline`

sublist **`[COMPOUND]`**
Elemental compound definition. See [COMP][COMPOUND] (page 110).

Default (empty sublist)

command **`elements`**
Create compounds from natural abundances of the given elements.

Creates compound

deprecated **`force_scl`**
Deprecated entry `force_scl` has been renamed to `load_scl`.

Update to load_scl

parameter **`input`**
Path to the HDF5 file containing compositions.

Type file path for reading (extension '.h5')

Applicable when `compgen` is `hdf5`

parameter **`load_scl`**

Load nuclides from the SCALE Standard Composition Library.

The SCALE standard composition library (SCL) provides a database of nuclides, elements, and compounds that can be used to simplify user composition input.

Exnihilo uses a global database of nuclide data (number densities, names, atomic numbers, etc.) for construction of compositions. This same database is also used to drive SCALE's multigroup cross section builder Fulcrum. If using the SCALE cross section builder (`xsgen processed`), the names in the database must correspond to the names SCALE expects.

Some model types (Geant4, Lava) are able to load nuclide metadata independently of the SCALE SCL; this can interfere with cross section generation. The `load_scl` option preferentially loads SCALE's nuclide definitions.

This option is also useful if using a composition source (hdf5 or inline) that has incomplete nuclide data but is being used for depletion. For example, since only nuclides in use by the current composition set are written to the composition output, it may not be sufficient to use those compositions/nuclides in a depletion run (since additional depletion nuclides will be added to the composition and their nuclide data may be missing).

Note that changing the nuclide data source will change the relationship between composition number densities and weight fractions, so output values may change.

Default True when using 'processed' MG physics, CE physics, or HDF5/inline materials

Type boolean

Applicable when 'SCALE_StdCompLib' is enabled in this build

sublist **`[MATERIAL]`**

Composition definition. See [COMP][MATERIAL] (page 109).

Applicable when `compgen` is `inline`

database **`[NUCLIDES]`**

Nuclide definitions. See [COMP][NUCLIDES] (page 110).

Optional

parameter **`output`**

Save compositions to the output file.

Default `True`

Type boolean

parameter **`sclib_path`**

Path to the SCALE standard composition library.

Default `'/.../scale.rev40.sclib'`

Type file path for reading (extension '.sclib')

Applicable when `load_scl` is `True`

3.19.1 [COMP][MATERIAL]

The material block is for defining an individual composition. Providing *any* materials will override *all* compositions that may be present in the model (page 43).

parameter **`deplete`**
parameter **`depl`**

Flag the material as depletable.

Marking a material as “depletable” tells Shift to enable ORIGEN depletion for this material unless the user overrides this using the options in the [DEPLETION] database.

The default value of “auto” will set this property to true if and only if it is marked as fissionable.

Default `auto`

Type `auto`, `true`, or `false`

parameter **`fission`**
parameter **`fiss`**

Flag the material as fissionable.

Marking a material as “fissionable” sets whether (by default) fission gammas and neutrons will be produced during fixed-source transport. In other words, setting this value to *false* will (again, by default) suppress secondary neutrons or gamma yields from the material.

Note that this option is *ignored* for fission site sampling in kcode/eigenvalue mode: all fissionable nuclides have a chance to create fission sites.

The default value of “auto” will set this property to true if any fissionable nuclide is present, and false if not.

Default `auto`

Type `auto`, `true`, or `false`

parameter **`matid`**

Internal matid number.

The `matid` is a [0,N)-indexed internal numbering system. The matids used by Shift typically differ from the material names used in the problem physics input (for example, *m10* in an MCNP input deck might correspond to matid=1). Currently, the only way to guarantee that this corresponds to a particular material in the geometry input is to use an input that specifies matids explicitly (RTK or mesh geometry). However, by viewing the matid-to-label mapping given in an Omnibus post-process output for a SCALE or MCNP input geometry, it is possible to determine what matid corresponds to what material in a particular problem input.

Type non-negative integer

parameter **`name`**

Label for the material.

Type non-empty string

parameter **`nd`**

Number densities of each nuclide.

Units $\frac{\text{atom}}{(\text{b}\cdot\text{cm})}$

Type list in which each element is a positive real number

postprocessor
The parameters `nd` and `zaid` must have the same length.

parameter **`temperature`**
parameter **`tmp`**
Material temperature.

Units K

Type non-negative real number

parameter **`zaid`**
Element/nuclide IDs (MZZZAAA) in this material.

Type list in which each element is a positive integer

3.19.2 [COMP][NUCLIDES]

Define properties for a given nuclide ID. This enables custom ZAID values in input files such as multigroup cross section data. These properties will override any existing masses loaded from the SCALE SCL.

parameter **`mass`**
Atomic masses of nuclides.

Type list in which each element is a positive real number

postprocessor
The parameters `name`, `zaid`, and `mass` must have the same length.

parameter **`name`**
Names of nuclides.

Type list in which each element is a string

parameter **`zaid`**
Nuclide IDs (MZZZAAA).

Type list in which each element is a positive integer

3.19.3 [COMP][COMPOUND]

Define compounds or natural-abundance elements. Any ZAID in the user model or composition definitions corresponding to the value of `czaid` will be expanded into the `zaid` values provided for this compound. These will override any compound defined by the SCALE SCL.

parameter **`czaid`**
Compound ZAID (e.g., 1000 for elemental hydrogen).

Type positive integer

parameter **`name`**
Descriptive name of the compound.

Type string without special characters

parameter **`wtfrac`**
Weight fraction of each constituent.

Type list in which each element is a positive real number

postprocessor

The parameters `wtfrac` and `zaid` must have the same length.

parameter **`zaid`**

Consitutent nuclide IDs (MZZZAAA).

Type list in which each element is a positive integer

3.20 RESPONSES: [RESPONSE]

The RESPONSE block is for defining energy- and particle-dependent responses such as dose conversion factors. Each response can be used multiple times in the tallies.

Table 22: Available types for the [RESPONSE] database

Type	Description	Applicability
histogram (page 111)	Histogram response	
interpolated (page 112)	Interpolation between values	
xs (page 112)	Microscopic cross section multiplier	

3.20.1 [RESPONSE=HISTOGRAM]

The "histogram" response is effectively a piecewise constant cross section. The response is the specified value of the response (page 111) parameter inside the corresponding energy (page 111) bin for the given particle type (page 111). The response is zero for other particle types or outside the given energy range.

parameter **`description`**

Optional longer descriptive string.

Default `''`

Type string

parameter **`energy`**

parameter **`e`**

Lowest bound plus upper bounds for the histograms.

Units eV

Type monotonically increasing list (each element is a real number)

parameter **`name`**

Short title or label for response.

Type string without special characters

parameter **`particle_type`**

parameter **`pt`**

Particle type to apply this response.

Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter **`response`**

parameter **`r`**

Histogram response values.

Type list in which each element is a real number

postprocessor

Size of energy bounds must be one greater than the number of response values.

3.20.2 [RESPONSE=INTERPOLATED]

Interpolation between values.

parameter **`description`**
: Optional longer descriptive string.

  Default `''`

  Type string

parameter **`energy`**
parameter **`e`**
: Energy points.

  Units eV

  Type monotonically increasing list (each element is a positive real number)

parameter **`interpolation_type`**
parameter **`interp`**
: Type of interpolated response.

  Type `linear`, `log_lin`, `lin_log`, or `log_log`

parameter **`name`**
: Short title or label for response.

  Type string without special characters

parameter **`particle_type`**
parameter **`pt`**
: Particle type to apply this response.

  Type particle type (`n`, `neutron`, `p`, or `photon`)

parameter **`response`**
parameter **`r`**
: Response values at energy points.

  Type list in which each element is a real number

postprocessor
: Response must be positive for log_log or log_lin.

postprocessor
: The parameters `energy` and `response` must have the same length.

3.20.3 [RESPONSE=XS]

Microscopic cross section multiplier.

parameter **`density`**
: Density multiplier for response calculation.

  Default `1.0`

  Type positive real number

parameter **`description`**

Optional longer descriptive string.

> **Default** `''`
>
> **Type** string

parameter **`mt`**

Reaction to tally.

> **Type** MT number or name (e.g., N_GAMMA, 102)

parameter **`name`**

Short title or label for response.

> **Type** string without special characters

parameter **`nuclide`**

Nuclide ID for the cross section.

> **Type** nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

parameter **`particle_type`**

parameter **`pt`**

Particle type to apply this response.

> **Type** particle type (`n`, `neutron`, `p`, or `photon`)

parameter **`physics`***(advanced)*

Name of the physics DB to use for the source data.

> **Default** the name of the CE physics database
>
> **Type** string without special characters

parameter **`temperature`**

parameter **`tmp`**

Temperature of nuclide.

> **Type** positive real number
>
> **Applicable when** `particle_type` is `n`

3.21 TALLIES: [TALLY]

Be aware that unless otherwise specified, tallies in Shift:

- are *replicated*, even if domain decomposition is requested;
- use history-based statistics to estimate variance;
- provide volume-averaged reaction rates if the tally region's volume is known;
- are path length estimators.

Many tallies support a common set of attributes, including a name and optional description, a list of reactions to tally, a list of [RESPONSE] (page 111) objects, and neutron and photon energy bin boundaries.

Note: Unlike other Monte Carlo transport codes, the bin boundaries in Omnibus are truly boundaries, not upper or lower energies. Therefore, the number of energy bins will be one less than the number of bounds. To reproduce the behavior of MCNP and Monaco, which tally from the cutoff energy to the lowest given energy, the user must explicitly add the cutoff energy as the lowest energy bound.

The cell and mesh tallies produce volume averaged quantities when volumes are available for the region being tallied. Therefore, a reaction rate is output as a reaction rate density (units of $\frac{\text{reaction}}{\text{s}-\text{cm}^3}$). If volumes are not provided (explicitly by the user or automatically by the geometry) for cell tallies, a warning will be issued and the tally result will be cell-integrated.

Warning: Many geometries define the volume of a cell to be the volume for an *instance* of that cell. If the cell is replicated (e.g., a pin cell in an assembly), then the volume being used to normalize the tally *might not* correspond to the total volume being tallied. This is because all instances of a cell will contribute to the same tally.

Because of the potential ambiguities that may occur with volume normalization, it is **highly** recommended that users check the `volumes` field output alongside cell tallies. A volume entry of `0` means that the volume was not provided, so that the corresponding tally will have units of $\frac{\text{reaction}}{\text{s}}$ as though the tally region had unit volume.

sublist **`[BATCH_MESH]`***(advanced)*

Tally reaction rates using batch statistics (*experimental*!). See [TALLY][BATCH_MESH] (page 160).

Applicable when problem mode is `kcode`

Optional

sublist **`[BIRTH_SPECTRUM]`**

Tally the energy distribution of particles at birth in geometry cells. See [TALLY][BIRTH_SPECTRUM] (page 158).

Optional

Applicable when solver is ‘shift’

sublist **`[CELL]`**

Tally reaction rates in geometry cells and unions of cells. See [TALLY][CELL] (page 130).

Optional

sublist **`[CYLMESH]`**

Tally reaction rates in cylindrical cells. See [TALLY][CYLMESH] (page 123).

Optional

sublist **`[DIAGNOSTIC]`**

Singleton tallies used for transport diagnostic purposes. See [TALLY][DIAGNOSTIC] (page 140).

Applicable when solver is ‘shift’

Default (empty sublist)

sublist **[HEXMESH]**
Tally reaction rates on a hexagonal grid. See [TALLY][HEXMESH] (page 127).

Optional

sublist **[HEXNODAL]**
Tally integral quantities on a hexagonal mesh for nodal calculations. See [TALLY][HEXNODAL] (page 150).

Applicable when solver is ‘shift’

Optional

sublist **[MEAN_SCATTER_ANGLE]**
Tally the mean scattering angle in geometry cells. See [TALLY][MEAN_SCATTER_ANGLE] (page 156).

Optional

Applicable when solver is ‘shift’

sublist **[MESH]**
Tally reaction rates on a domain-decomposed Cartesian mesh. See [TALLY][MESH] (page 116).

Optional

sublist **[MESH_SURFACE]**
Tally reaction rates and partial currents on mesh faces. See [TALLY][MESH_SURFACE] (page 121).

Optional

sublist **[MICRO]**
Tally flux and microscopic cross sections in materials. See [TALLY][MICRO] (page 138).

Applicable when

- solver is ‘shift’; and
- physics is CE

Optional

sublist **[MIGRATION_AREA]**
Tally particle migration area on a Cartesian mesh. See [TALLY][MIGRATION_AREA] (page 154).

Applicable when solver is ‘shift’

Optional

sublist **[NODAL]**
Tally integral quantities on a Cartesian mesh for nodal calculations. See [TALLY][NODAL] (page 146).

Applicable when solver is ‘shift’

Optional

sublist **[SCATTERING_PROB_MATRIX]**
Tally the group-to-group scattering probability matrix in geometry cells. See [TALLY][SCATTERING_PROB_MATRIX] (page 157).

Optional

Applicable when solver is 'shift'

database `[SENSITIVITY]`
Tally sensitivities for use in uncertainty quantification. See [TALLY][SENSITIVITY] (page 144).

Optional

Applicable when

- physics is CE; and
- 'Sensitivity' is enabled in this build

sublist `[SHADOW]`
Tally arbitrary cells in an overlaid but non-interacting geometry. See [TALLY][SHADOW] (page 135).

Applicable when 'GG' is enabled in this build

Optional

sublist `[SURFACE_CENSUS]`
Tally individual particle properties as they cross a geometry surface. See [TALLY][SURFACE_CENSUS] (page 159).

Applicable when solver is 'shift'

Optional

database `[SWORD]`
Include tally definitions from SWORD input. See [TALLY][SWORD] (page 141).

Optional

Applicable when model is 'sword'

sublist `[VERA]`
Tally in cells in a VERA model. See [TALLY][VERA] (page 134).

Optional

3.21.1 [TALLY][MESH]

Shift supports multiple structured Cartesian path length mesh tallies. The mesh can be defined over all or part of the physical problem geometry. If domain decomposition is enabled in Shift, only the part of the mesh tally that is present on a spatial domain will be transported on.

parameter `cycles`
The kcode problem phase in which this tally is active.

Default `active`

Type `active` or `inactive`

Applicable when problem mode is `kcode`

parameter `delta_x`
Length of mesh tally cell on the X axis.

Units cm

Type positive real number

Applicable when `type` is `global`

parameter **`delta_y`**

Length of mesh tally cell on the Y axis.

Units cm

Type positive real number

Applicable when `type` is `global`

parameter **`delta_z`**

Length of mesh tally cell on the Z axis.

Units cm

Type positive real number

Applicable when `type` is `global`

command **`deltas`**

Expand into parameters `delta_x`, `delta_y`, and `delta_z`.

Creates delta_x

Creates delta_y

Creates delta_z

parameter **`description`**

parameter **`desc`**

Optional longer descriptive string.

Default `''`

Type string

database **`[FILTERS]`**

Tally filtering options. See [TALLY][MESH][FILTERS] (page 161).

Optional

parameter **`macro_mt`**

ENDF reactions for partial macroscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`macro_mt_zaid`**

Nuclide IDs for partial macroscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`macro_rxn`**

Special reactions for macroscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

parameter **`macro_rxn_zaid`**

Nuclide IDs for macroscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_mt`**

ENDF reactions for microscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor

The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter **`micro_mt_zaid`**

Nuclide IDs for microscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_rxn`**

Special reactions for microscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor
The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

Applicability physics is CE

parameter **`micro_rxn_zaid`**
Nuclide IDs for microscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

deprecated **`micro_zaid`**
Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

Update to micro_mt_zaid

parameter **`mt`**
Additional macroscopic reaction rates to tally.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`name`**
Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**
Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**
Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`photon_bins`**
parameter **`pbins`**
Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number) *parameter* **`reactions`**

parameter **`rxn`**

Reactions to calculate for this tally.

Default `flux`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

parameter **`responses`**

parameter **`resp`**

Responses for this tally.

Default `---`

Type list in which each element is a string

postprocessor

Validate response names against [RESPONSE] blocks.

parameter **`type`**

Type of mesh tally.

Default `grid`

Type `grid` or `global`

parameter **`x`**

Tally grid coordinates along the X axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

parameter **`y`**

Tally grid coordinates along the Y axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

parameter **`z`**

Tally grid coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

3.21.2 [TALLY][MESH_SURFACE]

The Cartesian mesh *surface* tally can calculate surface flux, current, or partial current on each face of the mesh. The allowed reactions for this tally differ from the volumetric mesh tally (page 116) reactions.

parameter **`cycles`**
The kcode problem phase in which this tally is active.

> **Default** `active`
>
> **Type** `active` or `inactive`
>
> **Applicable when** solver is 'shift'

parameter **`delta_x`**
Length of mesh current tally cell on the X axis.

> **Units** cm
>
> **Type** positive real number
>
> **Applicable when** `type` is `global`

parameter **`delta_y`**
Length of mesh current tally cell on the Y axis.

> **Units** cm
>
> **Type** positive real number
>
> **Applicable when** `type` is `global`

parameter **`delta_z`**
Length of mesh current tally cell on the Z axis.

> **Units** cm
>
> **Type** positive real number
>
> **Applicable when** `type` is `global`

command **`deltas`**
Expand into parameters `delta_x`, `delta_y`, and `delta_z`.

> **Creates** delta_x
>
> **Creates** delta_y
>
> **Creates** delta_z

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

> **Default** `''`
>
> **Type** string

database **`[FILTERS]`**
Tally filtering options. See [TALLY][MESH][FILTERS] (page 161).

> **Optional**

parameter **`name`**
: Short title or label for the tally.

  Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**
: Energy bin boundaries for neutrons.

  Default `---`

  Units eV

  Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**
: Constant multiplicative factor to apply to tally results.

  Default `1.0`

  Type positive real number

parameter **`photon_bins`**
parameter **`pbins`**
: Energy bin boundaries for photons.

  Default `---`

  Units eV

  Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`reactions`**
parameter **`rxn`**
: Type of mesh surface tally.

  Default `flux`

  Type list in which each element is a `flux`, `current`, `partial_current_negative`, or `partial_current_positive`

parameter **`type`**
: Type of mesh surface tally.

  Default `grid`

  Type `grid` or `global`

parameter **`x`**
: Mesh current tally coordinates along the X axis.

  Units cm

  Type monotonically increasing list with at least two values (each element is a real number)

  Applicable when `type` is `grid`

parameter **`y`**
: Mesh current tally coordinates along the Y axis.

  Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

parameter **`z`**

Mesh current tally coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

3.21.3 [TALLY][CYLMESH]

Particles can be tracked on a translated, rotated cylinder broken into (r, z, θ) mesh cells.

parameter **`cycles`**

The kcode problem phase in which this tally is active.

Default `active`

Type `active` or `inactive`

Applicable when problem mode is `kcode`

parameter **`description`**
parameter **`desc`**

Optional longer descriptive string.

Default `''`

Type string

parameter **`macro_mt`**

ENDF reactions for partial macroscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`macro_mt_zaid`**

Nuclide IDs for partial macroscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`macro_rxn`**

Special reactions for macroscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

parameter `macro_rxn_zaid`
Nuclide IDs for macroscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter `micro_mt`
ENDF reactions for microscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor
The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter `micro_mt_zaid`
Nuclide IDs for microscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter `micro_rxn`
Special reactions for microscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor
The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

Applicability physics is CE

parameter `micro_rxn_zaid`
Nuclide IDs for microscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

deprecated **`micro_zaid`**

Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

Update to micro_mt_zaid

parameter **`mt`**

Additional macroscopic reaction rates to tally.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`name`**

Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**

Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**

Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`photon_bins`**
parameter **`pbins`**

Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`r`**

Radial mesh coordinates.

Units cm

Type monotonically increasing list with at least two values, starting with zero (each element is a real number)

parameter **`reactions`**
parameter **`rxn`**

Reactions to calculate for this tally.

Default `flux`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

parameter **`responses`**
parameter **`resp`**
Responses for this tally.

Default `---`

Type list in which each element is a string

postprocessor
Validate response names against [RESPONSE] blocks.

parameter **`rotate`**
parameter **`rot`**
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

parameter **`theta`**
Theta mesh coordinates.

Default `0.0 1.0`

Units revolution

Type monotonically increasing list with at least two values, starting with zero and ending with one [revolution] (each element is a real number)

parameter **`translate`**
parameter **`trans`**
Translation vector (applied after rotation).

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter **`z`**
Mesh coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

3.21.4 [TALLY][HEXMESH]

Tally volumetric path lengths on a hexagonal (triangular-pitch) mesh. This tally is meant for nodal data calculations and should generally not be used. The mesh boundaries must encompass the entirety of the transportable problem domain.

parameter **`apothem`**
Distance from hex center to face center.

Units cm

Type positive real number

parameter **`center_hex`**
(x,y) centroid of center hex.

Units cm

Type length-2 float vector (each element is a real number)

parameter **`cycles`**
The kcode problem phase in which this tally is active.

Default `active`

Type `active` or `inactive`

Applicable when problem mode is `kcode`

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

database **`[FILTERS]`**
Tally filtering options. See [TALLY][MESH][FILTERS] (page 161).

Optional

parameter **`macro_mt`**
ENDF reactions for partial macroscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`macro_mt_zaid`**
Nuclide IDs for partial macroscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`macro_rxn`**

Special reactions for macroscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

parameter **`macro_rxn_zaid`**

Nuclide IDs for macroscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_mt`**

ENDF reactions for microscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor

The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter **`micro_mt_zaid`**

Nuclide IDs for microscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_rxn`**

Special reactions for microscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor
The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

Applicability physics is CE

parameter **`micro_rxn_zaid`**
Nuclide IDs for microscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

deprecated **`micro_zaid`**
Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

Update to micro_mt_zaid

parameter **`mt`**
Additional macroscopic reaction rates to tally.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`name`**
Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**
Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**
Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`num_rings`**
Number of rings around the central hex.

Type non-negative integer

parameter **`photon_bins`**
parameter **`pbins`**
Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **reactions**
parameter **rxn**
Reactions to calculate for this tally.

Default `flux`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

parameter **responses**
parameter **resp**
Responses for this tally.

Default `---`

Type list in which each element is a string

postprocessor
Validate response names against [RESPONSE] blocks.

parameter **z**
Mesh coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

3.21.5 [TALLY][CELL]

Geometry cells and unions of cells are tallied using a hash table, allowing constant-time scaling with respect to the number of total cells being tallied.

The recommended way to tally multiple particle spectra in the same cell is to use a single tally.

```
[TALLY][CELL energybinned]
description "5n3g energy-binned tally."
reactions flux
cells 1 100 4:5:6
neutron_bins  1e7 1e6 1e3 10 1 1e-3
photon_bins   2e7 1e6 1e5 1e3
```

command **cells**
Generate 'union_cells' and 'union_lengths' from colon-separated unions.

Creates union_cells

Creates union_lengths

parameter **cycles**
The kcode problem phase in which this tally is active.

Default `active`

Type `active` or `inactive`

Applicable when problem mode is `kcode`

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

database **`[FILTERS]`**
Tally filtering options. See [TALLY][MESH][FILTERS] (page 161).

Optional

parameter **`macro_mt`**
ENDF reactions for partial macroscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`macro_mt_zaid`**
Nuclide IDs for partial macroscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`macro_rxn`**
Special reactions for macroscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

parameter **`macro_rxn_zaid`**
Nuclide IDs for macroscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_mt`**

ENDF reactions for microscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor

The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter **`micro_mt_zaid`**

Nuclide IDs for microscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_rxn`**

Special reactions for microscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor

The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

Applicability physics is CE

parameter **`micro_rxn_zaid`**

Nuclide IDs for microscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

deprecated **`micro_zaid`**

Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

The `micro_zaid` and `micro_mt` parameters are used to tally microscopic reaction rates for nuclides *in the material being tallied*. That is, if the user requests reaction rates for tungsten absorption in a cell that has pure water, the tally result for that cell will be zero. This allows the user (for example) to input trace nuclides in depletion calculations and only have nonzero reaction rates when the transport nuclide density is nonzero.

Example:

```
micro_zaid :micro_mt
      1001   N_TOTAL
      8016   N_TOTAL
      8016   N_ELASTIC
      8016   N_INELASTIC
```

Update to micro_mt_zaid

parameter **mt**

Additional macroscopic reaction rates to tally.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **name**

Short title or label for the tally.

Type string without special characters

parameter **neutron_bins**

parameter **nbins**

Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **normalization**

Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **photon_bins**

parameter **pbins**

Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **reactions**

parameter **rxn**

Reactions to calculate for this tally. See reactions (page 119) in [TALLY][MESH].

parameter **responses**

parameter **resp**

Responses for this tally.

Default `---`

Type list in which each element is a string

postprocessor
Validate response names against [RESPONSE] blocks.

parameter **`union_cells`***(advanced)*
Flattened list of cells in each union.

Type list of cell names (each element is a string)

parameter **`union_lengths`***(advanced)*
Number of cells per union in the above list.

Type list in which each element is a integer

3.21.6 [TALLY][VERA]

If using a VERA model input, this will create a cell tally for the outermost cell of the vessel, which can then be optimized for when running in hybrid mode.

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

parameter **`name`**
Short title or label for the tally.

Type string without special characters

parameter **`normalization`**
Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`reactions`**
parameter **`rxn`**
Reactions to calculate for this tally.

Default `flux`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

3.21.7 [TALLY][SHADOW]

"Shadow" path length tallies track through a secondary geometry during normal transport. Particles do not interact with this "shadow geometry," but they are tallied spatially over the cells in the shadow geometry. The shadow geometry is defined by an external Geometria/GG input file, distinct from the primary tracking geometry.

During transport, a fast test is performed at the beginning of every particle track to determine whether the track intersects with the bounding box of the geometry. If so, the particle's location inside the shadow geometry is determined, distances to boundaries are calculated, and the particle's track is tallied on top of the shadow geometry cells.

Every cell in the shadow geometry is tallied; however, due to the underlying geometry implementation, some cells will never receive a score. For example, a "cell" representing the outside of the universe is always created, but since the tally is not accumulated if the particle is outside the shadow geometry, that cell is never scored.

parameter **`cycles`**

The kcode problem phase in which this tally is active.

> **Default** `active`
>
> **Type** `active` or `inactive`
>
> **Applicable when** problem mode is `kcode`

parameter **`description`**
parameter **`desc`**

Optional longer descriptive string.

> **Default** `''`
>
> **Type** string

command **`input`**

Generate a Geometria XML representation from an `.gg.omn` input.

> **Creates** xml_path

parameter **`macro_mt`**

ENDF reactions for partial macroscopic cross section tallying.

> **Default** `---`
>
> **Type** list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))
>
> **Applicable when** physics is CE

parameter **`macro_mt_zaid`**

Nuclide IDs for partial macroscopic cross section tallying.

> **Default** `---`
>
> **Type** list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)
>
> **Applicable when** physics is CE

parameter **`macro_rxn`**

Special reactions for macroscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

parameter **`macro_rxn_zaid`**

Nuclide IDs for macroscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_mt`**

ENDF reactions for microscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor

The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter **`micro_mt_zaid`**

Nuclide IDs for microscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_rxn`**

Special reactions for microscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor
The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

> **Applicability** physics is CE

parameter **`micro_rxn_zaid`**
Nuclide IDs for microscopic 'special reaction' cross section tallying.

> **Default** `---`
>
> **Type** list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)
>
> **Applicable when** physics is CE

deprecated **`micro_zaid`**
Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

> **Update to** micro_mt_zaid

parameter **`mt`**
Additional macroscopic reaction rates to tally.

> **Default** `---`
>
> **Type** list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))
>
> **Applicable when** physics is CE

parameter **`name`**
Short title or label for the tally.

> **Type** string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**
Energy bin boundaries for neutrons.

> **Default** `---`
>
> **Units** eV
>
> **Type** nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**
Constant multiplicative factor to apply to tally results.

> **Default** `1.0`
>
> **Type** positive real number

parameter **`photon_bins`**
parameter **`pbins`**
Energy bin boundaries for photons.

> **Default** `---`
>
> **Units** eV
>
> **Type** nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`reactions`**
parameter **`rxn`**

Reactions to calculate for this tally.

> **Default** `flux`
>
> **Type** list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

parameter **`responses`**
parameter **`resp`**

Responses for this tally.

> **Default** `---`
>
> **Type** list in which each element is a string

postprocessor

Validate response names against [RESPONSE] blocks.

parameter **`xml_path`***(advanced)*

Path to the Geometria XML input file.

> **Type** file path for reading (extension '.xml')

3.21.8 [TALLY][MICRO]

The "micro" tally is primarily used for depletion coupling. It calculates material-averaged, flux-weighted cross sections for multiple materials, nuclides, and reactions. The user specifies a list of materials to tally, as well as a list of nuclide/reaction pairs. During the tally setup phase in Shift, a list is constructed of all the possible nuclide/reaction pairs in each mix table, and nuclides or reactions that are absent in each mixture are elided.

Note that the volumes of all cells that contain the given materials must be specified. If any of these are absent, an error will be issued that enumerates the needed cells with missing volumes.

If no particles are sampled in one of the requested materials, the flux is zero and the microscopic cross section will be set to the sentinel flag of -1.

parameter **`description`**
parameter **`desc`**

Optional longer descriptive string.

> **Default** `''`
>
> **Type** string

parameter **`materials`**
parameter **`mats`**

Materials in which to tally.

> **Type** list in which each element is a non-empty string

postprocessor

At least one *micro_mt_zaid:micro_mt* pair must be set.

parameter **`micro_mt`**

ENDF reactions for microscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor

The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter **`micro_mt_zaid`**

Nuclide IDs for microscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_rxn`**

Special reactions for microscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor

The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

Applicability physics is CE

parameter **`micro_rxn_zaid`**

Nuclide IDs for microscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

deprecated **`micro_zaid`**

Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

Update to micro_mt_zaid

parameter **`name`**

Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**

Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**

Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`photon_bins`**
parameter **`pbins`**

Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

3.21.9 [TALLY][DIAGNOSTIC]

Table 23: Available types for the [DIAGNOSTIC] database

Type	Description	Applicability
pathlength (page 162)	Measure distributions of step lengths traveled in the transporter	
collision (page 162)	Measure the materials and nuclides in which collisions occur	physics is CE
source (page 162)	Measure the particle source distribution	
history (page 163)	Write out all events that occur for a history or series of histories	
debug_history (page 163)	Write events for failed particle histories	
debug (page 163)	Track common transport statistics	
history_time (page 163)	Write transport time for each particle history	
fiss_site (page 163)	Write cycle-to-cycle fission event locations	problem mode is `kcode`
split (page 163)	Write particle variance reduction splitting locations	problem mode is `hybrid`
roulette (page 163)	Write particle variance reduction rouletting locations	problem mode is `hybrid`

3.21.10 [TALLY][SWORD]

When using a SWORD model input, this will import SWORD tally cells into the problem.

parameter **`cycles`**

The kcode problem phase in which this tally is active.

Default `active`

Type `active` or `inactive`

Applicable when problem mode is `kcode`

parameter **`description`**
parameter **`desc`**

Optional longer descriptive string.

Default `''`

Type string

parameter **`macro_mt`**

ENDF reactions for partial macroscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`macro_mt_zaid`**

Nuclide IDs for partial macroscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`macro_rxn`**

Special reactions for macroscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

parameter **`macro_rxn_zaid`**

Nuclide IDs for macroscopic ‘special reaction’ cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_mt`**
ENDF reactions for microscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor
The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter **`micro_mt_zaid`**
Nuclide IDs for microscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_rxn`**
Special reactions for microscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor
The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

Applicability physics is CE

parameter **`micro_rxn_zaid`**
Nuclide IDs for microscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

deprecated **`micro_zaid`**
Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

Update to micro_mt_zaid

parameter **`mt`**
Additional macroscopic reaction rates to tally.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`name`**
Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**
Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**
Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`photon_bins`**
parameter **`pbins`**
Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`reactions`**
parameter **`rxn`**
Reactions to calculate for this tally.

Default `flux`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

parameter **`responses`**
parameter **`resp`**
Responses for this tally.

Default `---`

Type list in which each element is a string

postprocessor
Validate response names against [RESPONSE] blocks.

3.21.11 [TALLY][SENSITIVITY]

The sensitivity tally calculates eigenvalue sensitivities to cross sections and to ratios of cross sections.

parameter **binned**
Store fully binned tallies.

Default `False`

Type boolean

parameter **constrained_chi**
Calculate constrained chi values.

Default `True`

Type boolean

parameter **covariance**
Use the covariance between tallies and the normalization factor when calculating final sensitivity variance.

Default `True`

Type boolean

parameter **cycles_per_batch**
Number of kcode cycles in a statistical batch.

Default `1`

Type positive integer

parameter **eint**
Store energy-integrated tallies.

Default `False`

Type boolean

parameter **latent_generations**
parameter **cfp**
Number of latent generations.

Default `5`

Type positive integer

Applicable when `method` is `ifp` or `gpt`

parameter **materials**
parameter **mats**
Materials in which to tally sensitivities.

A single asterisk (as a wild card) will cause sensitivities for all materials to be tallied:

```
materials *
```

Default `'*'`

Type list in which each element is a non-empty string

parameter **`meint`**

Store energy- and material-integrated tallies.

Default `True`

Type boolean

parameter **`method`**
parameter **`cet`**

Sensitivity coefficient calculation mode.

Default `clutch`

Type `clutch`, `ifp`, or `gpt`

parameter **`mint`**

Store material-integrated tallies.

Default `True`

Type boolean

parameter **`mts`**
parameter **`mt`**

MT reactions to tally.

Default `-1`

Type list in which each element is a MT name or ZAID, or '*' for default reactions

parameter **`neutron_bins`**
parameter **`nbins`**

Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`nuclides`**
parameter **`nucl`**

Nuclide IDs for microscopic cross section tallying.

A single asterisk (as a wild card) will cause sensitivities for all nuclides to be tallied:

```
nuclides *
```

Default `-1`

Type list in which each element is a Nuclide name or ZAID, or '*' for all nuclides

sublist **`[RATIO]`**

Define a ratio of two responses to calculate. See [TALLY][SENSITIVITY][RATIO] (page 165).

Applicable when `method` is `gpt`

sublist **`[RESPONSE]`**

Define a sensitivity response. See [TALLY][SENSITIVITY][RESPONSE] (page 164).

Applicable when `method` is `gpt`

3.21.12 [TALLY][NODAL]

Tally integral quantities on a Cartesian mesh for nodal calculations.

parameter **`birth_spectrum`**
Tally birth spectrum of particles.

Type boolean

parameter **`cycles`**
The kcode problem phase in which this tally is active.

Default `active`

Type `active` or `inactive`

Applicable when problem mode is `kcode`

parameter **`delta_x`**
Length of mesh tally cell on the X axis.

Units cm

Type positive real number

Applicable when `type` is `global`

parameter **`delta_y`**
Length of mesh tally cell on the Y axis.

Units cm

Type positive real number

Applicable when `type` is `global`

parameter **`delta_z`**
Length of mesh tally cell on the Z axis.

Units cm

Type positive real number

Applicable when `type` is `global`

command **`deltas`**
Expand into parameters `delta_x`, `delta_y`, and `delta_z`.

Creates delta_x

Creates delta_y

Creates delta_z

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

parameter `diffusion_coefficients`
Tally diffusion coefficients.

Type boolean

parameter `eddington_factors`
Tally the eddington factors.

Type boolean

database `[FILTERS]`
Tally filtering options. See [TALLY][MESH][FILTERS] (page 161).

Optional

parameter `macro_mt`
ENDF reactions for partial macroscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter `macro_mt_zaid`
Nuclide IDs for partial macroscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter `macro_rxn`
Special reactions for macroscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

parameter `macro_rxn_zaid`
Nuclide IDs for macroscopic ‘special reaction’ cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter `mean_transfer_angle`
Tally mean transfer angle.

Type boolean

parameter **`micro_mt`**

ENDF reactions for microscopic cross section tallying.

Default ---

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor

The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter **`micro_mt_zaid`**

Nuclide IDs for microscopic cross section tallying.

Default ---

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_rxn`**

Special reactions for microscopic cross section tallying.

Default ---

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor

The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

Applicability physics is CE

parameter **`micro_rxn_zaid`**

Nuclide IDs for microscopic 'special reaction' cross section tallying.

Default ---

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

deprecated **`micro_zaid`**

Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

Update to micro_mt_zaid

parameter **`mt`**

Additional macroscopic reaction rates to tally.

Default ---

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter `name`

Short title or label for the tally.

Type string without special characters

parameter `neutron_bins`

parameter `nbins`

Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter `normalization`

Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter `photon_bins`

parameter `pbins`

Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter `reactions`

parameter `rxn`

Reactions to calculate for this tally.

Default `flux`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

parameter `responses`

parameter `resp`

Responses for this tally.

Default `---`

Type list in which each element is a string

postprocessor

Validate response names against [RESPONSE] blocks.

parameter **`transfer_matrices`**

Tally the P0 and P1 transfer matrices.

Type boolean

parameter **`type`**

Type of mesh tally.

Default `grid`

Type `grid` or `global`

parameter **`x`**

Tally grid coordinates along the X axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

parameter **`y`**

Tally grid coordinates along the Y axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

parameter **`z`**

Tally grid coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

3.21.13 [TALLY][HEXNODAL]

Tally integral quantities on a hexagonal mesh for nodal calculations.

parameter **`apothem`**

Distance from hex center to face center.

Units cm

Type positive real number

parameter **`birth_spectrum`**

Tally birth spectrum of particles.

Type boolean

parameter **`center_hex`**

(x,y) centroid of center hex.

Units cm

Type length-2 float vector (each element is a real number)

parameter **`cycles`**

The kcode problem phase in which this tally is active.

> **Default** `active`
>
> **Type** `active` or `inactive`
>
> **Applicable when** problem mode is `kcode`

parameter **`description`**
parameter **`desc`**

Optional longer descriptive string.

> **Default** `''`
>
> **Type** string

parameter **`diffusion_coefficients`**

Tally diffusion coefficients.

> **Type** boolean

parameter **`eddington_factors`**

Tally the eddington factors.

> **Type** boolean

database **`[FILTERS]`**

Tally filtering options. See [TALLY][MESH][FILTERS] (page 161).

> **Optional**

parameter **`macro_mt`**

ENDF reactions for partial macroscopic cross section tallying.

> **Default** `---`
>
> **Type** list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))
>
> **Applicable when** physics is CE

parameter **`macro_mt_zaid`**

Nuclide IDs for partial macroscopic cross section tallying.

> **Default** `---`
>
> **Type** list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)
>
> **Applicable when** physics is CE

parameter **`macro_rxn`**

Special reactions for macroscopic cross section tallying.

> **Default** `---`
>
> **Type** list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

parameter **`macro_rxn_zaid`**
Nuclide IDs for macroscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`mean_transfer_angle`**
Tally mean transfer angle.

Type boolean

parameter **`micro_mt`**
ENDF reactions for microscopic cross section tallying.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

postprocessor
The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

Applicability physics is CE

parameter **`micro_mt_zaid`**
Nuclide IDs for microscopic cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

parameter **`micro_rxn`**
Special reactions for microscopic cross section tallying.

Default `---`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

Applicable when physics is CE

postprocessor
The parameters `micro_rxn_zaid` and `micro_rxn` must have the same length.

Applicability physics is CE

parameter **`micro_rxn_zaid`**
Nuclide IDs for microscopic 'special reaction' cross section tallying.

Default `---`

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

Applicable when physics is CE

deprecated **`micro_zaid`**

Deprecated entry `micro_zaid` has been renamed to `micro_mt_zaid`.

Update to micro_mt_zaid

parameter **`mt`**

Additional macroscopic reaction rates to tally.

Default `---`

Type list of MT numbers or names (each element is a MT number or name (e.g., N_GAMMA, 102))

Applicable when physics is CE

parameter **`name`**

Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**

Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**

Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`num_rings`**

Number of rings around the central hex.

Type non-negative integer

parameter **`photon_bins`**
parameter **`pbins`**

Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`reactions`**
parameter **`rxn`**

Reactions to calculate for this tally.

Default `flux`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

parameter **`responses`**
parameter **`resp`**
Responses for this tally.

Default `---`

Type list in which each element is a string

postprocessor
Validate response names against [RESPONSE] blocks.

parameter **`transfer_matrices`**
Tally the P0 and P1 transfer matrices.

Type boolean

parameter **`z`**
Mesh coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

3.21.14 [TALLY][MIGRATION_AREA]

Tally particle migration area on a Cartesian mesh.

parameter **`delta_x`**
Length of mesh tally cell on the X axis.

Units cm

Type positive real number

Applicable when `type` is `global`

parameter **`delta_y`**
Length of mesh tally cell on the Y axis.

Units cm

Type positive real number

Applicable when `type` is `global`

parameter **`delta_z`**
Length of mesh tally cell on the Z axis.

Units cm

Type positive real number

Applicable when `type` is `global`

command **`deltas`**

Expand into parameters `delta_x`, `delta_y`, and `delta_z`.

Creates delta_x

Creates delta_y

Creates delta_z

parameter **`description`**

parameter **`desc`**

Optional longer descriptive string.

Default `''`

Type string

database **`[FILTERS]`**

Tally filtering options. See [TALLY][MESH][FILTERS] (page 161).

Optional

parameter **`name`**

Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**

parameter **`nbins`**

Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`type`**

Type of mesh tally.

Default `grid`

Type `grid` or `global`

parameter **`x`**

Tally grid coordinates along the X axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

parameter **`y`**

Tally grid coordinates along the Y axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

parameter **`z`**

Tally grid coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `type` is `grid`

3.21.15 [TALLY][MEAN_SCATTER_ANGLE]

Tally the mean scattering angle in geometry cells.

command **`cells`**

Generate 'union_cells' and 'union_lengths' from colon-separated unions.

Creates union_cells

Creates union_lengths

parameter **`description`**
parameter **`desc`**

Optional longer descriptive string.

Default `''`

Type string

parameter **`name`**

Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**

Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**

Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`photon_bins`**
parameter **`pbins`**

Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

postprocessor
The parameters ``neutron_bins and photon_bins`` must not all be empty.

parameter **`union_cells`***(advanced)*
Flattened list of cells in each union.

Type list of cell names (each element is a string)

parameter **`union_lengths`***(advanced)*
Number of cells per union in the above list.

Type list in which each element is a integer

3.21.16 [TALLY][SCATTERING_PROB_MATRIX]

Tally the group-to-group scattering probability matrix in geometry cells.

command **`cells`**
Generate 'union_cells' and 'union_lengths' from colon-separated unions.

Creates union_cells

Creates union_lengths

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

parameter **`name`**
Short title or label for the tally.

Type string without special characters

parameter **`neutron_bins`**
parameter **`nbins`**
Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`normalization`**
Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **`photon_bins`**
parameter **`pbins`**
Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

postprocessor
The parameters ``neutron_bins and photon_bins`` must not all be empty.

parameter **union_cells***(advanced)*
Flattened list of cells in each union.

Type list of cell names (each element is a string)

parameter **union_lengths***(advanced)*
Number of cells per union in the above list.

Type list in which each element is a integer

3.21.17 [TALLY][BIRTH_SPECTRUM]

Tally the energy distribution of particles at birth in geometry cells.

command **cells**
Generate 'union_cells' and 'union_lengths' from colon-separated unions.

Creates union_cells

Creates union_lengths

parameter **description**
parameter **desc**
Optional longer descriptive string.

Default `''`

Type string

parameter **name**
Short title or label for the tally.

Type string without special characters

parameter **neutron_bins**
parameter **nbins**
Energy bin boundaries for neutrons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **normalization**
Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

parameter **photon_bins**

parameter `pbins`

Energy bin boundaries for photons.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

postprocessor

The parameters ``neutron_bins` and `photon_bins`` must not all be empty.

parameter `union_cells`*(advanced)*

Flattened list of cells in each union.

Type list of cell names (each element is a string)

parameter `union_lengths`*(advanced)*

Number of cells per union in the above list.

Type list in which each element is a integer

3.21.18 [TALLY][SURFACE_CENSUS]

The surface census tally records a particle's state (position, direction, type, energy) when crossing from the exiting cell to the target cell. The resulting data can be used for using a Shift calculation to generate a starting source for another transport code such as Geant4.

command `cells`

Map 'exiting_cells' to 'target_cells' from pairs or arrow-separated items.

Creates exiting_cells

Creates target_cells

parameter `description`

parameter `desc`

Optional longer descriptive string.

Default `''`

Type string

command `exiting_cells`

Generate 'union_exiting_cells' and 'union_exiting_lengths' from colon-separated unions.

Creates union_exiting_cells

Creates union_exiting_lengths

parameter `kill_particle`

Kill particle when tallied.

Default `True`

Type boolean

parameter `name`

Short title or label for the tally.

Type string without special characters

database **[TAGS]**

Particle tagging options. See [TALLY][SURFACE_CENSUS][TAGS] (page 165).

Optional

command **target_cells**

Generate 'union_target_cells' and 'union_target_lengths' from colon-separated unions.

Creates union_target_cells

Creates union_target_lengths

parameter **union_exiting_cells***(advanced)*

Flattened list of exiting cells in each union.

Type list of cell names (each element is a string)

parameter **union_exiting_lengths***(advanced)*

Number of cells per union in the exiting surface list.

Type list in which each element is a integer

parameter **union_target_cells***(advanced)*

Flattened list of target cells in each union.

Type list of cell names (each element is a string)

parameter **union_target_lengths***(advanced)*

Number of cells per union in the target surface list.

Type list in which each element is a integer

3.21.19 [TALLY][BATCH_MESH]

Tally reaction rates using batch statistics (*experimental*!).

parameter **description**
parameter **desc**

Optional longer descriptive string.

Default `''`

Type string

parameter **name**

Short title or label for the tally.

Type string without special characters

parameter **normalization**

Constant multiplicative factor to apply to tally results.

Default `1.0`

Type positive real number

database **[OUTPUT]**

Output method for the batch tallies. See [TALLY][BATCH_MESH][OUTPUT] (page 166).

Default (empty `hdf5` database)

parameter **`reactions`**
parameter **`rxn`**
Reactions to calculate for this tally.

Default `flux nu_fission`

Type list in which each element is a `flux`, `pos_partial_current_x`, `neg_partial_current_x`, `pos_partial_current_y`, `neg_partial_current_y`, `pos_partial_current_z`, `neg_partial_current_z`, `total`, `absorption`, `scattering`, `transfer_1n`, `transfer_2n`, `transfer_3n`, `transfer_4n`, `fission`, `nu_fission`, `kappa_sigma`, `kappa_sigma_f`, or `kappa_sigma_c`

parameter **`x`**
Mesh tally coordinates along the X axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

parameter **`y`**
Mesh tally coordinates along the Y axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

parameter **`z`**
Mesh tally coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

3.21.20 [TALLY][MESH][FILTERS]

Tally filtering options.

parameter **`birth_cells`**
Only tallies particles born in the given cells.

Default `---`

Type list in which each element is a string

parameter **`birth_energy_range`**
parameter **`be_range`**
Lower and upper birth energy of particles to tally.

Default `---`

Units eV

Type monotonically increasing list (each element is a positive real number)

parameter **`birth_matids`**
Only tallies particles born in the given materials.

Default `---`

Type list in which each element is a positive integer

parameter **`particle_type`**
parameter **`pt`**

Only tallies particles of the given type.

Default `---`

Type list in which each element is a particle type (`n`, `neutron`, `p`, or `photon`)

parameter **`source_names`**

Only tallies particles born in the given sources.

Default `---`

Type list in which each element is a string

3.21.21 [TALLY][DIAGNOSTIC=PATHLENGTH]

The path length diagnostic produces a distribution of the path length traveled by a particle between events. Note that this is not the same as the true path length distribution (distance between collisions), as the events considered by Shift include material boundary crossings, problem boundary crossings, etc.

parameter **`event_bins`**

Lower bin boundaries for the number of events per history.

Type monotonically increasing list (each element is a non-negative integer)

parameter **`pl_bins`**

Lower bin boundaries for the traversed path lengths in each event.

Type monotonically increasing list (each element is a positive real number)

3.21.22 [TALLY][DIAGNOSTIC=COLLISION]

The collision diagnostic tallies the number of collisions per history as a function of material, nuclide, and reaction ID.

3.21.23 [TALLY][DIAGNOSTIC=SOURCE]

This diagnostic tally is provided to calculate the source density binned into spatial cells. It also calculates the *particle* source density (i.e., binning $n(\vec{r})$ rather than $wn(\vec{r})$) to assist in the construction of biased sources.

parameter **`x`**

Mesh tally coordinates along the X axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

parameter **`y`**

Mesh tally coordinates along the Y axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

parameter **`z`**

Mesh tally coordinates along the Z axis.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

3.21.24 [TALLY][DIAGNOSTIC=HISTORY]

The history diagnostic tallies every event in a particle's lifetime. Currently, all particle histories are tallied, and only one processor writes the histories.

parameter **`begin_history`**
First history for which events will be saved.

Default `0`

Type non-negative integer

parameter **`domain`**
Domain on which history events will be saved.

Default `0`

Type non-negative integer

parameter **`end_history`**
Last + 1 history for which events will be saved.

Default `0`

Type non-negative integer

3.21.25 [TALLY][DIAGNOSTIC=DEBUG_HISTORY]

Write events for failed particle histories.

3.21.26 [TALLY][DIAGNOSTIC=DEBUG]

The debug diagnostic currently records the number of events per particle history, but it will be extended to provide other useful high-level debug information.

3.21.27 [TALLY][DIAGNOSTIC=HISTORY_TIME]

Write transport time for each particle history.

3.21.28 [TALLY][DIAGNOSTIC=FISS_SITE]

The fission site diagnostic records the locations where fission occurs for every kcode cycle provided by write_cycles. These are written to the

parameter **`write_cycles`**
parameter **`wc`**
List of cycles in which to write the fission source.

Default `---`

Type list in which each element is a non-negative integer

3.21.29 [TALLY][DIAGNOSTIC=SPLIT]

Write particle variance reduction splitting locations.

3.21.30 [TALLY][DIAGNOSTIC=ROULETTE]

Write particle variance reduction rouletting locations.

3.21.31 [TALLY][SENSITIVITY][RESPONSE]

Define a sensitivity response.

parameter `description`
parameter `desc`
Optional longer descriptive string.

Default `''`

Type string

parameter `emax`
parameter `ehigh`
Upper energy threshold for this response.

Optional

Units eV

Type positive real number

parameter `emax_out`
Upper exiting energy window for this response.

Optional

Units eV

Type positive real number

parameter `emin`
parameter `elow`
Lower energy threshold for this response.

Optional

Units eV

Type positive real number

parameter `emin_out`
Lower exiting energy window for this response.

Optional

Units eV

Type positive real number

parameter `materials`
parameter `mats`
Material names to include in this response.

Default `'*'`

Type list in which each element is a string

parameter `name`
Short title or label for the response.

Type string without special characters

parameter **`nuclide`**
Nuclide to include in this response.

Type Nuclide name or ZAID, or '*' for all nuclides

parameter **`reaction`**
Nuclide reaction MTs to include in this response.

Default `18`

Type MT number or name, or 0 for FLUX (e.g., N_GAMMA, 102)

3.21.32 [TALLY][SENSITIVITY][RATIO]

Define a ratio of two responses to calculate.

parameter **`denom`**
Denominator's response name.

Type string without special characters

parameter **`description`**
parameter **`desc`**
Optional longer descriptive string.

Default `''`

Type string

parameter **`name`**
Short title or label for the system response.

Type string without special characters

parameter **`numer`**
Numerator's response name.

Type string without special characters

3.21.33 [TALLY][SURFACE_CENSUS][TAGS]

Particle tagging options.

parameter **`birth_angle`**
parameter **`brth_dir`**
Tag each particle with its birth angle.

Default `False`

Type boolean

parameter **`birth_cell_label`**
parameter **`brth_cell`**
Tag each particle with its birth cell label.

Default `False`

Type boolean

parameter **`birth_energy`**
parameter **`brth_e`**
Tag each particle with its birth energy.

Default `False`

Type boolean

parameter **`birth_mat_label`**
parameter **`brth_mat`**
Tag each particle with its birth material label.

Default `False`

Type boolean

parameter **`birth_position`**
parameter **`brth_pos`**
Tag particles with its birth position.

Default `False`

Type boolean

parameter **`source_name`**
parameter **`src_name`**
Tag each particle with the name of its originating source.

Default `False`

Type boolean

3.21.34 [TALLY][BATCH_MESH][OUTPUT]

Table 24: Available types for the [OUTPUT] database

Type	Description	Applicability
hdf5 (page 166)	Write to the standard serial HDF5 file	
adios (page 166)	Write to an independent ADIOS file	'ADIOS' is enabled in this build

3.21.35 [TALLY][BATCH_MESH][OUTPUT=HDF5]

Write to the standard serial HDF5 file.

3.21.36 [TALLY][BATCH_MESH][OUTPUT=ADIOS]

Write to an independent ADIOS file.

parameter **`bufsize`**
ADIOS buffer size.

Default `4194304`

Units kB

Type positive integer

parameter `output`

Output filename.

Type file path to write (extension '.bp')

parameter `time_bufsize`

ADIOS time aggregation size.

Optional

Units kB

Type positive integer

parameter `transport`

Aggregation and write method.

Default MPI, or if using a Lustre PFS, MPI_LUSTRE

Type string

parameter `transport_params`

Parameters to pass to the transport method.

Default `''`

Type string

parameter `verbosity`

ADIOS log verbosity.

Default `warning`

Type `silent`, `error`, `warning`, `info`, or `debug`

3.22 SHIFT MONTE CARLO SOLVER: [SHIFT]

Shift is the Monte Carlo radiation transport code in Exnihilo. Like all Monte Carlo methods, the output is an *estimation* of the true solution (the mean of a tally), and a reported error bound provides an *estimation* of the error in this estimate. In accordance with the central limit theorem, as the number of transported particles increases, the output will converge to the true solution, and the variance will diminish proportionally to the square root of the number of particles.

Two classes of problems can be solved with Shift: eigenvalue ("kcode") solutions for steady-state fissionable systems, and fixed-source solutions for problems with a constant source of particles. The eigenvalue solution technique is described in [SHIFT][KCODE] (page 169). The only option in Shift that does not apply to `kcode` mode is num_histories (page 169). However, fixed-source problems are also the only ones that support hybrid methods.

The [SHIFT][DECOMPOSITION] (page 169) block enables Shift's domain decomposition feature for large problems. Currently, only mesh tallies are decomposed; compositions, cell tallies, and the problem geometry are all replicated. Some diagnostic tallies and other features may not be usable when domain decomposition is enabled.

Shift also supports an experimental GPU mode when built with CUDA support. It supports a limited subset of Shift features, restricting the available tallies, models, and physics options.

The behavior of Shift is strongly affected by the [HYBRID] (page 224) block corresponding to the `hybrid` fixed-source problem mode. Hybrid methods provide weight windows for variance reduction in Shift, and they can additionally bias the sources (page 56) to improve the chance that an emitted particle contributes to the user's tallies.

With the exception of the automatic *k*-effective tally and associated diagnostics in eigenvalue mode, Shift's tallies are specified in the [TALLY] (page 113) database.

parameter **`arch`**

Architecture type.

Default `cpu`

Type `cpu` or `gpu`

Applicable when 'SHIFT_CUDA' is enabled in this build

parameter **`batch_size`**

Number of particles per batch for computing tally statistics.

Optional

Type positive integer

Applicable when

- `arch` is `gpu`; and
- problem mode is `adjoint`, `forward`, or `hybrid`

database **`[DECOMPOSITION]`**

Domain decomposition options. See [SHIFT][DECOMPOSITION] (page 169).

Default (empty `none` database)

parameter **`device_id`**

Device id of GPU.

Default `0`

Type non-negative integer

Applicable when `arch` is `gpu`

parameter **`do_transport`***(advanced)*

Transport particles instead of merely setting up the problem.

Setting `do_transport` to `false` is a way to ensure problem integrity without running an expensive transport calculation. It disables transport itself but allows the rest of the code (including building sources, tallies, and physics) to run. This is similar to `parm=check` in SCALE.

Default `True`

Type boolean

parameter **`gpu_vector_size`**

Maximum size of GPU particle vector.

Optional

Type positive integer

database **[KCODE]**

Eigenvalue solution options. See [SHIFT][KCODE] (page 169).

Applicable when problem mode is `kcode`

parameter **num_histories**

parameter **np**

Number of particle histories.

Type positive integer

Applicable when problem mode is `adjoint`, `forward`, or `hybrid`

parameter **physics***(advanced)*

Name of the physics DB to use.

Default the name of the last physics database

Type string without special characters

database **[TRANSPORTER]**

Transport communication options. See [SHIFT][TRANSPORTER] (page 171).

Default (empty database)

database **[VR]**

Variance reduction options. See [SHIFT][VR] (page 172).

Default (empty database)

3.22.1 [SHIFT][DECOMPOSITION]

This database determines how the Shift Monte Carlo problem is spatially decomposed. If not present, the problem will be fully replicated.

Table 25: Available types for the [DECOMPOSITION] database

Type	Description	Applicability
none (page 174)	Fully domain-replicated	
bmesh (page 175)	Boundary mesh for domain decomposition	

3.22.2 [SHIFT][KCODE]

Criticality (or eigenvalue, or kcode) calculations involve iteratively sampling and transporting "generations" of fission neutrons. Several different parameters are needed to specify these generations.

The power iteration method used by Shift (and traditional Monte Carlo codes) may require many particle generations before the fission source converges. The generation at which the fission source converges can be estimated with the help of two diagnostics that Shift tallies by default:

- Shannon entropy, which provides a scalar value summarizing the distribution of occupied spatial cells in the problem, and
- Spatial moments, which provide a low-order approximation of the global particle distribution and shape.

parameter **`convergence_method`**

Kcode cycle convergence criteria for inactive and active cycles.

Shift supports different convergence criteria for switching from inactive to active cycles and for completing the kcode solve. Currently, two traditional methods are supported. The number of inactive cycles is always fixed by the user and specified with the `num_inactive_cycles` parameter; this number should be high enough that the fission source distribution is converged before tallying begins.

If the convergence method is set to `count`, then the number of active cycles is also set by the user with the `num_cycles` parameter, which is the total of inactive plus active cycles. This method should be used if a certain number of particles is needed to be run before finishing the problem (e.g., if a mesh tally is to be used).

The second implemented option is `count_ksig`, in which a counted number of inactive cycles is run, but the batch-estimated standard deviation of k_{eff} is used to stop the active cycles.

Default `count`

Type `count` or `count_ksig`

parameter **`entropy_mesh`***(advanced)*

How the entropy mesh is specified.

The default entropy grid uses the Shift decomposition (which by default is the problem's extents, which are automatically calculated in some geometry types) as its outer extents. If unspecified, Shift tries to build a mesh with:

$$N_{\text{cells}} = \max(N_{\text{p}}/10, 64),$$

where N_{p} is the number of particles per cycle.

Default `manual` when entropy mesh input is given

Type `automatic` or `manual`

parameter **`initial_keff`**
parameter **`initk`**

Initial keff value.

Default `1.0`

Type positive real number

parameter **`keff_sigma_active`**
parameter **`sig`**

Standard deviation of keff at which to stop active cycles.

Type positive real number

Applicable when `convergence_method` is `count_ksig`

parameter **`num_cycles`**
parameter **`nk`**

Number of active + inactive kcode cycles.

Type integer

parameter **`num_histories_per_cycle`** *parameter* **`npk`**

Number of histories per cycle.

Type positive integer

parameter **`num_inactive_cycles`**
parameter **`nik`**

Number of inactive kcode cycles.

Type integer

parameter **`x_entropy`**

Boundaries in x for the Shannon entropy mesh.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `entropy_mesh` is `manual`

parameter **`y_entropy`**

Boundaries in y for the Shannon entropy mesh.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `entropy_mesh` is `manual`

parameter **`z_entropy`**

Boundaries in z for the Shannon entropy mesh.

Units cm

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when `entropy_mesh` is `manual`

3.22.3 [SHIFT][TRANSPORTER]

Transport communication options.

parameter **`bank_size_warnings`**

Initial bank size warnings to print per domain.

Default `2000`

Type non-negative integer

parameter **`error_tolerance`**

Fraction of lost particles to tolerate before aborting.

Some especially complex models occasionally have nearly undetectable geometry errors. However, when running enough particles, inevitably some will be lost. To support transport on these models despite any errors, the tolerance parameter can be set to a higher value. This number is multiplied into the total number of particles to be run (in the case of an eigenvalue problem, the number of particles in a single generation) and divided amongst all the parallel processes. When that number is reached, the transport run will be aborted. The tolerance is rounded upward so that each domain will accept at least one lost particle.

Setting the error tolerance too high (a statistically significant number of particles in an important part of the problem) will result in erroneous tally results.

Finally, note that because of particle splitting, multiple particles could be lost per actual source particle.

Default `1e-06`

Type real number inside (0, 1)

database **`[GENERATIONS]`**

Synchronous DD control. See [SHIFT][TRANSPORTER][GENERATIONS] (page 175).

Default (empty `constant` database)

Applicable when Shift spatial partitioning is domain decomposed

parameter **`max_local_warnings`**

Max number of lost particle warnings to print per domain.

On complex inputs with known modeling errors, it may be infeasible to correct the model for a test run, but running a trillion particles may produce a million error messages, which (on large parallel systems) will slow down program execution significantly due to the increased I/O.

Setting this value will suppress warnings after the counter is reached.

Default `10`

Type non-negative integer

parameter **`method`**

Domain-decomposed transport method.

Default `sync`

Type `sync`

Applicable when Shift spatial partitioning is domain decomposed

parameter **`verbosity`**

How often to print about particles being transported.

Default `none` if kcode, `low` otherwise

Type `none`, `low`, or `high`

3.22.4 [SHIFT][VR]

Variance reduction is key to making Monte Carlo calculations tractable. Although Shift supports a fully analog mode, in which particles have a weight of either one or zero to mimic the physical event-by-event behavior, the Monte Carlo solution is almost exclusively used with some form of variance reduction.

The key concept behind variance reduction is adding a dimension to the phase space of the transport equation: weight. The weight-averaged Monte Carlo particle density is an estimate of the true particle density because a single Monte Carlo particle can now represent an *average* of multiple physical particles.

The simplest form of variance reduction, implicit capture, prevents particles from being physically absorbed. Instead, the weight of the particle is reduced proportionally to the chance that it would have been absorbed during its step. When a particle reaches a sufficiently small weight, it no longer contributes meaningfully to the solution but still requires equal computational resources as an important (high-weight) particle. To reduce the number of low-weight particles in the problem, the *Russian roulette* (or simply *roulette*) method will probabilistically kill particles below a specified weight. The weight of particles that survive the roulette increases proportionally to the inverse of the fraction of particles that survive the roulette process, maintaining a “fair game” and the resulting solution.

A more complex variance reduction method is that of *weight windows*, which introduces a spatially dependent "target weight" rather than a constant value as with Russian roulette. Besides killing particles of low weight, weight windows will also *split* particles that have high weight into multiple particles closer to the target weight so that multiple potential pathways for a particle's behavior can be averaged into the final result. Weight windows can be provided as input or generated automatically by Denovo. The weight window options are provided in the Hybrid methodology: [HYBRID] (page 224) documentation.

The Consistent Adjoint Driven Importance Sampling (CADIS) family of methods extends the weight window method by biasing particle sources so that the weight of a particle at birth corresponds to the weight window at its point in phase space. Consequently, particles are more likely to be born in the important regions of a problem rather than being rouletted or split immediately at birth. CADIS was originally designed for importance maps generated by a single tally of interest, but biased sources can be constructed "consistently" for any provided weight window map. Source biasing can be enabled for each source using the Particle source definitions: [SOURCE] (page 56) options.

deleted **`apply_ww`**

Entry `apply_ww` has been deleted: Weight windows are now applied at a set of events specified by the `vr_events` parameter.

parameter **`method`**
parameter **`vr`**

Variance reduction method.

Default 'ww' when hybrid, otherwise 'roulette'

Type `ww`, `analog`, or `roulette`

parameter **`minimum_thickness`**
parameter **`min_thick`**

Minimum window optical thickness above which to perform VR.

Default `0.01`

Type non-negative real number

Applicable when Weight window lookup *vr_events* has enabled *tracking*

parameter **`output`**

Write weight window centers to the output file.

Default `True`

Type boolean

Applicable when `method` is `ww`

parameter **`vr_events`**

When to apply weight windows.

This entry specifies which transport events should trigger a weight window lookup, thereby potentially initiating a particle splitting or rouletting. A weight window lookup is always performed after a collision. Additional lookup events are *precollision*, which causes a weight window lookup before a collision, *surface*, which causes a weight window lookup every time a geometric surface is crossed, *mfp*, which causes a weight window lookup every time a particle streams a mean free path, and *tracking*, which causes a particle to track through the weight window grid and look up the weight windows every time a weight window grid plane is crossed. These different lookup events may be used in any combination.

Default `tracking`

Type list in which each element is a `precollision`, `mfp`, `surface`, or `tracking`

Applicable when `method` is `ww`

parameter **`weight_cutoff`**
parameter **`wc`**
Particle weight cutoff for roulette.

Default `0.25`

Type non-negative real number

Applicable when `method` is `roulette`

parameter **`weight_survival`**
parameter **`ws`**
Particle weight survival for roulette.

Default `0.5`

Type non-negative real number

Applicable when `method` is `roulette`

parameter **`ww_decomp`**
Whether the weight window adjoint flux should be decomposed.

Default `full`

Type `full` or `separable`

Applicable when `method` is `ww`

parameter **`ww_lower_factor`**
parameter **`wwlow`**
Lower weight window ratio.

Default `0.5`

Type real number inside (0, 1)

Applicable when `method` is `ww`

parameter **`ww_upper_factor`**
parameter **`wwhigh`**
Upper weight window ratio.

Default `2.5`

Type real number greater than 1

Applicable when `method` is `ww`

3.22.5 [SHIFT][DECOMPOSITION=NONE]

Fully domain-replicated.

3.22.6 [SHIFT][DECOMPOSITION=BMESH]

Boundary mesh for domain decomposition.

parameter **`boundary_condition`**

Boundary condition for each side of the boundary mesh.

> **Default** `vacuum vacuum vacuum vacuum vacuum vacuum`
>
> **Type** list of boundary conditions on -X,+X,-Y,+Y,-Z,+Z (each element is a `vacuum`, `reflect`, `rotate`, or `periodic`)

parameter **`overlap`**

Fraction of DD domain overlap.

> **Default** `0.0`
>
> **Type** real number inclusive [0.0, 1.0]
>
> **Applicable when** Shift spatial partitioning is domain decomposed

parameter **`subblock_procs`**

Processor allocation for blocks of the boundary mesh.

> **Default** `---`
>
> **Type** list in which each element is a positive integer

postprocessor

Ensure that the Shift spatial decomposition is compatible with the number of processors if using a [RUN] block.

postprocessor

Check to make sure that Tpetra is enabled in build for DD decompositions.

> **Applicability** Shift spatial partitioning is domain decomposed

parameter **`x_partition`**

parameter **`x`**

Boundary mesh along the X axis.

> **Type** monotonically increasing list with at least two values (each element is a real number)

parameter **`y_partition`**

parameter **`y`**

Boundary mesh along the Y axis.

> **Type** monotonically increasing list with at least two values (each element is a real number)

parameter **`z_partition`**

parameter **`z`**

Boundary mesh along the Z axis.

> **Type** monotonically increasing list with at least two values (each element is a real number)

3.22.7 [SHIFT][TRANSPORTER][GENERATIONS]

Table 26: Available types for the [GENERATIONS] database

Type	Description	Applicability
constant (page 176)	Same number of iterations per cycle	
three_component (page 176)	Advanced iteration flexibility	

3.22.8 [SHIFT][TRANSPORTER][GENERATIONS=CONSTANT]

Same number of iterations per cycle.

parameter **`num_iterations`**
Number of iterations per generation.

Default `100`

Type positive integer

3.22.9 [SHIFT][TRANSPORTER][GENERATIONS=THREE_COMPONENT]

Advanced iteration flexibility.

parameter **`bound1`**
First boundary of three-component generations.

Default `20.0`

Type non-negative real number

parameter **`bound2`**
Second boundary of three-component generations.

Default `50.0`

Type positive real number

parameter **`exponent`**
Exponential decay constant of three-component generations.

Default `0.025`

Type non-negative real number

parameter **`intercept`**
Intercept of first component of three-component generations.

Default `100.0`

Type positive real number

parameter **`minimum`**
Minimum iterations of three-component generations.

Default `100.0`

Type positive real number

parameter **`slope`**
Slope of first component of three-component generations.

Default `5.0`

Type non-negative real number

3.23 DENOVO DETERMINISTIC SOLVER: [DENOVO]

Denovo is the parallel deterministic solver inside the Exnihilo code suite. It solves the steady-state Boltzmann transport equation by discretizing it in space, angle, and energy. The [DENOVO] database specifies these discretization parameters as well as numerical solver parameters.

3.23.1 DENOVO APPLICATIONS

Denovo is often used to generate importance maps for variance reduction, typically using the [HYBRID] (page 224) block. The figure of merit of a tally,

$$\text{FOM} = \frac{1}{\sigma^2 T} ,$$

where σ^2 is the variance of the tally in question and T is the time to solution, can improve by orders of magnitude given a good approximation to the importance map. However, even with a *bad* approximation to an adjoint transport solution for an importance map, the expected value of the Shift solution *will not change* as a result of the Denovo solver parameters. The figure of merit will simply be lowered, and the estimation of the variance for an unconverged solution may also be affected. This principle of hybrid methods means that coarse and fast Denovo solves can be adequate to improve the convergence rate of a Shift calculation.

In contrast to hybrid applications, using any discrete ordinates code to generate final results for an analysis usually requires a great deal of care and experience to produce accurate solutions. Significant errors can be introduced by poor approximations to:

- the spatial grid (e.g., by not capturing a streaming pathway);
- the spatial integration method (e.g., by using a difference method for optically thick cells) (see the method parameter (page 180));
- the energy discretization (e.g., by failing to capture self-shielding effects) (see Multigroup physics: [PHYSICS=mg] (page 96)); and
- the angular discretization (e.g., by ray effects in optically thin regions) (see [DENOVO][QUADRATURE] (page 184)).

Warning: The default settings for Denovo are generally for obtaining *qualitatively* accurate answers for use in hybrid schemes or for initial problem scoping. Obtaining accurate answers for most realistic problems typically requires a good deal of experience, parametric studies, and finesse.

Denovo has two categories of options for the angular discretization: discrete ordinates (S_N), in which particles are constrained to travel along specific angular directions; and spherical harmonics (SP_N), which is similar in treatment to the diffusion approximation. The method parameter (page 180) chooses between the two. The various S_N discretization closure equations are described in the equations parameter (page 179).

3.23.2 SOLVER OVERVIEW

The linear algebraic formulation of these deterministic approximations to the transport equation require numerical methods to solve. (Analytically solving the exact representation of the discretized transport equation is intractable except for toy problems.) The solution methodology will vary depending on whether the input is a "fixed source" problem

$$Ax = b$$

or an k-eigenvalue problem

$$FAx = \frac{1}{k} x .$$

Fixed-source problems without upscattering can be solved exactly with a series of consecutive within-group solutions: the solution vector is the flux (and higher-order moments) whose components are coupled by the spatial and angular behavior of the problem. This solution is the within-group (page 200) solve and can be performed with several numerical methods.

Upscattering introduces a dependency between multiple within-group solutions and therefore generally requires an outer level of iteration. The solvers that converge this multigroup solution are described in [DENOVO][SOLVER][UPSCATTER] (page 198). It is important to note that to support more advanced methods and to improve the parallelism of Denovo solves, there is an option to treat *all* groups as upscatter groups (even if the cross sections physically prevent upscatter) in order to solve the groups simultaneously. This option is discussed in the upscatter_groups parameter (page 194).

Finally, the convergence of an eigenvalue problem generally requires an *additional* level of iteration. The options for converging the eigenvalue (a measure of criticality of the problem) and eigenvector (the distribution of neutrons at a critical state) are described in [DENOVO][SOLVER=eigenvalue] (page 195).

For a more detailed discussion of Denovo's solution methodology and discrete ordinate methodology in general, see [4] and [11] and the references therein.

3.23.3 PERFORMANCE CONSIDERATIONS

The number of degrees of freedom D in a Denovo S_N calculation is

$$D = N_u \times N_c \times N_m \times N_a \times N_g \ ,$$

where N_u is the number of spatial unknowns (cf. the equations parameter (page 179)), N_c is the number of cells (determined by the spacing of `x`, `y`, and `z`), N_m is the number of moments (cf. the pn_order physics parameter (page 102)), N_a is the number of discrete angles (see [DENOVO][QUADRATURE] (page 184)), and N_g is the number of energy groups. This value is proportional to the number of floating point operations per transport sweep when all groups are being swept simultaneously (upscatter_groups (page 194) is set to "all").

A more important figure for some users will be the *memory consumption* of Denovo rather than the time to solution. The Denovo state vector (or solution vector) does *not* store angular fluxes; rather, it stores angular *moments* up to the specified maximum scattering order. It therefore contains M elements, with

$$M = N_u \times N_c \times N_m \times N_g \ .$$

This state vector is distributed across all MPI processes in a parallel run (see [DENOVO][DECOMPOSITION] (page 183)). In most problems, the state vector dominates memory usage. However, in problems with an unusually large number of groups, it is important to be aware of the memory footprint of scattering matrices:

$$M_{\mathrm{xs}} \propto N_g^2 N_{\mathrm{mixtures}}$$

The number of mixtures depends both on the original compositions of the input model *and* on the mix tolerance (page 187) used in the model ray tracing. Also critically important is that the number of mixtures on each domain depends on the complexity of the spatial region local to that domain! Since Denovo spatially partitions the problem to equally distribute the number of cells along the *xy* plane, some complex domains may end up with a hundred times as many mixtures as the simpler domains, and *that* memory requirement could contribute significantly to the total Denovo memory usage.

parameter **arch**

Architecture type.

Default `cpu`

Type `cpu` or `gpu`

Applicable when

- 'KBA_CUDA' is enabled in this build; and
- problem mode is `forward` or `kcode`; and
- Denovo discretization method is `ld` or `sc`

database **`[BOUNDARY]`**
Boundary condition specification. See [DENOVO][BOUNDARY] (page 183).

Default (empty `vacuum` database)

database **`[DECOMPOSITION]`**
Denovo space-energy decomposition. See [DENOVO][DECOMPOSITION] (page 183).

Default (empty database)

parameter **`dimension`***(advanced)*
Spatial dimension of the problem.

Default based on spatial discretization equations

Type integer 2 or 3

parameter **`disable`**
Choose to skip the 'solve' step or both 'solve' and construction.

Default `none`

Type `none`, `transport`, or `state`

parameter **`equations`**
parameter **`eq`**
Closure equations for the S_N approximation in a cell.

Like most options for deterministic methods, the choice of spatial discretization (closure equations for the S_N approximation) involves a trade-off between performance and accuracy. In this case, inaccuracy can result in numerical instability and negativities in the computed solution. The performance varies by discretization partly due to the solution method (e.g., the exponential function evaluations in step characteristics) and the increased memory costs of discretizations that have more unknowns per spatial cell.

The following spatial discretizations are available for 3D problems:

Table 27: Denovo spatial discretization options.

Value	Discretization	Unknowns
`sc`	Step characteristics	1
`ld`	Linear discontinuous finite element	4
`tld`	Trilinear discontinuous finite element	8
`twd`	Theta-weighted diamond difference	1
`wdd`	Weighted diamond difference	1
`wdd_ff`	Weighted diamond difference with flux fixup	1

Additionally, for 2D problems, a step characteristics `sc_2d` (1 unknown) option and a bilinear discontinuous `bld_2d` (4 unknowns) finite element discretization are available.

The step characteristics (SC) equations guarantee positive solutions and offer good accuracy for a wide range of problems. This should be the preferred method for difficult shielding problems and for problems in which a coarse spatial mesh must be used.

The linear discontinuous (LD) finite element method (FEM) is often more accurate than SC, but it does not guarantee positivity of the solution. The trilinear discontinuous (TLD) FEM is more accurate and rigorous in the asymptotic limit of diffusive cells, but it still does not guarantee positivity. For this reason, the FEM group of methods is not usually recommended for difficult shielding problems or problems where the spatial mesh does not adequately resolve the physics of the problem. They are most appropriate for problems that are not prone to negative solutions (such as reactors) and problems in which a finely resolved spatial mesh is possible.

The diamond difference methods, `twd`, `wdd`, and `wdd_ff`, are available primarily for direct comparisons to legacy radiation transport solvers and are not recommended.

Default `sc`

Type `sc`, `sc_2d`, `bld_2d`, `ld`, `tld`, `twd`, `wdd`, or `wdd_ff`

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

parameter **`first_group`**

The first energy group to solve.

Optional

Type non-negative integer

parameter **`last_group`**

The last energy group to solve.

Optional

Type non-negative integer

postprocessor

Check `first_group` and `last_group` for consistency.

parameter **`log_memory`***(advanced)*

Periodically print memory usage to screen.

Default value of `log_memory` in `[OUTPUT]`

Type boolean

command **`logically_uniform_grid`**

Generate a grid (approximately uniform in num cells) from the given extents.

Creates x

Creates y

Creates z

preprocessor (advanced)

Change deprecated SN ‘method’ values to ‘equations.’

parameter **`method`**

Deterministic solution method.

This parameter chooses between the discrete ordinates (S_N) and simplified spherical harmonics (SP_N) methods.

The discrete ordinates method is suitable for a variety of shielding applications and for accelerating Monte Carlo transport by estimating the global (space and energy) importance field with the adjoint flux. It is subject to discretization error not only by the spatial grid but also by the angular quadrature. Converging to a true monoenergetic transport solution requires simultaneous refinement in both angle and space.

The Simplified P_N finite volume discretization approach (SP_N) provides fast, accurate solutions primarily for light water reactor eigenvalue problems. The SP_N equations introduce approximations not present in other discretizations and are not recommended for general purpose (i.e., non-reactor) problems. In particular, problems with void or near-void regions cannot be handled accurately by this method. It should also be noted that, unlike the more rigorous P_N approximation, solutions with increasing SP_N order will *not* converge to the actual transport solution.

Full details on the mathematical methods used in Denovo can be found in the Exnihilo methods manual.

Default `sn`

Type `spn` or `sn`

Applicable when transporter state is constructed

database **`[OUTPUT]`**

HDF5 output options. See [DENOVO][OUTPUT] (page 189).

Default (empty database)

parameter **`output_spn_matrices`***(advanced)*

Output SP_N matrices for analysis.

Default `False`

Type boolean

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`

preprocessor (advanced)

Set `disable state` for `mode raytrace`.

parameter **`physics`**

Name of the associated MG physics database.

Default the name of the MG physics database

Type string without special characters

database **`[QUADRATURE]`**

Discrete ordinates quadrature. See [DENOVO][QUADRATURE] (page 184).

Default (empty database)

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

database **[RAYTRACE]**
Problem discretization options. See [DENOVO][RAYTRACE] (page 187).

Default (empty database)

Applicable when model type is not 'mesh'

database **[SILO]**
Silo output options. See [DENOVO][SILO] (page 190).

Default (empty database)

Applicable when 'silo' is enabled in this build

database **[SOLVER]**
Linear algebraic solver options. See [DENOVO][SOLVER] (page 192).

Default (empty database)

Applicable when transporter state is constructed

database **[SOURCE]**
Source discretization options. See [DENOVO][SOURCE] (page 188).

Default (empty database)

Applicable when problem mode is `adjoint`, `forward`, or `hybrid`

parameter **spn_order**
Discretization order of SP$_N$.

Default `1`

Type positive integer

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`

command **uniform_grid**
Generate a grid (approximately uniform in cell size) from the given extents.

This command is primarily for scalability testing. It will generate a mesh with approximately uniform cells, limited by the provided number of cells. An optional parameter snaps the grid lengths to the nearest multiple (i.e., the number of cells in each direction will be divisible by this number).

It accepts the following sequence of arguments

```
xmin, xmax, ymin, ymax, zmin, zmax, num_cells [, multiple]
```

Creates x

Creates y

Creates z

parameter **x**
Mesh coordinates along the X axis.

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when model type is not 'mesh'

parameter **`y`**

Mesh coordinates along the Y axis.

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when model type is not 'mesh'

parameter **`z`**

Mesh coordinates along the Z axis.

Type monotonically increasing list with at least two values (each element is a real number)

Applicable when

- model type is not 'mesh'; and
- Problem is 3-D

postprocessor

Print the number of cells in the mesh.

Applicability model type is not 'mesh'

Applicability Problem is 3-D

3.23.4 [DENOVO][BOUNDARY]

Table 28: Available types for the [BOUNDARY] database

Type	Description	Applicability
vacuum (page 192)	Vacuum boundaries	
reflect (page 193)	Reflecting and vacuum boundaries	
isotropic (page 193)	One or more isotropic incident boundaries	

3.23.5 [DENOVO][DECOMPOSITION]

The Denovo decomposition determines how the solution is distributed across the computational resources. The KBA decomposition splits the Denovo mesh into columns along an *xy* grid specified by dividing the number of mesh cells evenly by `x_blocks` and `y_blocks`. For problems with upscattering, the energy domain can also be decomposed into an orthogonal dimension using `energy_sets`. The number of processors being used must equal the product of these three parameters:

$$N_p = N_x N_y N_E \, .$$

If using a [RUN] block (page 29), Omnibus will automatically provide reasonable values for the decomposition.

parameter **`energy_sets`**

The number of energy sets.

Default `1`

Type non-negative integer

preprocessor (advanced)

If a [RUN] block is present, come up with a logically square KBA decomposition.

parameter **`x_blocks`**

parameter **`x`**

The number of spatial partitions along the x axis.

Type non-negative integer

parameter **`y_blocks`**

parameter **`y`**

The number of spatial partitions along the y axis.

Type non-negative integer

postprocessor

Ensure Denovo decomposition is compatible with number of processors.

parameter **`z_blocks`**

parameter **`z`**

The number of pipelining blocks along the z axis.

Default Default z_blocks to min(nx,ny)

Type non-negative integer

Applicable when

- Problem is 3-D; and
- `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

3.23.6 [DENOVO][QUADRATURE]

The runtime of an S_N calculation is proportional to the number of quadrature angles, in the limit of a large number of angles. To summarize from the ADVANTG 3.0 manual [7]:

- Level-symmetric quadratures have historically been used most often. These consist of rotationally symmetric quadratures that have positive weights up to S_{20}. In three dimensions, there are $N \times (N+2)/8$ angles per octant, where N is the order of the quadrature. Therefore, the order of these quadratures must be even. These quadratures tend to exhibit the most ray effects.
- Gauss-Legendre product quadratures are formed by taking the Cartesian product of a set of uniformly distributed azimuthal angles and a 1D GaussLegendre quadrature in the polar angle.
- Quadruple range (QR) product quadratures exactly integrate maximal-order products of sines and cosines of the polar and azimuthal angles [12]. These quadratures generally perform well across a broad range of transport problems and tend to exhibit far less ray effects than level-symmetric quadratures.
- Linear-discontinuous finite element (LDFE) quadratures approximate the angular flux using direction cosines [13]. They are determined by requiring that the integration of the basis functions is equal to the surface area of a unit sphere. The advantage of these LDFE sets is that they have positive weights and are rotationally symmetric about the x, y, and z axes. For a quadrature of order N, there are $4^{(N+1)}$ angles per octant, so the order can be even or odd.

parameter **`construction`**

Construction methodology for the quadrature set.

Table 29: Denovo quadrature construction options.

Construction	Description
`levelsym`	Level-symmetric quadrature set, which features rotationally invariant angular positions and weights
`product`	Product quadrature set, which has a specified number of azimuthal angles per polar angle and a specified number of polar angles.
`product_vec`	A specialization of the product quadrature set that allows the number of azimuthal angles to be different at each polar angle.

Each quadrature set only supports a limited subset of construction options.

Table 30: Denovo quadrature availability matrix.

Quadrature	levelsym	product	product_vec
levelsym	×		
glproduct		×	
qr	×	×	×

Default based on quadrature type

Type `levelsym`, `product`, or `product_vec`

Applicable when `quadrature` is `levelsym`, `glproduct`, or `qr`

postprocessor

Validate `construction` of quadrature sets.

parameter **`input`**

User-specified quadrature set file.

The Denovo quadrature may be manually input as an ASCII file. The format is:

- Optional comments have a # at the beginning of the line
- Each line contains the whitespace-separated tuple (μ, η, ξ, w), which is the *xyz* projection of the angle tied to the angle's associated weight.
- Angles for just a single octant (or quadrant if 2D) may be defined, or all angles in all octants may be defined. (This is checked by summing the weights over the input angles.)

An example input for S_2 is

```
# S2 quadrature input
0.57735026919 0.57735026919 0.57735026919 1.0
```

Type file path for reading

Applicable when `quadrature` is `userdefined`

parameter **`ldfe_order`**

Order for the LDFE quadrature set.

Default `1`

Type positive integer

Applicable when `quadrature` is `ldfe`

parameter **`num_azi`**

Number of azimuthal angles per level per octant.

Default `4`

Type positive integer

Applicable when `construction` is `product`

parameter **`num_azi_vec`**

List of the number of azimuthal angles per polar angle per octant, ordered from pole to equator.

Default `---`

Type list in which each element is a positive integer

Applicable when `construction` is `product_vec`

parameter **`num_polar`**

Number of polar angles per level per octant.

Default `4`

Type positive integer

Applicable when `construction` is `product` or `product_vec`

parameter **`order`**

Level-symmetric quadrature set order.

Default `10`

Type non-negative integer

Applicable when `construction` is `levelsym`

parameter **`polar_axis`**

Axis of rotation for product quadrature sets.

Default `z`

Type `x`, `y`, or `z`

Applicable when `construction` is `product` or `product_vec`

parameter **`quadrature`**

Discrete ordinates quadrature set class.

Default *‘qr’* unless *input* or *ldfe_order* are given

Type `levelsym`, `glproduct`, `qr`, `ldfe`, or `userdefined`

3.23.7 [DENOVO][RAYTRACE]

Denovo's Cartesian "brick mesh" spatial discretization requires cross sections to be homogenized within each spatial cell (a rectangular prism). Whereas legacy solvers required the user to specify a material for each spatial cell, Denovo can assist by using the same particle tracking engine as Shift (page 167) to map the continuous-in-space geometry specification of a model (page 43) to the Denovo mesh.

This raytracing is performed in parallel, with each local Denovo KBA decomposition generating an independent set of local materials and mixtures.

The options in this block determine how ray tracing is performed.

parameter `axes`

Axis/axes along which to fire rays for ray trace.

Default `xyz`

Type axis or axes ('x','zy','xyz')

parameter `error_tolerance`

Fraction of lost rays to tolerate before aborting.

Default `1e-05`

Type real number inside (0, 1)

parameter `max_local_warnings`

Max number of lost ray warnings to print per domain.

Default `10`

Type non-negative integer

parameter `mix_tolerance`

Tolerance for collapsing similar mixed materials into one.

To reduce memory requirements (see Performance considerations (page 178)), mixed cells with similar contents are collapsed to a single mixture on the fly [14]. A higher "mix tolerance" will reduce both memory consumption and accuracy for coarsely discretized problems. "Coarse" is relative to the length scale of the finest features of the input model.

Warning: Because the mixture collapsing is done locally on each KBA domain and not globally, different KBA decompositions will result in different discretized Denovo solutions! Since hybrid applications are relatively insensitive to weight windows (the estimated mean should converge to the same value), this is generally ok for `hybrid` mode. However, the on-the-fly discretization provided by the [DENOVO][RAYTRACE] (page 187) capability might *not* be appropriate for standalone solutions. The make-denovo-model (page 21) tool can be used to convert an initial raytraced Denovo run into a reproducible, more efficient model for comparison between multiple Denovo runs.

Default `0.05`

Type real number inside (0, 1)

parameter `rays_deterministic`

Use face midpoints rather than stratified sampling.

Default `False`

Type boolean

parameter **`rays_per_face`**

Number of ray trace rays to be fired per mesh face.

Default `4`

Type positive square integer

parameter **`void_matid`***(advanced)*

Material ID to be used when raytrace is outside the problem.

Default `0`

Type integer

parameter **`z_loc`**

The z coordinate for the ray trace.

Type real number

Applicable when Problem is 2-D

3.23.8 [DENOVO][SOURCE]

The `[SOURCE]` database controls discretization of Shift sources. Source strengths, including the `WGT` card for MCNP sources, are taken into account when creating the discrete source.

parameter **`mc_num_particles`**

Number of uncollided source particles to sample.

Type positive integer

Applicable when `uncflux` is `mc`

parameter **`mc_uncf_sets`**

Number of Denovo blocks per uncollided flux decomposition.

Default `1`

Type positive integer

Applicable when

- `uncflux` is `mc`; and
- ‘Tpetra’ is enabled in this build

preprocessor

Sources must be the same type when using Denovo.

parameter **`uncflux`**

parameter **`uncf`**

Uncollided flux treatment.

The uncollided flux treatment can reduce ray effects from point sources or other small sources. It currently applies only to separable sources, mesh problem sources (defined in an HDF5 input file), and SWORD sources.

The default is to treat all sources by discretizing them onto the Denovo grid as S_N sources.

If the "analytic" option is chosen, all point sources will be used as analytic uncollided flux sources. Ray traces are performed through the underlying geometry from each point source to quadrature points on each Denovo mesh cell to determine the uncollided flux contribution inside that cell.

The "mc" option is only valid when a single source is present. If selected, the source will be converted into a Monte Carlo uncollided flux source.

Default `analytic`

Type `none`, `analytic`, or `mc`

Applicable when

- not using an MCNP source; and
- `../decomposition/energy_sets` is 1

3.23.9 [DENOVO][OUTPUT]

HDF5 output options.

parameter **`angular_flux`**

Write the full angular flux.

Default `False`

Type boolean

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

postprocessor

Flux output is *not* automatically disabled when transport is disabled.

Applicability `/denovo/disable` is `state` or `transport`

parameter **`angular_mesh`**

Write the quadrature angles and weights.

Default `True`

Type boolean

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

parameter **`block`**

Write the KBA domain for each cell.

Default `True`

Type boolean

parameter **`current`**

Write the current (first angular moment).

Default `False`

Type boolean

Applicable when

- scattering order is not isotropic (pn_order > 0); and
- transporter state is constructed

deprecated `fc_source`

Deprecated entry `fc_source` has been renamed to `uncflux`.

Update to uncflux

parameter `flux`

Write the scalar flux.

Default True when performing transport

Type boolean

Applicable when transporter state is constructed

parameter `mat`

Write materials and mix tables.

Default True when the model type is not 'mesh'

Type boolean

parameter `source`

Write the energy-dependent source term.

Default True when performing transport and model is not 'mesh'

Type boolean

Applicable when problem mode is `adjoint`, `forward`, or `hybrid`

parameter `uncflux`

Write the uncollided flux if present.

Default True when performing transport

Type boolean

Applicable when

- `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`; and
- problem mode is `adjoint`, `forward`, or `hybrid`; and
- when uncflux is enabled

3.23.10 [DENOVO][SILO]

Silo output options.

parameter `blocks_per_file`

Number of KBA blocks written to each SILO output file.

Increasing this number will reduce the number of files in the `_silo` output directory, and each file will be correspondingly larger. The number of files can affect the output bandwidth, depending on the parallel file system being used.

Default `1`

Type positive integer

parameter **`current`**
Write the current (first angular moment).

Default `False`

Type boolean

Applicable when

- writing output; and
- scattering order is not isotropic (pn_order > 0); and
- transporter state is constructed

deprecated **`fc_source`**
Deprecated entry `fc_source` has been renamed to `uncflux`.

Update to uncflux

parameter **`flux`**
Write the scalar flux.

Default `False`

Type boolean

Applicable when

- writing output; and
- transporter state is constructed

parameter **`mat`**
Write materials.

Default `True`

Type boolean

parameter **`mixed_mats`***(advanced)*
Write material volume fractions rather than mixed matids.

Default `True`

Type boolean

Applicable when `mat` is `True`

parameter **`output`**
Name of Silo output file (without extension).

Default `denovo_output`

Type string without special characters

parameter **`power`**
Write power to the output Silo file.

Default `False`

Type boolean

Applicable when

- writing output; and
- problem mode is `kcode`; and
- transporter state is constructed

parameter **`source`**

Write the energy-dependent source term.

Default `False`

Type boolean

Applicable when

- writing output; and
- problem mode is `adjoint`, `forward`, or `hybrid`; and
- transporter state is constructed

parameter **`uncflux`**

Write the uncollided flux if present.

Default `False`

Type boolean

Applicable when

- writing output; and
- `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`; and
- problem mode is `adjoint`, `forward`, or `hybrid`; and
- transporter state is constructed

3.23.11 [DENOVO][SOLVER]

Table 31: Available types for the [SOLVER] database

Type	Description	Applicability
fixed (page 194)	Fixed-source solver options	problem mode is `adjoint`, `forward`, or `hybrid`
eigenvalue (page 195)	Solver options for eigenvalue problems	problem mode is `kcode`

3.23.12 [DENOVO][BOUNDARY=VACUUM]

Vacuum boundaries.

3.23.13 [DENOVO][BOUNDARY=REFLECT]

Reflecting and vacuum boundaries.

parameter `reflect`
Mark each exterior face of the problem as reflecting.

Default reflecting on all dimensions

Type list of boundary conditions for -X,+X,-Y,+Y,[-Z,+Z] (each element is a integer 0 or 1)

postprocessor
Reflect array length must be compatible with dimension.

3.23.14 [DENOVO][BOUNDARY=ISOTROPIC]

One or more isotropic incident boundaries.

parameter `minus_x`
Flux for each energy group on the -X boundary surface.

Optional

Type list in which each element is a real number

parameter `minus_y`
Flux for each energy group on the -Y boundary surface.

Optional

Type list in which each element is a real number

parameter `minus_z`
Flux for each energy group on the -Z boundary surface.

Optional

Type list in which each element is a real number

parameter `plus_x`
Flux for each energy group on the +X boundary surface.

Optional

Type list in which each element is a real number

parameter `plus_y`
Flux for each energy group on the +Y boundary surface.

Optional

Type list in which each element is a real number

parameter `plus_z`
Flux for each energy group on the +Z boundary surface.

Optional

Type list in which each element is a real number

postprocessor
Check number of groups and for one non-empty surface.

3.23.15 [DENOVO][SOLVER=FIXED]

The `fixed` solver database type specifies the solvers and options to use when solving a forward, adjoint, or hybrid problem through Denovo. The [DENOVO][SOLVER][WITHIN_GROUP] (page 200) database controls the solver options for solving within each energy group. The `upscatter` database controls the solver options for solving multiple coupled groups; some of the upscatter solution methods additionally have an inner iteration of within-group solves.

The `tolerance` parameter sets an overall desired convergence tolerance. The tolerances of any embedded solvers will be set accordingly to achieve a solution to this given accuracy. (The upscatter and within-group databases default to the same tolerance as the overall solver.)

parameter **`tolerance`**
parameter **`tol`**

Convergence tolerance to govern solver accuracy.

The default tolerance in most cases is to converge to a factor of ten tighter than the parent database. However, in the case of fixed-source problems, the tolerance of the within-group and upscatter databases is set to the value of the fixed-source solver database (with no additional multiplier). These default values are always written to the screen as a diagnostic.

Default `0.001`

Type real number inside (0, 1)

database **`[UPSCATTER]`**

Upscatter block solver options. See [DENOVO][SOLVER][UPSCATTER] (page 198).

Default (empty database)

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`; upscattering is enabled; or `upscatter_groups` is `all`

parameter **`upscatter_groups`**

Which groups to treat as upscatter groups during solve.

This parameter controls which energy groups to treat as upscatter when solving. If set to `all`, all energy groups are treated as upscatter during the solve. If set to `thermal`, only the thermal groups are treated as upscatter during the solve.

The `upscatter_groups` parameter has dependencies on other solver options:

- If the method (page 180) is `spn`, this parameter is not used as SP$_N$ *always* solves simultaneously over all groups.
- If the eigenvalue solver (page 195) is `rayleigh_quotient`, which must simultaneously solve all groups, it must be set to `all`.
- If `use_cuda` is True, it must be `all`. Increasing the amount of simultaneous work by transporting over all groups at once is critical to performant GPU code.
- If the number of energy set decompositions (page 183) is one, the default is to solve only thermal groups. Otherwise, increased parallelism is needed and the default changes to `all`.

Default `thermal` unless `arch` is `gpu`, eigenvalue solver is `rayleigh_quotient`, `energy_sets` > 1,‘‘method‘‘ is `spn`, or upscatter `preconditioner` is `multilevel`

Type `all` or `thermal`

postprocessor
CUDA sweeper, `rayleigh_quotient` solver, SPN, and `multilevel` upscatter preconditioner require all upscatter groups.

postprocessor
Warn if using downscatter-only physics with `upscatter all` unless needed.

Applicability `upscatter_groups` is `all`

database **`[WITHIN_GROUP]`**
One-group transport solver options. See [DENOVO][SOLVER][WITHIN_GROUP] (page 200).

Default (empty database)

Applicable when `upscatter_groups` is `thermal`

3.23.16 [DENOVO][SOLVER=EIGENVALUE]

The `eigenvalue` database specifies the solvers and options to use for solving an eigenvalue problem (mode `kcode`) through Denovo. Along with the within-group (page 200) and upscatter (page 198) databases described below, this database also sets the solver and options for the eigenvalue solve.

The `tolerance` parameter which controls the l_2 convergence tolerance of the eigenvalue solve can be used to set an overall desired convergence tolerance. Inner iteration tolerances will be set accordingly to achieve a solution with this accuracy.

The verbosity (page 198) setting determines the output level within the linear algebraic solver.

parameter **`acceleration_method`**
Type of power iteration acceleration.

Default `none`

Type `none` or `rebalance`

Applicable when `solver` is `power_iteration`

parameter **`calculate_flux_moments`**
Calculate the flux moments during Arnoldi iteration.

Default `True`

Type boolean

Applicable when `solver` is `arnoldi`

parameter **`fission_tolerance`**
Tolerance for infinity norm of flux.

Default `1.0`

Type real number inclusive [0.0, 1.0]

Applicable when `solver` is `power_iteration`

parameter **`k_tolerance`**
Tolerance for relative error of k-eff eigenvalue.

Default `1e-05`

Type real number inclusive [0.0, 1.0]

Applicable when `solver` is `power_iteration` or `rayleigh_quotient`

parameter **`max_iterations`**
parameter **`maxitr`**

Max number of iterations for this solver.

Default `1000`

Type non-negative integer

parameter **`shift`**

Shift parameter for RQI.

Default `-1.0`

Type real number

Applicable when `solver` is `rayleigh_quotient`

parameter **`solver`**

Solver used for eigenvalue iteration.

The Arnoldi solver offers fast, robust convergence for almost all problems. Like the GMRES (Generalized Minimal RESidual method) linear solver, Arnoldi is a subspace solver and therefore incurs some extra memory usage. To reduce memory usage, it is possible to use a variation of this solver that turns off energy dependence, which will reduce the memory used by the solver in exchange for some extra computational work at the end of the solve.

Power Iteration is a robust eigenvalue solver, but it suffers from extremely slow convergence and long computational times for many problems. It has minimal memory requirements; however, using the energy independent Arnoldi solver typically results in only a small extra memory cost and should be preferred for most problems.

Rayleigh Quotient Iteration (RQI) offers superior performance to Arnoldi for certain very challenging problems. However, this solver often results in very high memory usage, and the stability is not as well understood as for Arnoldi and Power Iteration. RQI should be considered experimental and is not recommended for most users.

The Davidson solver offers extremely fast convergence, but it is currently only available when using the SP_N discretization. Although all of the above solvers are also available with SP_N, use of the Davidson solver is always preferred.

With the exception of the Davidson solver, all eigenvalue solvers require the solution of a fixed-source sub-problem as part of the iterative solution process. See the multigroup (page 198) and within-group (page 200) sections for details on the inner loops of the solution process.

Default `arnoldi` for SN, `davidson` for SPN

Type `power_iteration`, `arnoldi`, `rayleigh_quotient`, or `davidson`

postprocessor

Cannot set `solver` to `arnoldi`, `davidson`, or `rayleigh_quotient` unless ‘equations’ discretization is linear (not ‘twd’ or ‘wdd_ff’).

postprocessor
Cannot set solver to davidson unless /denovo/disable is none or transport and /denovo/method is spn.

parameter **subspace_size**
Max subspace size for this solver.

Default 20

Type non-negative integer

Applicable when solver is gmres, arnoldi, or davidson

parameter **tolerance**
parameter **tol**
L2 convergence tolerance for this solver.

Default 0.001

Type real number inside (0, 1)

parameter **tolerance_relax_factor**
Inner tolerance relaxation factor for Arnoldi iteration.

Default 1.0

Type real number inclusive [1.0, 10.0]

Applicable when

- solver is arnoldi; and
- tolerance_relaxer is constant

parameter **tolerance_relaxer**
Type of inner tolerance relaxer for Arnoldi iteration.

Default none

Type none or constant

Applicable when solver is arnoldi

database **[UPSCATTER]**
Upscatter block solver options. See [DENOVO][SOLVER][UPSCATTER] (page 198).

Default (empty database)

Applicable when /denovo/disable is none or transport and /denovo/method is spn; upscattering is enabled; or upscatter_groups is all

parameter **upscatter_groups**
Which groups to treat as upscatter groups during solve.

Default thermal unless arch is gpu, eigenvalue solver is rayleigh_quotient, energy_sets > 1,‘‘method‘‘ is spn, or upscatter preconditioner is multilevel

Type all or thermal

postprocessor

CUDA sweeper, `rayleigh_quotient` solver, SPN, and `multilevel` upscatter preconditioner require all upscatter groups.

postprocessor

Warn if using downscatter-only physics with `upscatter all` unless needed.

Applicability `upscatter_groups` is `all`

parameter **`use_energy_dependent`**

Use energy-dependent Arnoldi iteration.

Default `True`

Type boolean

Applicable when `solver` is `arnoldi`

parameter **`verbosity`**

Solver verbosity.

Table 32: Denovo solver verbosity options.

Level	Description
`none`	Output only warnings from the solver.
`low`	Additionally, output a diagnostic summary of each (typically within-group) transport solution.
`medium`	Additionally, output information about the convergence tests (residual, iteration count) for each solve.
`high`	Additionally, output diagnostic information about each solver iteration.

Default `low`

Type `none`, `low`, `medium`, or `high`

database **`[WITHIN_GROUP]`**

One-group transport solver options. See [DENOVO][SOLVER][WITHIN_GROUP] (page 201).

Default (empty database)

Applicable when `upscatter_groups` is `thermal`

3.23.17 [DENOVO][SOLVER][UPSCATTER]

The parameters and sub-databases in this database control the solve options for the multigroup solve. If `method` is `spn`, this database is required and is used to determine all solve options since the SP$_N$ representation used by Denovo is an explicit multigroup sparse matrix rather than an implicit operator such as S$_N$.

The available multigroup solvers in Denovo are GMRES (the default) and Gauss–Seidel. These solvers are only used to converge inter-group coupling. When the upscatter (page 194) parameter is set to `all`, *all* energy groups are coupled. For problems that have no upscatter and use the `thermal` coupling option, this database is not used. If the upscatter option is set to `thermal`, the within-group (page 200) solver settings determine how the high-energy (uncoupled) groups are solved, and this database applies only to the coupled low-energy groups.

Gauss–Seidel, the traditional multigroup iterative solution method, offers the smallest possible memory footprint of the upscatter solvers at a cost of significantly degraded convergence behavior for many problems. Gauss–Seidel is essentially an extra level of iteration over the upscattering groups.

The GMRES upscatter convergence option typically offers the most rapid, robust convergence. Its solution vector comprises the entire upscatter flux. Consequently, since multiple Krylov vectors are necessary for the method, its memory requirements are higher than Gauss–Seidel. It should also be noted that since the GMRES option is currently incompatible with other features of Denovo such as adjoint solutions and first-collision sources. The Omnibus input processor should fail informatively if these incompatible conditions are requested.

parameter **`max_iterations`**
parameter **`maxitr`**
Max number of iterations for this solver.

Default 1000, or 3 when SPN + multilevel

Type non-negative integer

database **`[PRECONDITIONER]`**
Upscatter preconditioner type. See [DENOVO][SOLVER][UPSCATTER][PRECONDITIONER] (page 203).

Default (empty `none` database)

parameter **`solver`**
Solver used for the multigroup block solve.

Default ‘gmres’ unless mode is adjoint or a nonlinear spatial discretization is being used

Type `gauss_seidel` or `gmres`

postprocessor
Cannot set `solver` to `gmres` unless ‘equations’ discretization is linear (not ‘twd’ or ‘wdd_ff’).

postprocessor
Cannot set `solver` to `gmres` unless problem mode is `forward`, `hybrid`, `kcode`, or `raytrace` or `/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`.

postprocessor
Cannot set `solver` to `gauss_seidel` unless CUDA sweeper is disabled.

parameter **`subspace_size`**
Max subspace size for this solver.

Default `20`

Type non-negative integer

Applicable when `solver` is `gmres`, `arnoldi`, or `davidson`

parameter **`tolerance`**
parameter **`tol`**
Convergence tolerance for this solver.

Default typically 0.1 * parent database tolerance

Type real number inside (0, 1)

postprocessor

Tolerance must be less than or equal to tolerance of parent solver database.

parameter **`verbosity`**

Solver verbosity.

Default low, or none when SPN + multilevel

Type `none`, `low`, `medium`, or `high`

database **`[WITHIN_GROUP]`**

One-group transport solver options. See [DENOVO][SOLVER][UPSCATTER][WITHIN_GROUP] (page 203).

Default (empty database)

Applicable when `solver` is `gauss_seidel`

3.23.18 [DENOVO][SOLVER][WITHIN_GROUP]

The parameters and sub-databases in this database control the solver options for single-group solves embedded in the multigroup iteration schemes. The available within-group solvers in Denovo are GMRES (the default), BiCGStab, and source iteration (SI).

GMRES (Generalized Minimal RESidual method) offers fast, robust convergence for most problems. GMRES is a subspace solver, so multiple vectors must be stored simultaneously which results in additional memory requirements. Because a downscatter-only problem solves only a single energy group at a time, the extra memory required is typically small compared to the cost of storing the solution vector over all energy groups.

The performance of BiCGStab (BiConjugate Gradient Stabilized method) is generally similar to that of GMRES. Memory requirements for BiCGStab are smaller than for GMRES, at a cost of typically slightly slower convergence leading to longer runtimes. BiCGStab may be suitable for problems where memory usage must be minimized.

Source iteration offers minimal memory requirements at a cost of significantly worse convergence behavior. It is only recommended for problems in which memory usage is at an absolute premium; it should be expected that run times will be significantly longer when using this method.

parameter **`matrix_output`***(advanced)*

Matrix output file for Krylov solver.

Default `A.h5`

Type file path to write (extension '.h5')

Applicable when `solver` is `matrixwriter`

parameter **`max_iterations`**

parameter **`maxitr`**

Max number of iterations for this solver.

Default `1000`

Type non-negative integer

database **`[PRECONDITIONER]`**

Within-group preconditioner type. See [DENOVO][SOLVER][WITHIN_GROUP][PRECONDITIONER] (page 204).

Default (empty none database)

parameter **`solver`**

Solver used in each within_group solve.

Default *gmres* if using a linear discretization, otherwise *si*

Type `gmres`, `gmres_r`, `si`, `bicgstab`, `stratimikos`, or `matrixwriter`

postprocessor

Cannot set `solver` to `bicgstab`, `gmres`, `gmres_r`, `matrixwriter`, or `stratimikos` unless 'equations' discretization is linear (not 'twd' or 'wdd_ff').

parameter **`subspace_size`**

Max subspace size for this solver.

Default `20`

Type non-negative integer

Applicable when `solver` is `gmres`, `arnoldi`, or `davidson`

parameter **`tolerance`**
parameter **`tol`**

Convergence tolerance for this solver.

Default typically 0.1 * parent database tolerance

Type real number inside (0, 1)

postprocessor

Tolerance must be less than or equal to tolerance of parent solver database.

unvalidated-database **`[TRILINOS]`**

Advanced Trilinos solver options. See [DENOVO][SOLVER][WITHIN_GROUP][TRILINOS] (page 204).

Optional

parameter **`verbosity`**

Solver verbosity.

Default `low`

Type `none`, `low`, `medium`, or `high`

3.23.19 [DENOVO][SOLVER][WITHIN_GROUP]

One-group transport solver options.

parameter **`matrix_output`***(advanced)*

Matrix output file for Krylov solver.

Default `A.h5`

Type file path to write (extension '.h5')

Applicable when `solver` is `matrixwriter`

parameter **`max_iterations`**

parameter **`maxitr`**

Max number of iterations for this solver.

Default `1000`

Type non-negative integer

database **`[PRECONDITIONER]`**

Within-group preconditioner type. See [DENOVO][SOLVER][WITHIN_GROUP][PRECONDITIONER] (page 204).

Default (empty `none` database)

parameter **`solver`**

Solver used in each within_group solve.

Default *gmres* if using a linear discretization, otherwise *si*

Type `gmres`, `gmres_r`, `si`, `bicgstab`, `stratimikos`, or `matrixwriter`

postprocessor

Cannot set `solver` to `bicgstab`, `gmres`, `gmres_r`, `matrixwriter`, or `stratimikos` unless ‘equations’ discretization is linear (not ‘twd’ or ‘wdd_ff’).

parameter **`subspace_size`**

Max subspace size for this solver.

Default `20`

Type non-negative integer

Applicable when `solver` is `gmres`, `arnoldi`, or `davidson`

parameter **`tolerance`**
parameter **`tol`**

Convergence tolerance for this solver.

Default typically 0.1 * parent database tolerance

Type real number inside (0, 1)

postprocessor

Tolerance must be less than or equal to tolerance of parent solver database.

unvalidated-database **`[TRILINOS]`**

Advanced Trilinos solver options. See [DENOVO][SOLVER][WITHIN_GROUP][TRILINOS] (page 204).

Optional

parameter **`verbosity`**

Solver verbosity.

Default `low`

Type `none`, `low`, `medium`, or `high`

3.23.20 ...[SOLVER][UPSCATTER][PRECONDITIONER]

Table 33: Available types for the [PRECONDITIONER] database

Type	Description	Applicability
none (page 204)	No preconditioner	
multilevel (page 205)	Multilevel preconditioner	`solver` is `gmres`
twogrid (page 206)	Two-grid energy preconditioner	`/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn` and `solver` is `gauss_seidel`
ifpack (page 206)	ifpack energy preconditioner	`/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`
ml (page 206)	ml energy preconditioner	`/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`

3.23.21 ...[SOLVER][UPSCATTER][WITHIN_GROUP]

One-group transport solver options.

parameter **`matrix_output`***(advanced)*

Matrix output file for Krylov solver.

Default `A.h5`

Type file path to write (extension '.h5')

Applicable when `solver` is `matrixwriter`

parameter **`max_iterations`**
parameter **`maxitr`**

Max number of iterations for this solver.

Default `1000`

Type non-negative integer

database **`[PRECONDITIONER]`**

Within-group preconditioner type. See [DENOVO][SOLVER][WITHIN_GROUP][PRECONDITIONER] (page 204).

Default (empty `none` database)

parameter **`solver`**

Solver used in each within_group solve.

Default *gmres* if using a linear discretization, otherwise *si*

Type `gmres`, `gmres_r`, `si`, `bicgstab`, `stratimikos`, or `matrixwriter`

postprocessor

Cannot set `solver` to `bicgstab`, `gmres`, `gmres_r`, `matrixwriter`, or `stratimikos` unless 'equations' discretization is linear (not 'twd' or 'wdd_ff').

parameter **`subspace_size`**

Max subspace size for this solver.

Default `20`

Type non-negative integer

Applicable when `solver` is `gmres`, `arnoldi`, or `davidson`

parameter **`tolerance`**
parameter **`tol`**

Convergence tolerance for this solver.

Default typically 0.1 * parent database tolerance

Type real number inside (0, 1)

postprocessor

Tolerance must be less than or equal to tolerance of parent solver database.

unvalidated-database **`[TRILINOS]`**

Advanced Trilinos solver options. See [DENOVO][SOLVER][WITHIN_GROUP][TRILINOS] (page 204).

Optional

parameter **`verbosity`**

Solver verbosity.

Default `low`

Type `none`, `low`, `medium`, or `high`

3.23.22 …[SOLVER][WITHIN_GROUP][PRECONDITIONER]

Table 34: Available types for the [PRECONDITIONER] database

Type	Description	Applicability
none (page 206)	No preconditioner	

3.23.23 …[SOLVER][WITHIN_GROUP][TRILINOS]

Advanced Trilinos solver options.

Note: This database passes its input through exactly as given. If it is defined in an ASCII (.omn) input file, all embedded parameters will be propagated as strings, which is usually not the desired behavior. Users should only include this database when the input file is a Python script or JSON file (or alternatively using the advanced Python interface to modify an ASCII input).

3.23.24 …[SOLVER][UPSCATTER][PRECONDITIONER=NONE]

No preconditioner.

3.23.25 ...[SOLVER][UPSCATTER][PRECONDITIONER=MULTILEVEL]

Multilevel preconditioner.

parameter **`depth_v_cycle`**
: Level of depth.

    Default $\log_2(N_g - 1) + 2$

    Type positive integer

    Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

parameter **`num_v_cycles`**
: Number of V-cycles.

    Default `1`

    Type positive integer

    Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

database **`[QUADRATURE]`**
: Discrete ordinates quadrature. See [DENOVO][QUADRATURE] (page 184).

    Default (empty database)

    Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

parameter **`relax_count`**
: Number of rounds of weighted richardson iterations.

    Default `1`

    Type positive integer

    Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

parameter **`relax_weight`**
: Weight for richardson iteration.

    Default `1.0`

    Type positive real number

    Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

database **`[SMOOTHER]`**
: Multigrid smoother. See [DENOVO][SOLVER][UPSCATTER][PRECONDITIONER][SMOOTHER] (page 207).

    Optional

    Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`

3.23.26 …[SOLVER][UPSCATTER][PRECONDITIONER=TWOGRID]

Two-grid energy preconditioner.

database **`[QUADRATURE]`**
Discrete ordinates quadrature. See [DENOVO][QUADRATURE] (page 184).

Default (empty database)

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

database **`[WITHIN_GROUP]`**
One-group transport solver options. See [DENOVO][SOLVER][UPSCATTER][PRECONDITIONER][WITHIN_GROU
(page 207).

Default (empty database)

3.23.27 …[SOLVER][UPSCATTER][PRECONDITIONER=IFPACK]

ifpack energy preconditioner.

database **`[QUADRATURE]`**
Discrete ordinates quadrature. See [DENOVO][QUADRATURE] (page 184).

Default (empty database)

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

database **`[WITHIN_GROUP]`**
One-group transport solver options. See [DENOVO][SOLVER][UPSCATTER][PRECONDITIONER][WITHIN_GROU
(page 209).

Default (empty database)

3.23.28 …[SOLVER][UPSCATTER][PRECONDITIONER=ML]

ml energy preconditioner.

database **`[QUADRATURE]`**
Discrete ordinates quadrature. See [DENOVO][QUADRATURE] (page 184).

Default (empty database)

Applicable when `/denovo/disable` is `none` or `transport` and `/denovo/method` is `sn`

database **`[WITHIN_GROUP]`**
One-group transport solver options. See [DENOVO][SOLVER][UPSCATTER][PRECONDITIONER][WITHIN_GROU
(page 210).

Default (empty database)

3.23.29 …[SOLVER][WITHIN_GROUP][PRECONDITIONER=NONE]

No preconditioner.

3.23.30 ...[UPSCATTER][PRECONDITIONER][SMOOTHER]

Multigrid smoother.

parameter **`max_iterations`**
parameter **`maxitr`**
Max number of iterations for this solver.

Default `1000`

Type non-negative integer

database `[PRECONDITIONER]`
Smoother preconditioner type. See [DENOVO][SOLVER][UPSCATTER][PRECONDITIONER][SMOOTHER][PREC
(page 211).

Default (empty `none` database)

parameter **`solver`**
Solver used for smoother solve.

Default `gmres`

Type `gmres`, `si`, `bicgstab`, or `stratimikos`

parameter **`subspace_size`**
Max subspace size for this solver.

Default `20`

Type non-negative integer

Applicable when `solver` is `gmres`, `arnoldi`, or `davidson`

parameter **`tolerance`**
parameter **`tol`**
Convergence tolerance for this solver.

Default typically 0.1 * parent database tolerance

Type real number inside (0, 1)

postprocessor
Tolerance must be less than or equal to tolerance of parent solver database.

parameter **`verbosity`**
Solver verbosity.

Default `low`

Type `none`, `low`, `medium`, or `high`

3.23.31 ...[UPSCATTER][PRECONDITIONER][WITHIN_GROUP]

One-group transport solver options.

parameter **`matrix_output`***(advanced)*
Matrix output file for Krylov solver.

Default `A.h5`

Type file path to write (extension '.h5')

Applicable when `solver` is `matrixwriter`

parameter **`max_iterations`**
parameter **`maxitr`**
Max number of iterations for this solver.

Default `1000`

Type non-negative integer

database **`[PRECONDITIONER]`**
Within-group preconditioner type. See [DENOVO][SOLVER][WITHIN_GROUP][PRECONDITIONER] (page 204).

Default (empty `none` database)

parameter **`solver`**
Solver used in each within_group solve.

Default *gmres* if using a linear discretization, otherwise *si*

Type `gmres`, `gmres_r`, `si`, `bicgstab`, `stratimikos`, or `matrixwriter`

postprocessor
Cannot set `solver` to `bicgstab`, `gmres`, `gmres_r`, `matrixwriter`, or `stratimikos` unless 'equations' discretization is linear (not 'twd' or 'wdd_ff').

parameter **`subspace_size`**
Max subspace size for this solver.

Default `20`

Type non-negative integer

Applicable when `solver` is `gmres`, `arnoldi`, or `davidson`

parameter **`tolerance`**
parameter **`tol`**
Convergence tolerance for this solver.

Default typically 0.1 * parent database tolerance

Type real number inside (0, 1)

postprocessor
Tolerance must be less than or equal to tolerance of parent solver database.

unvalidated-database **`[TRILINOS]`**
Advanced Trilinos solver options. See [DENOVO][SOLVER][WITHIN_GROUP][TRILINOS] (page 204).

Optional

parameter **`verbosity`**
Solver verbosity.

Default `low`

Type `none`, `low`, `medium`, or `high`

3.23.32 ... [UPSCATTER][PRECONDITIONER][WITHIN_GROUP]

One-group transport solver options.

parameter **`matrix_output`***(advanced)*
Matrix output file for Krylov solver.

Default `A.h5`

Type file path to write (extension '.h5')

Applicable when `solver` is `matrixwriter`

parameter **`max_iterations`**
parameter **`maxitr`**
Max number of iterations for this solver.

Default `1000`

Type non-negative integer

database **`[PRECONDITIONER]`**
Within-group preconditioner type. See [DENOVO][SOLVER][WITHIN_GROUP][PRECONDITIONER] (page 204).

Default (empty `none` database)

parameter **`solver`**
Solver used in each within_group solve.

Default *gmres* if using a linear discretization, otherwise *si*

Type `gmres`, `gmres_r`, `si`, `bicgstab`, `stratimikos`, or `matrixwriter`

postprocessor
Cannot set `solver` to `bicgstab`, `gmres`, `gmres_r`, `matrixwriter`, or `stratimikos` unless 'equations' discretization is linear (not 'twd' or 'wdd_ff').

parameter **`subspace_size`**
Max subspace size for this solver.

Default `20`

Type non-negative integer

Applicable when `solver` is `gmres`, `arnoldi`, or `davidson`

parameter **`tolerance`**
parameter **`tol`**
Convergence tolerance for this solver.

Default typically 0.1 * parent database tolerance

Type real number inside (0, 1)

postprocessor
Tolerance must be less than or equal to tolerance of parent solver database.

unvalidated-database **`[TRILINOS]`**
Advanced Trilinos solver options. See [DENOVO][SOLVER][WITHIN_GROUP][TRILINOS] (page 204).

Optional

parameter **`verbosity`**
Solver verbosity.

Default `low`

Type `none`, `low`, `medium`, or `high`

3.23.33 ...[UPSCATTER][PRECONDITIONER][WITHIN_GROUP]

One-group transport solver options.

parameter **`matrix_output`***(advanced)*
Matrix output file for Krylov solver.

Default `A.h5`

Type file path to write (extension '.h5')

Applicable when `solver` is `matrixwriter`

parameter **`max_iterations`**
parameter **`maxitr`**
Max number of iterations for this solver.

Default `1000`

Type non-negative integer

database **`[PRECONDITIONER]`**
Within-group preconditioner type. See [DENOVO][SOLVER][WITHIN_GROUP][PRECONDITIONER] (page 204).

Default (empty `none` database)

parameter **`solver`**
Solver used in each within_group solve.

Default *gmres* if using a linear discretization, otherwise *si*

Type `gmres`, `gmres_r`, `si`, `bicgstab`, `stratimikos`, or `matrixwriter`

postprocessor
Cannot set `solver` to `bicgstab`, `gmres`, `gmres_r`, `matrixwriter`, or `stratimikos` unless 'equations' discretization is linear (not 'twd' or 'wdd_ff').

parameter **`subspace_size`**
Max subspace size for this solver.

Default `20`

Type non-negative integer

Applicable when `solver` is `gmres`, `arnoldi`, or `davidson`

parameter **`tolerance`**
parameter **`tol`**
Convergence tolerance for this solver.

Default typically 0.1 * parent database tolerance

Type real number inside (0, 1)

postprocessor
Tolerance must be less than or equal to tolerance of parent solver database.

unvalidated-database `[TRILINOS]`
Advanced Trilinos solver options. See [DENOVO][SOLVER][WITHIN_GROUP][TRILINOS] (page 204).

Optional

parameter **`verbosity`**
Solver verbosity.

Default `low`

Type `none`, `low`, `medium`, or `high`

3.23.34 ...[PRECONDITIONER][SMOOTHER][PRECONDITIONER]

Table 35: Available types for the [PRECONDITIONER] database

Type	Description	Applicability
none (page 211)	No preconditioner	
ifpack (page 211)	IFPACK algebraic preconditioner	`/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`
ml (page 211)	ML multi-level preconditioner	`/denovo/disable` is `none` or `transport` and `/denovo/method` is `spn`

3.23.35 ...[PRECONDITIONER][SMOOTHER][PRECONDITIONER=NONE]

No preconditioner.

3.23.36 ...[PRECONDITIONER][SMOOTHER][PRECONDITIONER=IFPACK]

IFPACK algebraic preconditioner.

unvalidated-database `[TRILINOS]`
Advanced Trilinos solver options. See [DENOVO][SOLVER][WITHIN_GROUP][TRILINOS] (page 204).

Optional

3.23.37 ...[PRECONDITIONER][SMOOTHER][PRECONDITIONER=ML]

ML multi-level preconditioner.

unvalidated-database `[TRILINOS]`
Advanced Trilinos solver options. See [DENOVO][SOLVER][WITHIN_GROUP][TRILINOS] (page 204).

Optional

3.24 ORIGEN DEPLETION SOLVER: [DEPLETION]

Omnibus couples Shift and ORIGEN, a depletion/transmutation analysis code, using ORIGEN's new C++ API and CRAM solver [20]. This new in-memory API avoids the prohibitive cost (on HPC systems) of writing to disk between transport and depletion steps, and it also enables each depletion step to be performed on each depletable region in parallel. Shift uses the same approach as the VESTA code to obtain microscopic per-nuclide reaction rates. This approach tallies ultra-fine-group fluxes in each depletion region and then uses these fluxes to collapse the microscopic continuous-energy cross sections into one-group reaction rates. Shift then sends these reaction rates to ORIGEN for a depletion calculation.

In order to optimize the parallel efficiency of the depletion calculation, the depletable regions on each block are distributed among the available processors, thereby minimizing the number of depletion solves performed on each core. After every core has calculated the new concentrations for its depletion regions, the results are broadcast to every other core on the block.

Shift provides several different transport-depletion coupling schemes and renormalization methods for the burnup calculations, with additional parameters to fine tune the coupling. Only `coupling_method` should need to be selected in everyday applications. The other coupling parameters (`depletion_method`, `renormalization_method`, `predictor_substeps`, `corrector-substeps`, `predictor_renormalization`, `calculate_depletion_energy`, and `cram_internal_substeps`) get reasonable defaults, some of which depend on the coupling scheme. Altering them should be considered an advanced feature.

Note: Depletion is currently supported *only* when using Shift with continuous energy. Deterministic and multigroup depletion are not implemented.

---

parameter **`always_transport`**

Always run transport for each timestep, even during decay.

Default `True`

Type boolean

parameter **`burn_length`**
parameter **`burn`**

Burnup lengths for each input step.

Units day

Type list of non-negative floats (each element is a non-negative real number)

parameter **`calculate_depletion_energy`**
parameter **`calc_de`**

Calculate energy released in depletion to get accurate burnups.

Default `True`

Type boolean

parameter **`constant_flux_per_step`**
parameter **`flux`**

Constant flux to be applied per burnup step.

Default `---`

Units $\frac{\mathrm{n}}{\mathrm{cm}^2}$

Type list of non-negative floats (each element is a non-negative real number)

parameter **`corrector_substeps`**

Number of substeps on the corrector.

The `corrector_substeps` parameter specifies the number of depletion substeps to use on the corrector (if applicable). See `predictor_substeps` for more details. The default value of this parameter depends on the depletion solver, coupling scheme, and renormalization.

Default heuristic values based on coupling method and solver

Type positive integer

Applicable when `coupling_method` is `middlestep`, `ce/li`, `le/li`, `le/qi`, `triton`, or `polaris`

postprocessor

Cannot set `renormalization_method` to `energy` unless `calculate_depletion_energy` is `True`.

postprocessor

Cannot set `renormalization_method` to `origen` unless `coupling_method` is `fully_explicit`, `middlestep`, `ce`, `triton`, or `polaris`.

postprocessor

Energy-based renormalization is unreliable with the MATREX depletion solver.

parameter **`coupling_method`**

parameter **`method`**

Method used to solve the coupled depletion-transport problem.

The `coupling_method` parameter specifies which method to use for selecting the cross sections over each depletion step or predicting their behavior over the step (when not assumed constant). The same treatment is used for the spatial distribution of the neutron flux. The behavior of the methods is further controlled by the `predictor_substeps`, `corrector_substeps` and `predictor_renormalization` parameters. The options (methods) and their descriptions are the following:

`fully_explicit` On the predictor, transport is solved at the beginning of step (BOS), and the BOS cross sections are used for the entire step. No corrector.

`middlestep` A two-transport-solutions-per-step version of the middlestep method. Predictor uses BOS cross sections and flux to obtain middle-of-step compositions. Corrector uses MOS cross sections and flux to deplete for the entire step.

`ce` A newer implementation of the `fully_explicit` method.

`le` On the predictor, transport is solved at BOS and the cross sections are linearly interpolated through the previous step values and the BOS values. No corrector.

`ce/li` Predictor works as `ce`. On the corrector, transport is solved at the end of step (EOS), and the cross sections are interpolated linearly through the BOS and EOS values.

`le/li` Predictor works as `le`. On the corrector, transport is solved at the end of step (EOS), and the cross sections are interpolated linearly through the BOS and EOS values.

`le/qi` Predictor works as `le`. On the corrector, transport is solved at the end of step (EOS), and the cross sections are interpolated quadratically through the previous step, BOS, and EOS values.

`triton` As `middlestep` except that after the first step, there is no transport calculation on the predictor. Instead, the cross sections and flux from the middle of the previous step are used. Note that this method outputs on a different time grid than the others.

`polaris` Predictor works as `ce`. On the corrector, transport is solved at the end of step (EOS), and the EOS cross sections and flux are used to re-deplete the materials. The average of the EOS compositions obtained on the predictor and corrector becomes the initial composition for the next step.

The labels `ce`, `le`, `li`, and `qi` come from constant extrapolation, linear extrapolation, linear interpolation, and quadratic interpolation, respectively. They stand for the approximation used for the time development of the cross sections and flux on the predictor or corrector.

The methods `le`, `le/li`, and `le/qi` are more accurate than the rest but also sensitive to large (factor of 35 or more) changes in step lengths. These methods will default to lower-order methods when previous step data is not available, or is not applicable due to changed normalization. `le/li` and `le/qi` are the most accurate, but if steps need to be short due to desired output, `le` might be preferable as it takes half as long per step (but needs more then twice as many steps to reach given accuracy).

Regardless of the choice of `coupling_method`, pure decay steps with zero flux will always be solved with `ce`, as it is the simplest method and still exact in the absence of neutron flux.

Default `fully_explicit`

Type `fully_explicit`, `middlestep`, `ce`, `le`, `ce/li`, `le/li`, `le/qi`, `triton`, or `polaris`

parameter **`cram_internal_substeps`**

Number of internal substeps in the CRAM depletion solver.

This option is only applied when there are fewer coupling substeps.

The `cram_internal_substeps` parameter specifies the minimum number of substeps that CRAM depletion solver should use on each step for depletion accuracy purposes. If this amount is larger than the number of regular substeps, the CRAM solver uses a feature called internal substeps to meet the amount specified here.

Internal substeps do not involve different cross sections or renormalization, but they are much faster than regular substeps. The number of internal substeps to apply on each regular substep is selected so that the total number of internal substeps over all substeps adds up to at least `cram_internal_substeps`.

The default value is 2.

Default `2`

Type positive integer

Applicable when `depletion_solver` is `cram`

parameter **`cram_order`**

Order of the CRAM depletion solver.

Default `16`

Type positive integer

Applicable when `depletion_solver` is `cram`

parameter **`decay_length`**
parameter **`decay`**

Decay lengths for each input step.

Default `---`

Units day

Type list of non-negative floats (each element is a non-negative real number)

parameter **`deplete_cells`**
parameter **`cells`**

Labels of cells to deplete instead of all fissionable cells, or * to indicate all cells.

By default, when depletion is enabled, all “depletable” cells will be tracked and depleted. (Depletable cells correspond to materials with fissionable materials, or if a `[COMP]` block is used, materials with the depletable flag set.) This parameter overrides this default: cells with the listed labels will have their materials depleted.

Default `---`

Type list of cell names (each element is a string)

parameter **`deplete_nuclides`**
parameter **`nuclides`**

List of nuclides to deplete. All cells containing these nuclides will be depleted. Can be used together with ‘deplete_cells.’

Default `---`

Type list of nuclides in the TRITON nuclide set (each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1))

parameter **`depletion_solver`**

Depletion solver type.

Default `cram`

Type `cram` or `matrex`

parameter **`group_bounds`**

Energy bin boundaries for depletion tally.

Default `---`

Units eV

Type nonnegative floats in decreasing order (each element is a non-negative real number)

parameter **`jeff_library`**

Filepath to an ORIGEN JEFF multigroup file.

Default `'/.../origen.rev01.jeff252g'`

Type library path

parameter **`kappa_library`**

Filepath to an HDF5 file containing kappa values.

Optional

Type file path for reading (extension '.h5')

parameter **`max_burn_substep_size`**

Maximum substep size for an ORIGEN time step of non-zero power/flux.

Default `40.0`

Units day

Type non-negative real number

parameter **`max_decay_substep_size`**

Maximum substep size for an ORIGEN time step of zero power/flux.

Default `75.0`

Units day

Type non-negative real number

parameter **`max_step`**

Maximum time before automatically increasing the number of steps.

Default `400.0`

Units day

Type non-negative real number

database **`[MICRO]`**

Tally microscopic cross sections. See [DEPLETION][MICRO] (page 223).

Optional

sublist **`[MOVE]`**

Time-dependent geometry movement. See [DEPLETION][MOVE] (page 223).

Optional

parameter **`nuclide_filter_threshold`**

Threshold at which nuclides below are removed from transport.

Default appropriate filtering threshold for the filter type

Type non-negative real number

Applicable when filtering nuclides

parameter **`nuclide_filter_type`**

How to filter nuclides for transport calculations.

Default `none`

Type `none`, `number_density`, `absorption`, or `total` *parameter* **`num_burn_steps`**

Number of steps to take for each burn length entry.

The `num_burn_steps` parameter must have the same length as `burn_length` and `decay_length`. It is the number of constant-flux calculations per entry. Increasing the number will increase the accuracy of the answer by having better approximations of the depleted concentrations during the transport step, but it will increase the computational cost because more transport calculations must be performed.

Default `---`

Type list in which each element is a non-negative integer

parameter **`num_decay_steps`**

Number of steps to take for each decay length entry.

Default `---`

Type list in which each element is a non-negative integer

parameter **`origen_library`**

Filepath to an ORIGEN library file.

Default `'/.../pwr.rev03.orglib'`

Type library path

parameter **`power`**

Constant power to be applied per burnup step.

Default `---`

Units MW

Type list of non-negative floats (each element is a non-negative real number)

postprocessor

The parameters `burn_length`, `decay_length`, `power`, `num_burn_steps`, and `num_decay_steps` must have the same length. Empty lists are ignored.

parameter **`predictor_renormalization`**

Perform renormalization on the predictor.

Default `true` only if using Polaris coupling

Type boolean

Applicable when `coupling_method` is `middlestep`, `ce/li`, `le/li`, `le/qi`, `triton`, or `polaris`

parameter **`predictor_substeps`**

Number of substeps on the predictor.

The `predictor_substeps` parameter specifies the number of depletion substeps to use on the predictor. Substeps are always equidistant except for long zero- flux steps with MATREX, in which case each substep will be thrice as long as the previous.

Substeps serve two roles:

1. The depletion for each substep uses cross sections and flux averaged over that substeps from the prediction made in the coupling scheme.

2. The neutron flux is renormalized at each substep using the compositions, cross sections, and flux/power distribution for that substep.

In addition, the number of substeps affects the depletion solver's accuracy. The MATREX depletion solver requires a sufficient number of substeps that are not too long. The number of substeps is automatically incremented on a step-by-step basis to meet these requirements. Decay steps with the CRAM solver always use one only substep. See the parameter `cram_internal_substeps`.

The default value of this parameter depends on the depletion solver, coupling scheme, and renormalization.

Default heuristic values based on coupling method and solver

Type positive integer

parameter **`print_filtering`**
Print statistics about nuclide filtering.

Default `False`

Type boolean

parameter **`renormalization_method`**
How to renormalize the flux at each substep.

Which renormalization method (if any) to use on each substep of depletion calculations. The following options are available:

`none` No renormalization is performed.

`boss` Beginning-of-substep cross sections and compositions are used for the renormalization. This method is inaccurate and should not be used.

`moss` Middle-of-substep cross sections and compositions are used for the renormalization.

`energy` Renormalization is based on the energy released during depletion. This method is very accurate with CRAM, although the difference to `moss` has no practical significance if substeps are used. There is no proof that this would always be accurate with MATREX.

`origen` ORIGEN-style renormalization where power distribution is assumed to remain constant through the step.

The default is `energy` if using CRAM and `moss` if using MATREX or if `calculate_depletion_energy` is false.

Default `energy` if allowable, else `moss`

Type `none`, `boss`, `moss`, `energy`, or `origen`

parameter **`reset_inactive_cycles`**
Number of inactive cycles to run for all transport calculations except the initial calculation.

Default `-1`

Type integer

parameter **`tracking_nuclides`**
Nuclides that will be tracked for depletion.

Default `---`

Type list of nuclides in the TRITON nuclide set (each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1))

command **`tracking_set`**

append a set of TRITON nuclides to `tracking_nuclides`.

The `tracking_set` command exposes the TRITON `addnux` option to the user.

`tracking_set none` adds no extra nuclides to track (the default).

`tracking_set addnux1` corresponds to `addnux=1` and adds:

U-234, U-235, U-236, U-238, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-242, Am-243, Cm-242, Cm-243

`tracking_set addnux-2` corresponds to `addnux=-2` and adds the above nuclides as well as:

H-1, B-10, B-11, N-14, O-16, Kr-83, Zr-94, Nb-93, Mo-95, Tc-99, Ru-106, Rh-103, Rh-105, Ag-109, Sn-126, I-135, Xe-131, Xe-135, Cs-133, Cs-134, Cs-135, Cs-137, Ce-144, Pr-143, Nd-143, Nd-145, Nd-146, Nd-147, Nd-148, Pm-147, Pm-148, Pm-149, Sm-147, Sm-149, Sm-150, Sm-151, Sm-152, Eu-151, Eu-153, Eu-154, Eu-155, Gd-152, Gd-154, Gd-155, Gd-156, Gd-157, Gd-158, Gd-160, Cm-244

`tracking_set addnux2` corresponds to `addnux=2` and adds the above nuclides as well as:

Zr-91, Zr-93, Zr-95, Zr-96, Nb-95, Mo-97, Mo-98, Mo-99, Mo-100, Ru-101, Ru-102, Ru-103, Ru-104, Pd-105, Pd-107, Pd-108, Cd-113, In-115, I-127, I-129, Xe-133, Ba-140, La-139, Ce-141, Ce-142, Ce-143, Pr-141, Nd-144, Sm-153, Eu-156

`tracking_set addnux3` corresponds to `addnux=3` and adds the above nuclides as well as:

Ge-72, Ge-73, Ge-74, Ge-76, As-75, Se-76, Se-77, Se-78, Se-80, Se-82, Br-79, Br-81, Kr-80, Kr-82, Kr-84, Kr-85, Kr-86, Rb-85, Rb-86, Rb-87, Sr-84, Sr-86, Sr-87, Sr-88, Sr-89, Sr-90, Y-89, Y-90, Y-91, Zr-90, Zr-92, Nb-94, Mo-92, Mo-94, Mo-96, Ru-96, Ru-98, Ru-99, Ru-100, Ru-105, Pd-102, Pd-104, Pd-106, Pd-110, Ag-107, Ag-111, Cd-106, Cd-108, Cd-110, Cd-111, Cd-112, Cd-114, Cd-115m, Cd-116, In-113, Sn-112, Sn-114, Sn-115, Sn-116, Sn-117, Sn-118, Sn-119, Sn-120, Sn-122, Sn-123, Sn-124, Sn-125, Sb-121, Sb-123, Sb-124, Sb-125, Sb-126, Te-120, Te-122, Te-123, Te-124, Te-125, Te-126, Te-127m, Te-128, Te-129m, Te-130, Te-132, I-130, I-131, Xe-124, Xe-126, Xe-128, Xe-129, Xe-130, Xe-132, Xe-134, Xe-136, Cs-136, Ba-134, Ba-135, Ba-136, Ba-137, Ba-138, La-140, Ce-140, Pr-142, Nd-142, Nd-150, Pm-151, Sm-144, Sm-148, Sm-154, Eu-152, Eu-157, Tb-159, Tb-160, Dy-160, Dy-161, Dy-162, Dy-163, Dy-164, Ho-165, Er-166, Er-167, Lu-175, Lu-176, Ta-181, W-182, W-183, W-184, W-186, Re-185, Re-187, Au-197, Th-230, Th-232, Pa-231, Pa-233, U-232, U-233

`tracking_set addnux4` corresponds to `addnux=4` and adds the above nuclides as well as:

H-2, H-3, He-3, He-4, Li-6, Li-7, Be-7, Be-9, N-15, O-17, F-19, Na-23, Mg-24, Mg-25, Mg-26, Al-27, Si-28, Si-29, Si-30, P-31, S-32, S-33, S-34, S-36, Cl-35, Cl-37, Ar-36, Ar-38, Ar-40, Ka-39, Ka-40, Ka-41, Ca-40, Ca-42, Ca-43, Ca-44, Ca-46, Ca-48, Sc-45, Ti-46, Ti-47, Ti-48, Ti-49, Ti-50, Cr-50, Cr-52, Cr-53, Cr-54, Mn-55, Fe-54, Fe-56, Fe-57, Fe-58, Co-58m, Co-58, Co-59, Ni-58, Ni-59, Ni-60, Ni-61, Ni-62, Ni-64, Cu-63, Cu-65, Ga-69, Ga-71, Ge-70, As-74, Se-74, Se-79, Kr-78, Ag-110m, Sn-113, Xe-123, Ba-130, Ba-132, Ba-133, La-138, Ce-136, Ce-138, Ce-139, Pm-148m, Gd-153, Dy-156, Dy-158, Ho-166m, Er-162, Er-164, Er-168, Er-170, Hf-174, Hf-176, Hf-177, Hf-178, Hf-179, Hf-180, Ta-182, Ir-191, Ir-193, Hg-196, Hg-198, Hg-199, Hg-200, Hg-201, Hg-202, Hg-204, Pb-204, Pb-206, Pb-207, Pb-208, Bi-209, Ra-223, Ra-224, Ra-225, Ra-226, Ac-225, Ac-226, Ac-227, Th-227, Th-228, Th-229, Th-233, Th-234, Pa-232, U-237, U-239, U-240, U-241, Np-235, Np-236, Np-238, Np-239, Pu-236, Pu-237, Pu-243, Pu-244, Pu-246, Am-242m, Am-244, Am-244m, Cm-241, Cm-245, Cm-246, Cm-247, Cm-248, Cm-249, Cm-250, Bk-249, Bk-250, Cf-249, Cf-250, Cf-251, Cf-252, Cf-253, Cf-254, Es-253, Es-254, Es-255

`tracking_set all` contains all the nuclides available in ORIGEN, which are the above nuclides as well as:

H-4, He-5, He-6, He-8, Li-8, Li-9, Be-8, Be-10, Be-11, Be-12, B-12, C-0, C-12, N-13, N-16, O-18, O-19, F-20, Ne-20, Ne-21, Ne-22, Ne-23, Na-22, Na-24, Na-24m, Na-25, Mg-27, Mg-28, Al-26, Al-28, Al-29, Al-30, Si-31, Si-32, P-32, P-33, P-34, S-25, S-35, S-37, Cl-36, Cl-38, Cl-38m, Ar-37, Ar-39, Ar-41, Ar-42, Ka-42, Ka-43, Ka-44, Ca-41, Ca-45, Ca-47, Ca-49, Sc-44, Sc-44m, Sc-45m, Sc-46, Sc-46m, Sc-47, Sc-48, Sc-49, Sc-50, Ti-44, Ti-45, Ti-51, V-48, V-49, V-50, V-51, V-52, V-53, V-54, Cr-48, Cr-49, Cr-51, Cr-55, Cr-66, Cr-67, Mn-52, Mn-53, Mn-54, Mn-56, Mn-57, Mn-58, Mn-66, Mn-67, Mn-68, Mn-69, Fe-55, Fe-59, Fe-60, Fe-65, Fe-66, Fe-67, Fe-68, Fe-69, Fe-70, Fe-71, Fe-72, Co-55, Co-56, Co-57, Co-60, Co-60m, Co-61, Co-62, Co-65, Co-66, Co-67, Co-68, Co-69, Co-70, Co-71, Co-72, Co-73, Co-74, Co-75, Ni-56, Ni-57, Ni-63, Ni-65, Ni-66, Ni-67, Ni-68, Ni-69, Ni-70, Ni-71, Ni-72, Ni-73, Ni-74, Ni-75, Ni-76, Ni-77, Ni-78, Cu-62, Cu-64, Cu-66, Cu-67, Cu-68, Cu-68m, Cu-69, Cu-70, Cu-70m, Cu-71, Cu-72, Cu-73, Cu-74, Cu-75, Cu-76, Cu-77, Cu-78, Cu-79, Cu-80, Cu-81, Zn-63, Zn-64, Zn-65, Zn-66, Zn-67, Zn-68, Zn-69, Zn-69m, Zn-70, Zn-71, Zn-71m, Zn-72, Zn-73, Zn-74, Zn-75, Zn-76, Zn-77, Zn-78, Zn-79, Zn-80, Zn-81, Zn-82, Zn-83, Ga-66, Ga-67, Ga-68, Ga-70, Ga-72, Ga-72m, Ga-73, Ga-74, Ga-74m, Ga-75, Ga-76, Ga-77, Ga-78, Ga-79, Ga-80, Ga-81, Ga-82, Ga-83, Ga-84, Ga-85, Ga-86, Ge-66, Ge-67, Ge-68, Ge-69, Ge-71, Ge-71m, Ge-73m, Ge-75, Ge-75m, Ge-77, Ge-77m, Ge-78, Ge-79, Ge-79m, Ge-80, Ge-81m, Ge-81, Ge-82, Ge-83, Ge-84, Ge-85, Ge-86, Ge-87, Ge-88, Ge-89, As-69, As-71, As-72, As-73, As-75m, As-76, As-77, As-78, As-79, As-80, As-81, As-82, As-82m, As-83, As-84, As-84m, As-85, As-86, As-87, As-88, As-89, As-90, As-91, As-92, Se-72, Se-73, Se-73m, Se-75, Se-77m, Se-79m, Se-81, Se-81m, Se-83m, Se-83, Se-84, Se-85, Se-86, Se-87, Se-88, Se-89, Se-90, Se-91, Se-92, Se-93, Se-94, Br-75, Br-76, Br-77, Br-77m, Br-78, Br-79m, Br-80, Br-80m, Br-82, Br-82m, Br-83, Br-84, Br-84m, Br-85, Br-86, Br-87, Br-88, Br-89, Br-90, Br-91, Br-92, Br-93, Br-94, Br-95, Br-96, Br-97, Kr-76, Kr-77, Kr-79m, Kr-79, Kr-81, Kr-81m, Kr-83m, Kr-85m, Kr-87, Kr-88, Kr-89, Kr-90, Kr-91, Kr-92, Kr-93, Kr-94, Kr-95, Kr-96, Kr-97, Kr-98, Kr-99, Kr-100, Rb-79, Rb-81, Rb-82, Rb-83, Rb-84, Rb-86m, Rb-88, Rb-89, Rb-90, Rb-90m, Rb-91, Rb-92, Rb-93, Rb-94, Rb-95, Rb-96, Rb-97, Rb-98, Rb-99, Rb-100, Rb-101, Rb-102, Sr-82, Sr-83, Sr-85, Sr-85m, Sr-87m, Sr-91, Sr-92, Sr-93, Sr-94, Sr-95, Sr-96, Sr-97, Sr-98, Sr-99, Sr-100, Sr-101, Sr-102, Sr-103, Sr-104, Sr-105, Y-85, Y-86, Y-87, Y-87m, Y-88, Y-89m, Y-90m, Y-91m, Y-92, Y-93, Y-93m, Y-94, Y-95, Y-96, Y-96m, Y-97, Y-97m, Y-98, Y-98m, Y-99, Y-100, Y-101, Y-102, Y-103, Y-104, Y-105, Y-106, Y-107, Y-108, Zr-86, Zr-87, Zr-88, Zr-89, Zr-89m, Zr-90m, Zr-97, Zr-98, Zr-99, Zr-100, Zr-101, Zr-102, Zr-103, Zr-104, Zr-105, Zr-106, Zr-107, Zr-108, Zr-109, Zr-110, Nb-89, Nb-90, Nb-91, Nb-91m, Nb-92, Nb-92m, Nb-93m, Nb-94m, Nb-95m, Nb-96, Nb-97, Nb-97m, Nb-98, Nb-98m, Nb-99, Nb-99m, Nb-100, Nb-100m, Nb-101, Nb-102, Nb-102m, Nb-103, Nb-104, Nb-104m, Nb-105, Nb-106, Nb-107, Nb-108, Nb-109, Nb-110, Nb-111, Nb-112, Nb-113, Mo-90, Mo-91, Mo-93, Mo-93m, Mo-101, Mo-102, Mo-103, Mo-104, Mo-105, Mo-106, Mo-107, Mo-108, Mo-109, Mo-110, Mo-111, Mo-112, Mo-113, Mo-114, Mo-115, Tc-93, Tc-95, Tc-95m, Tc-96, Tc-97, Tc-97m, Tc-98, Tc-99m, Tc-100, Tc-101, Tc-102, Tc-102m, Tc-103, Tc-104, Tc-105, Tc-106, Tc-107, Tc-108, Tc-109, Tc-110, Tc-111, Tc-112, Tc-113, Tc-114, Tc-115, Tc-116, Tc-117, Tc-118, Ru-95, Ru-97, Ru-107, Ru-108, Ru-109, Ru-109m, Ru-110, Ru-111, Ru-112, Ru-113, Ru-114, Ru-115, Ru-116, Ru-117, Ru-118, Ru-119, Ru-120, Rh-99, Rh-99m, Rh-100, Rh-101, Rh-101m, Rh-102, Rh-102m, Rh-103m, Rh-104, Rh-104m, Rh-105m, Rh-106, Rh-106m, Rh-107, Rh-108, Rh-108m, Rh-109, Rh-109m, Rh-110, Rh-110m, Rh-111, Rh-112, Rh-113, Rh-114, Rh-115, Rh-116, Rh-117, Rh-118, Rh-119, Rh-120, Rh-121, Rh-122, Rh-123, Pd-99, Pd-100, Pd-101, Pd-103, Pd-107m, Pd-109, Pd-109m, Pd-111, Pd-111m, Pd-112, Pd-113, Pd-114, Pd-115, Pd-116, Pd-117, Pd-118, Pd-119, Pd-120, Pd-121, Pd-122, Pd-123, Pd-124, Pd-125, Pd-126, Ag-103, Ag-105, Ag-105m, Ag-106, Ag-106m, Ag-107m, Ag-108, Ag-108m, Ag-109m, Ag-110, Ag-111m, Ag-112, Ag-113, Ag-113m, Ag-114, Ag-115, Ag-115m, Ag-116, Ag-116m, Ag-117, Ag-117m, Ag-118, Ag-118m, Ag-119, Ag-120, Ag-120m, Ag-121, Ag-122, Ag-122m, Ag-123, Ag-124, Ag-125, Ag-126, Ag-127, Ag-128, Ag-129, Ag-130, Cd-105, Cd-107, Cd-109, Cd-111m, Cd-113m, Cd-115, Cd-117, Cd-117m, Cd-118, Cd-119, Cd-119m, Cd-120, Cd-121, Cd-121m, Cd-122, Cd-123, Cd-123m, Cd-124, Cd-125, Cd-126, Cd-127, Cd-128, Cd-129, Cd-130, Cd-131, Cd-132, In-107, In-109, In-111m, In-111, In-112, In-112m, In-113m, In-114m, In-114, In-115m, In-116m, In-116, In-117m, In-117, In-118m, In-118, In-119m, In-119, In-120m, In-120, In-121m, In-121, In-122m, In-122, In-123m, In-123, In-124m, In-124, In-125m, In-125, In-126m, In-126, In-127m, In-127, In-128m, In-128, In-129m, In-129, In-130m, In-130, In-131m, In-131, In-132, In-133, In-134, In-135, Sn-111, Sn-113m, Sn-117m, Sn-119m, Sn-121, Sn-121m, Sn-123m, Sn-125m, Sn-127, Sn-127m, Sn-128, Sn-128m, Sn-129, Sn-129m, Sn-130, Sn-130m, Sn-131, Sn-131m, Sn-132, Sn-133, Sn-134, Sn-135, Sn-136, Sn-137, Sb-113, Sb-115m, Sb-115, Sb-117, Sb-118m, Sb-118, Sb-119, Sb-120m, Sb-120, Sb-122m, Sb-122, Sb-124m, Sb-126m, Sb-127, Sb-128m, Sb-128, Sb-129, Sb-130m, Sb-130, Sb-131, Sb-132m, Sb-132, Sb-133, Sb-134m, Sb-134, Sb-135, Sb-136, Sb-137, Sb-138, Sb-139, Te-115, Te-117, Te-118, Te-119m, Te-119, Te-121, Te-121m, Te-123m, Te-125m, Te-127, Te-129, Te-131, Te-131m, Te-133, Te-133m, Te-134, Te-135, Te-136, Te-137, Te-138, Te-139, Te-140, Te-141, Te-142, I-121, I-122, I-123, I-124, I-125, I-126, I-128, I-130m, I-132, I-132m, I-133, I-133m, I-134m, I-134, I-136m, I-136, I-137, I-138, I-139, I-140, I-141, I-142, I-143, I-144, I-145, Xe-122, Xe-125, Xe-125m, Xe-127m, Xe-127, Xe-129m, Xe-131m, Xe-133m, Xe-134m, Xe-135m, Xe-137, Xe-138, Xe-139, Xe-140, Xe-141, Xe-142, Xe-143, Xe-144, Xe-145, Xe-145m, Xe-146, Xe-147, Cs-127, Cs-128, Cs-129, Cs-130, Cs-131, Cs-132, Cs-134m, Cs-135m, Cs-136m, Cs-138m, Cs-138, Cs-139, Cs-140, Cs-141, Cs-142, Cs-143, Cs-144, Cs-145, Cs-146, Cs-147, Cs-148, Cs-149, Cs-150, Cs-151, Ba-128, Ba-129, Ba-131, Ba-131m, Ba-133m, Ba-135m, Ba-136m, Ba-137m, Ba-139, Ba-141, Ba-142, Ba-143, Ba-144, Ba-145, Ba-146, Ba-147, Ba-148, Ba-149, Ba-150, Ba-151, Ba-152, Ba-153, La-133, La-134, La-135, La-136, La-137, La-141, La-142, La-143, La-144, La-145, La-146m, La-146, La-147, La-148, La-149, La-150, La-151, La-152, La-153, La-154, La-155, Ce-134, Ce-135, Ce-137m, Ce-137, Ce-139m, Ce-145, Ce-146, Ce-147, Ce-148, Ce-149, Ce-150, Ce-151, Ce-152, Ce-153, Ce-154, Ce-155, Ce-156, Ce-157, Pr-139, Pr-140, Pr-142m, Pr-144m, Pr-144, Pr-145, Pr-146, Pr-147, Pr-148m, Pr-148, Pr-149, Pr-150, Pr-151, Pr-152, Pr-153, Pr-154, Pr-155, Pr-156, Pr-157, Pr-158, Pr-159, Nd-140, Nd-141, Nd-149, Nd-151, Nd-152, Nd-153, Nd-154, Nd-155, Nd-156, Nd-157, Nd-158, Nd-159, Nd-160, Nd-161, Pm-141, Pm-143, Pm-144, Pm-145, Pm-146, Pm-150, Pm-152m, Pm-152, Pm-153, Pm-154m, Pm-154, Pm-155, Pm-156, Pm-157, Pm-158, Pm-159, Pm-160, Pm-161, Pm-162, Pm-163, Sm-143, Sm-143m, Sm-145, Sm-146, Sm-155, Sm-156, Sm-157, Sm-158, Sm-159, Sm-160, Sm-161, Sm-162, Sm-163, Sm-164, Sm-165, Eu-145, Eu-146, Eu-147, Eu-148, Eu-149, Eu-150m, Eu-150, Eu-152m, Eu-154m, Eu-158, Eu-159, Eu-160, Eu-161, Eu-162, Eu-163, Eu-164, Eu-165, Eu-166, Eu-167, Gd-146, Gd-147, Gd-148, Gd-149, Gd-150, Gd-151, Gd-153m, Gd-155m, Gd-159, Gd-161, Gd-162, Gd-163, Gd-164, Gd-165, Gd-166, Gd-167, Gd-168, Gd-169, Tb-151, Tb-152, Tb-153, Tb-154m, Tb-154, Tb-155, Tb-156m, Tb-156, Tb-157, Tb-158m, Tb-158, Tb-161, Tb-162, Tb-163, Tb-164, Tb-165, Tb-166, Tb-167, Tb-168, Tb-169, Tb-170, Tb-171, Dy-154, Dy-155, Dy-157, Dy-159, Dy-165, Dy-165m, Dy-166, Dy-167, Dy-168, Dy-169, Dy-170, Dy-171, Dy-172, Ho-159m, Ho-159, Ho-160m, Ho-160, Ho-161m, Ho-161, Ho-162m, Ho-162, Ho-163m, Ho-163, Ho-164m, Ho-164, Ho-166, Ho-167, Ho-168, Ho-169, Ho-170m, Ho-170, Ho-171, Ho-172, Er-160, Er-161, Er-163, Er-165, Er-167m, Er-169, Er-171, Er-172, Tm-165, Tm-166, Tm-167, Tm-168, Tm-169, Tm-170m, Tm-170, Tm-171, Tm-172, Tm-173, Yb-166, Yb-167, Yb-168, Yb-169m, Yb-169, Yb-170, Yb-171, Yb-172, Yb-173, Yb-174, Yb-175m, Yb-175, Yb-176, Yb-177, Lu-169m, Lu-169, Lu-170, Lu-171m, Lu-171, Lu-172m, Lu-172, Lu-173, Lu-174m, Lu-174, Lu-176m, Lu-177m, Lu-177, Hf-170, Hf-171, Hf-172, Hf-173, Hf-175, Hf-178m, Hf-179m, Hf-180m, Hf-181, Hf-182, Ta-177, Ta-178, Ta-179, Ta-180m, Ta-180, Ta-182m, Ta-183, W-178, W-180, W-181, W-183m, W-185, W-185m, W-187, W-188, W-189, Re-181, Re-182, Re-182m, Re-183, Re-184, Re-184m, Re-186, Re-186m, Re-188, Re-188m, Re-189, Os-182, Os-183, Os-184, Os-185, Os-186, Os-187, Os-188, Os-189, Os-189m, Os-190, Os-190m, Os-191, Os-191m, Os-192, Os-193, Os-194, Ir-185, Ir-186, Ir-188, Ir-189, Ir-189m, Ir-190, Ir-191m, Ir-192, Ir-192m, Ir-193m, Ir-194, Ir-194m, Ir-196, Ir-196m, Pt-188, Pt-189, Pt-190, Pt-191, Pt-192, Pt-193, Pt-193m, Pt-194, Pt-195, Pt-195m, Pt-196, Pt-197, Pt-197m, Pt-198, Pt-199, Pt-199m, Pt-200, Au-193, Au-194, Au-195, Au-195m, Au-196, Au-198, Au-198m, Au-199, Au-199m, Au-200, Au-200m, Hg-193m, Hg-193, Hg-194, Hg-195m, Hg-195, Hg-197, Hg-197m, Hg-199m, Hg-203, Hg-205, Hg-206, Tl-200, Tl-201, Tl-202, Tl-203, Tl-204, Tl-205, Tl-206, Tl-207, Tl-208, Tl-209, Tl-210, Pb-200, Pb-202, Pb-203, Pb-205, Pb-205m, Pb-207m, Pb-209, Pb-210, Pb-211, Pb-212, Pb-214, Bi-205, Bi-206, Bi-207, Bi-208, Bi-210, Bi-210m, Bi-211, Bi-212, Bi-212m, Bi-213, Bi-214, Po-206, Po-207, Po-208, Po-209, Po-210, Po-211, Po-211m, Po-212, Po-213, Po-214, Po-215, Po-216, Po-218, At-216, At-217, At-218, Rn-216, Rn-217, Rn-218, Rn-219, Rn-220, Rn-222, Fr-220, Fr-221, Fr-222, Fr-223, Ra-220, Ra-222, Ra-227, Ra-228, Ac-224, Ac-228, Th-226, Th-231, Pa-228, Pa-229, Pa-230, Pa-234, Pa-234m, Pa-235, U-230, U-231, Np-234, Np-236m, Np-240, Np-240m, Np-241, Pu-237m, Pu-245, Pu-247, Am-239, Am-240, Am-245, Am-246, Am-247, Cm-240, Cm-251, Bk-245, Bk-246, Bk-247, Bk-248, Bk-248m, Bk-251, Cf-246, Cf-248, Cf-255, Es-251, Es-252, Es-254m

These tables are available in the SCALE 6.1 manual.

Creates tracking_nuclides

parameter **`write_mixtables`***(advanced)*

Write the transport mixtables.

Default `False`

Type boolean

parameter **`write_predictor_data`**

parameter **`write_p`**

Write predictor data.

Default `False`

Type boolean

Applicable when `coupling_method` is `middlestep`, `ce/li`, `le/li`, `le/qi`, `triton`, or `polaris`

parameter **`write_xs`**

Write the collapsed origen XS.

Default `False`

Type boolean

parameter **`yield_library`**

Filepath to an ORIGEN fission yields library file.

Default `'/.../origen.rev05.yields.data'`

Type library path

3.24.1 [DEPLETION][MOVE]

Time-dependent geometry movement.

parameter **`delta`**

Distance to move surfaces at the beginning of each step.

Type list in which each element is a real number

postprocessor

Number of movement steps should match depletion steps.

parameter **`name`**

Name of the surface group.

Type string without special characters

postprocessor

Move name must correspond to a movable geometry name.

3.24.2 [DEPLETION][MICRO]

This creates a "micro" tally to calculate reaction rates for depletion and calculates the material-averaged, flux-weighted cross sections for multiple materials, nuclides, and reactions. The user specifies a list of materials to tally, as well as a list of nuclide/reaction pairs.

The multibinning method is used to calculate any additional rates which are not specified in this tally.

Note: Micro tallies can currently only calculate reaction rates for nuclides that are present in the material.

parameter **`materials`**

parameter **`mats`**

Materials in which to tally.

Type list in which each element is a non-empty string

parameter **`micro_mt`**

ENDF reactions for microscopic cross section tallying.

Type list in which each element is a MT number or name (e.g., N_GAMMA, 102)

postprocessor

The parameters `micro_mt_zaid` and `micro_mt` must have the same length.

parameter **`micro_mt_zaid`**

Nuclide IDs for microscopic cross section tallying.

Type list in which each element is a nuclide specifier (e.g., U-235, 92235, u235, u-235m1)

3.25 HYBRID METHODOLOGY: [HYBRID]

In computational nuclear engineering, the term "hybrid" describes methods that couple two different classes of approximate methods to obtain a more accurate or faster solution. The primary hybrid method in Exnihilo is to use an approximate Denovo deterministic adjoint solution to generate an important map that reduces the variance of a Shift Monte Carlo calculation using weight windows.

Table 36: Available types for the [HYBRID] database

Type	Description	Applicability
cadis (page 224)	CADIS hybrid method	solver is 'denovo'
fwcadis (page 224)	FW-CADIS hybrid method	solver is 'denovo'
ww (page 226)	Manually input weight windows	Shift is enabled and Denovo is not

3.25.1 [HYBRID=CADIS]

Consistent Adjoint Driven Importance Sampling (CADIS) goes beyond the use of weight windows by also applying source biasing. Full details on the theory of this method can be found in [16]. This variance reduction technique is useful when considering local quantities of interest.

In Shift, a Denovo adjoint calculation is first performed to generate the adjoint flux. This adjoint flux is used to automatically generate weight windows and also to consistently bias the source used in the subsequent Shift fixed source calculation. See Shift Omnibus hybrid cadis input section (page 224) for specific input options available when running CADIS with Shift. Also see the Denovo Omnibus input section (page 176) for the input options for Denovo adjoint calculations.

parameter **`tallies`**

Tallies to optimize.

Type list in which each element is a string

postprocessor

Validate tally names against [TALLY] blocks.

3.25.2 [HYBRID=FWCADIS]

Forward-Weighted Consistent Adjoint Driven Importance Sampling (FW–CADIS) takes the CADIS method a step further by weighting the adjoint source by the inverse of the forward flux. Full details on the theory of this method can be found in [17]. This variance reduction technique is useful for reducing variance of global quantities of interest.

In Shift, first, a Denovo forward calculation is performed to optimize a response. The forward flux solution is used to determine the adjoint source for the following Denovo adjoint calculation. The procedure then follows the same as that used for CADIS. The adjoint source can be built to optimize for both energy-binned and energy-integrated responses using the energy_treatment (page 225) parameter. Furthermore, two types of weightings are applied: `global` and `pathlength`, as determined by the tally_weighting (page 226) parameter. The adjoint source construction for each weighting and energy treatment is as follows:

`global` weighting, `integrated` energy treatment

$$q^{\dagger}(\mathbf{r}, E) = \frac{g(\mathbf{r})\sigma_{\mathrm{d}}(E)}{\int_E \sigma_{\mathrm{d}}(E)\phi(\mathbf{r}, E)\, dE}$$

`global` weighting, `binned` energy treatment

$$q^{\dagger}(\mathbf{r}, E) = \frac{g(\mathbf{r})}{\phi(\mathbf{r}, E)}$$

`pathlength` weighting, `integrated` energy treatment

$$q^{\dagger}(\mathbf{r}, E) = \frac{g(\mathbf{r})\sigma_{\mathrm{d}}(E)}{\int_E \sigma_{\mathrm{d}}(E) \int_V \phi(\mathbf{r}, E)\, dV dE}$$

`pathlength` weighting, `binned` energy treatment

$$q^{\dagger}(\mathbf{r}, E) = \frac{g(\mathbf{r})}{\int_V \phi(\mathbf{r}, E)\, dV}$$

In the `pathlength` weightings, the volume integrals are over the cell tally volume (in the case of cell tallies) or over **each** tally mesh cell volume (for mesh tallies). Also, $g(\mathbf{r})$ is the volume fraction of a Denovo mesh cell subtended by the tally region. Thus, Denovo cells that are completely enclosed by V have $g = 1$, whereas cells completely outside the tally region have $g = 0$. For `flux` tally optimization (see multipliers (page 225)), the detector response is $\sigma_{\mathrm{d}} = 1$.

See Shift Omnibus hybrid cadis input section (page 224) for specific input options that are available when running FW–CADIS with Shift along with the input options for Denovo adjoint and forward calculations in the Denovo Omnibus input section (page 176).

parameter **`energy_treatment`**

Optimize for energy-integrated or -binned responses.

Default `integrated`

Type `integrated` or `binned`

parameter **`multipliers`**

Multipliers to optimize for each tally.

Default Flux for each tally

Type list in which each element is a string

postprocessor

Validate tally multipliers.

parameter **`tallies`**

Tallies to optimize.

If a cell tally is specified, each cell union will be treated as a separate tally to optimize.

Type list in which each element is a string

postprocessor

Validate tally names against [TALLY] blocks.

parameter **`tally_weighting`**

parameter **`weighting`**

Flux weighting to use for each tally.

The tally weighting can be specified as `default`, `global`, or `pathlength`. The `default` option is replaced by `global` for mesh tallies and by `pathlength` for cell tallies.

Default Default flux weighting for each tally

Type list in which each element is a `default`, `global`, or `pathlength`

postprocessor

Validate tally weighting.

3.25.3 [HYBRID=WW]

Importance maps to accelerate Shift calculations can be set manually from a previous Omnibus output file. The `field_type` parameter selects a field to read from that input file.

deleted **`field`**

Entry `field` has been deleted: Use ‘field_type’ instead.

parameter **`field_type`**

Dataset from which to calculate weight windows.

Table 37: Weight window input options.

Option	Description
`auto`	Automatically select from the following options based on the contents of the HDF5 file. This will prefer `ww` to `adjoint` to `forward`.
`ww`	Use previously calculated weight windows in the `hybrid/ww` group.
`adjoint`	Use a Denovo solution in `denovo-adjoint/flux` as an importance map, setting weight window centers to the inverse of the adjoint flux.
`forward`	Use a Denovo solution in `denovo-forward/flux` directly as weight window centers, the Cooper–Larsen method.

The default field type is `auto`, which will build from previously built weight windows if they are present in the file. If not, the weight windows will be built from the adjoint flux in the file. If neither weight windows nor an adjoint flux is present, the weight windows will be built proportional to the forward flux.

Default `auto`

Type `auto`, `forward`, `adjoint`, or `ww`

parameter **`input`**

Manual weight window HDF5 file.

Type file path for reading (extension '.h5')

deleted **`method`**

Entry `method` has been deleted: Use 'field_type' instead.

parameter **`normalization`**
parameter **`norm`**

Multiplicative normalization for weight windows.

Default `1.0`

Type positive real number

Applicable when `normalization_method` is `manual`

parameter **`normalization_method`**
parameter **`norm_method`**

How to normalize weight window centers based on source responses.

Default `cadis`

Type `manual` or `cadis`

3.26 PRE-EXECUTION UTILITIES: [PRE]

These utilities are run via *omnibus-run* on the local system *before* the Omnibus executable is launched.

sublist **`[PLOT]`**

Generate a raytraced slice of the model. See [PRE][PLOT] (page 227).

Default (empty sublist)

Applicable when

- 'ENABLE_PYTHON_WRAPPERS' is enabled in this CMake build; and
- The 'matplotlib' python package is installed

3.26.1 [PRE][PLOT]

This experimental feature uses the Exnihilo python bindings to generate raytraced images of the problem geometry. To generate more customized outputs, the interested user should use the direct Python bindings (see the examples).

Tip: For example, this entry in the front end will generate three slices showing the materials at $z = -10, -5, 0$, with the lower left coordinate at $(x, y) = (-15, -20)$ and the upper right coordinate at $(15, 20)$:

```
[PRE]

[.][PLOT levels]
origin -15 -20 0
axis  z
size 30 40
slice -10 -5 0
```

parameter `axis`

Axis orthogonal to the image.

Default `2`

Type axis (‘x’,’y’,’z’)

parameter `check`

Use error checking during raytrace.

Default `False`

Type boolean

parameter `cmap`*(advanced)*

Color map for plotting.

Default `rainbow` if `trace cell` else `Set3`

Type string without special characters

parameter `name`

Base name of the output file.

Default `plot`*`NNN`*

Type string without special characters

parameter `origin`

Lower-left corner of the image.

Units cm

Type length-3 float vector (each element is a real number)

parameter `render`

Save as a standalone rendered PNG.

Default `False`

Type boolean

Applicable when The ‘PIL’ python package is installed

parameter `resolution`

Maximum number of pixels along one axis of the image.

Default `1024`

Type positive integer

parameter `size`

Width and height of the image slice.

Units cm

Type pair of floats (each element is a positive real number)

parameter `slice`

Positions along ‘axis’ to take slices, relative to ‘origin.’

Default `0.0`

Type non-empty float list (each element is a real number)

parameter **`trace`**

Model property to raytrace.

Default `mat`

Type `cell` or `mat`

3.27 POST-PROCESSING: [POST]

The [POST] block controls post-processing of Omnibus output. It extracts data from the HDF5 output file and formats it to be more human-accessible.

database **`[DENOVO]`**

Denovo post-processing options. See [POST][DENOVO] (page 230).

Default (empty database)

Applicable when solver is 'denovo'

database **`[DEPLETION]`**

Depletion post-processing options. See [POST][DEPLETION] (page 231).

Default (empty database)

Applicable when solver is 'depletion'

parameter **`html`**

Convert the ReStructured Text problem summary to HTML.

Default `False`

Type boolean

Applicable when `rst` is `True`

database **`[HYBRID]`**

Shift post-processing options. See [POST][HYBRID] (page 231).

Default (empty database)

Applicable when problem mode is `hybrid`

parameter **`rst`**

Write a ReStructured Text problem summary.

Default `True`

Type boolean

database **`[TALLY]`**

Tally post-processing options. See [POST][TALLY] (page 230).

Default (empty database)

Applicable when

- solver is 'shift'; and
- `/shift/do_transport` is `True`

3.27.1 [POST][TALLY]

Tally post-processing options.

parameter **`cell_csv`**
Generate CSV files from cell tallies.

Default `True`

Type boolean

parameter **`kcode_plots`**
Generate keff and convergence plots.

Default `True`

Type boolean

Applicable when problem mode is `kcode`

parameter **`max_csv_size`***(advanced)*
Maximum allowed size of average CSV output file.

Default `500.0`

Units kB

Type positive real number

Applicable when `cell_csv` is `True`

parameter **`mesh_xdmf`**
Generate XDMF files from mesh tallies.

Default `True`

Type boolean

3.27.2 [POST][DENOVO]

Denovo post-processing options.

sublist **`[SPECTRUM]`**
Save spectra from a list of x/y/z points. See [POST][DENOVO][SPECTRUM] (page 231).

Default (empty sublist)

Applicable when `/denovo/disable` is `none`

parameter **`xdmf`**
Create an XDMF file for visualization.

Default `True`

Type boolean

Applicable when `/denovo/disable` is `none`

3.27.3 [POST][HYBRID]

Shift post-processing options.

parameter **`ww_xdmf`**

Create an XDMF file for weight windows.

Default `True`

Type boolean

Applicable when `/shift/vr/output` is `True`

3.27.4 [POST][DEPLETION]

Depletion post-processing options.

parameter **`max_csv_size`***(advanced)*

Maximum allowed size of average CSV output file.

Default `500.0`

Units kB

Type positive real number

Applicable when `nd_csv` is `True` or `xs_csv` is `True`

parameter **`nd_csv`**

Write Excel-compatible CSV files with number densities.

Default `True`

Type boolean

parameter **`xs_csv`**

Write CSV files with cross sections.

Default `True`

Type boolean

Applicable when `/depletion/write_xs` is `True`

3.27.5 [POST][DENOVO][SPECTRUM]

Save spectra from a list of x/y/z points.

parameter **`field`**

Output field from which to save spectra.

Default `flux`

Type `flux`, `source`, or `uncflux`

postprocessor

The requested `field` must be enabled in the Denovo output block.

parameter **`name`**

Short title or label for the source.

Default `spectrum`*`NNN`*

Type string without special characters

parameter `normalization`

Constant multiplicative factor to apply to spectra.

Default `1.0`

Type positive real number

parameter `on_disk`*(advanced)*

Refrain from loading the solution into memory.

Default `False`

Type boolean

parameter `points`

List of x/y/z points.

Type List of space-separated x/y/z tuples (each element is a real number)

4. GEOMETRIA INPUT DESCRIPTION

The Geometria input format is identical to the Omnibus input format and is split into a hierarchy of blocks. All input blocks are described in the following sections.

Note: This documentation was generated automatically with the following version of Exnihilo:

version 6.3.pre-b13 (branch 'master' on 'upstream', r729: #9809b44f on 2020JUL16)

date 2020-07-16 22:02:43

4.1 GEOMETRIA INPUT FILE CONTENTS

Each of the top-level blocks (and the overall problem input file) are described here.

database `[GEOMETRY]`
Global geometry options. See [GEOMETRY] (page 233).

sublist `[UNIVERSE]`
Universes. See [UNIVERSE] (page 234).

postprocessor
Universe names in `/geometry/global` must already have been defined.

4.1.1 [GEOMETRY]

Global geometry options.

parameter `check_overlapping_volumes`
Perform extra (and slow) geometry validation checks during transport.

Default `False`

Type boolean

parameter `composition`
parameter `comp`
Provide an optional explicit mapping for composition names.

Default `---`

Type list in which each element is a string

command `comps`
Map 'comp' to 'matid' from pairs or arrow-separated items.

Creates comp

Creates matid

parameter `deduplication_warning`
parameter `dedupe_warn`
Warn about duplicate surfaces being elided.

Default `False`

Type boolean

parameter **`global`**
Name of the global universe.

Type string without special characters

parameter **`length_scale`**
Characteristic length scale of the problem.

Default `1.0`

Type positive real number

parameter **`matid`**
Matids corresponding to the given commposition names.

Default `---`

Type list in which each element is a non-negative integer

postprocessor
The parameters `composition` and `matid` must have the same length.

parameter **`tolerance`**
parameter **`tol`**
Global tolerance for geometry construction and particle bumping.

Default `1e-08`

Type real number inside (0, 1)

parameter **`write_kdtree`***(advanced)*
Output the k-D tree representation for each universe.

Default `False`

Type boolean

4.2 UNIVERSE DEFINITIONS: [UNIVERSE]

Universes are analogous to 'units' in KENO: an independent, complete definition of the problem within some region of space. Universes can be reused multiple times via holes (page 243) and arrays (page 237).

Table 38: Available types for the [UNIVERSE] database

Type	Description	Applicability
general (page 235)	General universe	
keno6 (page 235)	KENO6 universe	
random (page 237)	Randomly constructed universe	
array (page 237)	Rectangular array	
hexarray (page 239)	Hexagonal array	
dodarray (page 241)	Dodecahedral array	
rtk (page 242)	Insert an RTK geometry from an external file	
core (page 243)	Insert a VERA-defined reactor core	
rtkarray	Alias to `rtk` type	—

4.2.1 [UNIVERSE=GENERAL]

The "general" universe is a constructive solid geometry universe, essentially equivalent to a "unit" in KENO. Its components are "cells", solid bodies with a single fill material, and "holes", which are other universes embedded into this general universe.

command `boundary`
: Create an `interior` parameter for a single bounding shape.

  Creates interior

sublist `[CELL]`
: Cell definition. See [UNIVERSE][CELL] (page 244).

  Default (empty sublist)

sublist `[HOLE]`
: Inserted sub-universes. See [UNIVERSE][HOLE] (page 243).

  Optional

parameter `interior`
: Senses and shape names defining the interior of this universe.

  Type list in which each element is a shape with optional leading +- sense

postprocessor
: Check that `interior` shapes have been defined.

parameter `name`
: Name of the universe.

  Type string without special characters

sublist `[SHAPE]`
: Geometry shapes. See [UNIVERSE][SHAPE] (page 246).

  Default (empty sublist)

4.2.2 [UNIVERSE=KENO6]

The "KENO" universe activates features necessary to build KENO geometry definitions using GG. Unlike GG, KENO continually tracks on many geometry layers simultaneously, so that the "topmost" layer's cells are used. This allows holes and arrays to be defined without integrating them into the daughter universes – they simply override whatever is there.

GG's tracking engine operates differently: it tracks on only one universe at a time, so that in any universe, a single point in space corresponds to exactly one logical position in that universe, or else it is in the "exterior" of that universe. Particles hitting the exterior are transported to another universe (except in the outermost universe where the boundary condition is applied).

To unify these two tracking types, this special universe uses intersection tests to *automatically modify* the cell definitions. It uses shape-to-shape intersection tests to determine whether any of the specified holes, arrays, or external boundaries modify the cells interior to the problem. The test for shape *A* intersecting shape *B* can return one of five results:

Separate *A* and *B* do not intersect.

Identical *A* and *B* are exactly the same shape: their logical definition and surfaces are identical.

Encloses The region in *A* is a superset of the region of *B*

Enclosed by The region in *B* is a superset of the region of *A*

Overlaps The two regions *may* intersect (or one may even enclose the other). This result increases geometry complexity but is the most conservative.

Some of the shape-to-shape intersection tests are more accurate than others. Spheres, aligned cylinders, cuboids, and planes can tell their exact relationship to shapes of the same kind, but it's not always possible to tell the exact intersection result for some shapes. The conservative case extends cell definitions to exclude the shapes in question.

sublist **`[ARRAY]`**
Implicitly truncated arrays. See [UNIVERSE][ARRAY] (page 244).

Optional

command **`boundary`**
Create an `interior` parameter for a single bounding shape.

Creates interior

sublist **`[CELL]`**
Cell definition. See [UNIVERSE][CELL] (page 244).

Default (empty sublist)

sublist **`[HOLE]`**
Inserted sub-universes. See [UNIVERSE][HOLE] (page 243).

Optional

parameter **`interior`**
Senses and shape names defining the interior of this universe.

Type list in which each element is a shape with optional leading +- sense

postprocessor
Check that `interior` shapes have been defined.

parameter **`name`**
Name of the universe.

Type string without special characters

sublist **`[SHAPE]`**
Geometry shapes. See [UNIVERSE][SHAPE] (page 246).

Default (empty sublist)

4.2.3 [UNIVERSE=RANDOM]

The "random" universe is a procedurally generated universe filled with a given volume fraction of spheres. It is used for HTGRs to model pebbles and TRISO particles.

It is defined by specifying one or more previously defined spherical universes (e.g. particles with different compositions) that will be replicated inside the universe. The number of embedded particles is determined by specifying a volume fraction v such that $N_i = \frac{\mathrm{vf}_i V_T}{V_i}$ for particle type i which has volume V_i inside an object of volume V_t.

The region outside the sampled particles is filled with the single composition `composition`. (If the random universe is a fuel pebble and the particles are TRISO particles, this composition will be the graphite matrix.)

Currently, the only shapes supported as bounding shapes are a single cuboid, sphere, and cylinder without any rotations or translations applied.

parameter **`composition`**
parameter **`comp`**
Composition outside of the particles (the matrix).

Type non-empty string

parameter **`fill`**
Names of particle universes to emplace.

Type list in which each element is a string without special characters

postprocessor
Universe names in `fill` must already have been defined.

parameter **`name`**
Name of the universe.

Type string without special characters

database **`[OPTIONS]`**
Random universe construction options. See [UNIVERSE][OPTIONS] (page 245).

database **`[SHAPE]`**
Geometry shapes. See [UNIVERSE][SHAPE] (page 246).

parameter **`volume_fraction`**
parameter **`vf`**
Names of particle universes to emplace.

Type fractions that sum to less than one (each element is a real number inside (0, 1))

4.2.4 [UNIVERSE=ARRAY]

Rectangular array.

command **`boundary`**
Create an `interior` parameter for a single bounding shape.

Creates interior

parameter **`clip_composition`**

parameter **`clip`**
: Composition that will replace any clipped array cell.

    Optional

    Type non-empty string

parameter **`fill`**
: Names of array universe fills, indexed as ZUV.

    Type list in which each element is a string without special characters

postprocessor
: Universe names in `fill` must already have been defined.

sublist **`[HOLE]`**
: Inserted sub-universes. See [UNIVERSE][HOLE] (page 243).

    Optional

parameter **`interior`**
: Sense/shapes defining the interior of the array.

    Optional

    Type list in which each element is a shape with optional leading +- sense

postprocessor
: Check that `interior` shapes have been defined.

parameter **`name`**
: Name of the universe.

    Type string without special characters

parameter **`nx`**
: Number of units in the X direction.

    Type positive integer

parameter **`ny`**
: Number of units in the Y direction.

    Type positive integer

parameter **`nz`**
: Number of units in the Z direction.

    Default `1`

    Type positive integer

postprocessor
: Check array sizes.

parameter **`origin`**
: Location of the lower-left corner of the array bounds.

    Default `0.0 0.0 0.0`

    Type length-3 float vector (each element is a real number)

parameter **`origin_is`**

Whether `origin` is the array lower-left or a unit origin.

Default 'array' unless the 'place' parameter is present

Type `array` or `unit`

parameter **`place`**

Location of the lower-left corner of the array bounds.

Type length-3 logical position vector (each element is a non-negative integer)

Applicable when `origin_is` is `unit`

sublist **`[SHAPE]`**

Geometry shapes. See [UNIVERSE][SHAPE] (page 246).

Default (empty sublist)

4.2.5 [UNIVERSE=HEXARRAY]

Hexagonal array.

command **`boundary`**

Create an `interior` parameter for a single bounding shape.

Creates interior

parameter **`clip_composition`**
parameter **`clip`**

Composition that will replace any clipped array cell.

Optional

Type non-empty string

parameter **`fill`**

Names of array universe fills, indexed as ZUV.

Type list in which each element is a string without special characters

postprocessor

Universe names in `fill` must already have been defined.

sublist **`[HOLE]`**

Inserted sub-universes. See [UNIVERSE][HOLE] (page 243).

Optional

parameter **`interior`**

Sense/shapes defining the interior of the array.

Type list in which each element is a shape with optional leading +- sense

postprocessor

Check that `interior` shapes have been defined.

parameter **`layout`**

Layout of the hex array elements.

Default `rhomb`

Type `rhomb` or `rect`

parameter **`name`**
Name of the universe.

Type string without special characters

parameter **`nu`**
Number of units in the U direction.

Type positive integer

parameter **`nv`**
Number of units in the V direction.

Type positive integer

parameter **`nz`**
Number of units in the Z direction.

Default `1`

Type positive integer

postprocessor
Check array sizes.

parameter **`origin`**
Location of the lower-left corner of the array bounds.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

parameter **`origin_is`**
Whether `origin` is the array lower-left or a unit origin.

Default 'array' unless the 'place' parameter is present

Type `array` or `unit`

parameter **`place`**
Location of the lower-left corner of the array bounds.

Type length-3 logical position vector (each element is a non-negative integer)

Applicable when `origin_is` is `unit`

sublist **`[SHAPE]`**
Geometry shapes. See [UNIVERSE][SHAPE] (page 246).

Default (empty sublist)

4.2.6 [UNIVERSE=DODARRAY]

Dodecahedral array.

command **`boundary`**
Create an `interior` parameter for a single bounding shape.

Creates interior

parameter **`clip_composition`**
parameter **`clip`**
Composition that will replace any clipped array cell.

Optional

Type non-empty string

parameter **`fill`**
Names of array universe fills, indexed as ZUV.

Type list in which each element is a string without special characters

postprocessor
Universe names in `fill` must already have been defined.

sublist **`[HOLE]`**
Inserted sub-universes. See [UNIVERSE][HOLE] (page 243).

Optional

parameter **`interior`**
Sense/shapes defining the interior of the array.

Type list in which each element is a shape with optional leading +- sense

postprocessor
Check that `interior` shapes have been defined.

parameter **`name`**
Name of the universe.

Type string without special characters

parameter **`nx`**
Number of units in the X direction.

Type positive integer

parameter **`ny`**
Number of units in the Y direction.

Type positive integer

parameter **`nz`**
Number of units in the Z direction.

Default `1`

Type positive integer

postprocessor
Check array sizes.

parameter **`origin`**
Location of the lower-left corner of the array bounds.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

parameter **`origin_is`**
Whether `origin` is the array lower-left or a unit origin.

Default ‘array’ unless the ‘place’ parameter is present

Type `array` or `unit`

parameter **`place`**
Location of the lower-left corner of the array bounds.

Type length-3 logical position vector (each element is a non-negative integer)

Applicable when `origin_is` is `unit`

sublist **`[SHAPE]`**
Geometry shapes. See [UNIVERSE][SHAPE] (page 246).

Default (empty sublist)

4.2.7 [UNIVERSE=RTK]

Insert an RTK geometry from an external file.

command **`boundary`**
Create an `interior` parameter for a single bounding shape.

Creates interior

sublist **`[HOLE]`**
Inserted sub-universes. See [UNIVERSE][HOLE] (page 243).

Optional

parameter **`input`**
Path to the RTK geometry XML file.

Type file path for reading (extension ‘.xml’)

parameter **`interior`**
Sense/shapes defining the interior of the array.

Type list in which each element is a shape with optional leading +- sense

postprocessor
Check that `interior` shapes have been defined.

parameter **`name`**
Name of the universe.

Type string without special characters

sublist **`[SHAPE]`**
Geometry shapes. See [UNIVERSE][SHAPE] (page 246).

Default (empty sublist)

4.2.8 [UNIVERSE=CORE]

The core universe can only be used when running a VERA (Virtual Environment for Reactor Applications) model in Omnibus or when run externally through the VERA code suite. It inserts the analyst-defined reactor design into a Geometria input for external dosimetry applications.

parameter **`name`**

Name of universe.

Type string without special characters

4.2.9 [UNIVERSE][HOLE]

Inserted sub-universes.

command **`euler`**

Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter **`fill`**

Name of the universe to fill this hole with.

Type string without special characters

postprocessor

Universe names in `fill` must already have been defined.

parameter **`name`**

Name of the shape that this hole creates.

Type string without special characters

parameter **`rotate`**

Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)

Squelch identity rotations and null translations.

parameter **`translate`**

Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.2.10 [UNIVERSE][CELL]

Cells are defined as the intersection of one or more regions defined by shapes and holes. Each shape separates space into two half-spaces: "inside" the shape, with a "negative" sense, and "outside" the shape with a "positive" sense. For a shape called `sphere`, these two senses are written as `-sphere` (inside) and `+sphere` (outside). When another universe is placed into this general universe via a hole, it implicitly creates a shape – the external boundary of the embedded universe – that can be referenced when defining cells.

The choice for the signs is based on the standard form of the quadric equations, such as the surface of a sphere:

$$x^2 + y^2 + z^2 - R^2 = 0$$

When the left-hand side of this equation is positive (+), the point (x, y, z) is outside the sphere; when negative (-), the point is inside. We think of surfaces and shapes as having outward-facing normals; when the projection of a point onto the surface is negative, the point is inside.

parameter **`composition`**
parameter **`comp`**
Name of the composition that fills this cell.

Type non-empty string

deleted **`matid`**
Entry `matid` has been deleted: 'matid' has been replaced with 'comp', the name of the composition.

parameter **`name`**
Name of the cell.

Type string without special characters

parameter **`shapes`**
Senses and shape names defining this cell.

Type list in which each element is a shape with optional leading +- sense

postprocessor
Check that `shapes` have been defined.

parameter **`volume`**
Add a pre-calculated volume for this cell.

Optional

Type real number

4.2.11 [UNIVERSE][ARRAY]

Implicitly truncated arrays.

command **`euler`**
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter `fill`

Name of the universe to fill this hole with.

Type string without special characters

postprocessor

Universe names in `fill` must already have been defined.

parameter `name`

Name of the shape that this hole creates.

Type string without special characters

parameter `rotate`

Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)

Squelch identity rotations and null translations.

parameter `translate`

Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.2.12 [UNIVERSE][OPTIONS]

Random universe construction options.

parameter `failure_batch_size`

Number of samples per batch to test.

Default `100000`

Type positive integer

parameter `failure_tolerance`

Fraction of samples per batch that must be rejected to fail.

Default `0.99999`

Type real number inside (0, 1)

parameter `insert_method`

Method for attempting to insert particles into a pebble.

The `naive` method is the simplest and slowest way to instantiate a loosely packed particle universe. It samples random points inside the universe and rejects them if the sphere around that particle intersects with any particle previously sampled. The naive collision detection scales with $O(N^2)$ for N particles, and the rejection fraction approaches 1 very quickly.

When sampling with the `naive` method, batches of `failure_batch_size` samples are tallied; if the fraction of failed samples exceeds `failure_tolerance` then an error will be raised.

Default `naive`

Type `naive`

parameter **`seed`**

Seed value for instantiating this universe.

The seed is used to choose an independent random number stream when instantiating a universe. Different universes' particle placements will be uncorrelated even if they share a seed, but changing the universe's name will change the particle placements, as the actual computational seed value is a combination of the seed given by this parameter and the name of this universe.

Default `0`

Type non-negative integer

4.3 SHAPE DEFINITIONS: [UNIVERSE][SHAPE]

Shapes are primitive solid bodies, the constituents of cells. Although this manual does not yet include helpful images for the shape descriptions, the KENO-VI shape description section of the SCALE user manual [2] is essentially equivalent to the input quantities in Geometria. For example, the wedge construction example gives `wedge label xbase xpt ypt zlng`, and the wedge input block (page 256) defines `zlng` as an alias for `height`, `xbase` as an alias for `width`, and `xy` as an alias for `corner_pt`.

Each shape is the intersection of half-spaces defined by primitive quadric surfaces. When a geometry is instantiated, the shapes are decomposed into their surfaces and volumes are expressed by a logical representation of these surfaces using boolean logic as is typical with a constructive solid geometry definition.

The coordinate system of the shape is defined using a rotation matrix and translation vector: rotations are applied to the shape about its origin, then translations moves the daughter shape relative to the parent universe. The transformation from a point in the shape's coordinate system into the universe's system is

$$\mathbf{x}_u = \mathbf{R}\mathbf{x}_s + \mathbf{t}\,,$$

Where the subscripts u, s refer to the universe and shape coordinate systems, respectively. The vector $\mathbf{t}$ is a translation vector. To transform from the parent into the daughter system we apply the inverse:

$$\mathbf{x}_s = \mathbf{R}^T(\mathbf{x}_u - \mathbf{t})\,.$$

(Note that because $\mathbf{R}$ is unitary, the transpose is equal to the inverse.)

The surfaces created by each shape have unique names that can be used to reference them later, or to create reflecting outer boundaries during construction.

Most shapes share many of the same parameters such as "reflect" and "rotate". To reduce duplication, the more detailed documentation is provided for the "cuboid" shape:

- euler (page 247)
- rotate (page 248)
- reflect (page 248)

Table 39: Available types for the [SHAPE] database

Type	Description	Applicability
cuboid (page 247)	Box shape	
box	Alias to `cuboid` type	—
sphere (page 249)	Sphere shape	
cyl (page 250)	Cylinder shape	
cylsegment (page 251)	Cylinder segment shape	
pad	Alias to `cylsegment` type	—
ring (page 252)	Cylindrical shell shape	
cylshell	Alias to `ring` type	—
prism (page 253)	Regular prism shape	
slab (page 255)	Infinite slab shape	
plane (page 255)	Infinite half-space	
wedge (page 256)	Wedge shape	
cone (page 257)	Cone shape	
ellipsoid (page 258)	Ellipsoid shape	
hopper (page 259)	Hopper shape	
righttet (page 260)	Right tetrahedron shape	
triprism (page 261)	Triangular prism shape	
ecylinder (page 261)	Elliptical cylinder shape	
rhombdod (page 262)	Rhombic dodecahedron shape	
ppiped (page 263)	Parallelepiped	
quadric (page 264)	General quadric	

4.3.1 [UNIVERSE][SHAPE=CUBOID]

The possible reflecting faces for the cuboid (chosen via `reflect`) are:

Face	Description
mx	lower x face
px	upper x face
my	lower y face
py	upper y face
mz	lower z face
pz	upper z face

command **`euler`**

Perform an Euler rotation about the z, x', z'' axes.

See [the Euler angles wikipedia page](https://en.wikipedia.org/wiki/Euler_angles#Definition_by_intrinsic_rotations) for a graphic representation of the z, x', z'' rotation. This command simply generates a rotation matrix.

Units revolution

Creates rotate

command **`faces`**

Expand into parameters `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax`.

Creates xmin

Creates xmax

Creates ymin

Creates ymax

Creates zmin

Creates zmax

parameter `name`
: Name of the shape.

Type string without special characters

parameter `reflect`
: Reflecting boundary surfaces.

The `reflect` option allows a subset of faces on a shape to specularly reflect particles. Enter the single value * to reflect all faces for the given shape.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`
: Rotation matrix.

The rotation matrix

$$\mathbf{R} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

is applied to a point in the shape's coordinate system as a column vector

$$\mathbf{R}\mathbf{x}_s = \mathbf{R}\begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

The input to the code is the row-major flattened list $[a, b, c, d, e, f, g, h, i]$.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
: Squelch identity rotations and null translations.

parameter `translate`
parameter `origin`
: Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

parameter **`xmax`**
Maximum x-coordinate of box source.

Type real number

postprocessor
Parameter `xmin` must be less than `xmax`.

parameter **`xmin`**
Minimum x-coordinate of box source.

Type real number

parameter **`ymax`**
Maximum y-coordinate of box source.

Type real number

postprocessor
Parameter `ymin` must be less than `ymax`.

parameter **`ymin`**
Minimum y-coordinate of box source.

Type real number

parameter **`zmax`**
Maximum z-coordinate of box source.

Type real number

postprocessor
Parameter `zmin` must be less than `zmax`.

parameter **`zmin`**
Minimum z-coordinate of box source.

Type real number

4.3.2 [UNIVERSE][SHAPE=SPHERE]

Sphere shape.

command **`euler`**
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter **`name`**
Name of the shape.

Type string without special characters

parameter **`radius`**
parameter **`r`**
Radius of sphere.

Type real number

parameter **`reflect`**
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter **`rotate`**
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter **`translate`**
parameter **`origin`**
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.3 [UNIVERSE][SHAPE=CYL]

Cylinder shape.

parameter **`axis`**
Axis along the cylinder.

Type axis (‘x’,’y’,’z’)

command **`euler`**
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter **`extents`**
Negative and positive position along the given axis.

Type (min, max) extent values (each element is a real number)

parameter **`name`**
Name of the shape.

Type string without special characters

parameter **`radius`**
parameter **`r`**
Radius of cylinder.

Type real number

parameter **`reflect`**
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter `translate`
parameter `origin`
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.4 [UNIVERSE][SHAPE=CYLSEGMENT]

Cylinder segment shape.

parameter `angle`
parameter `a`
Beginning angle CCW from $x = 0$.

Units revolution

Type real number inclusive [0.0, 1.0]

parameter `arc`
parameter `da`
Angle subtended by cylindrical segment.

Units revolution

Type real number in [0.0, 0.5]

deleted `begin_angle`
deleted `ba`
Entry `begin_angle` has been deleted: Replaced by 'angle' in turns not radians.

command `euler`
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter `extents`
Negative and positive position along the z-axis.

Type (min, max) extent values (each element is a real number)

parameter `inner_radius`

parameter **`ri`**

Inner radius.

Type positive real number

parameter **`name`**

Name of the shape.

Type string without special characters

parameter **`outer_radius`**
parameter **`ro`**

Outer radius.

Type positive real number

postprocessor

Parameter `inner_radius` must be less than `outer_radius`.

parameter **`reflect`**

Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter **`rotate`**

Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)

Squelch identity rotations and null translations.

deleted **`solid_angle`**
deleted **`sa`**

Entry `solid_angle` has been deleted: Replaced by 'arc' in turns not radians.

parameter **`translate`**
parameter **`origin`**

Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.5 [UNIVERSE][SHAPE=RING]

Cylindrical shell shape.

command **`euler`**

Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter **`extents`**

Negative and positive position along the Z axis.

Type (min, max) extent values (each element is a real number)

parameter **`inner_radius`**

parameter **`ri`**

Inner radius.

Type real number

parameter **`name`**

Name of the shape.

Type string without special characters

parameter **`outer_radius`**

parameter **`ro`**

Outer radius.

Type real number

postprocessor

Parameter `inner_radius` must be less than `outer_radius`.

parameter **`reflect`**

Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter **`rotate`**

Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)

Squelch identity rotations and null translations.

parameter **`translate`**

parameter **`origin`**

Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.6 [UNIVERSE][SHAPE=PRISM]

The possible reflecting faces for a prism depend on the number of sides:

Face	Description
pN	for integer N in [0, *num_sides*), CCW from x=0
mz	lower z face
pz	upper z face

parameter `apothem`
parameter `r`

Inner radius of the prism.

Type real number

command `euler`

Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter `extents`

Negative and positive position along the Z axis.

Type (min, max) extent values (each element is a real number)

parameter `name`

Name of the shape.

Type string without special characters

parameter `num_sides`

Number of sides on the prism.

Type integer >= 3

parameter `reflect`

Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`

Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)

Squelch identity rotations and null translations.

parameter `rotfrac`

Angle (fraction of the angle spanned by one face) to rotate.

Default `0.0`

Type real number inclusive [0.0, 1.0]

parameter `translate`
parameter `origin`

Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.7 [UNIVERSE][SHAPE=SLAB]

Infinite slab shape.

parameter **`axis`**
: Axis along the slab.

  Type axis (‘x’,’y’,’z’)

command **`euler`**
: Perform an Euler rotation about the z, x', z'' axes.

  Units revolution

  Creates rotate

parameter **`extents`**
: Negative and positive position along the slab axis.

  Type (min, max) extent values (each element is a real number)

parameter **`name`**
: Name of the shape.

  Type string without special characters

parameter **`reflect`**
: Reflecting boundary surfaces.

  Default `---`

  Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter **`rotate`**
: Rotation matrix.

  Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

  Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
: Squelch identity rotations and null translations.

parameter **`translate`**
parameter **`origin`**
: Local-to-global translation vector.

  Default `0.0 0.0 0.0`

  Type length-3 float vector (each element is a real number)

4.3.8 [UNIVERSE][SHAPE=PLANE]

Infinite half-space.

command **`euler`**
: Perform an Euler rotation about the z, x', z'' axes.

  Units revolution

  Creates rotate

parameter **`name`**
Name of the shape.

Type string without special characters

parameter **`normal`**
Vector (possibly unnormalized) point outward from the plane.

Type length-3 float vector (each element is a real number)

parameter **`point`**
A point somewhere on the plane.

Type length-3 float vector (each element is a real number)

parameter **`reflect`**
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter **`rotate`**
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter **`translate`**
parameter **`origin`**
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.9 [UNIVERSE][SHAPE=WEDGE]

Wedge shape.

parameter **`corner_pt`**
parameter **`xy`**
XY location of the right-angle corner of the wedge.

Type length-2 (x,y) position (each element is a positive real number)

command **`euler`**
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter **`height`**
parameter **`zlng`**
Height of the wedge (along Z axis).

Type positive real number

parameter `name`
Name of the shape.

Type string without special characters

parameter `reflect`
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter `translate`
parameter `origin`
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

parameter `width`
parameter `xbase`
Length of the hypotenuse of the wedge (along the X axis).

Type positive real number

4.3.10 [UNIVERSE][SHAPE=CONE]

Cone shape.

parameter `axis`
Axis along the centerline of the cone.

Type axis (‘x’,’y’,’z’)

command `euler`
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter `extents`
Negative and positive base positions along the given axis.

Type (min, max) extent values (each element is a real number)

parameter `name`
Name of the shape.

Type string without special characters

parameter `radii`
parameter `r`
Radii at the top and bottom.

Type 2 positive floats (each element is a positive real number)

parameter `reflect`
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter `translate`
parameter `origin`
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.11 [UNIVERSE][SHAPE=ELLIPSOID]

Ellipsoid shape.

command `euler`
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter `name`
Name of the shape.

Type string without special characters

parameter `radii`
parameter `r`
Radii in the x, y, and z directions.

Type 3 positive floats (each element is a positive real number)

parameter `reflect`
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter `translate`
parameter `origin`
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.12 [UNIVERSE][SHAPE=HOPPER]

Hopper shape.

command `euler`
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter `extents`
Negative and positive base positions along the Z axis.

Type (min, max) extent values (each element is a real number)

parameter `lower_pt`
parameter `lo`
X and Y half-lengths on the low side of the hopper.

Type length-2 (x,y) position (each element is a positive real number)

parameter `name`
Name of the shape.

Type string without special characters

parameter `reflect`
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter `translate`
parameter `origin`
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

parameter `upper_pt`
parameter `hi`
X and Y half-lengths on the high side of the hopper.

Type length-2 (x,y) position (each element is a positive real number)

4.3.13 [UNIVERSE][SHAPE=RIGHTTET]

Right tetrahedron shape.

command `euler`
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter `lengths`
Length of the tetrahedron edges along the x, y, and z axes.

Type 3 positive floats (each element is a positive real number)

parameter `name`
Name of the shape.

Type string without special characters

parameter `reflect`
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter `translate`
parameter `origin`
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.14 [UNIVERSE][SHAPE=TRIPRISM]

Triangular prism shape.

command **`euler`**
: Perform an Euler rotation about the z, x', z'' axes.

  Units revolution

  Creates rotate

parameter **`lengths`**
: Length of the triangular prism's bounding box.

  Type 3 positive floats (each element is a positive real number)

parameter **`name`**
: Name of the shape.

  Type string without special characters

parameter **`reflect`**
: Reflecting boundary surfaces.

  Default `---`

  Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter **`rotate`**
: Rotation matrix.

  Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

  Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
: Squelch identity rotations and null translations.

parameter **`translate`**
parameter **`origin`**
: Local-to-global translation vector.

  Default `0.0 0.0 0.0`

  Type length-3 float vector (each element is a real number)

4.3.15 [UNIVERSE][SHAPE=ECYLINDER]

Elliptical cylinder shape.

command **`euler`**
: Perform an Euler rotation about the z, x', z'' axes.

  Units revolution

  Creates rotate

parameter **`extents`**
: Negative and positive position along the given axis.

  Type (min, max) extent values (each element is a real number)

parameter **`name`**

Name of the shape.

Type string without special characters

parameter **`radii`**
parameter **`r`**

Radii in the x and y directions.

Type length-2 (x,y) position (each element is a positive real number)

parameter **`reflect`**

Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter **`rotate`**

Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)

Squelch identity rotations and null translations.

parameter **`translate`**
parameter **`origin`**

Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.16 [UNIVERSE][SHAPE=RHOMBDOD]

The faces of a rhombic dodecahedron are ordered so that face n connects to $n + 6 \mod 12$ of an adjacent lattice cell. For a dodecahedron with interior radius 1, these faces are:

Face	Description
px	Plane: x=1
py	Plane: y=1
p0	Plane: n=(0.5 0.5 0.707107), d=1
p1	Plane: n=(0.5 -0.5 -0.707107), d=-1
p2	Plane: n=(0.5 -0.5 0.707107), d=1
p3	Plane: n=(0.5 0.5 -0.707107), d=-1
mx	Plane: x=-1
my	Plane: y=-1
p4	Plane: n=(0.5 0.5 0.707107), d=-1
p5	Plane: n=(0.5 -0.5 -0.707107), d=1
p6	Plane: n=(0.5 -0.5 0.707107), d=-1
p7	Plane: n=(0.5 0.5 -0.707107), d=1

parameter **`apothem`**
parameter **`r`**
Inner radius of the dodecahedron.

Type positive real number

command **`euler`**
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter **`name`**
Name of the shape.

Type string without special characters

parameter **`reflect`**
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter **`rotate`**
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter **`translate`**
parameter **`origin`**
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

4.3.17 [UNIVERSE][SHAPE=PPIPED]

Parallelepiped.

command **`euler`**
Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter **`lengths`**
Length of the x, xy, and xyz edges.

Type 3 positive floats (each element is a positive real number)

parameter **`name`**
Name of the shape.

Type string without special characters

parameter `reflect`
Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`
Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)
Squelch identity rotations and null translations.

parameter `translate`
parameter `origin`
Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

parameter `xy_angle`
parameter `phi`
Angle between xy component of xyz edge and x axis (phi).

Units revolution

Type real number in [0,.25)

parameter `xyz_angle`
parameter `theta`
Angle between xyz edge and z axis (theta).

Units revolution

Type real number in [0,.25)

parameter `y_angle`
parameter `psi`
Angle between xy edge and y axis (psi).

Units revolution

Type real number in [0,.25)

4.3.18 [UNIVERSE][SHAPE=QUADRIC]

General quadric.

parameter `cross`
parameter `def`
Second-order cross coefficients $dXY + eYZ + fXZ$.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

command `euler`

Perform an Euler rotation about the z, x', z'' axes.

Units revolution

Creates rotate

parameter `first`
parameter `ghi`

First-order coefficients $gX + hY + iZ$.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

parameter `name`

Name of the shape.

Type string without special characters

parameter `reflect`

Reflecting boundary surfaces.

Default `---`

Type list of shape surfaces (e.g. mx, co) (each element is a string without special characters)

parameter `rotate`

Rotation matrix.

Default `1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0`

Type length-9 row-major rotation matrix (each element is a real number)

postprocessor (advanced)

Squelch identity rotations and null translations.

parameter `scalar`
parameter `j`

Scalar coefficient j.

Default `0.0`

Type real number

parameter `second`
parameter `abc`

Second-order coefficients $aX^2 + bY^2 + cZ^2$.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

parameter `translate`
parameter `origin`

Local-to-global translation vector.

Default `0.0 0.0 0.0`

Type length-3 float vector (each element is a real number)

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[18] https://doi.org/10.1016/S0168-9002(03)01368-8
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5. ACKNOWLEDGMENTS

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Appendix A. EXAMPLES

Appendix A. EXAMPLES

The following examples demonstrate many of the capabilities in Exnihilo, such as:

- creating and running a problem in Omnibus,
- postprocessing the data with the included Python tools, and
- interacting with nuclear data using the Exnihilo Python bindings.

Caution: This LaTeX version of the documentation is not able to render some of the postprocessed output datasets. The HTML version of this document includes the missing inline tables. A future revision to this manual will improve the typesetting to better distinguish user input, system output, and Jupyter notebook results. Also, since the figures are the result of inline computations, they are presented as inline text rather than figures with captions.

A.1 VISUALIZATION

These examples demonstrate basic problem visualization techniques for Denovo and Shift input.

A.1.1 OMNIBUS GEOMETRY VISUALIZATION

This example shows how to process and visualize an MCNP input and its compositions, using both the interactive Python 2-D ray tracer and the executable 3-D Silo-based ray tracer (using `mode=raytrace`). We also save the compositions to a separate HDF5 input file; they can later be used to override the compositions provided by MCNP.

```
# Set up example environment
import os
from exnihilotools.matplotlib import screen_style
%matplotlib inline
screen_style()
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
%load_ext wurlitzer
```

Visualizing the MCNP input requires first loading the geometry. The `load_mcnp` command accepts either an existing `runtpe` filename or the path to an MCNP input (which must have a `.inp`, `.i`, or `.mcnp` extension). Generating a runtpe file requires an MCNP5 executable, since it invokes `mcnp5 ix`. The resulting `model` stores the geometry and a vector of loaded compositions.

```
from omnibus.raytrace.load import load_mcnp
model = load_mcnp(os.path.join(SOURCE_DIR, "data", "dv1a.mcnp"))
```

```
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file in 4.5 seconds
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
```

A.1.1.1 Construct a color table

Material visualization is more easily interpreted when the chosen color scheme associates physical properties with the materials.

The model stores a vector of wrapped C++ `Composition` objects. Their contents can be extracted through accessors such as `name` and `density`, or converted into a dictionary using the `_asdict` method. Omnibus includes a convenience class that mimics the C++ composition object but uses native python datatypes. Since this class's constructor accepts keyword arguments, it can be constructed by expanding each composition using `_asdict` and using the Python keyword argument expansion `**`.

```python
from omnibus.raytrace.composition import Composition
comps = [Composition(**c._asdict()) for c in model.compositions]
comps[1]
```

Each composition's name is constructed by default from the MCNP material numbers in the input deck. These can be changed to more descriptive names by using a convenience function that returns the MCNP `M` card identifiers that correspond to each composition.

```python
matno_to_name = { 0: "emptiness",
                 10: "fuel",
                 20: "gap",
                 30: "clad",
                 40: "mod"}
for c in comps:
    mno = model.matnum(c.matid)
    c.name = matno_to_name[mno]
```

The `ColorMap` class automatically applies colors for common reactor materials such as fuel, clad, control rods, and water. Colors from unknown materials are assigned from the `matplotlib` "Set3" color map[21].

```python
from omnibus.raytrace.colors import ColorMap
colors = ColorMap.from_compositions(comps)
colors[colors.unassigned] = 'Set3'
```

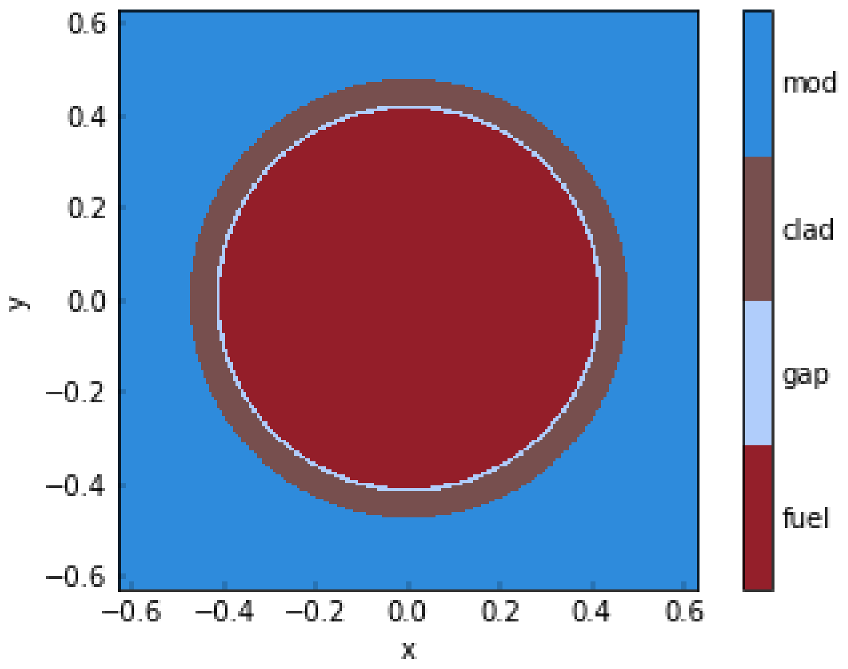
The raytracing `Imager` class renders the geometry to an image. The `lower` and `upper` coordinates are the 3-D points corresponding to the lower-left and upper-right corner of the visualization window. The `basis` vector completes the window specification by defining the rightward direction (`x` axis in the resulting plot) of the window. Increasing the pixel count increases rendering time but provides a sharper-resolution image when exporting. The `trace` option can be set to `cell` (plot the cell names obtained from the MCNP input) or `mat` (for plotting materials, the default). Colors and names can be assigned from the compositions and color map constructed above.

The raytracing engine uses the same particle tracking engine as Shift, so unlike the quadric-intersection-based method in MCNP's visualizer, it will catch actual tracking errors and is typically faster to render.

The `Imager`'s `plot` command returns a matplotlib plot displaying the cells or materials present along the ray-traced slice. Regions not encountered in this specific trace are not displayed, increasing the zoom level will decrease the number of materials.

[21] https://matplotlib.org/3.1.0/gallery/color/colormap_reference.html#sphx-glr-gallery-color-colormap-reference-py

```
from omnibus.raytrace.imager import Imager
imager = Imager(model.geometry,
                lower=(-.63, -.63, 0),
                upper=(.63, .63, 0),
                basis=(1, 0, 0),
                max_pixels=512)
imager.names = [c.name for c in comps]
imager.colors = colors
imager.plot();
```



Here, input files that contain the colors and the name mappings are written out so they can be imported into the raytrace input.

```
from omnibus.raytrace.colors import dump_colors
dump_colors("dv1a-colors.omn", comps, colors)
%cat "dv1a-colors.omn"
```

```
[COMP]
colors
    emptiness               #000000
    fuel                    #941e29
    gap                     #afccfb
    clad                    #774f4e
    mod                     #2e8bdc
```

```
# Save the MCNP name mapping
with open("dv1a-mcnp-names.omn", 'w') as f:
    f.write("! inside [MODEL=mcnp]\n")
    f.write("m")
```

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```
    for mno in sorted(matno_to_name):
        f.write("    {:>8} -> {:s}\n".format(mno, matno_to_name[mno]))
%cat "dv1a-mcnp-names.omn"
```

```
! inside [MODEL=mcnp]
m            0 -> emptiness
            10 -> fuel
            20 -> gap
            30 -> clad
            40 -> mod
```

A.1.1.2 Save compositions to HDF5

It is possible to manually load HDF5 compositions into Omnibus: composition input may be needed for some geometry types like GG or RTK, or it can be used to override compositions present in the model. For example, one could perturb the MCNP nuclide densities without modifying the original MCNP input file. The following block of code saves a composition HDF5 file from the compositions that were loaded from the model.

```
from omnibus.formats.comp import Compositions
from omnibus.data.group import MetadataGroup
import h5py

compout = Compositions.from_list(c._asdict() for c in comps)

with h5py.File("dv1a-comps.h5", 'w') as f:
    compout.dump(f)
    MetadataGroup.from_current_version().dump(f)
!h5ls -r dv1a-comps.h5
```

```
/                         Group
/compositions             Dataset {5}
/metadata                 Group
/metadata/datetime        Dataset {SCALAR}
/metadata/scale_rev       Dataset {SCALAR}
/metadata/scale_version   Dataset {SCALAR}
/metadata/system          Dataset {SCALAR}
```

A.1.1.3 Run the Omnibus 3D ray tracer

Now let’s execute the Omnibus raytracer (which uses the Shift geometry tracking engine to generate a Silo visualization file). Our input file uses `#include` to import the material names and composition colors we generated above.

```
!cp {SOURCE_DIR}/data/dv1a* .
%cat "dv1a-raytrace.omn"
!omnibus-run dv1a-raytrace.omn
```

```
[PROBLEM]
name "Pin cell ray trace example"
```

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```
mode raytrace

[MODEL=mcnp]
input "dv1a.mcnp"

! Import material names
#include "dv1a-mcnp-names.omn"

[DENOVO]
x -0.63 9i 0.63
y -0.63 9i 0.63
z -0.63 9i 0.63

[DENOVO][RAYTRACE]
rays_per_face 16

! Import the colors
#include "dv1a-colors.omn"

[DENOVO][OUTPUT]
block false

[RUN=mpi]
np 4

! Suppress output RST summary file
[POST]
rst false
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
 ↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at dv1a-raytrace.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
INFO: Deleting existing working directory at dv1a_run_mcnp
MCNP:  xact   is done            ...finished generating MCNP runtpe file in 4.7 seconds
INFO: Set default for 'physics' to '[{'_type': 'void'}]' in '/'
INFO: Set default for 'mode' to 'n' in '/physics/void'
INFO: Set default for 'load_scl' to 'False' in '/comp'
INFO: Set default for 'physics' to 'void' in '/denovo'
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Global Denovo mesh has 1000 cells
INFO: Writing Omnibus input ParameterList to dv1a-raytrace.inp.xml
INFO: Writing preprocessed file to dv1a-raytrace.pp.json
INFO: Writing processed ASCII input to 'dv1a-raytrace.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
```

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```
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading nuclide data from processed MCNP libraries
INFO: Loading compositions from MCNP input
INFO: Applying 5 user-provided composition colors
WARNING: Extents of MCNP geometry are extremely large or unknown; this may adversely␣
↪affect 'global' tallies, entropy mesh, etc.
Building physics 'void'
Building Denovo solver internals
Ray tracing Denovo mesh
Mixing Denovo cross sections
Building Denovo sources
Initializing Denovo solver
INFO: Skipping Denovo state construction due to user option
Skipping transport due to user option
Writing Denovo HDF5 output
Run complete
Cleaning up
            ...finished running Omnibus in 1.5 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'dv1a-raytrace.out.h5', problem name 'Pin cell ray␣
↪trace example', created on 2020MAR11 22:36 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'dv1a-raytrace.out.h5', problem name 'Pin cell ray␣
↪trace example', created on 2020MAR11 22:36 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```

Omnibus created one silo file (inside a subdirectory) for each KBA block (execution core), as well as one "master" silo file, which is what we'll open in VisIT.

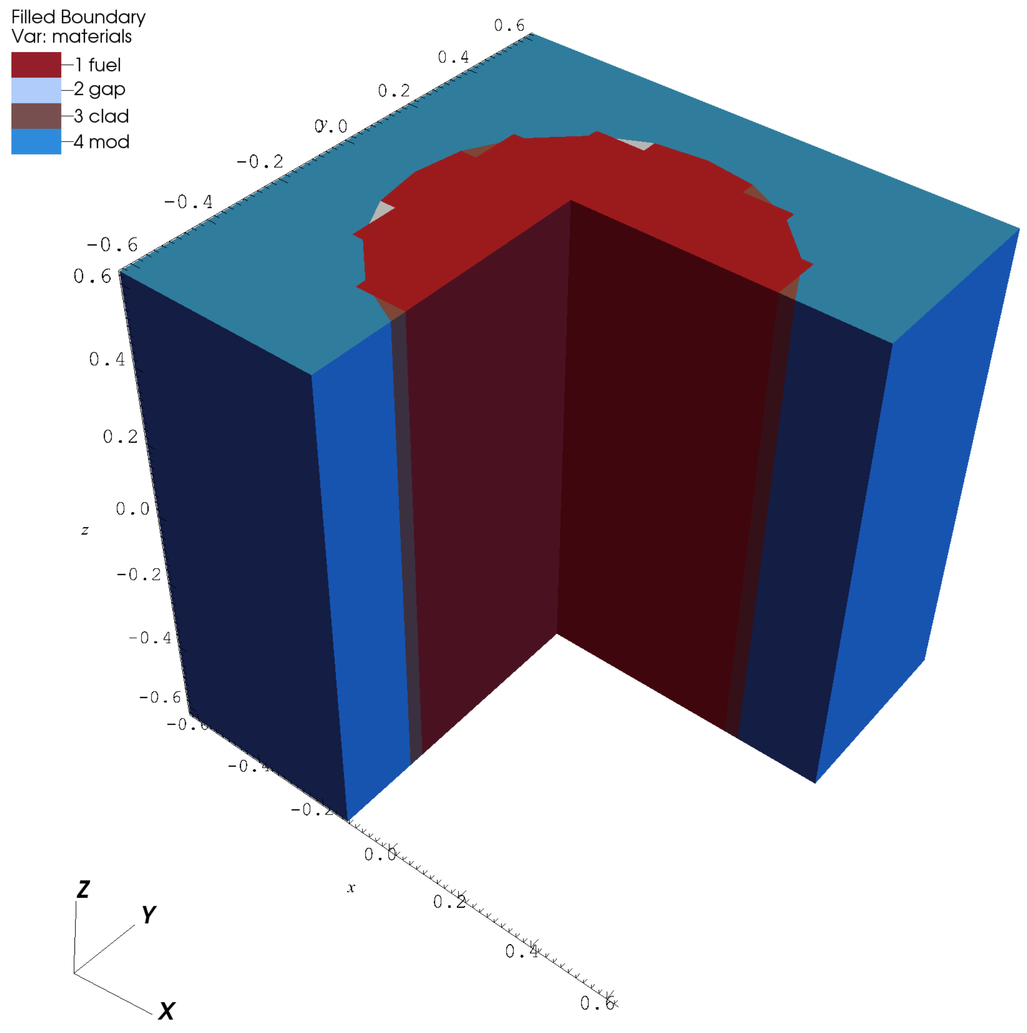
```
!ls *silo
# !visit denovo_output.silo
```

```
denovo_output.silo

denovo_output_silo:
denovo_output.0.silo denovo_output.2.silo
denovo_output.1.silo denovo_output.3.silo
```

A filled boundary plot lets us visualize the ray traced output. Note that the material interface reconstruction is imprecise because we used a relatively coarse mesh. Also note that the material colors and names have been correctly propagated.

```
from IPython.display import Image
Image(filename=os.path.join(SOURCE_DIR, "data", "dv1a-visit0000.png"))
```



A.2 DENOVO

This section provides examples, each of which demonstrates a different way to visualize, input, run, and/or post-process typical problems for Denovo to solve.

A.2.1 DISCRETIZED MCNP GODIVA

This example demonstrates post-processing and visualization for a simple criticality problem using the Denovo deterministic solver.

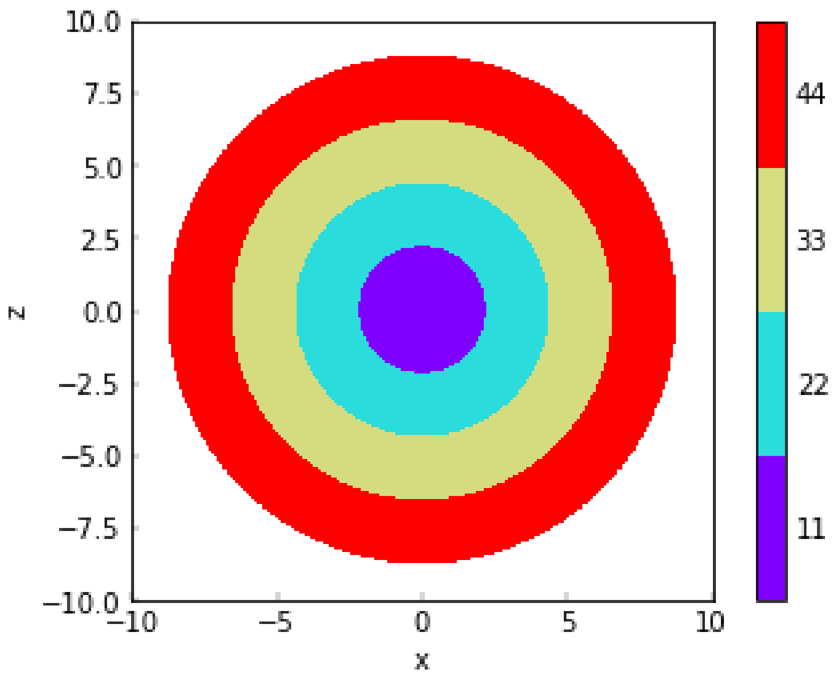
```
# Set up example environment
import os
from exnihilotools.matplotlib import screen_style
%matplotlib inline
screen_style()
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
```

The model and its cell IDs are previsualized using the Omnibus Python tools described in the geometry visualization example.

```
from omnibus.raytrace.load import load_mcnp
from omnibus.raytrace.imager import Imager

model = load_mcnp(os.path.join(SOURCE_DIR, "data", "godiva_multicell.mcnp"))
imager = Imager(model.geometry,
                lower=(-10, 0, -10),
                upper=(10, 0, 10),
                basis=(1, 0, 0),
                max_pixels=1024,
                trace='cell')
imager.plot();
```

```
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
```



A.2.1.1 Execute Omnibus

Running Denovo through Omnibus requires an Omnibus input with SCALE multigroup physics. The `kcode` mode specifies that this is an eigenvalue problem; the `[SOLVER=eigenvalue]` block specifies the numerical accuracy of the solver result.

```
%cat {SOURCE_DIR}/data/denovo-godiva.omn
!omnibus-run {SOURCE_DIR}/data/denovo-godiva.omn
```

```
[PROBLEM]
name "Godiva with SMG physics, MCNP geometry"
mode kcode

[MODEL=mcnp]
input "../data/godiva_multicell.mcnp"

[PHYSICS=mg]
mg_lib "test8g_v7.1"
pn_order 0

[DENOVO]
method sc
! Spatial grid with 'interpolation' keywords
x -9.0 9i 9.0
y -9.0 9i 9.0
z -9.0 9i 9.0

[DENOVO][SILO]
flux true
output "godiva_fluxes"

[DENOVO][SOLVER=eigenvalue]
tolerance 1e-06
verbosity none

[DENOVO][QUADRATURE]
quadrature levelsym
order 4

[RUN=mpi]
np 4
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-godiva.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
INFO: Set default for 'mode' to 'n' in '/physics/mg'
INFO: Set default for 'disable_upscattering' to 'False' in '/physics/mg'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
WARNING: The 'method' keyword is now 'equations' for SN discretization types. Changing␣
↪`method sc` to `equations sc`
```

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```
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'construction' to 'levelsym' in '/denovo/quadrature'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'solver' to 'arnoldi' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '1e-07' in '/denovo/solver/upscatter'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/
↪upscatter'
INFO: Set default for 'max_iterations' to '1000' in '/denovo/solver/upscatter'
INFO: Set default for 'verbosity' to 'low' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '1e-07' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 1000 cells
INFO: Writing Omnibus input ParameterList to denovo-godiva.inp.xml
INFO: Writing preprocessed file to denovo-godiva.pp.json
INFO: Writing processed ASCII input to 'denovo-godiva.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
INFO: Loading compositions from MCNP input
WARNING: Extents of MCNP geometry are extremely large or unknown; this may adversely␣
↪affect 'global' tallies, entropy mesh, etc.
Building physics 'mg'
INFO: Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
INFO: Retained 3 of 449 nuclides on the master AMPX library
INFO: Running XSProc on 4 cells
Building Denovo solver internals
Ray tracing Denovo mesh
```

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```
Mixing Denovo cross sections
Initializing Denovo solver
INFO: Constructing Denovo state vector with 8 groups, 1000 cells, 1 moments, 1 unknowns␣
 ↪per cell
Running Denovo transport calculation
INFO: Inner Krylov iterations in replicated group 0: 7 on node 0
INFO: Inner Krylov iterations in replicated group 1: 9 on node 0
INFO: Inner Krylov iterations in replicated group 2: 7 on node 0
INFO: Inner Krylov iterations in replicated group 3: 5 on node 0
The following inner iteration counts are for Arnoldi solve(wg tol = 1e...
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 0: 7 on node 0
Belos Block GMRES converged after 9 iterations.
>>> Inner Krylov iterations in replicated group 1: 9 on node 0
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 2: 7 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in replicated group 3: 5 on node 0
INFO: Inner Krylov iterations in partitioned groups 4-7 on set 0 and node 0: 5
INFO: Inner Krylov iterations in replicated group 0: 7 on node 0
INFO: Inner Krylov iterations in replicated group 1: 9 on node 0
INFO: Inner Krylov iterations in replicated group 2: 7 on node 0
INFO: Inner Krylov iterations in replicated group 3: 5 on node 0
INFO: Inner Krylov iterations in partitioned groups 4-7 on set 0 and node 0: 5
INFO: Inner Krylov iterations in replicated group 0: 7 on node 0
INFO: Inner Krylov iterations in replicated group 1: 9 on node 0
INFO: Inner Krylov iterations in replicated group 2: 7 on node 0
INFO: Inner Krylov iterations in replicated group 3: 5 on node 0
INFO: Inner Krylov iterations in partitioned groups 4-7 on set 0 and node 0: 5
INFO: Inner Krylov iterations in replicated group 0: 7 on node 0
INFO: Inner Krylov iterations in replicated group 1: 9 on node 0
INFO: Inner Krylov iterations in replicated group 2: 7 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in partitioned groups 4-7 on set 0 and nod...
The following inner iteration counts are for Arnoldi solve(wg tol = 1e...
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 0: 7 on node 0
Belos Block GMRES converged after 9 iterations.
>>> Inner Krylov iterations in replicated group 1: 9 on node 0
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 2: 7 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in replicated group 3: 5 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in partitioned groups 4-7 on set 0 and nod...
The following inner iteration counts are for Arnoldi solve(wg tol = 1e...
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 0: 7 on node 0
Belos Block GMRES converged after 9 iterations.
>>> Inner Krylov iterations in replicated group 1: 9 on node 0
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 2: 7 on node 0
```

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```
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in replicated group 3: 5 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in partitioned groups 4-7 on set 0 and nod...
The following inner iteration counts are for Arnoldi solve(wg tol = 1e...
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 0: 7 on node 0
Belos Block GMRES converged after 9 iterations.
>>> Inner Krylov iterations in replicated group 1: 9 on node 0
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 2: 7 on node 0
INFO: Inner Krylov iterations in replicated group 3: 5 on node 0
INFO: Inner Krylov iterations in partitioned groups 4-7 on set 0 and node 0: 5
INFO: Inner Krylov iterations in replicated group 0: 7 on node 0
INFO: Inner Krylov iterations in replicated group 1: 9 on node 0
INFO: Inner Krylov iterations in replicated group 2: 7 on node 0
INFO: Inner Krylov iterations in replicated group 3: 5 on node 0
INFO: Inner Krylov iterations in partitioned groups 4-7 on set 0 and node 0: 5
INFO: Inner Krylov iterations in replicated group 0: 8 on node 0
INFO: Inner Krylov iterations in replicated group 1: 10 on node 0
INFO: Inner Krylov iterations in replicated group 2: 7 on node 0
INFO: Inner Krylov iterations in replicated group 3: 5 on node 0
INFO: Inner Krylov iterations in partitioned groups 4-7 on set 0 and node 0: 5
INFO: Inner Krylov iterations in replicated group 0: 8 on node 0
INFO: Inner Krylov iterations in replicated group 1: 10 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in replicated group 3: 5 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in partitioned groups 4-7 on set 0 and nod...
The following inner iteration counts are for Arnoldi solve(wg tol = 1e...
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 0: 7 on node 0
Belos Block GMRES converged after 9 iterations.
>>> Inner Krylov iterations in replicated group 1: 9 on node 0
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 2: 7 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in replicated group 3: 5 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in partitioned groups 4-7 on set 0 and nod...
The following inner iteration counts are for Arnoldi solve(wg tol = 1e...
Belos Block GMRES converged after 8 iterations.
>>> Inner Krylov iterations in replicated group 0: 8 on node 0
Belos Block GMRES converged after 10 iterations.
>>> Inner Krylov iterations in replicated group 1: 10 on node 0
Belos Block GMRES converged after 7 iterations.
>>> Inner Krylov iterations in replicated group 2: 7 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in replicated group 3: 5 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in partitioned groups 4-7 on set 0 and nod...
The following inner iteration counts are for Arnoldi solve(wg tol = 1e...
```

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```
Belos Block GMRES converged after 8 iterations.
>>> Inner Krylov iterations in replicated group 0: 8 on node 0
Belos Block GMRES converged after 10 iterations.
>>> Inner Krylov iterations in replicated group 1: 10 on node 0
INFO: Inner Krylov iterations in replicated group 2: 8 on node 0
INFO: Inner Krylov iterations in replicated group 3: 5 on node 0
INFO: Inner Krylov iterations in partitioned groups 4-7 on set 0 and node 0: 5
INFO: Inner Krylov iterations in replicated group 0: 8 on node 0
INFO: Inner Krylov iterations in replicated group 1: 10 on node 0
INFO: Inner Krylov iterations in replicated group 2: 8 on node 0
INFO: Inner Krylov iterations in replicated group 3: 5 on node 0
INFO: Inner Krylov iterations in partitioned groups 4-7 on set 0 and node 0: 5
INFO: k-eff = 1.035583673
INFO: Writing Silo file to 4 concurrent files using material volume fractions
Writing Denovo HDF5 output
Run complete
Cleaning up
Belos Block GMRES converged after 8 iterations.
>>> Inner Krylov iterations in replicated group 2: 8 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in replicated group 3: 5 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in partitioned groups 4-7 on set 0 and nod...
The following inner iteration counts are for Arnoldi solve(wg tol = 1e...
Belos Block GMRES converged after 8 iterations.
>>> Inner Krylov iterations in replicated group 0: 8 on node 0
Belos Block GMRES converged after 10 iterations.
>>> Inner Krylov iterations in replicated group 1: 10 on node 0
Belos Block GMRES converged after 8 iterations.
>>> Inner Krylov iterations in replicated group 2: 8 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in replicated group 3: 5 on node 0
Belos Block GMRES converged after 5 iterations.
>>> Inner Krylov iterations in partitioned groups 4-7 on set 0 and nod...
            ...finished running Omnibus in 2.1 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-godiva.out.h5', problem name 'Godiva with␣
↪SMG physics, MCNP geometry', created on 2020MAR11 22:36 using SCALE version 6.3.pre-
↪b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-godiva.out.h5', problem name 'Godiva with␣
↪SMG physics, MCNP geometry', created on 2020MAR11 22:36 using SCALE version 6.3.pre-
↪b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to denovo-godiva.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to denovo-godiva.rst
            ...finished building RST summary
```

The run itself produces a single HDF5 file (or two HDF5 files if parallel HDF5 is in use). The post-processor creates a ReStructured Text file that summarizes the problem run, which can optionally be disabled in the [POST] post-processing block of the user input.

```python
# Print the first 35 lines of the text output
with open('denovo-godiva.rst') as f:
    for i in range(35):
        print(next(f).rstrip())
    print("...")
```

```
###########################################
Problem and system information (``system``)
###########################################

:Problem name:  Godiva with SMG physics, MCNP geometry
:Identifier:    ``2020-03-11-c639aa1c-3850-4e22-83f0-e0e43942b810``
:Input path:    ``denovo-godiva.inp.xml``

Software versions:

:SCALE version:      6.3.pre-b10 r539
:Release date:       2020 Mar 10
:SCALE data version: data (#13321298 on 2019APR11)

Software installation:

:Build date:       2020MAR10
:Build platform:   machine 'vostok' running Darwin version 18.7.0 (x86_64)
:Install dir:      /rnsdhpc/code/install/Exnihilo-examples

Runtime information:

:Host:          vostok
:# processors:  4
:Start time:    Wed Mar 11 22:36:34 2020
:Working dir:   /rnsdhpc/code/build/Exnihilo-examples/Exnihilo/packages/Omnibus/driver/
 ↪example/denovo-godiva

##########################################
Geometry and model information (``model``)
##########################################

****************************************
MCNP Geometry Description
****************************************


...
```

A.2.1.2 Postprocess Denovo eigenvalue results

The first step of data postprocessing is loading a wrapper for the Denovo output file. By default, this only references the data on disk; but since it is a small output file that will fit entirely in memory on our analysis computer, the `extract` method can be used immediately to load it into memory. However, for very large files it may be impossible to load the entire data file into memory, in which case the `extract` method should *not* be called. Instead, each time the output data is accessed, an HDF5 read operation will be performed on only the requested data (e.g., a single energy group). Thus these post-processing tools can be used efficiently even for very large files by processing data in smaller chunks.

The eigenvalue is stored in the Denovo block of the output file.

```
from omnibus.formats.output import load
from exnihilotools.unittest.comparer import Comparer

output = load("denovo-godiva.out.h5").extract()
keff = output['denovo']['keff'].data
print("Keff =", keff)

# Check that the calculated keff value is within 4% of the analytic solution
assertSoftEquiv = Comparer(float_tolerance=0.04)
assertSoftEquiv(1.0, keff)
```

```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-godiva.out.h5', problem name 'Godiva with␣
↪SMG physics, MCNP geometry', created on 2020MAR11 22:36 using SCALE version 6.3.pre-
↪b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```

```
Keff = 1.0355836734048962
```

The entire set of denovo results are readily available:

```
dnv = output['denovo']
dnv
```

The above table shows all the datasets and groups present in the original file. Note that since the data reside in memory, the `hdf_file` attribute is blank. The other attributes are blank because, by default, they are not written to the output. Additional entries to the `[DENOVO][OUTPUT]` block will cause them to be written to disk.

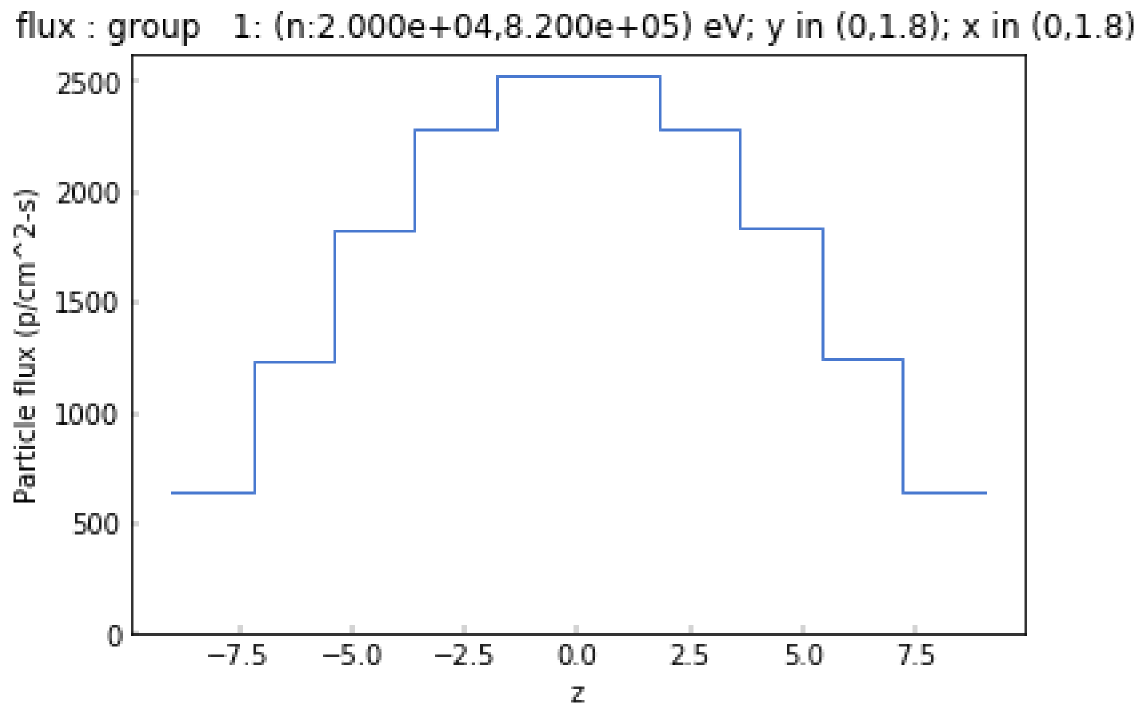
The `omnibus.field.Field` data wrappers allow easy indexing and slicing of the data: it is not necessary to manually determine integer indices in the output: the spatial or energy values can be used directly. Slicing is usually done by taking a "cross sectional" view (hence, `xs`) of the data. The `selection` attribute of a slice shows where the slice was taken from (i.e., what part of the original data is selected).

All the axes remain part of the sliced field, so each dataset always retains knowledge of its dimensions and name. The names of the sliced fields are used by `omnibus.plot` to automatically determine the kind of plot to produce.

The following command plots the flux along the z axis in cells where $x = y = 0$ in energy group $g = 1$:

```
from omnibus.data import plot

plots = plot(dnv['flux'].xs(x=0, y=0, g=1))
ax = plots['ax']
ax.set_ylim(0, None)
ax.set_title(ax.get_ylabel())
ax.set_ylabel("Particle flux (p/cm^2-s)");
```



Rendering a slice of the flux as a pseudocolor plot is similarly trivial. The options on the matplotlib LogNorm[22] class constrain the range of the color scale.

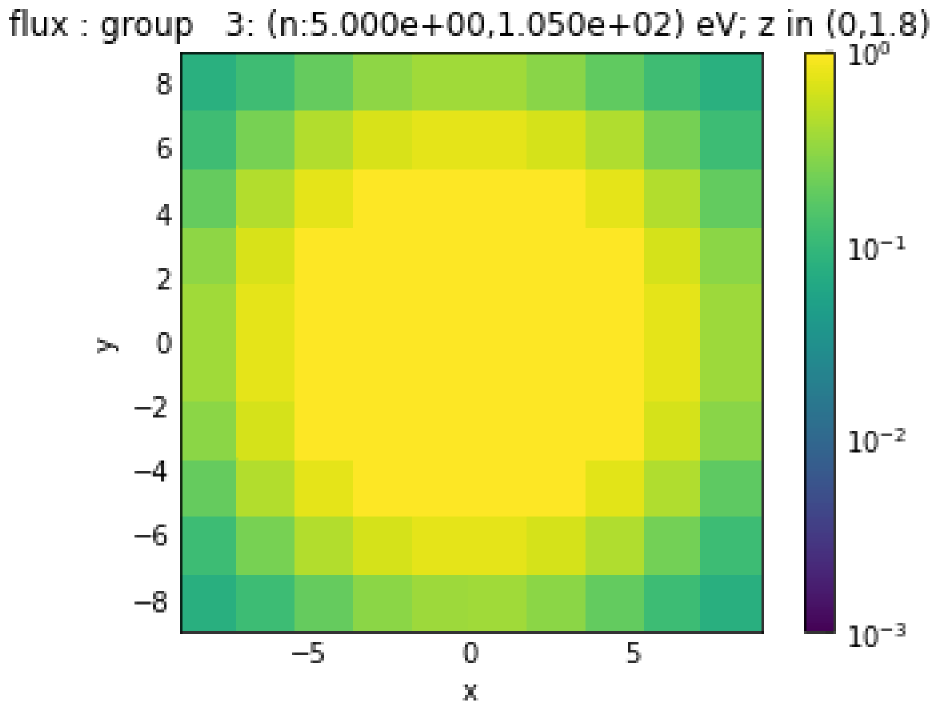
```
print("Max flux:", dnv.flux.xs(g=3, z=1.0).data.max())
print("Min flux:", dnv.flux.xs(g=4, z=1.0).data.min())
```

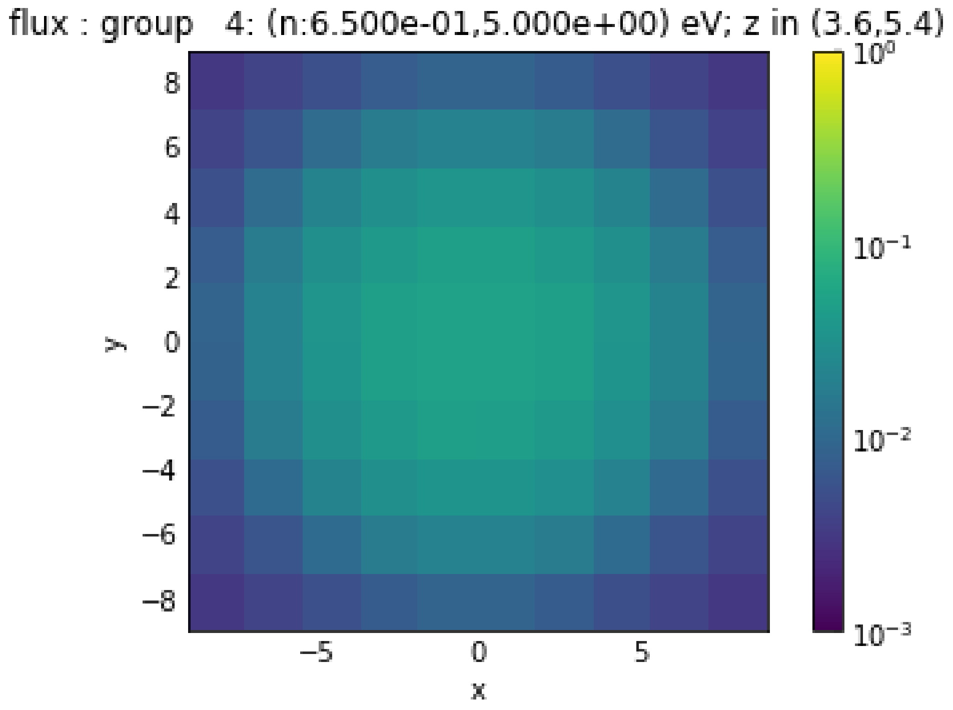
```
Max flux: 1.5522386128007388
Min flux: 0.003584260291936911
```

```
from matplotlib.colors import LogNorm

norm = LogNorm(vmin=1e-3, vmax=1)
plot(dnv.flux.xs(g=3, z=1.0), norm=norm)
plot(dnv.flux.xs(g=4, z=5.0), norm=norm);
```

[22] http://matplotlib.org/api/colors_api.html#matplotlib.colors.LogNorm



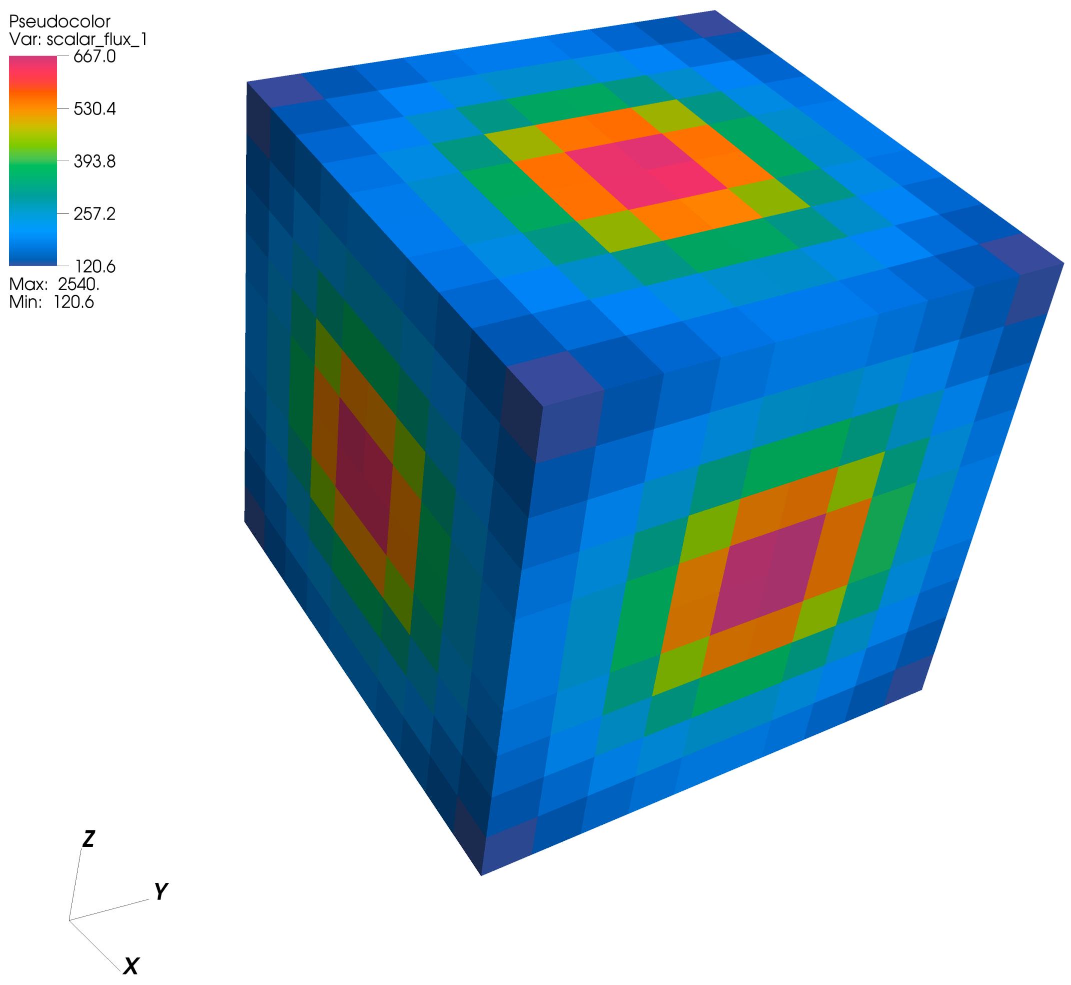


A.2.1.3 Visualize 3D data

The `denovo_godiva.omn` input is configured with a `[SILO]` block to create a Silo-format visualization file, `godiva_fluxes.silo`, containing a voxelized representation of the scalar flux and the materials. This is an alternate way to view and manipulate data produced from Omnibus.

Launch VisIt and open godiva_fluxes.silo to view this data. An image of the scalar flux has been pre-generated in VisIt an example:

```
from IPython.display import Image
Image(os.path.join(SOURCE_DIR, "data", "godiva_scalar_flux_1.png"),  width=600)
```



A.2.2 A TOY SHIELDING PROBLEM

This example demonstrates:

- Denovo's capability to directly discretize and use an MCNP source definition,
- the various Denovo spatial discretization methods, and
- post-processing/flux visualization for a criticality problem.

Three spatial discretization methods will be explored:

- a first order method, Step Characteristics (SC),
- a second order method, Linear Discontinuous (LD), and

- a diffusion-based method, the Simplified PN (SP$_N$) finite volume discretization.

The Denovo `method` parameter in this manual provides guidance on the choice of discretization scheme:

- SC guarantees positive solutions. It is the preferred method for difficult shielding problems and for problems where a coarse spatial mesh must be used.
- LD methods are often more accurate than SC methods, but they do not guarantee positivity of the solution. They are most appropriate for problems that are not prone to negative solutions (such as reactors).
- SP$_N$ provides fast, accurate solutions primarily for light water reactor eigenvalue problems.

This example uses the expedients of a reduced mesh resolution and a smaller multigroup library to decrease run time. The parameters here are not characteristic of a reliable analysis and should not be construed as such.

```
# Set up example environment
import os
from exnihilotools.matplotlib import screen_style
%matplotlib inline
screen_style()
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
```

A.2.2.1 Visualize the geometry

The `[PRE]` block in the input file generates images of the geometry before the Omnibus executable is run. It is automatically run when `omnibus-run` is called, but it can also be used with the standalone `omnibus-pre`.

In this input file, the `autoname` command is used to automatically set MCNP names based on the material compositions. (It substitutes “ss” for “m1” and “water” for “m2”).

```
!grep -A 4 "\[PRE\]" {SOURCE_DIR}/data/denovo-ironsphere.omn
!omnibus-pre {SOURCE_DIR}/data/denovo-ironsphere.omn
```

```
[PRE]
[PRE][PLOT]
origin -10 -10 0
size 20 20
axis z
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-ironsphere.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
MCNP:   xact   is done            ...finished generating MCNP runtpe file in 2.6 seconds
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
```

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```
INFO: Set default for 'disable_upscattering' to 'False' in '/physics/mg'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/upscatter'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/
↪upscatter'
INFO: Set default for 'max_iterations' to '1000' in '/denovo/solver/upscatter'
INFO: Set default for 'verbosity' to 'low' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 4096 cells
INFO: Writing Omnibus input ParameterList to denovo-ironsphere.inp.xml
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
Generating geometry image...
INFO: Saved geometry image at z=0 to 'plot000_z0.pdf'
            ...finished generating geometry image
INFO: Writing preprocessed file to denovo-ironsphere.pp.json
```

```
from IPython.display import display_pdf
with open('plot000_z0.pdf', 'rb') as f:
    display_pdf(f.read(), raw=True)
```

A.2.2.2 SC results

The following Omnibus input uses SCALE multigroup physics for the Denovo calculation. The forward mode specifies a fixed source problem for this shielding calculation; the [SOURCE=mcnp] uses the MCNP SDEF card to generate the source term; the DENOVO method specifies the spatial discretization; and the [SOLVER=fixed] block specifies an overall desired convergence tolerance for this fixed source problem.

To avoid repeating the same input file for the three different methods in this example, a “base” input file stores the common parameters. Each individual method uses a Python snippet to tweak the input. Calling omnibus-run on multiple input arguments allows them to modify a common input.

```
%cat {SOURCE_DIR}/data/denovo-ironsphere.omn {SOURCE_DIR}/data/denovo-ironsphere-sc.py
```

```
[PROBLEM]
name "Iron sphere"
mode forward

[MODEL=mcnp]
input "../data/ironsphere.mcnp"
autoname

[SOURCE=mcnp]

[PHYSICS=mg]
mg_lib "test8g_v7.1"
mode n
pn_order 3

[DENOVO]
! Need to add 'method' via a supplementary python input

! import numpy as np
! x = (np.logspace(0,1,9) - 0.9) * 20 / (10-0.9)
! y = np.concatenate([-x[::-1], x[1:]])
! print(" ".join('{:.6f}'.format(v) for v in y))
x  -20.000000 -14.503169 -10.381128 -7.290033 -4.972039 -3.233788 -1.930284
    -0.952794 -0.219780 0.952794 1.930284 3.233788 4.972039 7.290033 10.381128
    14.503169 20.000000
y  -20.000000 -14.503169 -10.381128 -7.290033 -4.972039 -3.233788 -1.930284
    -0.952794 -0.219780 0.952794 1.930284 3.233788 4.972039 7.290033 10.381128
    14.503169 20.000000
z  -20.000000 -14.503169 -10.381128 -7.290033 -4.972039 -3.233788 -1.930284
    -0.952794 -0.219780 0.952794 1.930284 3.233788 4.972039 7.290033 10.381128
    14.503169 20.000000

[DENOVO][SOLVER=fixed]
tolerance 1e-03

[.][WITHIN_GROUP]
verbosity none

[DENOVO][QUADRATURE]
quadrature qr
construction product
num_azi 4
num_polar 4

[RUN=mpi]
np 4

[PRE]
[PRE][PLOT]
origin -10 -10 0
```

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```
size 20 20
axis z
###############################################################################
# File  : Omnibus/driver/example/data/denovo-ironsphere-sc.py
# Date  : Fri Nov 18 14:03:23 2016
################################################################################
from __future__ import (division, absolute_import, print_function, )
#-----------------------------------------------------------------------------#

print("Running from inside the python script:", locals().keys())

# Modify the problem name
db['problem']['name'] += " (SC)"
db['output'] = {'output': 'denovo-ironsphere-sc.out.h5'}

# Set the method to 'sc'
db['denovo']['method'] = "sc"

###############################################################################
# end of Omnibus/driver/example/data/denovo-ironsphere-sc.py
###############################################################################
```

```
!omnibus-run {SOURCE_DIR}/data/denovo-ironsphere.omn {SOURCE_DIR}/data/denovo-ironsphere-
↪sc.py
```

```
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-ironsphere.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
Running from inside the python script: dict_keys(['db', '__builtins__', 'division',
↪'absolute_import', 'print_function'])
            ...finished loading problem db from Python file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
INFO: Set default for 'disable_upscattering' to 'False' in '/physics/mg'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
WARNING: The 'method' keyword is now 'equations' for SN discretization types. Changing␣
↪`method sc` to `equations sc`
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
```

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```
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/upscatter'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/
↪upscatter'
INFO: Set default for 'max_iterations' to '1000' in '/denovo/solver/upscatter'
INFO: Set default for 'verbosity' to 'low' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 4096 cells
INFO: Renaming existing file denovo-ironsphere.inp.xml to denovo-ironsphere.inp-20200311-
↪2237.xml
INFO: Writing Omnibus input ParameterList to denovo-ironsphere.inp.xml
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
Generating geometry image...
INFO: Saved geometry image at z=0 to 'plot000_z0.pdf'
            ...finished generating geometry image
INFO: Renaming existing file denovo-ironsphere.pp.json to denovo-ironsphere.pp-20200311-
↪2237.json
INFO: Writing preprocessed file to denovo-ironsphere.pp.json
INFO: Writing processed ASCII input to 'denovo-ironsphere.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
INFO: Loading compositions from MCNP input
WARNING: Extents of MCNP geometry are extremely large or unknown; this may adversely␣
↪affect 'global' tallies, entropy mesh, etc.
Building physics 'mg'
INFO: Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
```

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```
INFO: Retained 21 of 449 nuclides on the master AMPX library
INFO: Running XSProc on 2 cells
WARNING: Remapped 2 nuclide IDs: 6012->6000, 6013->6000
Building sources
Building Denovo solver internals
Ray tracing Denovo mesh
Mixing Denovo cross sections
Building Denovo sources
Constructing forward sources for Denovo
WARNING: MCNP source discretization is currently experimental: only a single isotropic␣
↪volumetric source will be treated correctly.
WARNING: Discretization of source (type MCNP) was undersampled (undersampling fraction 0.
↪999329).
WARNING: Consider increasing the number of samples per batch or decreasing the source␣
↪bounding box to (-0.952794,-0.952794,-0.952794) - (0.952794,0.952794,0.952794)
Initializing Denovo solver
INFO: Constructing Denovo state vector with 8 groups, 4096 cells, 16 moments, 1 unknowns␣
↪per cell
Running Denovo transport calculation
Forward group   0 finished in    3 Belos Block GMRES iterations in 1 s...
Forward group   1 finished in    4 Belos Block GMRES iterations in 1 s...
Forward group   2 finished in    5 Belos Block GMRES iterations in 1 s...
Forward group   3 finished in    3 Belos Block GMRES iterations in 1 s...
INFO: Forward groups 4-7 finished in   25 Belos Block GMRES iterations.
INFO: Writing Silo file to 4 concurrent files using material volume fractions
Writing Denovo HDF5 output
Run complete
Cleaning up
Belos Block GMRES converged after 25 iterations.
>>> Forward groups 4-7 finished in   25 Belos Block GMRES iterations.
            ...finished running Omnibus in 3.3 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-sc.out.h5', problem name 'Iron␣
↪sphere (SC)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-sc.out.h5', problem name 'Iron␣
↪sphere (SC)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to denovo-ironsphere-sc.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to denovo-ironsphere-sc.rst
            ...finished building RST summary
```

After executing Omnibus, the data can be extracted and visualized:

```
from omnibus.formats.output import load

dnv_sc = load("denovo-ironsphere-sc.out.h5")['denovo'].extract()
dnv_sc
```

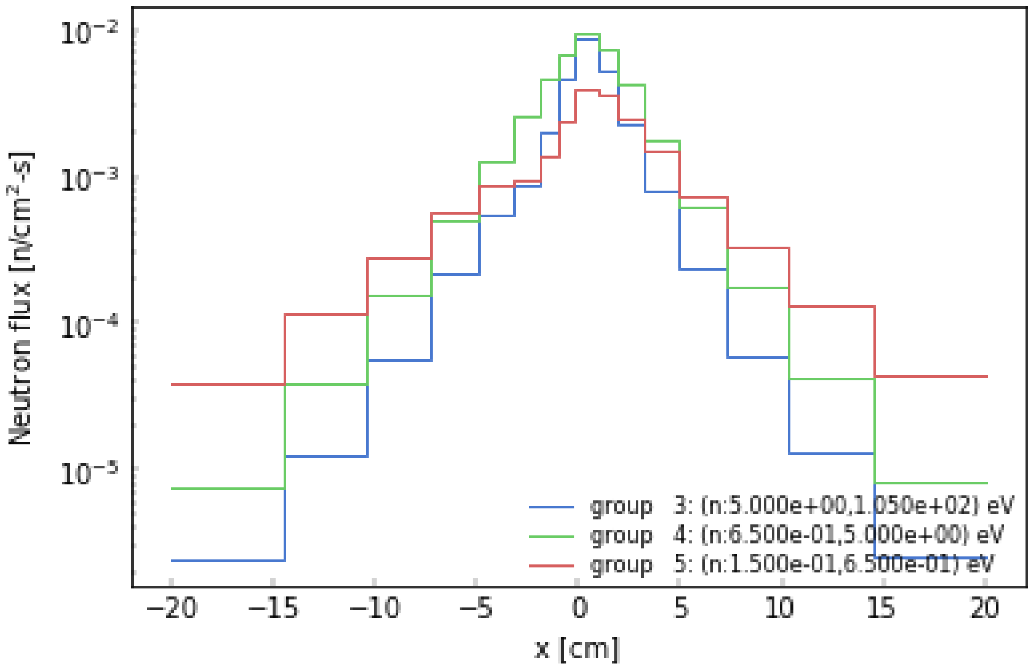
```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-sc.out.h5', problem name 'Iron␣
↪sphere (SC)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```

```
print(dnv_sc['flux'].shape)
print(dnv_sc['flux'].dims)
```

```
(8, 16, 16, 16)
['g', 'z', 'y', 'x']
```

```
# Print group-5 flux
flux_sc = dnv_sc.flux.xs(g=5)
flux_sc
```

```
from omnibus.data import plot

def plot_x_flux(flux, groups):
    """Plot multigroup wise fluxes along the x axis"""
    ax = None
    for g in groups:
        plots = plot(flux.xs(y=0.0, z=0.0, g=g), logy=True, ax=ax)
        ax = plots['ax']
        plots['plot'][0].set_label(flux.axis('g').describe_index(g))
    ax.legend(loc='lower right')
    ax.set_title("")
    ax.set_xlabel("x [cm]")
    ax.set_ylabel("Neutron flux [n/cm$^2$-s]")

plot_x_flux(dnv_sc['flux'], range(3, 6))
```



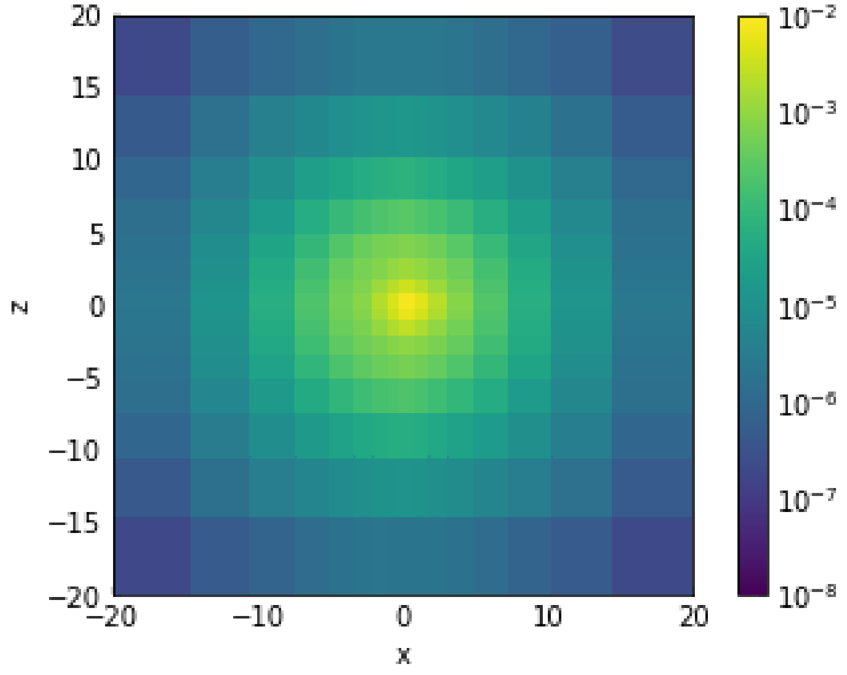
Two-dimensional pseudocolor plots of the flux are easy to render. Note that the ray effects seen in the following plot are characteristic of any discrete ordinate method, including SC.

```
flux_slice = dnv_sc['flux'].xs(g=5, y=0.0)
print("Flux spans {:.2e} to {:.2e}".format(
        flux_slice.data.min(),
        flux_slice.data.max()))
```

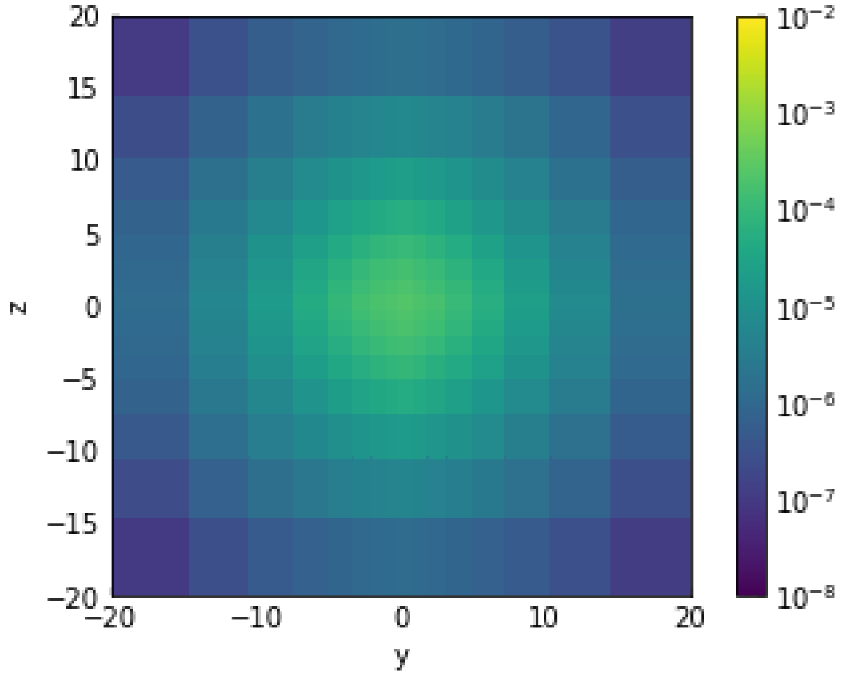
```
Flux spans 3.72e-06 to 3.88e-03
```

```
from matplotlib.colors import Normalize, LogNorm

def plot_pcolor(flux):
    norm = LogNorm(vmin=1e-8, vmax=1e-2)
    plots = plot(flux.xs(g=3, y=0.0), norm=norm)
    plots['ax'].title.set_position([.5, 1.05])
    plots = plot(flux.xs(g=3, x=5.0), norm=norm)
    plots['ax'].title.set_position([.5, 1.05])

plot_pcolor(dnv_sc['flux'])
```

flux : group 3: (n:5.000e+00,1.050e+02) eV; y in (-0.21978,0.952794)



flux : group 3: (n:5.000e+00,1.050e+02) eV; x in (4.97204,7.29003)



A.2.2.3 LD results

The following changes to the base input run Omnibus with LD instead of SC.

```
%cat {SOURCE_DIR}/data/denovo-ironsphere.ld.py
```

```
cat: /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/example/data/denovo-
↪ironsphere.ld.py: No such file or directory
```

```
!omnibus-run {SOURCE_DIR}/data/denovo-ironsphere.omn {SOURCE_DIR}/data/denovo-ironsphere-
↪ld.py
```

```
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-ironsphere.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
INFO: Set default for 'disable_upscattering' to 'False' in '/physics/mg'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
WARNING: The 'method' keyword is now 'equations' for SN discretization types. Changing␣
↪`method ld` to `equations ld`
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: ld
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: ld
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/upscatter'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/
↪upscatter'
INFO: Set default for 'max_iterations' to '1000' in '/denovo/solver/upscatter'
INFO: Set default for 'verbosity' to 'low' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: ld
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
```

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```
INFO: Equations: ld
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 4096 cells
INFO: Renaming existing file denovo-ironsphere.inp.xml to denovo-ironsphere.inp-20200311-
↪2237a.xml
INFO: Writing Omnibus input ParameterList to denovo-ironsphere.inp.xml
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
Generating geometry image...
INFO: Saved geometry image at z=0 to 'plot000_z0.pdf'
            ...finished generating geometry image
INFO: Renaming existing file denovo-ironsphere.pp.json to denovo-ironsphere.pp-20200311-
↪2237a.json
INFO: Writing preprocessed file to denovo-ironsphere.pp.json
INFO: Renaming existing file denovo-ironsphere.inp.omn to denovo-ironsphere.inp-20200311-
↪2237.omn
INFO: Writing processed ASCII input to 'denovo-ironsphere.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
INFO: Renaming existing file omnibus.out to omnibus-20200311-2237.out
INFO: Renaming existing file omnibus.err to omnibus-20200311-2237.err
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
INFO: Loading compositions from MCNP input
WARNING: Extents of MCNP geometry are extremely large or unknown; this may adversely␣
↪affect 'global' tallies, entropy mesh, etc.
Building physics 'mg'
INFO: Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
INFO: Retained 21 of 449 nuclides on the master AMPX library
INFO: Running XSProc on 2 cells
WARNING: Remapped 2 nuclide IDs: 6012->6000, 6013->6000
Building sources
Building Denovo solver internals
Ray tracing Denovo mesh
Mixing Denovo cross sections
Building Denovo sources
Constructing forward sources for Denovo
WARNING: MCNP source discretization is currently experimental: only a single isotropic␣
↪volumetric source will be treated correctly.
WARNING: Discretization of source (type MCNP) was undersampled (undersampling fraction 0.
↪999329).
WARNING: Consider increasing the number of samples per batch or decreasing the source␣
↪bounding box to (-0.952794,-0.952794,-0.952794) - (0.952794,0.952794,0.952794)
```

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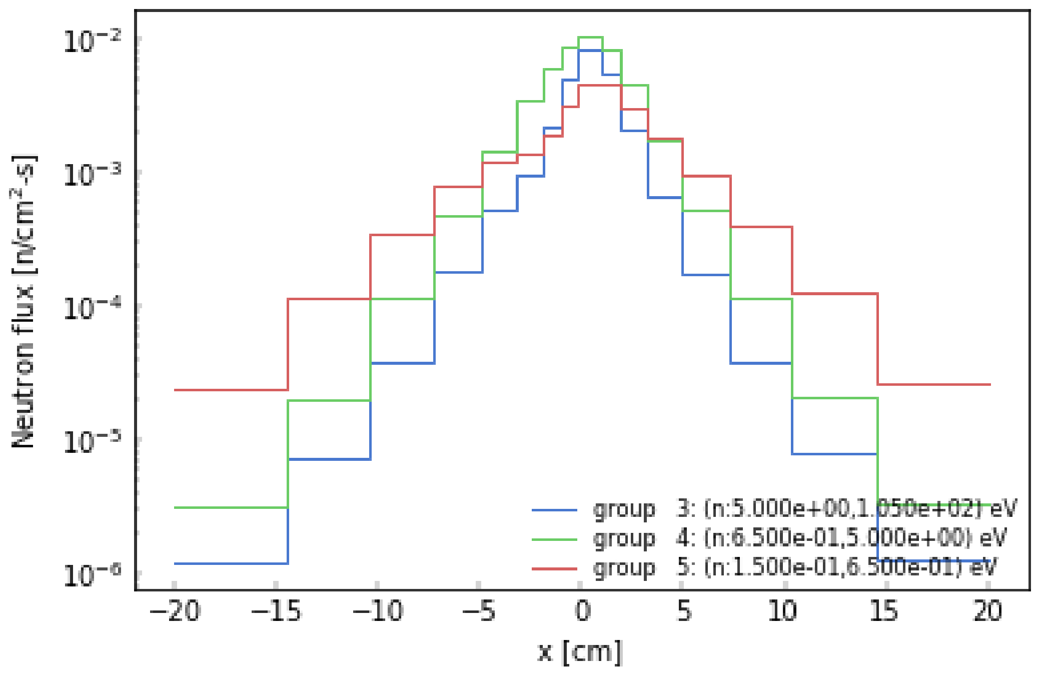
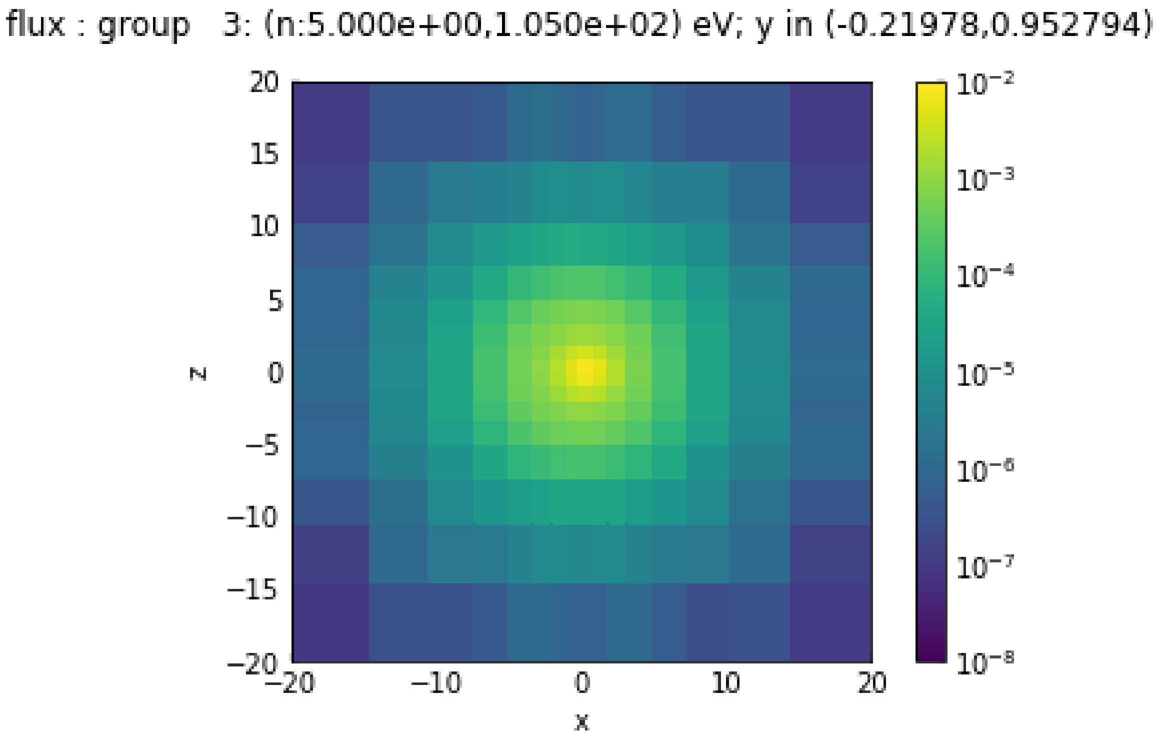
```
Initializing Denovo solver
INFO: Constructing Denovo state vector with 8 groups, 4096 cells, 16 moments, 4 unknowns␣
↪per cell
Running Denovo transport calculation
Forward group   0 finished in    3 Belos Block GMRES iterations in 1 s...
Forward group   1 finished in    4 Belos Block GMRES iterations in 1 s...
Forward group   2 finished in    5 Belos Block GMRES iterations in 1 s...
Forward group   3 finished in    4 Belos Block GMRES iterations in 1 s...
INFO: Forward groups 4-7 finished in   37 Belos Block GMRES iterations.
INFO: Writing Silo file to 4 concurrent files using material volume fractions
INFO: Removing SILO directory denovo_output_silo
Writing Denovo HDF5 output
Run complete
Cleaning up
Belos Block GMRES converged after 37 iterations.
>>> Forward groups 4-7 finished in   37 Belos Block GMRES iterations.
            ...finished running Omnibus in 6.1 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-ld.out.h5', problem name 'Iron␣
↪sphere (LD)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-ld.out.h5', problem name 'Iron␣
↪sphere (LD)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to denovo-ironsphere-ld.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to denovo-ironsphere-ld.rst
            ...finished building RST summary
```

```
dnv_ld = load("denovo-ironsphere-ld.out.h5")['denovo'].extract()
plot_x_flux(dnv_ld['flux'], range(3, 6))
plot_pcolor(dnv_ld['flux'])
```

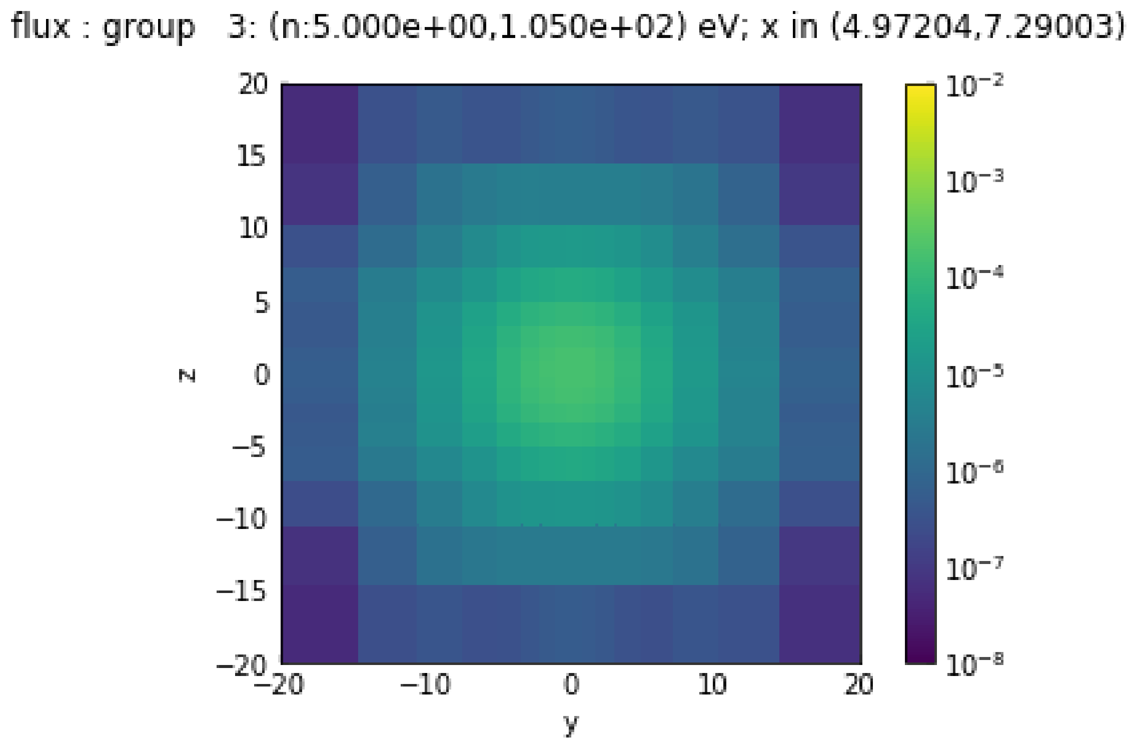
```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-ld.out.h5', problem name 'Iron␣
↪sphere (LD)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```



Neutron flux [n/cm²-s]
10⁻²
10⁻³
10⁻⁴
10⁻⁵
10⁻⁶
−20
−15
−10
−5
0
5
10
15
20
x [cm]
group 3: (n:5.000e+00,1.050e+02) eV
group 4: (n:6.500e-01,5.000e+00) eV
group 5: (n:1.500e-01,6.500e-01) eV



flux : group 3: (n:5.000e+00,1.050e+02) eV; y in (-0.21978,0.952794)
z
x
20
15
10
5
0
−5
−10
−15
−20
−20
−10
0
10
20
10⁻²
10⁻³
10⁻⁴
10⁻⁵
10⁻⁶
10⁻⁷
10⁻⁸



Again, notice the ray effects in the scalar flux plot below due to LD being a discrete ordinates method.

A.2.2.4 Run with SP$_N$

A final set of changes to the base input runs Omnibus with SP$_3$.

```
%cat {SOURCE_DIR}/data/denovo-ironsphere-spn.py
```

```
##############################################################################
# File  : Omnibus/driver/example/data/denovo-ironsphere-spn.py
# Date  : Fri Nov 18 14:03:23 2016
###############################################################################
from __future__ import (division, absolute_import, print_function, )
#-----------------------------------------------------------------------------#

# Modify the problem name
db['problem']['name'] += " (SPN)"
db['output'] = {'output': 'denovo-ironsphere-spn.out.h5'}

# Set the method to 'spn'
db['denovo']['method'] = "spn"
# Delete the inapplicable databases
del db['denovo']['quadrature']
del db['denovo']['solver']['within_group']

##############################################################################
# end of Omnibus/driver/example/data/denovo-ironsphere-spn.py
##############################################################################
```

```
!omnibus-run {SOURCE_DIR}/data/denovo-ironsphere.omn {SOURCE_DIR}/data/denovo-ironsphere-
↪spn.py
```

```
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-ironsphere.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
INFO: Set default for 'disable_upscattering' to 'False' in '/physics/mg'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'all' in '/denovo/solver'
INFO: Method: spn
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/upscatter'
INFO: Method: spn
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/upscatter'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/
↪upscatter'
INFO: Set default for 'max_iterations' to '1000' in '/denovo/solver/upscatter'
INFO: Set default for 'verbosity' to 'low' in '/denovo/solver/upscatter'
INFO: Global Denovo mesh has 4096 cells
INFO: Renaming existing file denovo-ironsphere.inp.xml to denovo-ironsphere.inp-20200311-
↪2237b.xml
INFO: Writing Omnibus input ParameterList to denovo-ironsphere.inp.xml
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
Generating geometry image...
INFO: Saved geometry image at z=0 to 'plot000_z0.pdf'
            ...finished generating geometry image
INFO: Renaming existing file denovo-ironsphere.pp.json to denovo-ironsphere.pp-20200311-
↪2237b.json
INFO: Writing preprocessed file to denovo-ironsphere.pp.json
INFO: Renaming existing file denovo-ironsphere.inp.omn to denovo-ironsphere.inp-20200311-
↪2237a.omn
INFO: Writing processed ASCII input to 'denovo-ironsphere.inp.omn'
```

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```
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
INFO: Renaming existing file omnibus.out to omnibus-20200311-2237a.out
INFO: Renaming existing file omnibus.err to omnibus-20200311-2237a.err
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
INFO: Loading compositions from MCNP input
WARNING: Extents of MCNP geometry are extremely large or unknown; this may adversely␣
↪affect 'global' tallies, entropy mesh, etc.
Building physics 'mg'
INFO: Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
INFO: Retained 21 of 449 nuclides on the master AMPX library
INFO: Running XSProc on 2 cells
WARNING: Remapped 2 nuclide IDs: 6012->6000, 6013->6000
Building sources
Building Denovo solver internals
Ray tracing Denovo mesh
Mixing Denovo cross sections
Building Denovo sources
Constructing forward sources for Denovo
WARNING: MCNP source discretization is currently experimental: only a single isotropic␣
↪volumetric source will be treated correctly.
WARNING: Discretization of source (type MCNP) was undersampled (undersampling fraction 0.
↪999329).
WARNING: Consider increasing the number of samples per batch or decreasing the source␣
↪bounding box to (-0.952794,-0.952794,-0.952794) - (0.952794,0.952794,0.952794)
Initializing Denovo solver
INFO: Built SPN FV Element LHS Matrix with 1333248 nonzero entries.
Running Denovo transport calculation
INFO: Writing Silo file to 4 concurrent files using material volume fractions
INFO: Removing SILO directory denovo_output_silo
Writing Denovo HDF5 output
Run complete
Cleaning up
Belos Block GMRES converged after 274 iterations.
            ...finished running Omnibus in 2.1 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-spn.out.h5', problem name 'Iron␣
↪sphere (SPN)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-spn.out.h5', problem name 'Iron␣
↪sphere (SPN)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
```

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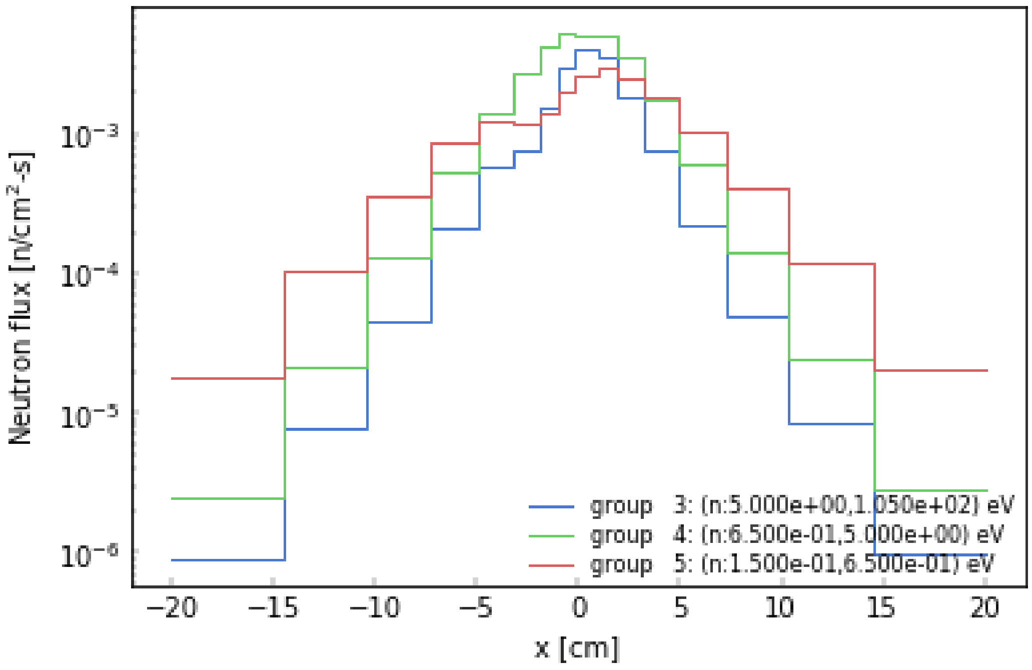
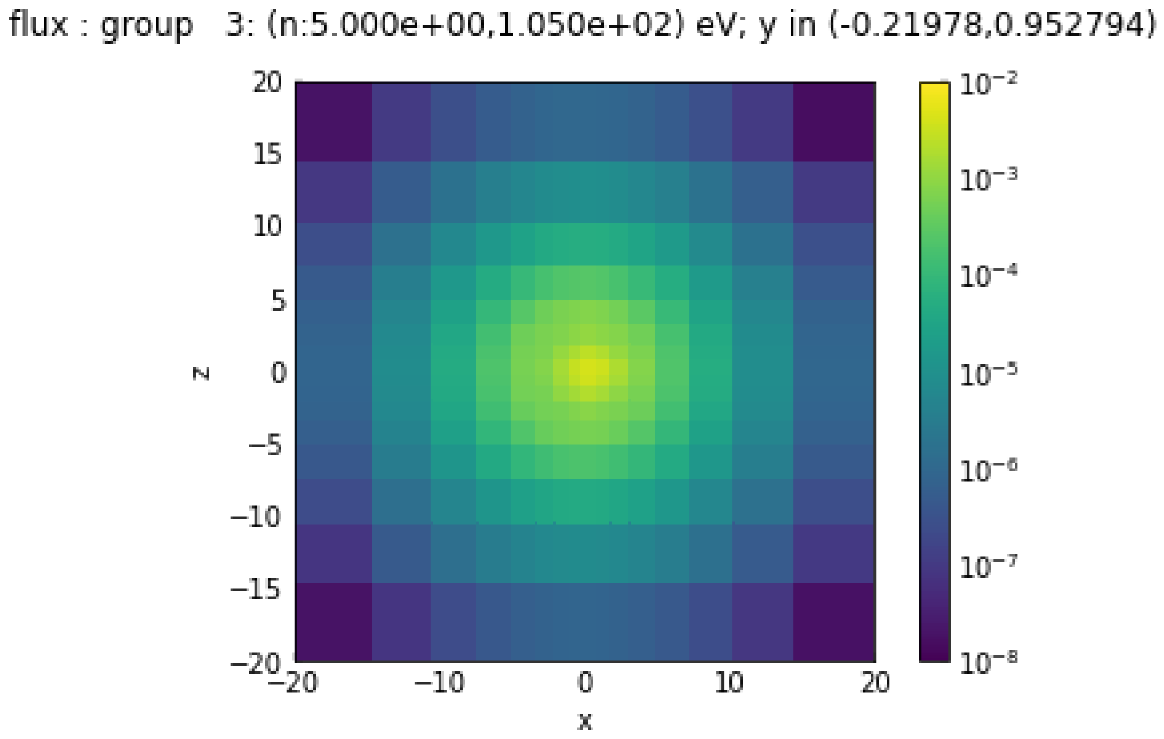
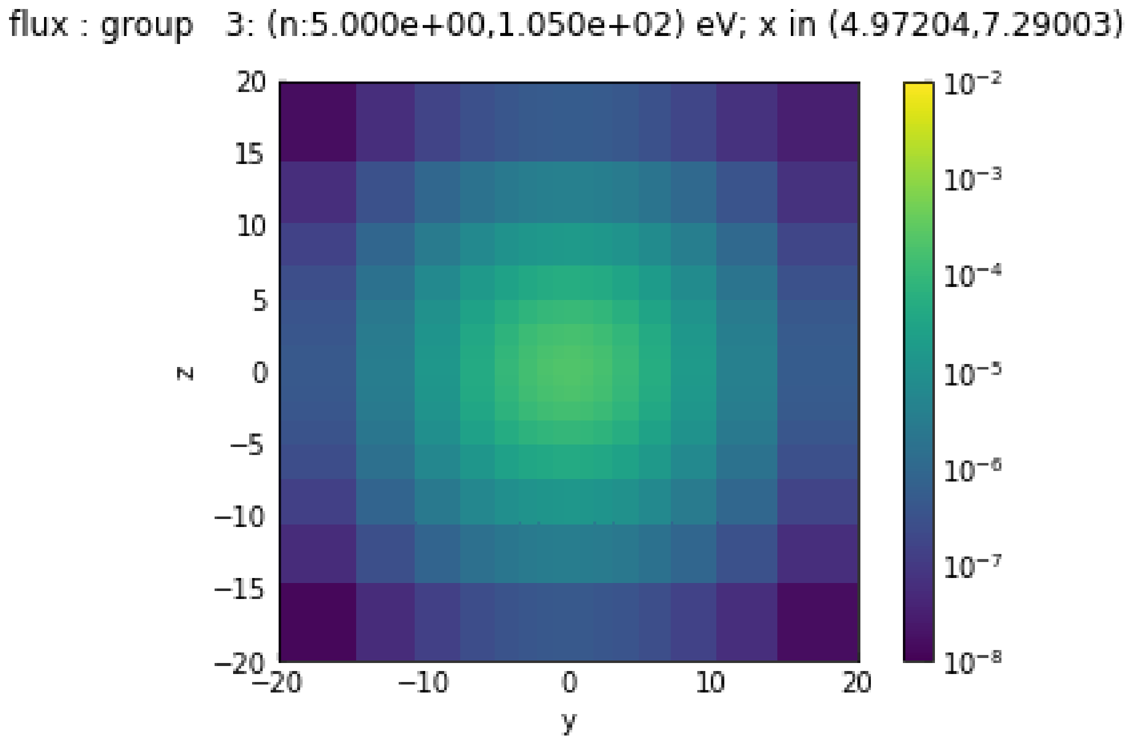
```
            ...finished loading HDF5 file
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to denovo-ironsphere-spn.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to denovo-ironsphere-spn.rst
            ...finished building RST summary
```

```
dnv_spn = load("denovo-ironsphere-spn.out.h5")['denovo'].extract()
plot_x_flux(dnv_spn['flux'], range(3, 6))
plot_pcolor(dnv_spn['flux'])
```

```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ironsphere-spn.out.h5', problem name 'Iron␣
↪sphere (SPN)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```







Note that the SP_N method demonstrates no ray effects since it is a spherical harmonics method rather than a discrete ordinates method.

A.2.2.5 Compare the three methods

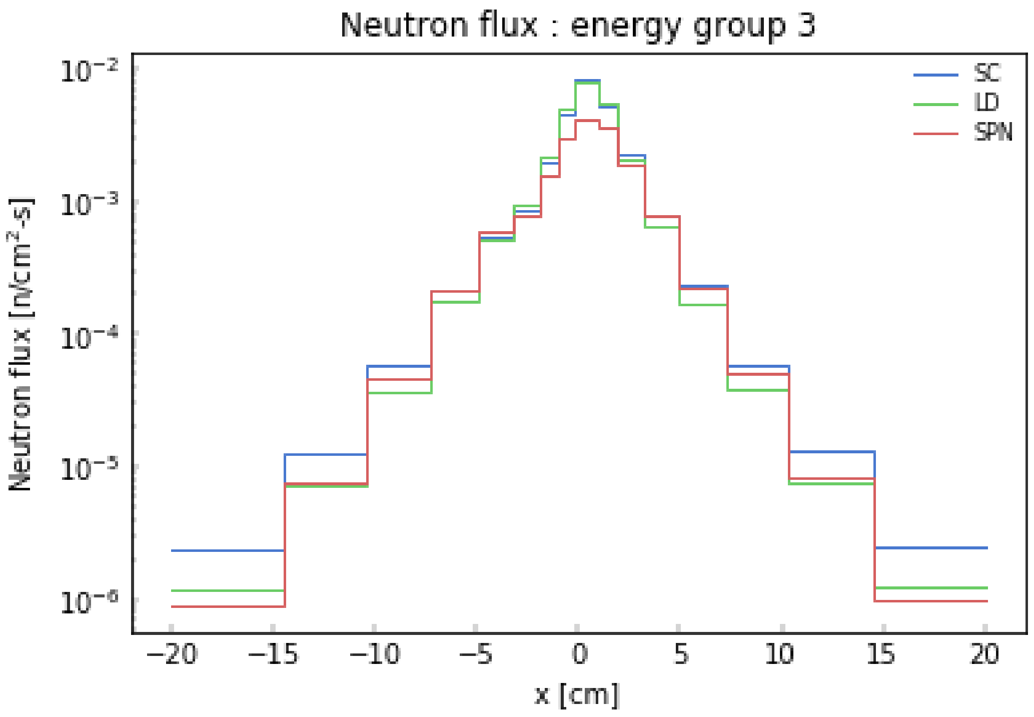
A final plot summarizes results from the three spatial discretization methods, plotting along the *x* axis (where $y = 0$ and $z = 0$).

The SP$_3$ solution is depressed at the source material bounary as expected.

All solutions agree well farther from the source.

```
labeled_data = [('SC', dnv_sc),
                ('LD', dnv_ld),
                ('SPN', dnv_spn)]
ax = None
for (label, data) in labeled_data:
    plots = plot(data.flux.xs(y=0.0, z=0.0, g=3), logy=True, ax=ax)
    plots['plot'][0].set_label(label)
    ax = plots['ax']

ax.set_xlabel("x [cm]")
ax.set_ylabel("Neutron flux [n/cm$^2$-s]")
ax.set_title("Neutron flux : energy group 3")
ax.legend();
```



A.2.3 KOBAYASHI PROBLEM 1.II

This example compares Denovo results to published transport benchmark results [1].

```
# Set up example environment
import os
from exnihilotools.matplotlib import screen_style
```

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```
%matplotlib inline
screen_style()
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
```

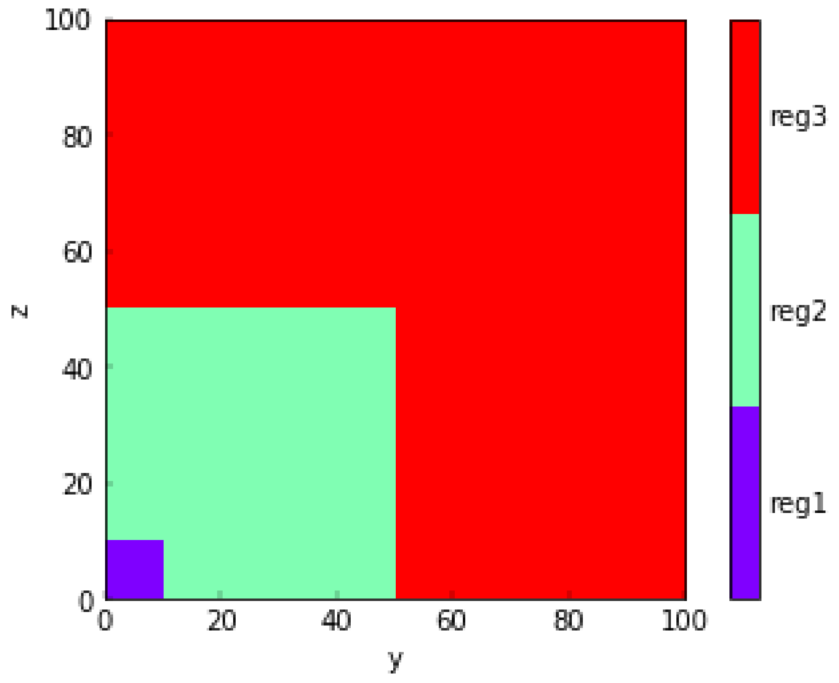
A.2.3.1 Visualizing geometry

The geometry is loaded from the GG input file to create a raytrace imager for visualizing the geometry. The `from_extents` method works for geometries that have bounding boxes (e.g., GG, SCALE, SWORD)..

```
from geometria import GG_Geometry
from omnibus.raytrace.imager import Imager
from omnibus.raytrace.load import load_gg

model = load_gg(os.path.join(SOURCE_DIR, "data", "kobp1.gg.omn"))
imager = Imager.from_extents(model.geometry, x=0, trace='cell')
imager.plot();
```

```
Generating Geometria XML input file from .gg.omn...
INFO: Starting Geometria preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/kobp1.gg.omn
            ...finished loading problem db from Omnibus ASCII file
INFO: Writing Geometria input ParameterList to kobp1.gg.xml
            ...finished generating Geometria XML input file from .gg.omn
```



A.2.3.2 Kobayashi Cross Sections

Now the Exnihilo python wrappers are used to generate analytic 1-group cross sections for the Kobayashi problem. The `Materials` class is a simple working multigroup cross section library container.

```
import robus
import numpy as np
from nemesis import make_const_view
from transcore import XML_Writer

# Create XS container
mats = robus.Materials()
mats.set_num_materials(4)

# Define names and values
num_groups = 1
pn_order = 0
reactions = [robus.TOTAL, robus.SCATTERING]
totals = [0.0, 0.1, 1.0e-5, 0.1]
names  = ['vaccum', 'region 1', 'region 2', 'region 3']
c = 0.5

# Construct cross sections
for (i, tot_xs) in enumerate(totals):
    mat = robus.Material_Downscatter(reactions, num_groups, pn_order)
    total = np.array([tot_xs])
    mat.set_sigma(make_const_view(total))
    scat = np.array([[[c * tot_xs]]])
    mat.set_sigma_s(make_const_view(scat))
    mat.complete()
    mats.set_material(i, mat)

mats.complete()

# Write to XS input file
writer = XML_Writer(mats, "kobayashi_ii.xs.xml", names)
writer.write()
```

A.2.3.3 Execute Omnibus

Because the cross sections we generated are in the working directory, the Omnibus input files must also be copied the working directory too, since paths in the input file are relative to the input file.

```
%cp {SOURCE_DIR}/data/denovo-kobayashi.omn .
%cp {SOURCE_DIR}/data/kobp1.gg.omn .
%cat denovo-kobayashi.omn
```

```
[PROBLEM]
name "Kobayashi Problem 1-ii"
mode forward

[MODEL=gg]
input "kobp1.gg.omn"
```

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```
[PHYSICS=mg]
pn_order 0
num_groups 1
neutron_bounds 2e7 1e-5 ! arbitrary
xml_path "kobayashi_ii.xs.xml"

[SOURCE=separable source]
q    1000.0
fis  False

[SOURCE][SHAPE=box]
xmin 0.0
xmax 10.0
ymin 0.0
ymax 10.0
zmin 0.0
zmax 10.0

[SOURCE][ENERGY=histogram]
e    1e-05 2e7
p       1.0
pt   n

[SOURCE][ANGLE=isotropic]

[DENOVO]
method sc
x 0.0 9i 100.0
y 0.0 9i 100.0
z 0.0 9i 100.0

[DENOVO][BOUNDARY=reflect]
reflect 1 0 1 0 1 0

[DENOVO][SOLVER=fixed]
tolerance 1e-03
[.][WITHIN_GROUP]
verbosity none

[DENOVO][QUADRATURE]
quadrature   glproduct
construction product
num_azi      2
num_polar    2

[RUN=mpi]
np 4
```

```
!omnibus-run denovo-kobayashi.omn
```

```
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at denovo-kobayashi.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating Geometria XML input file from .gg.omn...
INFO: Starting Geometria preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/build/Exnihilo-examples/Exnihilo/packages/
↪Omnibus/driver/example/denovo-kobayashi/kobp1.gg.omn
            ...finished loading problem db from Omnibus ASCII file
INFO: Renaming existing file kobp1.gg.xml to kobp1.gg-20200311-2236.xml
INFO: Writing Geometria input ParameterList to kobp1.gg.xml
            ...finished generating Geometria XML input file from .gg.omn
INFO: Set default for 'mode' to 'n' in '/physics/mg'
INFO: Set default for 'disable_upscattering' to 'False' in '/physics/mg'
INFO: Set default for 'load_scl' to 'False' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
WARNING: The 'method' keyword is now 'equations' for SN discretization types. Changing␣
↪`method sc` to `equations sc`
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'uncflux' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/upscatter'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/
↪upscatter'
INFO: Set default for 'max_iterations' to '1000' in '/denovo/solver/upscatter'
INFO: Set default for 'verbosity' to 'low' in '/denovo/solver/upscatter'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 1000 cells
INFO: Writing Omnibus input ParameterList to denovo-kobayashi.inp.xml
INFO: Writing preprocessed file to denovo-kobayashi.pp.json
```

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```
INFO: Writing processed ASCII input to 'denovo-kobayashi.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: No composition data is present in the GG model at '/rnsdhpc/code/build/Exnihilo-
↪examples/Exnihilo/packages/Omnibus/driver/example/denovo-kobayashi/kobp1.gg.xml'
INFO: Creating default boundary mesh from (0 0 0) to (100 100 100) for GG geometry
Building physics 'mg'
Building sources
Building Denovo solver internals
Ray tracing Denovo mesh
Mixing Denovo cross sections
Building Denovo sources
Constructing forward sources for Denovo
Initializing Denovo solver
INFO: Constructing Denovo state vector with 1 groups, 1000 cells, 1 moments, 1 unknowns␣
↪per cell
Running Denovo transport calculation
INFO: Writing Silo file to 4 concurrent files using material volume fractions
Writing Denovo HDF5 output
Run complete
Cleaning up
Forward group   0 finished in    6 Belos Block GMRES iterations in 1 s...
            ...finished running Omnibus in 1.2 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-kobayashi.out.h5', problem name 'Kobayashi␣
↪Problem 1-ii', created on 2020MAR11 22:36 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-kobayashi.out.h5', problem name 'Kobayashi␣
↪Problem 1-ii', created on 2020MAR11 22:36 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to denovo-kobayashi.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to denovo-kobayashi.rst
            ...finished building RST summary
```

The run generates several files, including an HDF5 file with the denovo solution data and a ReStructured Text file that summarizes the problem run.

```
assert os.path.exists("denovo-kobayashi.out.h5")
```

A.2.3.4 Check the source term

Verifying the computational input is an important step in analysis. Plotting the source region (again only in group zero) reveals that it has a single nonzero source mesh cell.

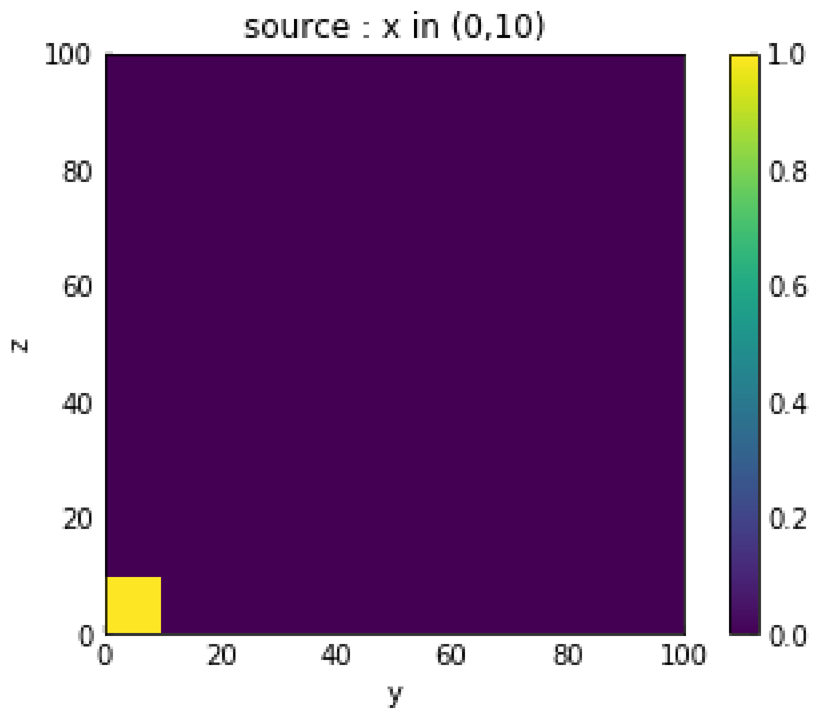
Since this is a one-group problem, it is easier to extract group zero at the beginning. Clearing the `hyperslice` field reduces clutter by discarding the metadata that this `source` object is group zero.

```
from omnibus.formats.output import load

dnv = load("denovo-kobayashi.out.h5")['denovo'].extract()

source = dnv.source.xs(g=0)
source.hyperslice = []
source
```

```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-kobayashi.out.h5', problem name 'Kobayashi␣
↪Problem 1-ii', created on 2020MAR11 22:36 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```

```
from omnibus.data import plot

print(np.count_nonzero(source))
plot(source.xs(x=5.0));
```

```
1
```

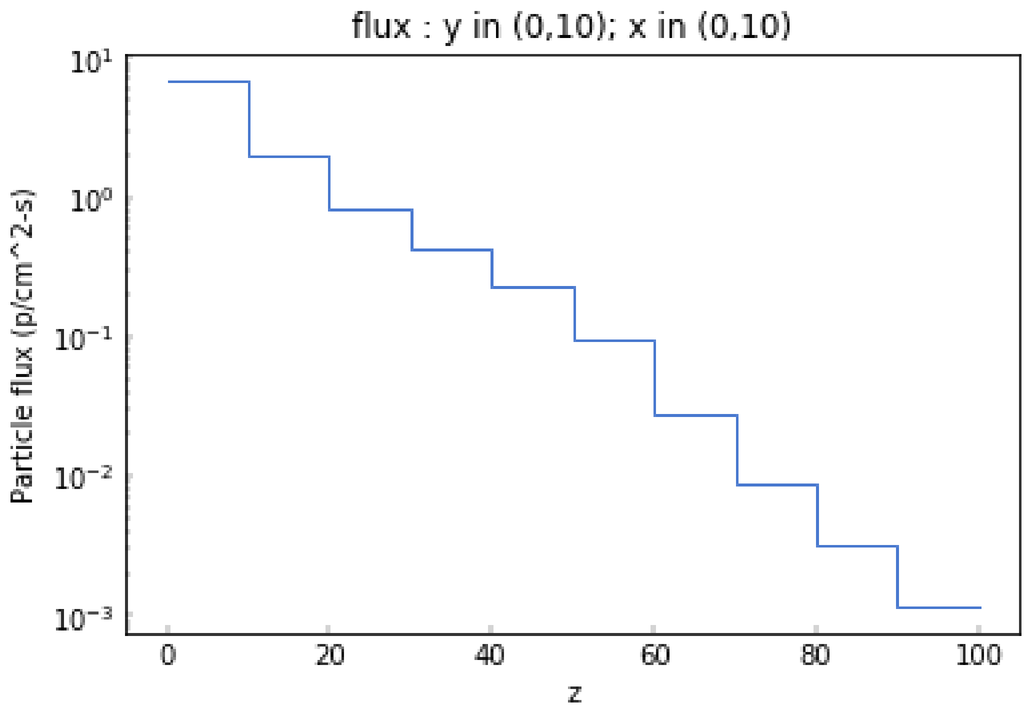


A.2.3.5 Visualize the flux

```
flux = dnv.flux.xs(g=0)
flux.hyperslice = []
flux
```

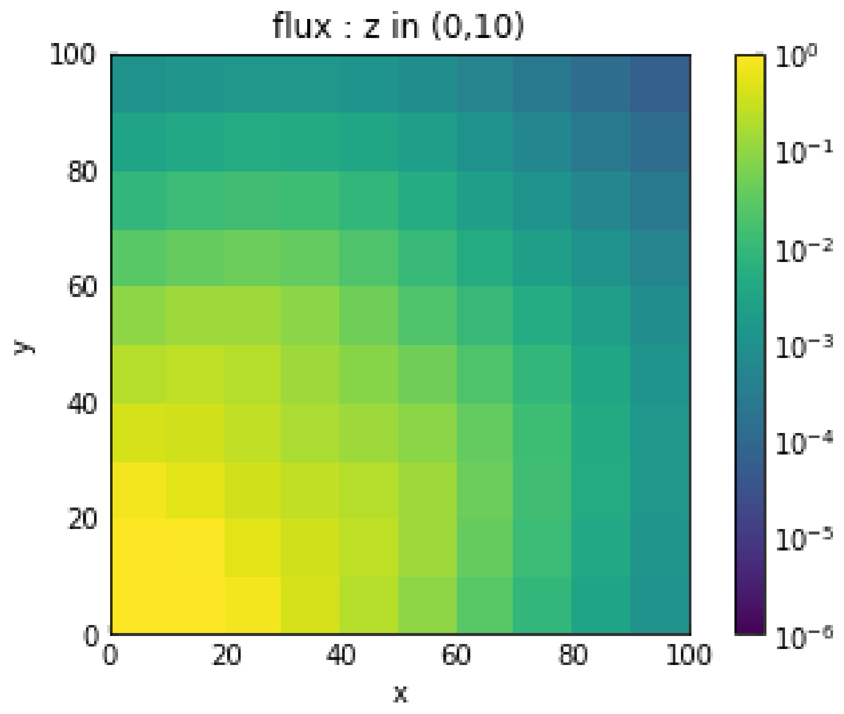
This code `plots` a lineout along the z axis in the cell where $x = y = 5$:

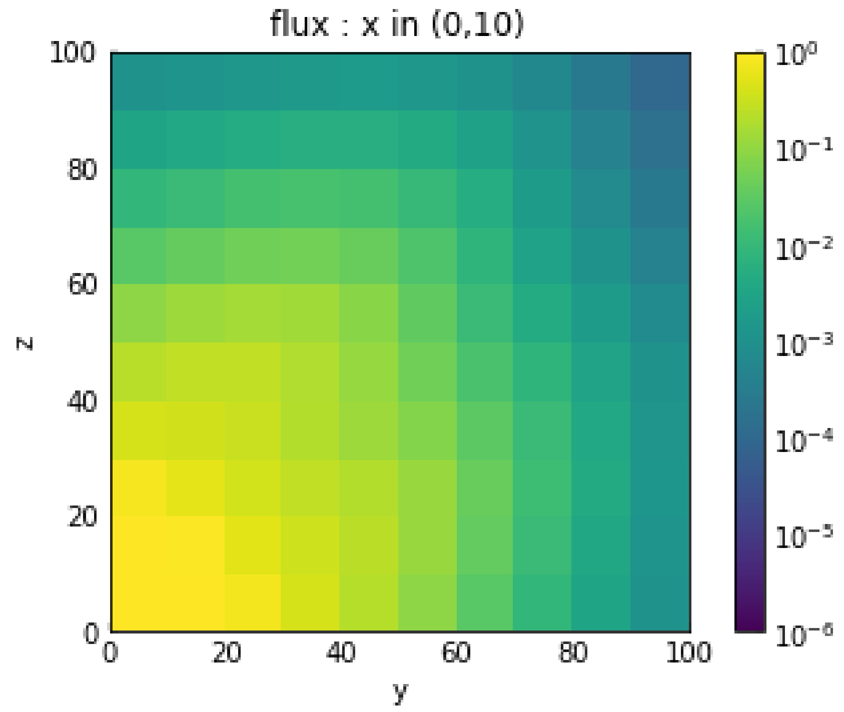
```
plots = plot(flux.xs(x=5, y=5), logy=True)
ax = plots['ax']
ax.set_title(ax.get_ylabel())
ax.set_ylabel("Particle flux (p/cm^2-s)");
```



A pseudocolor plot can visualize the flux. The options on the matplotlib `LogNorm` class constrain the range of the color scale.

```
from matplotlib.colors import LogNorm

norm = LogNorm(vmin=1e-6, vmax=1)
plot(flux.xs(z=5.0), norm=norm);
plot(flux.xs(x=5.0), norm=norm);
```





Compare against reference solutions

The reference data in the Kobayashi paper are point samples formatted as (x, y, z, ϕ). They comprise three lineouts: one along y, one along $x = y = z$, and one along x.

```
from six.moves import StringIO
import numpy as np

# X, Y, Z, reference
ref_y = """
5   5       5       8.29260E+00
5   15      5       1.87028E+00
5   25      5       7.13986E-01
5   35      5       3.84685E-01
5   45      5       2.53984E-01
5   55      5       1.37220E-01
5   65      5       4.65913E-02
5   75      5       1.58766E-02
5   85      5       5.47036E-03
5   95      5       1.85082E-03
"""
ref_xyz = """
5   5       5       8.29260E+00
15  15      15      6.63233E-01
25  25      25      2.68828E-01
35  35      35      1.56683E-01
45  45      45      1.04405E-01
55  55      55      3.02145E-02
65  65      65      4.06555E-03
75  75      75      5.86124E-04
85  85      85      8.66059E-05
95  95      95      1.12892E-05
"""
ref_x = """
5   55      5       1.37220E-01
15  55      5       1.27890E-01
25  55      5       1.13582E-01
35  55      5       9.59578E-02
45  55      5       7.82701E-02
55  55      5       5.67030E-02
65  55      5       1.88631E-02
75  55      5       6.46624E-03
85  55      5       2.28099E-03
95  55      5       7.93924E-04
"""
ref_y = np.loadtxt(StringIO(ref_y))
ref_xyz = np.loadtxt(StringIO(ref_xyz))
ref_x = np.loadtxt(StringIO(ref_x))
```

Since these are all physical points, it is easy to use the meshes to look up the points where the reference data is using the `xs` method.

```
import matplotlib.pyplot as plt

# Get a line-out of the actual flux
x_phi = flux.xs(y=55, z=5)
# Extract calculated points along the coordinate mesh
```

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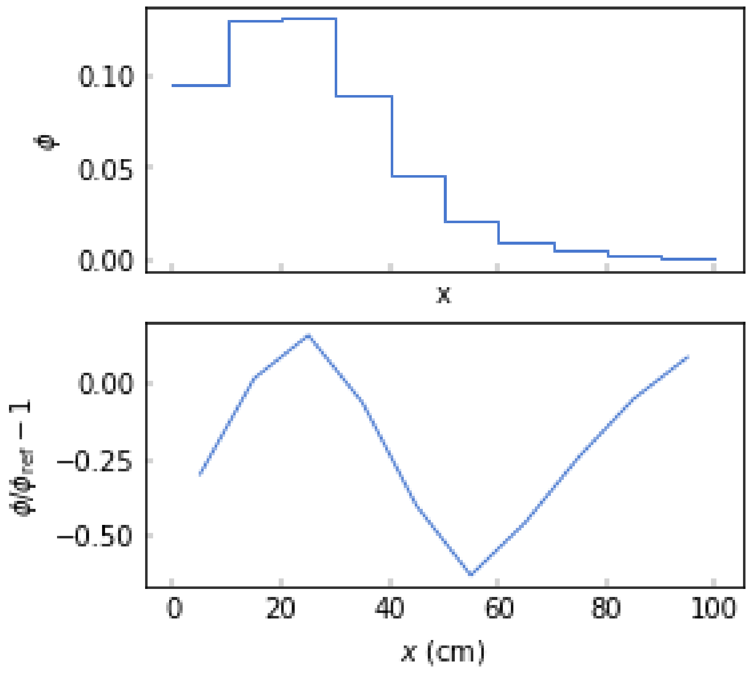
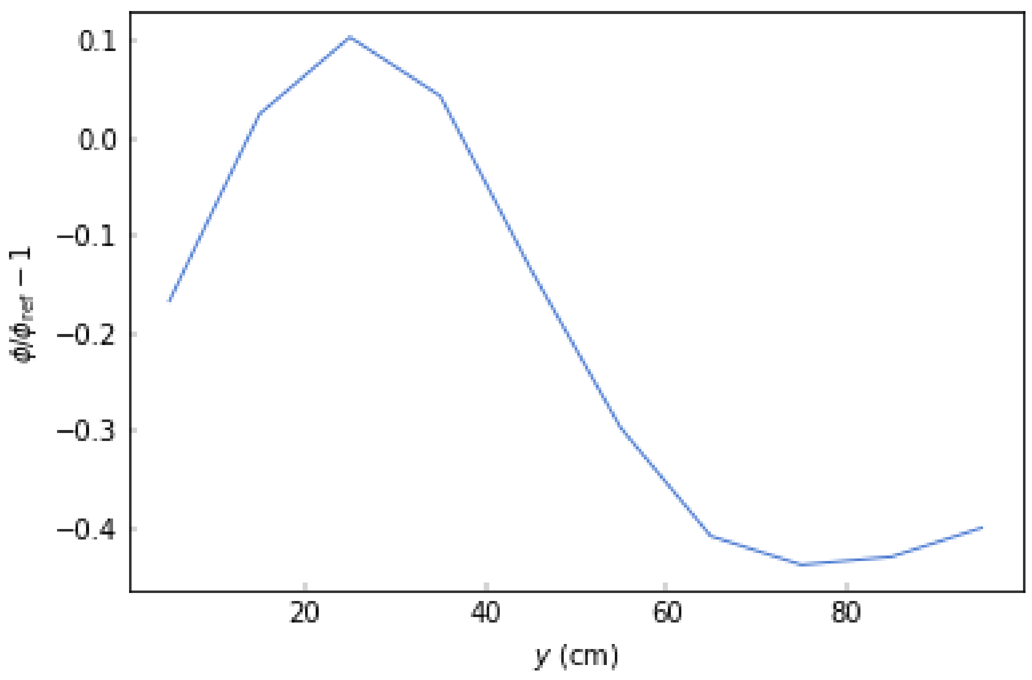
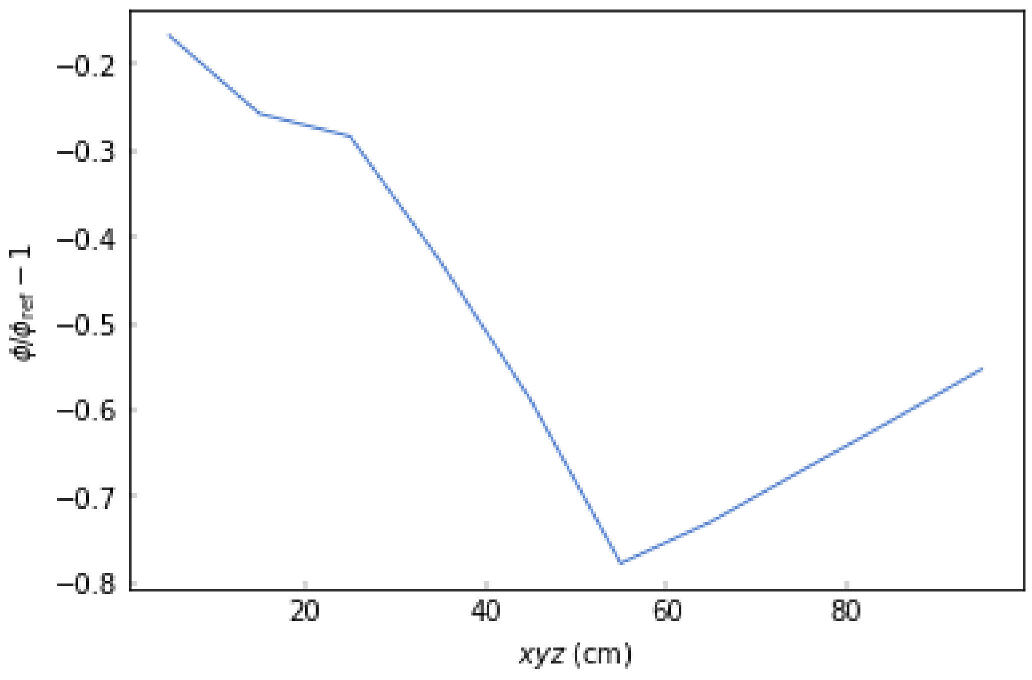
```
x_mesh = ref_x[:,0]
act = np.array([x_phi.xs(x=x).data for x in x_mesh])
# Get the reference values
ref = ref_x[:,3]

(fig, (flux_ax, ratio_ax)) = plt.subplots(2, 1, figsize=(4, 4), sharex=True)
# Plot the actual lineout
plot(x_phi, ax=flux_ax)
# Plot the ratios
ratio_ax.plot(x_mesh, act/ref - 1)

flux_ax.set_ylabel(r'$\phi$')
ratio_ax.set_xlabel("$x$ (cm)")
ratio_ax.set_ylabel(r"$\phi / \phi_{\mathrm{ref}} - 1$");
```



```
axis = ref_y[:,1]
y_phi = flux.xs(x=5, z=5)
act = np.array([y_phi.xs(y=y).data for y in axis])
ref = ref_y[:,3]

(fig, ax) = plt.subplots()
ax.plot(axis, act/ref - 1)
ax.set_xlabel("$y$ (cm)")
ax.set_ylabel("$\phi / \phi_{\mathrm{ref}} - 1$");
```



```
axis = ref_xyz[:,0]
act = np.array([flux.xs(x=v, y=v, z=v).data for v in axis])
ref = ref_xyz[:,3]

(fig, ax) = plt.subplots()
ax.plot(axis, act/ref - 1)
ax.set_xlabel("$xyz$ (cm)")
ax.set_ylabel("$\phi / \phi_{\mathrm{ref}} - 1$");
```



A.2.4 UEKI BENCHMARK PROBLEM

This example uses Denovo to determine a dose rate to the detector, and it demonstrates using the adjoint solution capability to obtain an importance function. Since this problem also contains a point source, it shows how an "uncollided flux" treatment can reduce ray effects. Two approximation methods for the uncollided flux source (uncf) will be explored: the "analytic" approximation, where the source is physically raytraced to every computational cell in the geometry; and a Monte Carlo approximation, where numerous samples from a stochastic point source generate the deterministic source term.

```
# Set up example environment
import os
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
%matplotlib inline
from exnihilotools.matplotlib import screen_style
screen_style()
```

A.2.4.1 Pre-visualize the geometry

The [PLOT][PRE] block in the input file generates a 2D image of the problem geometry for visualizing before actually executing the problem.

The Ueki problem consists of a neutron source is placed at the center of a block of paraffin with a 45 degree cone-shaped opening at the front. This opening points toward a graphite shield of varying thickness, with an ideal detector on the far side.

```
!grep -A 5 "\[PRE\]" {SOURCE_DIR}/data/denovo-ueki-adj.omn
!omnibus-pre {SOURCE_DIR}/data/denovo-ueki-adj.omn
```

```
[PRE]
[PRE][PLOT lateral]
origin -25 0 -40
size 127.5 80
axis y
render true
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-ueki-adj.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
MCNP:  xact   is done            ...finished generating MCNP runtpe file
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
WARNING: The 'method' keyword is now 'equations' for SN discretization types. Changing␣
↪`method sc` to `equations sc`
```

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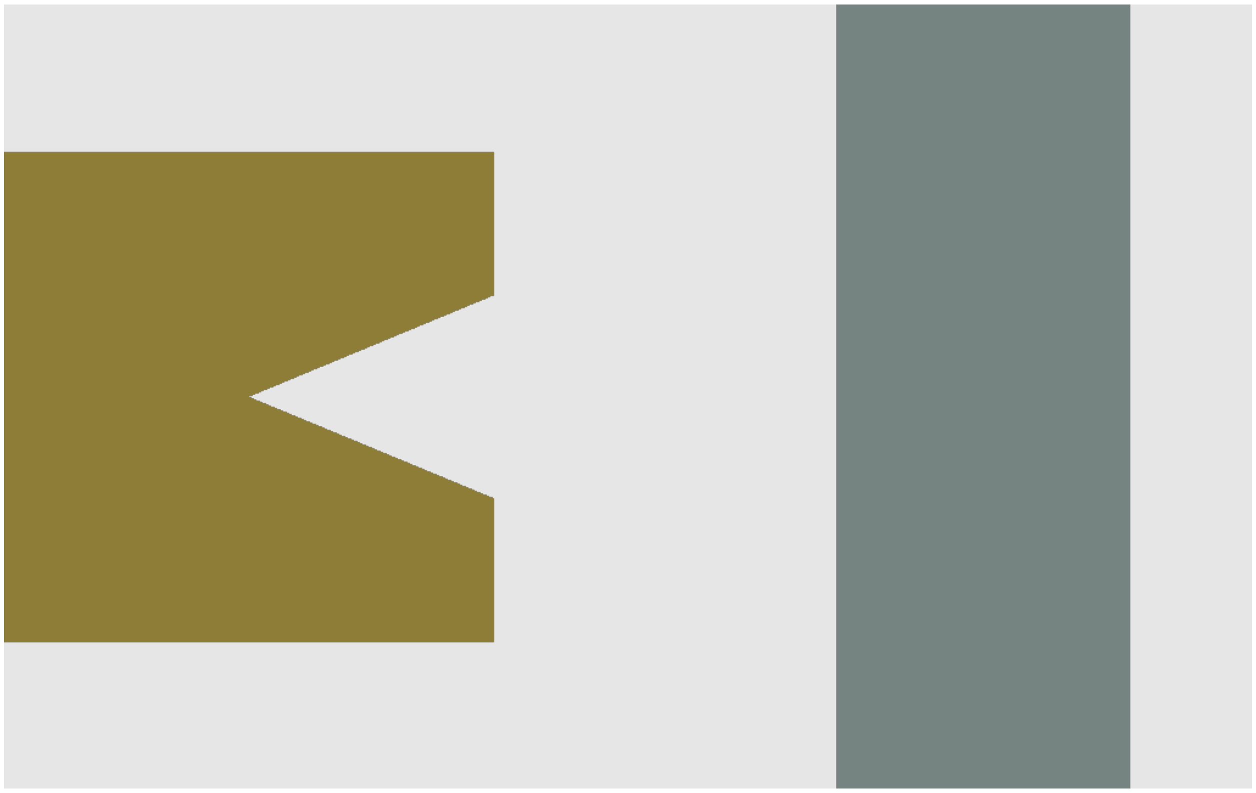
```
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'quadrature' to 'qr' in '/denovo/quadrature'
INFO: Set default for 'construction' to 'product' in '/denovo/quadrature'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'uncflux' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 4950 cells
INFO: Writing Omnibus input ParameterList to denovo-ueki-adj.inp.xml
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
Generating geometry image...
INFO: Saved geometry image at y=0 to 'lateral_y0.png'
            ...finished generating geometry image
INFO: Writing preprocessed file to denovo-ueki-adj.pp.json
```

```python
from IPython.display import display, Image
display(Image(filename="lateral_y0.png"))
```



A.2.4.2 Analytic uncollided flux results

The uncollided flux from a point source is the solution to a purely absorbing transport equation in each group:

$$\Omega \cdot \nabla \hat{\psi}_g + \sigma_g \hat{\psi}_g = \frac{q_g}{4\pi} \delta(r - r_0).$$

This equation has a simple Green's function solution:

$$\hat{\psi}_g = \delta(\Omega - \Omega_{0\rightarrow r}) \frac{q_g}{4\pi |r - r_0|^2} \mathrm{e}^{-\tau(r_0, r)}.$$

Denovo calculates the total optical thickness τ between the point source and every point on the grid cell, and using the source spectrum, constructs an analytic solution to the first-collision source. The `uncf analytic` option in the `[DENOVO][SOURCE]` block enables this feature.

```
%cat {SOURCE_DIR}/data/denovo-ueki-fwd-uncf-analytic.omn
```

```
[PROBLEM]
name "Ueki 30cm benchmark (analytic forward source)"
mode forward

[MODEL=mcnp]
input "../data/ueki.mcnp"

[SOURCE=separable cf252]
strength 4.05e7 ! neutrons/sec

```

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```
[SOURCE][SHAPE=point]
point 0.001 0 0

[SOURCE][ENERGY=watt]
a 1.025
b 2.926

[SOURCE][ANGLE=isotropic]

[PHYSICS=mg]
mg_lib "v7-28n19g"
pn_order 1
disable_upscattering true

[DENOVO]
method sc
x -25 5i 0 5i 60 5i 90 3i 112.5
y -40 2i -25 2i -2.5 2i 2.5 2i 25 2i 40
z -40 2i -25 2i -2.5 2i 2.5 2i 25 2i 40

[DENOVO][SOLVER=fixed]
[.][WITHIN_GROUP]
verbosity none

[DENOVO][SOURCE]
uncf analytic

[DENOVO][QUADRATURE]
num_azi 2
num_polar 2

[RUN=mpi]
np 4
```

```
!omnibus-run {SOURCE_DIR}/data/denovo-ueki-fwd-uncf-analytic.omn
```

```
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-ueki-fwd-uncf-analytic.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
INFO: Set default for 'fissionable_only' to 'False' in '/source/cf252'
INFO: Set default for 'mode' to 'n' in '/physics/mg'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
```

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```
WARNING: The 'method' keyword is now 'equations' for SN discretization types. Changing␣
↪`method sc` to `equations sc`
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'quadrature' to 'qr' in '/denovo/quadrature'
INFO: Set default for 'construction' to 'product' in '/denovo/quadrature'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'uncflux' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 4950 cells
INFO: Writing Omnibus input ParameterList to denovo-ueki-fwd-uncf-analytic.inp.xml
INFO: Writing preprocessed file to denovo-ueki-fwd-uncf-analytic.pp.json
INFO: Writing processed ASCII input to 'denovo-ueki-fwd-uncf-analytic.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
INFO: Loading compositions from MCNP input
INFO: Splitting compound 6000 into at% {6012: 0.9893, 6013: 0.0107}
INFO: Splitting compound 3006000 into at% {3006012: 0.9893, 3006013: 0.0107}
WARNING: Extents of MCNP geometry are extremely large or unknown; this may adversely␣
↪affect 'global' tallies, entropy mesh, etc.
Building physics 'mg'
INFO: Loading AMPX library at '/usr/local/scale/data/scale.rev12.xn28g19v7.1'
INFO: Retained 3 of 455 nuclides on the master AMPX library
INFO: Running XSProc on 2 cells
WARNING: Upscattering has been lumped into within-group scattering in the thermal groups
WARNING: Remapped 4 nuclide IDs: 6012->6000, 6013->6000, 3006012->3006000, 3006013->
↪3006000
INFO: Truncating cross sections to groups [0, 28)
Building sources
Building Denovo solver internals
Ray tracing Denovo mesh
WARNING: Number of Z blocks (2) is not divisible into the number of z cells 15; reducing␣
↪to 1
```

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```
Mixing Denovo cross sections
Building Denovo sources
Constructing forward sources for Denovo
Initializing Denovo solver
INFO: Constructing Denovo state vector with 28 groups, 4950 cells, 4 moments, 1 unknowns␣
↪per cell
Performing analytic first-collision source calculation on 1 sources
Running Denovo transport calculation
Forward group   0 finished in    4 Belos Block GMRES iterations.
Forward group   1 finished in    4 Belos Block GMRES iterations.
Forward group   2 finished in    4 Belos Block GMRES iterations.
Forward group   3 finished in    3 Belos Block GMRES iterations.
Forward group   4 finished in    4 Belos Block GMRES iterations.
Forward group   5 finished in    5 Belos Block GMRES iterations.
Forward group   6 finished in    5 Belos Block GMRES iterations.
Forward group   7 finished in    6 Belos Block GMRES iterations.
Forward group   8 finished in    6 Belos Block GMRES iterations.
Forward group   9 finished in    6 Belos Block GMRES iterations.
Forward group  10 finished in    6 Belos Block GMRES iterations.
Forward group  11 finished in    5 Belos Block GMRES iterations.
Forward group  12 finished in    4 Belos Block GMRES iterations.
Forward group  13 finished in    4 Belos Block GMRES iterations.
Forward group  14 finished in    4 Belos Block GMRES iterations.
Forward group  15 finished in    4 Belos Block GMRES iterations.
Forward group  16 finished in    3 Belos Block GMRES iterations.
Forward group  17 finished in    3 Belos Block GMRES iterations.
Forward group  18 finished in    3 Belos Block GMRES iterations.
Forward group  19 finished in    3 Belos Block GMRES iterations.
Forward group  20 finished in    4 Belos Block GMRES iterations.
Forward group  21 finished in    4 Belos Block GMRES iterations.
Forward group  22 finished in    4 Belos Block GMRES iterations.
Forward group  23 finished in    6 Belos Block GMRES iterations.
Forward group  24 finished in    8 Belos Block GMRES iterations.
Forward group  25 finished in    9 Belos Block GMRES iterations.
Forward group  26 finished in   13 Belos Block GMRES iterations.
INFO: Writing Silo file to 4 concurrent files using material volume fractions
Writing Denovo HDF5 output
Run complete
Cleaning up
Forward group  27 finished in   39 Belos Block GMRES iterations.
            ...finished running Omnibus in 3.3 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-fwd-uncf-analytic.out.h5', problem␣
↪name 'Ueki 30cm benchmark (analytic forward source)', created on 2020MAR11 22:36 using␣
↪SCALE version 6.3.pre-b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-fwd-uncf-analytic.out.h5', problem␣
↪name 'Ueki 30cm benchmark (analytic forward source)', created on 2020MAR11 22:36 using␣
↪SCALE version 6.3.pre-b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```

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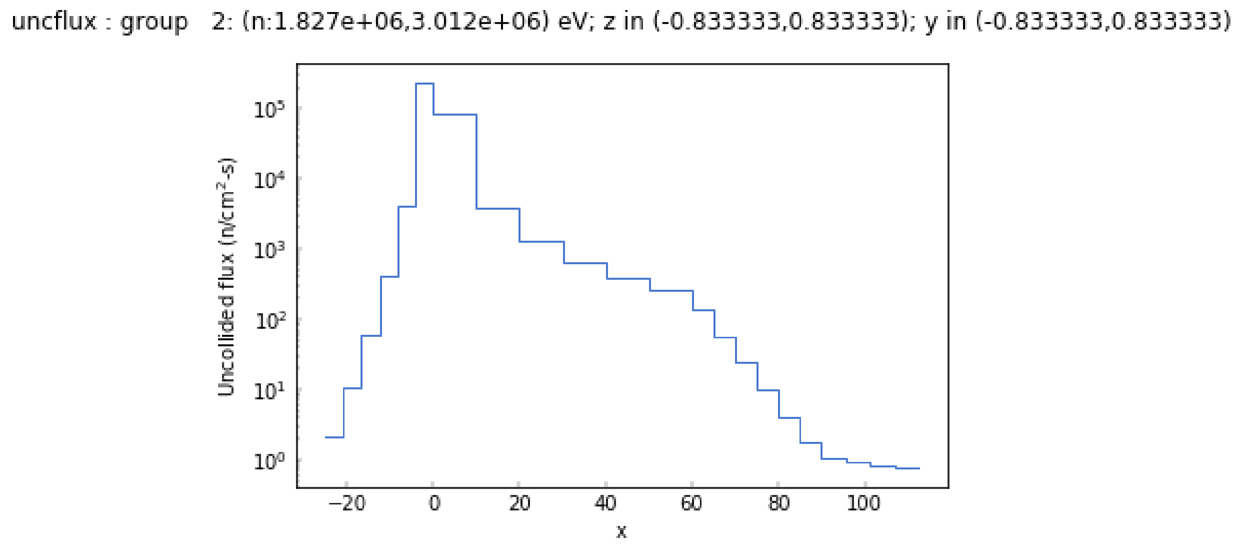
```
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to denovo-ueki-fwd-uncf-analytic.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to denovo-ueki-fwd-uncf-analytic.rst
            ...finished building RST summary
```

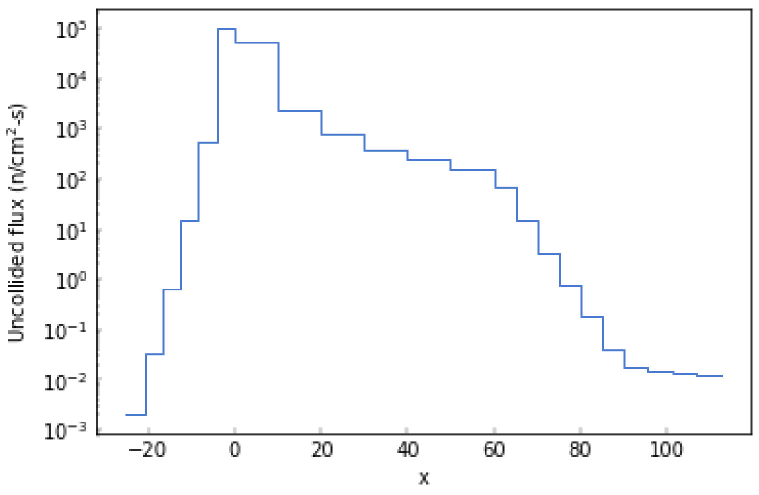
The first-collision method works by splitting the transport equation into uncollided and collided flux components. The uncollided flux is solved using an analytic approximation. Visualizing the uncollided flux term helps in verifying the problem setup.

```
from omnibus.data import plot
from omnibus.formats.output import load

dnv = load("denovo-ueki-fwd-uncf-analytic.out.h5")['denovo'].extract()
uncflux = dnv['uncflux']
for g in (2, 5):
    plots = plot(uncflux.xs(y=0.0, z=0.0, g=g), logy=True)
    ax = plots['ax']
    ax.set_title(ax.get_ylabel())
    ax.set_ylabel("Uncollided flux (n/cm$^2$-s)")
    ax.title.set_position([.5, 1.05]);
```

```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-fwd-uncf-analytic.out.h5', problem␣
↪name 'Ueki 30cm benchmark (analytic forward source)', created on 2020MAR11 22:36 using␣
↪SCALE version 6.3.pre-b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```



uncflux : group 5: (n:4.076e+05,9.072e+05) eV; z in (-0.833333,0.833333); y in (-0.833333,0.833333)

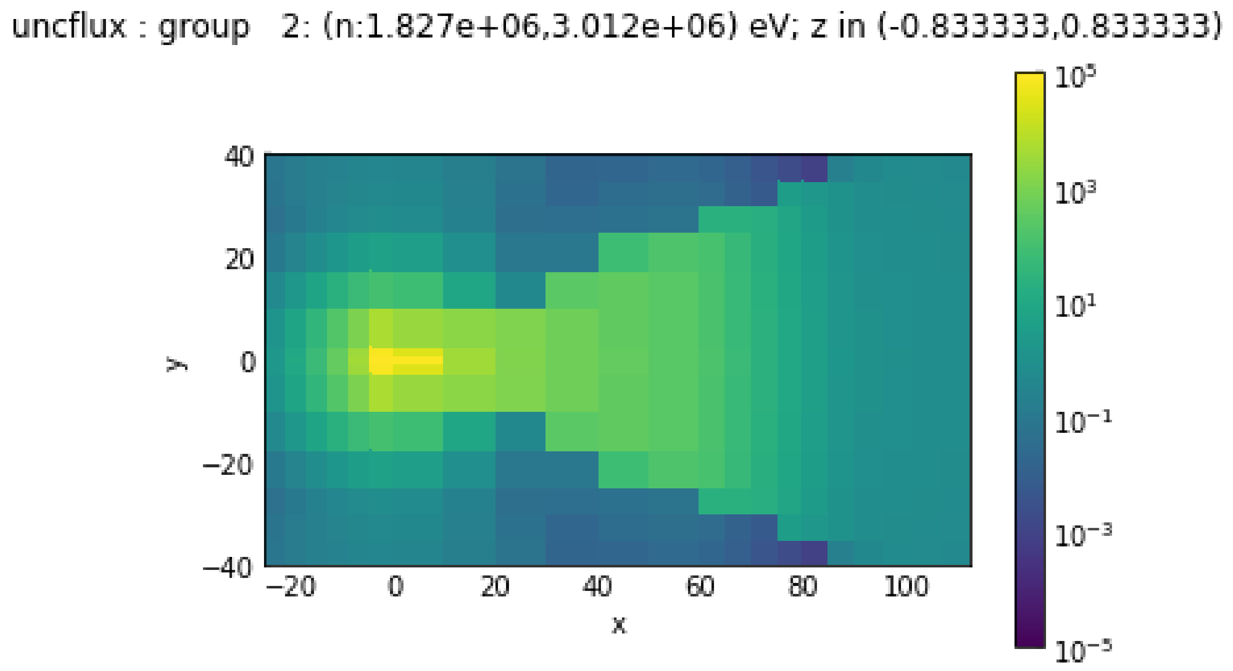


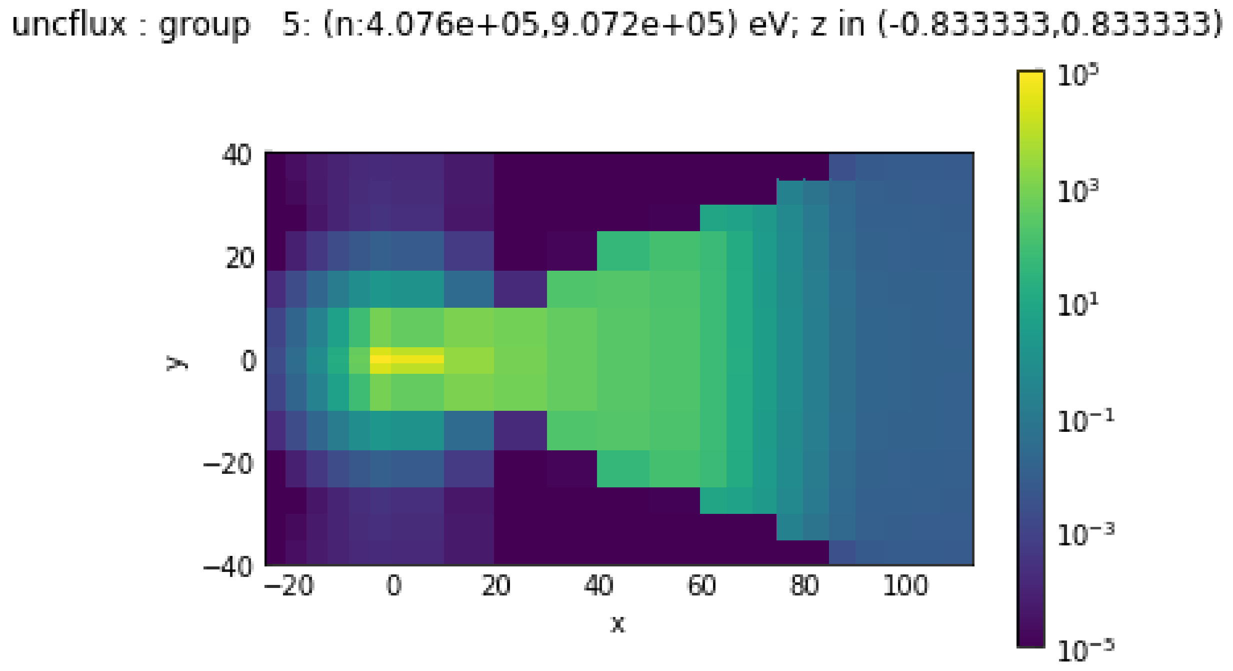
```
uncf_slice = uncflux.xs(g=2,z=0.0)
print("Flux spans {:.2e} to {:.2e}".format(
        uncf_slice.data.min(),
        uncf_slice.data.max()))
```

```
Flux spans 8.63e-04 to 2.39e+05
```

Pseudocolor plots show the attenuation of the source term through the material and through space. Since the material cross sections depend on energy group, the shape of the uncollided flux terms is different in groups 2 and 5.

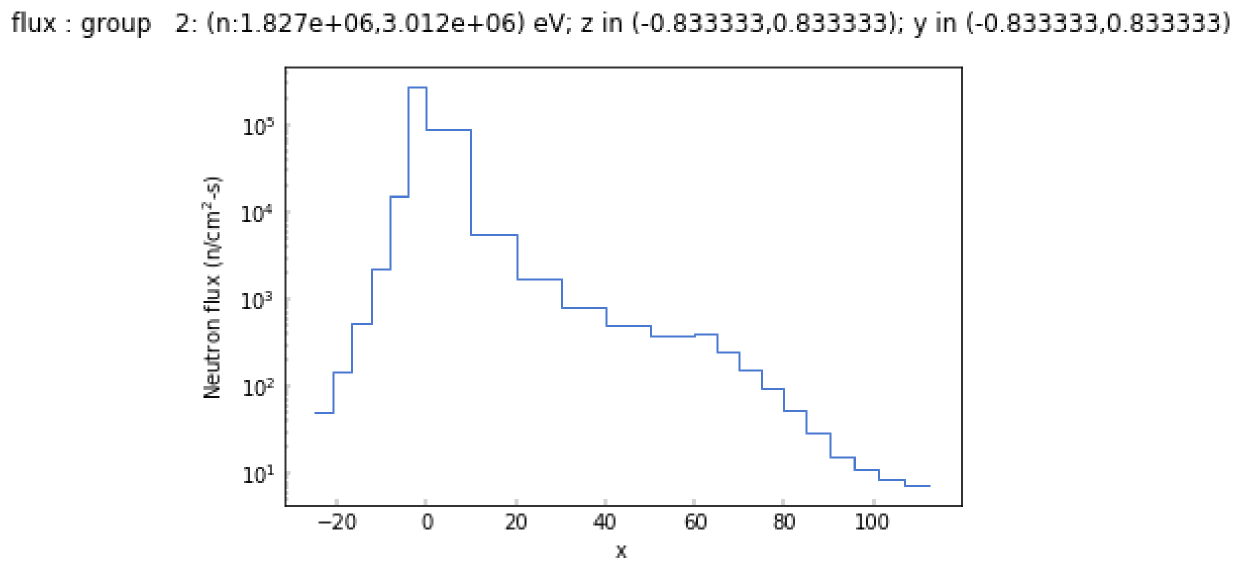
```
from matplotlib.colors import LogNorm

norm = LogNorm(vmin=1.0e-5, vmax=1e5)
for g in (2, 5):
    plots = plot(uncflux.xs(g=g,z=0.0), norm=norm)
    plots['ax'].title.set_position([.5, 1.25]);
```





The flux along the x axis in energy group 2 follows the uncollided flux contribution but also includes inscattering in the material from the higher-energy groups.

```
plots = plot(dnv['flux'].xs(g=2, y=0, z=0), logy=True)
ax = plots['ax']
ax.set_title(ax.get_ylabel())
ax.set_ylabel("Neutron flux (n/cm$^2$-s)")
ax.title.set_position([.5, 1.05]);
```



A.2.4.3 Calculate dose rates

The SCALE master library contains American National Standards Institute (ANSI) standard (1977) neutron flux-to-dose conversion factors (rem/hr)/(n/cm^2-s) (MT 9029). The PALEALE code module can be used to print out these conversion factors from the SCALE AMPX library.

```
import numpy as np
# neutron flux-to-dose conversion factors from ansl/ans 6.1.1 - 1977 02/09/11 (rem/hr)/
↪(n/cm^2-s)
flux_to_dose_factor = np.array([
    1.61496E-04, 1.44530E-04, 1.27035E-04, 1.28101E-04, 1.29832E-04, 1.00375E-04,
    4.53982E-05, 1.19215E-05, 3.72975E-06, 3.71969E-06, 4.00846E-06, 4.29442E-06,
    4.47304E-06, 4.55834E-06, 4.57702E-06, 4.55983E-06, 4.52102E-06, 4.48745E-06,
    4.46602E-06, 4.43429E-06, 4.33168E-06, 4.20288E-06, 4.09745E-06, 3.84414E-06,
    3.66980E-06, 3.67484E-06, 3.67484E-06, 3.67484E-06
])

print("The Denovo output has", len(dnv['flux'].axis('g')), "neutron energy bounds:")
print(dnv['flux'].axis('g').bounds.n.tolist())
```

```
The Denovo output has 28 neutron energy bounds:
[20000000.0, 6376300.0, 3011900.0, 1826800.0, 1422700.0, 907180.0, 407620.0, 111090.0,␣
↪15034.0, 3035.39990234375, 582.9500122070312, 101.30000305175781, 29.023000717163086,␣
↪10.677000045776367, 5.0, 3.059000015258789, 1.8553999662399292, 1.2999999523162842, 1.
↪1253000497817993, 1.0, 0.800000011920929, 0.41398999094963074, 0.32499998807907104, 0.
↪22499999403953552, 0.10000000149011612, 0.05000000074505806, 0.029999999329447746, 0.
↪009999999776482582, 9.999999747378752e-06]
```

```
from omnibus.data import Field

def weighted_energy_integrate(flux, weights, **kwargs):
    assert len(flux.axis('g')) == len(weights)
    assert flux.dims[0] == 'g'
```

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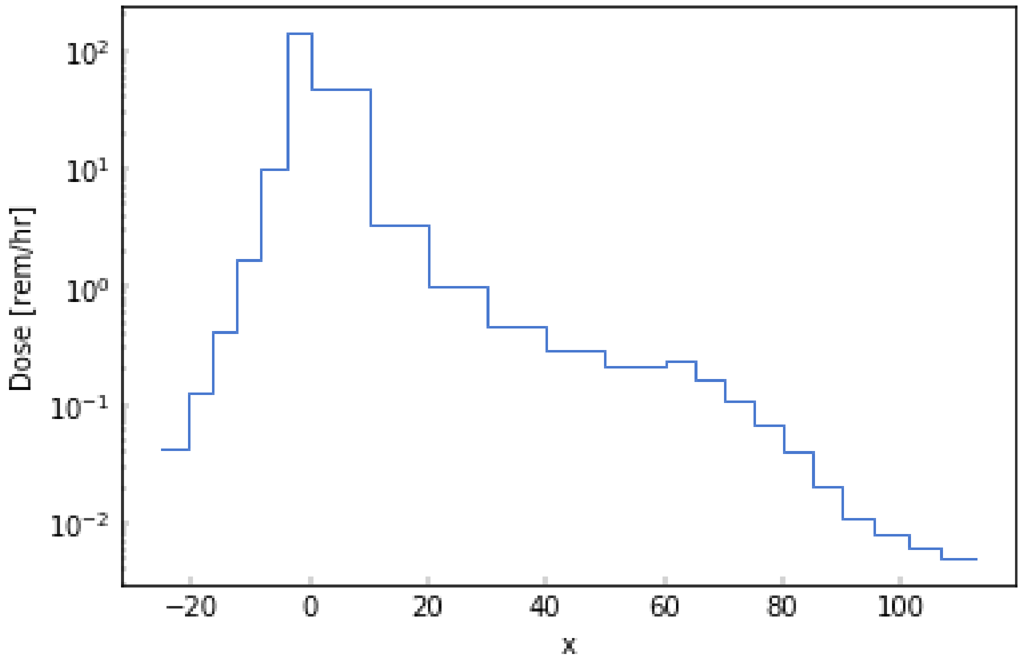
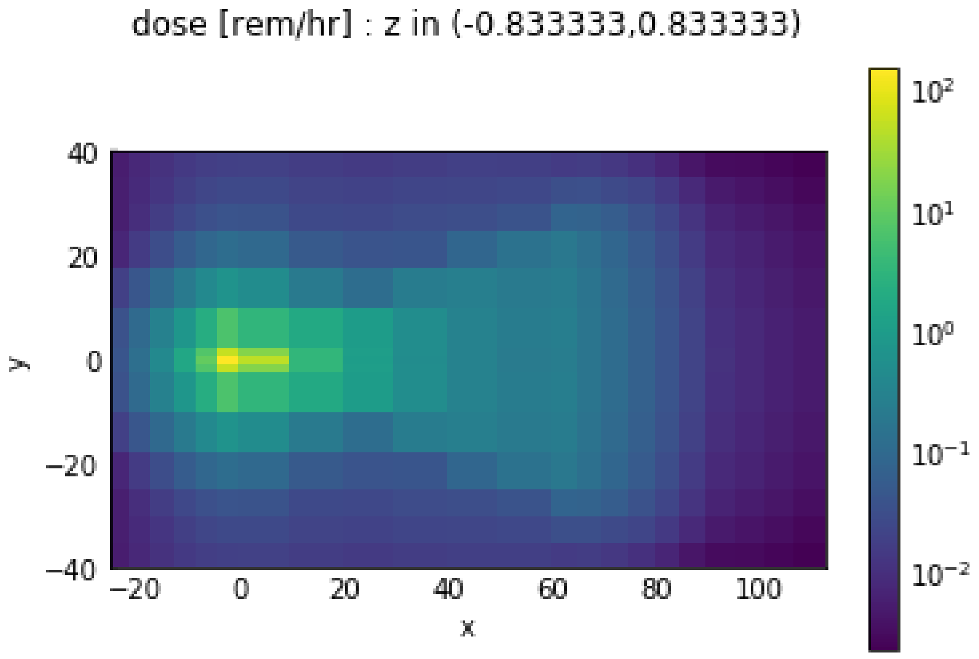
```
    axes = flux.axes[1:]
    result_data = np.zeros([len(ax) for ax in axes])
    result = Field(axes=axes, data=result_data, **kwargs)

    # Perform weighted integral
    flux_data = flux.data
    for g in range(len(flux.axis('g'))):
        result_data += weights[g] * flux_data[g]

    return result

dose = weighted_energy_integrate(dnv['flux'], flux_to_dose_factor, name='dose', units=
↪'rem/hr')
```

The 3D field of doses can be visualized by extracting lineouts or by coloring slices.

```
plots = plot(dose.xs(y=0, z=0), logy=True)
ax = plots['ax']
ax.set_ylabel("Dose [rem/hr]")

plots = plot(dose.xs(z=0.0), norm=LogNorm())
plots['ax'].title.set_position([.5, 1.25]);
```





A.2.4.4 Monte Carlo uncollided flux results

With the Monte Carlo approach, the first collision source (uncollided flux) is obtained by direct Monte Carlo sampling. Thus the resulting uncollided flux fluctuates around the mean. As the number of Monte Carlo particles simulated increases, the uncollided flux obtained from the Monte Carlo approach should approach the analytic uncollided flux. The `uncf mc` option in the `[DENOVO][SOURCE]` block enables this feature.

```
%cat {SOURCE_DIR}/data/denovo-ueki-fwd-uncf-mc.omn
```

```
[PROBLEM]
name "Ueki 30cm benchmark (MC forward source)"
mode forward

[MODEL=mcnp]
input "../data/ueki.mcnp"

[SOURCE=separable cf252]
strength 4.05e7 ! neutrons/sec

[SOURCE][SHAPE=point]
point 0.001 0 0

[SOURCE][ENERGY=watt]
a 1.025
b 2.926

[SOURCE][ANGLE=isotropic]

[PHYSICS=mg]
mg_lib "v7-28n19g"
```

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```
pn_order 1
disable_upscattering true

[DENOVO]
method sc
x -25 5i 0 5i 60 5i 90 3i 112.5
y -40 2i -25 2i -2.5 2i 2.5 2i 25 2i 40
z -40 2i -25 2i -2.5 2i 2.5 2i 25 2i 40

[DENOVO][SOLVER=fixed]
[.][WITHIN_GROUP]
verbosity none

[DENOVO][OUTPUT]

[DENOVO][SOURCE]
uncf mc
mc_num_particles  50000

[DENOVO][QUADRATURE]
num_azi 2
num_polar 2

[RUN=mpi]
np 4
```

```
!omnibus-run {SOURCE_DIR}/data/denovo-ueki-fwd-uncf-mc.omn
```

```
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-ueki-fwd-uncf-mc.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
INFO: Set default for 'fissionable_only' to 'False' in '/source/cf252'
INFO: Set default for 'mode' to 'n' in '/physics/mg'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
WARNING: The 'method' keyword is now 'equations' for SN discretization types. Changing␣
↪`method sc` to `equations sc`
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'quadrature' to 'qr' in '/denovo/quadrature'
INFO: Set default for 'construction' to 'product' in '/denovo/quadrature'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
```

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```
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'uncflux' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 4950 cells
INFO: Writing Omnibus input ParameterList to denovo-ueki-fwd-uncf-mc.inp.xml
INFO: Writing preprocessed file to denovo-ueki-fwd-uncf-mc.pp.json
INFO: Writing processed ASCII input to 'denovo-ueki-fwd-uncf-mc.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
INFO: Renaming existing file omnibus.out to omnibus-20200311-2236.out
INFO: Renaming existing file omnibus.err to omnibus-20200311-2236.err
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
INFO: Loading compositions from MCNP input
INFO: Splitting compound 6000 into at% {6012: 0.9893, 6013: 0.0107}
INFO: Splitting compound 3006000 into at% {3006012: 0.9893, 3006013: 0.0107}
WARNING: Extents of MCNP geometry are extremely large or unknown; this may adversely␣
↪affect 'global' tallies, entropy mesh, etc.
Building physics 'mg'
INFO: Loading AMPX library at '/usr/local/scale/data/scale.rev12.xn28g19v7.1'
INFO: Retained 3 of 455 nuclides on the master AMPX library
INFO: Running XSProc on 2 cells
WARNING: Upscattering has been lumped into within-group scattering in the thermal groups
WARNING: Remapped 4 nuclide IDs: 6012->6000, 6013->6000, 3006012->3006000, 3006013->
↪3006000
INFO: Truncating cross sections to groups [0, 28)
Building sources
Building Denovo solver internals
Ray tracing Denovo mesh
WARNING: Number of Z blocks (2) is not divisible into the number of z cells 15; reducing␣
↪to 1
Mixing Denovo cross sections
Building Denovo sources
Constructing forward sources for Denovo
Initializing Denovo solver
INFO: Constructing Denovo state vector with 28 groups, 4950 cells, 4 moments, 1 unknowns␣
↪per cell
```

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```
Performing Monte Carlo first-collision source calculation
Running Denovo transport calculation
Forward group   0 finished in   3 Belos Block GMRES iterations.
Forward group   1 finished in   4 Belos Block GMRES iterations.
Forward group   2 finished in   4 Belos Block GMRES iterations.
Forward group   3 finished in   3 Belos Block GMRES iterations.
Forward group   4 finished in   4 Belos Block GMRES iterations.
Forward group   5 finished in   4 Belos Block GMRES iterations.
Forward group   6 finished in   5 Belos Block GMRES iterations.
Forward group   7 finished in   6 Belos Block GMRES iterations.
Forward group   8 finished in   6 Belos Block GMRES iterations.
Forward group   9 finished in   6 Belos Block GMRES iterations.
Forward group  10 finished in   5 Belos Block GMRES iterations.
Forward group  11 finished in   5 Belos Block GMRES iterations.
Forward group  12 finished in   4 Belos Block GMRES iterations.
Forward group  13 finished in   4 Belos Block GMRES iterations.
Forward group  14 finished in   4 Belos Block GMRES iterations.
Forward group  15 finished in   4 Belos Block GMRES iterations.
Forward group  16 finished in   3 Belos Block GMRES iterations.
Forward group  17 finished in   3 Belos Block GMRES iterations.
Forward group  18 finished in   3 Belos Block GMRES iterations.
Forward group  19 finished in   3 Belos Block GMRES iterations.
Forward group  20 finished in   4 Belos Block GMRES iterations.
Forward group  21 finished in   4 Belos Block GMRES iterations.
Forward group  22 finished in   4 Belos Block GMRES iterations.
Forward group  23 finished in   6 Belos Block GMRES iterations.
Forward group  24 finished in   7 Belos Block GMRES iterations.
Forward group  25 finished in   8 Belos Block GMRES iterations.
Forward group  26 finished in  13 Belos Block GMRES iterations.
INFO: Writing Silo file to 4 concurrent files using material volume fractions
INFO: Removing SILO directory denovo_output_silo
Writing Denovo HDF5 output
Forward group  27 finished in  39 Belos Block GMRES iterations.
Run complete
Cleaning up
            ...finished running Omnibus in 3.7 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-fwd-uncf-mc.out.h5', problem name
↪'Ueki 30cm benchmark (MC forward source)', created on 2020MAR11 22:36 using SCALE␣
↪version 6.3.pre-b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-fwd-uncf-mc.out.h5', problem name
↪'Ueki 30cm benchmark (MC forward source)', created on 2020MAR11 22:36 using SCALE␣
↪version 6.3.pre-b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to denovo-ueki-fwd-uncf-mc.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to denovo-ueki-fwd-uncf-mc.rst
```

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```
             ...finished building RST summary
```

```
dnv_mc = load("denovo-ueki-fwd-uncf-mc.out.h5")['denovo'].extract()
```

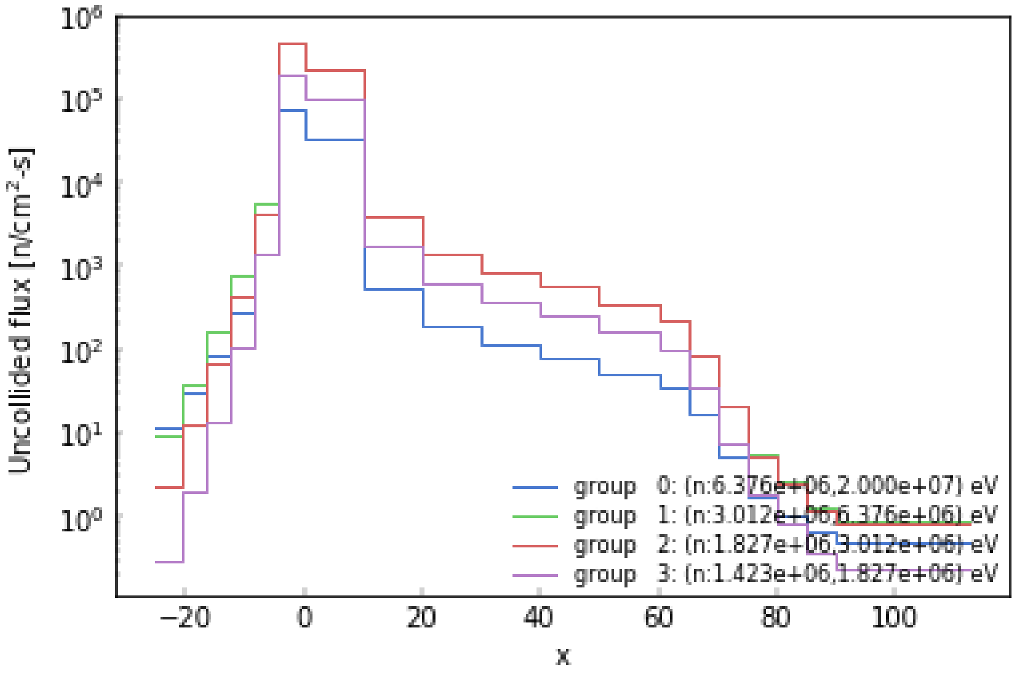
```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-fwd-uncf-mc.out.h5', problem name
↪'Ueki 30cm benchmark (MC forward source)', created on 2020MAR11 22:36 using SCALE␣
↪version 6.3.pre-b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
             ...finished loading HDF5 file
```

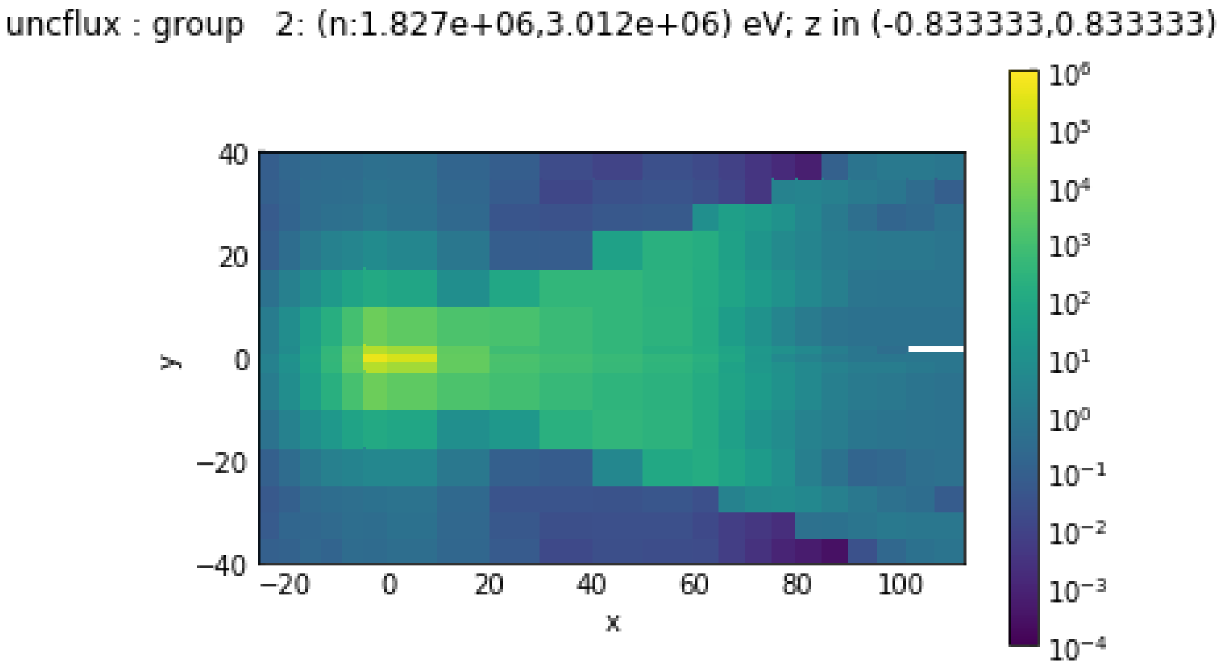
Here the uncollided flux is solved using the Monte Carlo approximation. Note that unlike the smooth exponential shape calculated by the analytic method, the MC approximation has statistical error (the uncollided term abruptly drops to zero in undersampled regions far from the source). The shapes for each group uncollided flux are similar because the energy discretization on the source is performed separately from the spatial tracking.

```
fc_source_mc = dnv_mc['uncflux']
```

```
ax = None;
for g in range(4):
    plots = plot(fc_source_mc.xs(y=0.0,z=0.0,g=g), logy=True, ax=ax)
    ax = plots['ax']
    plots['plot'][0].set_label(fc_source_mc.axis('g').describe_index(g))
ax.legend(loc='lower right')
ax.set_title("")
ax.set_ylabel("Uncollided flux [n/cm$^2$-s]");

norm = LogNorm(vmin=1e-4,vmax=1e6)
plots = plot(fc_source_mc.xs(g=2,z=0.0), norm=norm)
plots['ax'].title.set_position([.5, 1.25]);
```





A comparison of the calculated doses for the analytic and Monte Carlo solutions show good agreement away from the source, modulo some statistical noice.

```
dose_mc = weighted_energy_integrate(dnv_mc['flux'], flux_to_dose_factor,
                                    name='dose', units='rem/hr')

plots = plot(dose_mc.xs(y=0,z=0), logy=True)
plots['plot'][0].set_label("MC")
```

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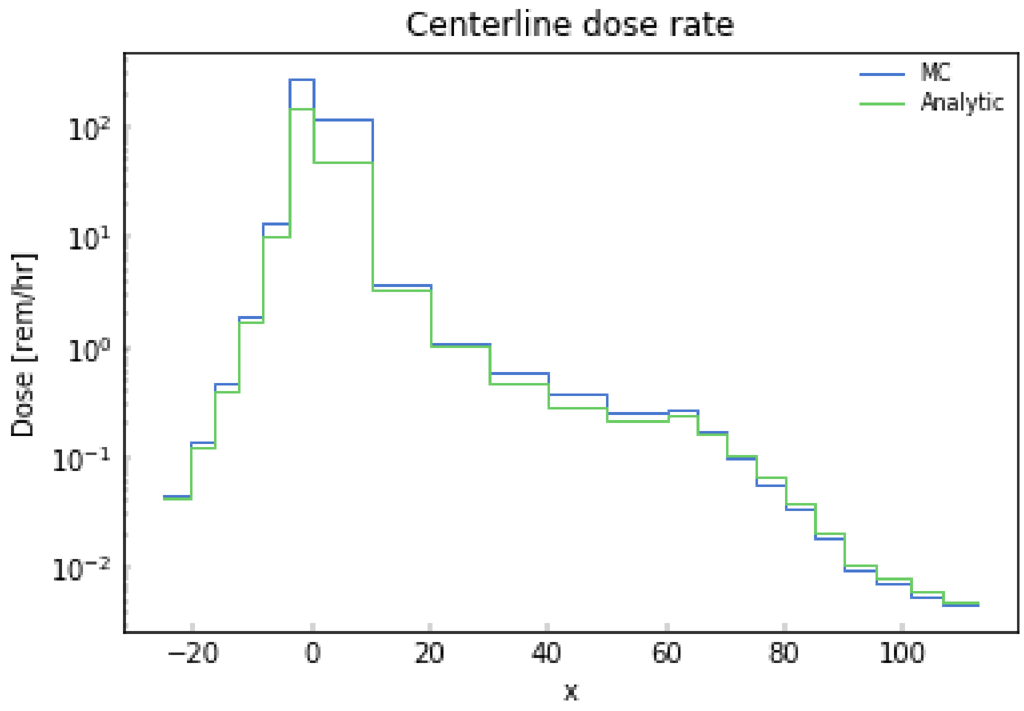
```
ax = plots['ax']

plots = plot(dose.xs(y=0,z=0), logy=True, ax=ax)
plots['plot'][0].set_label("Analytic")

ax.set_ylabel("Dose [rem/hr]")
ax.set_title("Centerline dose rate")
ax.legend();
```



A.2.4.5 Adjoint solutions

The solution of the adjoint transport equation (adjoint flux) is the expected contribution from the neutron source to the detector. In other words, the adjoint flux is a measurement of the importance of a particle's contribution to the detector tally.

```
%cat {SOURCE_DIR}/data/denovo-ueki-adj.omn
```

```
[PROBLEM]
name "Ueki 30cm benchmark (adjoint solution)"
mode adjoint
adjoint_source tally

[MODEL=mcnp]
input "../data/ueki.mcnp"
autoname
extents -25 112.5 -40 40 -40 40 ! Bounding box

[TALLY]
```

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```
[TALLY][CELL response]
cells 3

[PHYSICS=mg]
mg_lib "v7-28n19g"
mode n
pn_order 0
disable_upscattering true

[DENOVO]
method sc
x -25 5i 0 5i 60 5i 90 3i 112.5
y -40 2i -25 2i -2.5 2i 2.5 2i 25 2i 40
z -40 2i -25 2i -2.5 2i 2.5 2i 25 2i 40

[DENOVO][SOLVER=fixed]

[.][WITHIN_GROUP]
verbosity none
max_iterations 10

[DENOVO][QUADRATURE]
num_azi 2
num_polar 2

[RUN=mpi]
np 4

[PRE]
[PRE][PLOT lateral]
origin -25 0 -40
size 127.5 80
axis y
render true
```

```
!omnibus-run {SOURCE_DIR}/data/denovo-ueki-adj.omn
```

```
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/denovo-ueki-adj.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
>>> Loading nuclide data from processed MCNP libraries
>>> Loading compositions from MCNP input
>>> Loading nuclide data from processed MCNP libraries
```

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```
>>> Loading compositions from MCNP input
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
WARNING: The 'method' keyword is now 'equations' for SN discretization types. Changing␣
↪`method sc` to `equations sc`
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 2' and 'y_blocks 2'
INFO: Set default for 'z_blocks' to '2' in '/denovo/decomposition'
INFO: Set default for 'quadrature' to 'qr' in '/denovo/quadrature'
INFO: Set default for 'construction' to 'product' in '/denovo/quadrature'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'uncflux' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
INFO: Global Denovo mesh has 4950 cells
INFO: Renaming existing file denovo-ueki-adj.inp.xml to denovo-ueki-adj.inp-20200311-2236.
↪xml
INFO: Writing Omnibus input ParameterList to denovo-ueki-adj.inp.xml
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
Generating geometry image...
INFO: Saved geometry image at y=0 to 'lateral_y0.png'
            ...finished generating geometry image
INFO: Renaming existing file denovo-ueki-adj.pp.json to denovo-ueki-adj.pp-20200311-2236.
↪json
INFO: Writing preprocessed file to denovo-ueki-adj.pp.json
INFO: Writing processed ASCII input to 'denovo-ueki-adj.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
INFO: Renaming existing file omnibus.out to omnibus-20200311-2236a.out
INFO: Renaming existing file omnibus.err to omnibus-20200311-2236a.err
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
INFO: Loading compositions from MCNP input
INFO: Splitting compound 6000 into at% {6012: 0.9893, 6013: 0.0107}
INFO: Splitting compound 3006000 into at% {3006012: 0.9893, 3006013: 0.0107}
```

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```
INFO: Creating default boundary mesh from (-25 -40 -40) to (112.5 40 40) for MCNP␣
↪geometry
Building physics 'mg'
INFO: Loading AMPX library at '/usr/local/scale/data/scale.rev12.xn28g19v7.1'
INFO: Retained 3 of 455 nuclides on the master AMPX library
INFO: Running XSProc on 2 cells
WARNING: Upscattering has been lumped into within-group scattering in the thermal groups
WARNING: Remapped 4 nuclide IDs: 6012->6000, 6013->6000, 3006012->3006000, 3006013->
↪3006000
INFO: Truncating cross sections to groups [0, 28)
Building tallies
Building Denovo solver internals
Ray tracing Denovo mesh
WARNING: Number of Z blocks (2) is not divisible into the number of z cells 15; reducing␣
↪to 1
Mixing Denovo cross sections
Building Denovo sources
Constructing adjoint sources for Denovo
WARNING: Tally 'response' has no multiplier specified in the HYBRID block; a flat␣
↪adjoint spectrum will be used
Discretizing adjoint sources (1 cell tallies)
Initializing Denovo solver
INFO: Constructing Denovo state vector with 28 groups, 4950 cells, 1 moments, 1 unknowns␣
↪per cell
Running Denovo transport calculation
Adjoint group  27 finished in    5 Belos Block GMRES iterations.
Adjoint group  26 finished in    5 Belos Block GMRES iterations.
Adjoint group  25 finished in    5 Belos Block GMRES iterations.
Adjoint group  24 finished in    5 Belos Block GMRES iterations.
Adjoint group  23 finished in    4 Belos Block GMRES iterations.
Adjoint group  22 finished in    3 Belos Block GMRES iterations.
Adjoint group  21 finished in    3 Belos Block GMRES iterations.
Adjoint group  20 finished in    3 Belos Block GMRES iterations.
Adjoint group  19 finished in    3 Belos Block GMRES iterations.
Adjoint group  18 finished in    2 Belos Block GMRES iterations.
Adjoint group  17 finished in    2 Belos Block GMRES iterations.
Adjoint group  16 finished in    3 Belos Block GMRES iterations.
Adjoint group  15 finished in    3 Belos Block GMRES iterations.
Adjoint group  14 finished in    3 Belos Block GMRES iterations.
Adjoint group  13 finished in    3 Belos Block GMRES iterations.
Adjoint group  12 finished in    4 Belos Block GMRES iterations.
Adjoint group  11 finished in    4 Belos Block GMRES iterations.
Adjoint group  10 finished in    4 Belos Block GMRES iterations.
Adjoint group   9 finished in    4 Belos Block GMRES iterations.
Adjoint group   8 finished in    4 Belos Block GMRES iterations.
Adjoint group   7 finished in    4 Belos Block GMRES iterations.
Adjoint group   6 finished in    4 Belos Block GMRES iterations.
Adjoint group   5 finished in    3 Belos Block GMRES iterations.
Adjoint group   4 finished in    3 Belos Block GMRES iterations.
Adjoint group   3 finished in    2 Belos Block GMRES iterations.
Adjoint group   2 finished in    3 Belos Block GMRES iterations.
INFO: Writing Silo file to 4 concurrent files using material volume fractions
```

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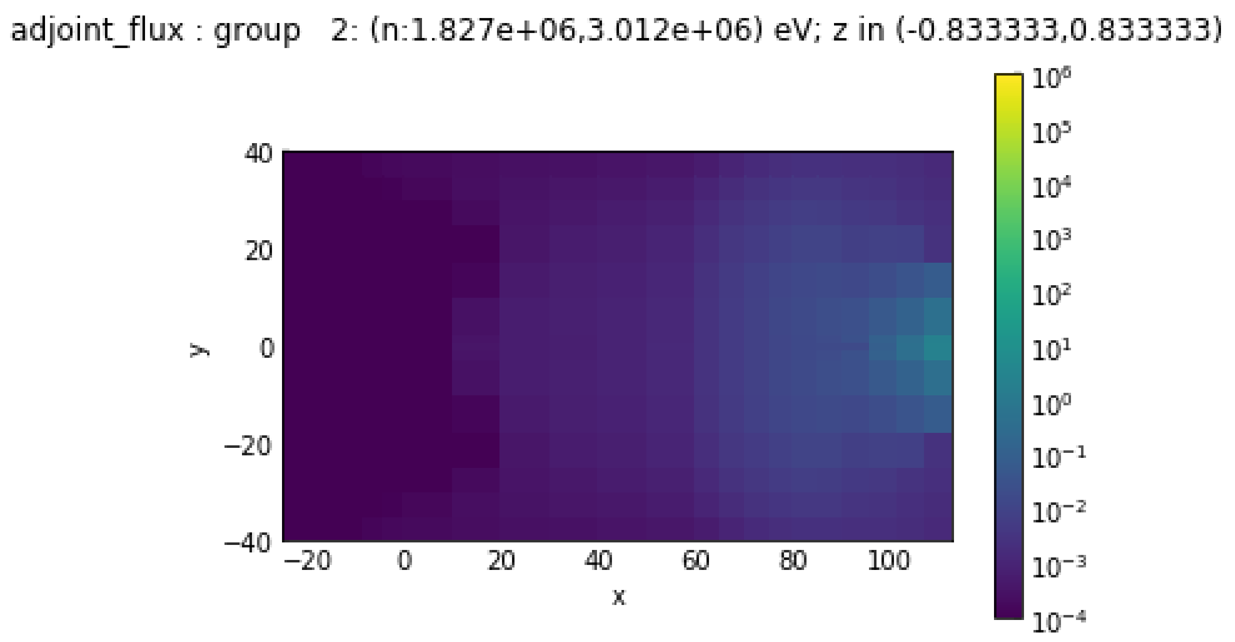
```
INFO: Removing SILO directory denovo_output_silo
Writing Denovo HDF5 output
Run complete
Cleaning up
Adjoint group   1 finished in    3 Belos Block GMRES iterations.
Adjoint group   0 finished in    3 Belos Block GMRES iterations.
            ...finished running Omnibus in 2.7 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-adj.out.h5', problem name 'Ueki 30cm␣
↪benchmark (adjoint solution)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-
↪b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-adj.out.h5', problem name 'Ueki 30cm␣
↪benchmark (adjoint solution)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-
↪b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to denovo-ueki-adj.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to denovo-ueki-adj.rst
            ...finished building RST summary
```

```
dnv = load("denovo-ueki-adj.out.h5")['denovo'].extract()
adj_flux = dnv['flux'].copy()
adj_flux.name ='adjoint_flux'
```

```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'denovo-ueki-adj.out.h5', problem name 'Ueki 30cm␣
↪benchmark (adjoint solution)', created on 2020MAR11 22:37 using SCALE version 6.3.pre-
↪b10 (branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```

Plotting the adjoint flux shows how likely it is for particles at each point in space to contribute to the detector. Denovo predicts that the flux is of lowest importance in the paraffin block and of highest importance behind the graphite shield.

```
plots = plot(adj_flux.xs(g=2,z=0.0), norm=norm)
plots['ax'].title.set_position([.5, 1.25]);
```



A.2.5 DENOVO/SWORD INTEGRATION

This example demonstrates how to load and visualize a SWORD input file, create an Omnibus Denovo input for it that writes the angular flux and current, and post-process the output.

```
# Set up example environment
import os
from exnihilotools.matplotlib import screen_style
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
%matplotlib inline
screen_style()
```

A.2.5.1 Visualize a GDML geometry

Loading a SWORD geometry reads a set of XML input files and calls Geant4 initialization routines to load a corresponding GDML geometry input.

```
from omnibus.raytrace.load import load_sword
model = load_sword(os.path.join(SOURCE_DIR, "data", "btest5", "btest5.sword"))
```

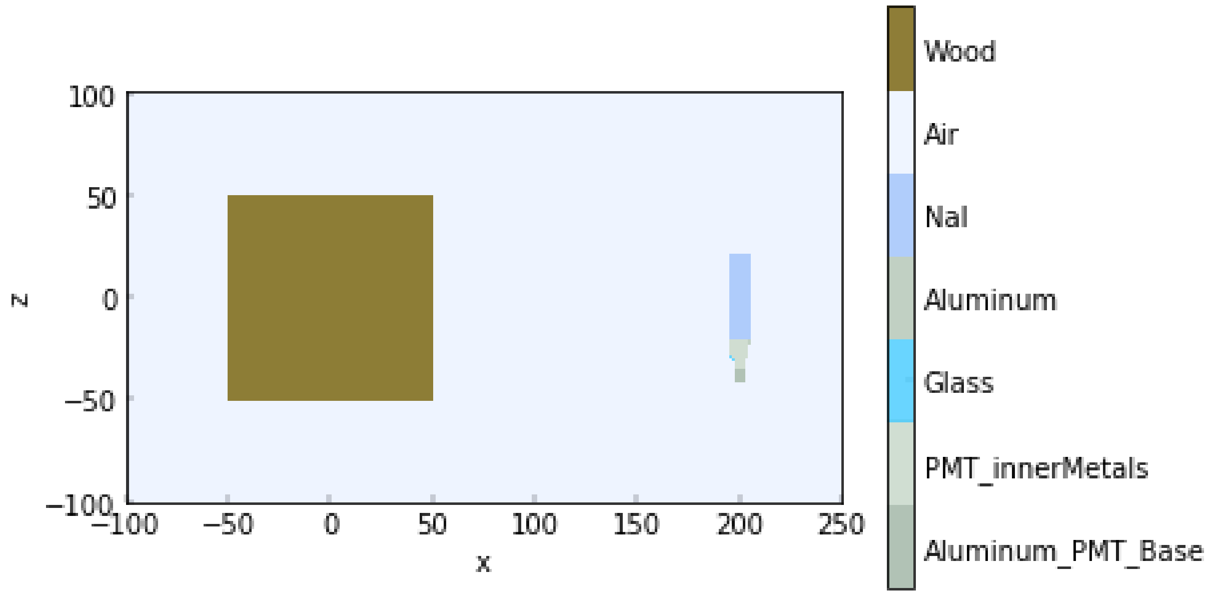
```
Generating serialized SWORD model...
INFO: Writing packed model to btest5.xdr
            ...finished generating serialized SWORD model
```

Omnibus includes tools to create color schemes based on the phyical compositions of the problem. The `ColorMap.from_compositions` method automatically assigns colors for common real-life materials such as air, carbon-based life forms, and detector materials. The individual compositions from the model can also be explored to validate that Denovo is seeing the right nuclides, weight fractions, etc.

```
from omnibus.raytrace.colors import ColorMap
colors = ColorMap.from_compositions(model.compositions)
colors.comps[1]._asdict()
```

```
{'name': 'PMT_innerMetals',
 'matid': 1,
 'density': 0.7,
 'temperature': 293.15,
 'zaid': array([ 6012,  6013, 13027, 15031, 16032, 16033, 16034, 16036, 24050,
        24052, 24053, 24054, 25055, 26054, 26056, 26057, 26058, 28058,
        28060, 28061, 28062, 28064, 29063, 29065, 42092, 42094, 42095,
        42096, 42097, 42098, 42100], dtype=uint32),
 'wtfrac': array([2.96790000e-05, 3.21000000e-07, 2.50000000e-01, 5.00000000e-05,
        4.74650000e-05, 3.80000000e-07, 2.14500000e-06, 1.00000000e-08,
        7.82100000e-04, 1.50820200e-02, 1.71018000e-03, 4.25700000e-04,
        1.70000000e-03, 4.11312650e-03, 6.45672898e-02, 1.49114030e-03,
        1.98443400e-04, 6.67153620e-03, 2.56986380e-03, 1.11710200e-04,
        3.56181000e-04, 9.07088000e-05, 8.64625000e-02, 3.85375000e-02,
        7.79100000e-02, 4.85625000e-02, 8.35800000e-02, 8.75700000e-02,
        5.01375000e-02, 1.26682500e-01, 5.05575000e-02]),
 'depletable': False,
 'fissionable': False}
```

```python
from omnibus.raytrace.imager import Imager
imager = Imager(model.geometry,
                lower=(-100, 0, -100),
                upper=(250, 0, 100),
                basis=(1, 0, 0),
                max_pixels=1024)
imager.names = [c.name for c in model.compositions]
imager.colors = colors
imager.plot();
```



Rendering produces a faster, higher-resolution image but doesn't show the extents or material names.

```
imager.render('rendered.png')
from IPython.display import Image
Image(filename='rendered.png')
```

A.2.5.2 Execute Omnibus

The Omnibus input to this problem uses ANISN data (the multigroup data distributed with ADVANTG) and the SWORD model loaded above. Inside the Denovo block it specifies to output both the current (first angular moment) and the angular flux (actual discrete ordinates solution at each angle).

```
%cat {SOURCE_DIR}/data/btest.omn
```

```
[PROBLEM]
name "Simple SWORD source-detector problem"
mode forward

[MODEL=sword]
input "btest5/btest5.sword"

[SOURCE=sword]

[PHYSICS=mg]
anisn_lib "27n19g"
pn_order 1
disable_upscattering true
omit_zaid 8018
mode p
pemax 662e3

```

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```
[DENOVO]
! Spatial grid with 'interpolation' keywords
x -100 2i -50 7i 50 8i 190 7i 210   2i  250
y -100 2i -50 2i -20    -6 3i 6     20 2i 50 2i 100
z -100 2i -50          -40 15i 40   50 2i 100

[DENOVO][OUTPUT]
current true
angular_flux true

[DENOVO][QUADRATURE]
order 16

[DENOVO][SOLVER=fixed]
[.][WITHIN_GROUP]
verbosity none

[RUN=serial]
```

```
!omnibus-run {SOURCE_DIR}/data/btest.omn
```

```
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/btest.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
Generating serialized SWORD model...
            ...finished generating serialized SWORD model
INFO: Setting ANISN libraries based on data at /usr/local/advantg-data/27n19g.bin
INFO: Set default for 'load_scl' to 'False' in '/comp'
INFO: Set default for 'physics' to 'mg' in '/denovo'
INFO: Set default for 'boundary' to '{'_type': 'vacuum'}' in '/denovo'
INFO: Set default 'x_blocks 1' and 'y_blocks 1'
INFO: Set default for 'z_blocks' to '1' in '/denovo/decomposition'
INFO: Set default for 'quadrature' to 'qr' in '/denovo/quadrature'
INFO: Set default for 'construction' to 'levelsym' in '/denovo/quadrature'
INFO: Set default for 'mat' to 'True' in '/denovo/output'
INFO: Set default for 'source' to 'True' in '/denovo/output'
INFO: Set default for 'uncflux' to 'True' in '/denovo/output'
INFO: Set default for 'flux' to 'True' in '/denovo/output'
INFO: Set default for 'upscatter_groups' to 'thermal' in '/denovo/solver'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'solver' to 'gmres' in '/denovo/solver/within_group'
INFO: Method: sn
INFO: Equations: sc
INFO: Set default for 'tolerance' to '0.001' in '/denovo/solver/within_group'
INFO: Set default for 'preconditioner' to '{'_type': 'none'}' in '/denovo/solver/within_
↪group'
```

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```
INFO: Global Denovo mesh has 13392 cells
INFO: Writing Omnibus input ParameterList to btest.inp.xml
INFO: Writing preprocessed file to btest.pp.json
INFO: Writing processed ASCII input to 'btest.inp.omn'
INFO: Launching Omnibus driver on 1 cores
Running Omnibus...
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
 ↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
 ↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
 ↪interpreted values match your input values.
Building model
INFO: Loading Geant problem from GDML file at /rnsdhpc/code/src/scale/Exnihilo/packages/
 ↪Omnibus/driver/example/data/btest5/sword.gdml
INFO: Loading 19 elements from Geant4
INFO: Loading nuclide data from Geant4 isotope libraries
INFO: Loading 48 isotopes from Geant4
WARNING: Nuclide data for 13027 was already set; ignoring and using existing data
WARNING: Nuclide data for 13027 was already set; ignoring and using existing data
INFO: Loading compositions from Geant4 material data
INFO: Creating default boundary mesh from (-12500 -12500 -12500) to (12500 12500 12500)␣
 ↪for Geant4 geometry
Building physics 'mg'
INFO: Loading ANISN attributes from /usr/local/advantg-data/27n19g.info
INFO: Loading ANISN zaid map from /usr/local/advantg-data/27n19g.zaid
INFO: Loading ANISN cross sections from /usr/local/advantg-data/27n19g.bin
WARNING: Upscattering has been lumped into within-group scattering in the thermal groups
WARNING: Remapped 2 nuclide IDs: 6012->6000, 6013->6000
WARNING: Omitted 1 nuclide IDs: 8018
INFO: Truncating cross sections to groups [39, 46)
Building sources
Building Denovo solver internals
Ray tracing Denovo mesh
Mixing Denovo cross sections
Building Denovo sources
Constructing forward sources for Denovo
Discretizing SWORD sources (1 points)
Initializing Denovo solver
INFO: Constructing Denovo state vector with 7 groups, 13392 cells, 4 moments, 1 unknowns␣
 ↪per cell
Performing analytic first-collision source calculation on 1 sources
Running Denovo transport calculation
Forward group   0 finished in    3 Belos Block GMRES iterations.
Forward group   1 finished in    3 Belos Block GMRES iterations.
Forward group   2 finished in    3 Belos Block GMRES iterations.
Forward group   3 finished in    4 Belos Block GMRES iterations.
Forward group   4 finished in    5 Belos Block GMRES iterations.
Forward group   5 finished in    7 Belos Block GMRES iterations.
INFO: Writing Silo file to 1 concurrent files using material volume fractions
Writing Denovo HDF5 output
Forward group   6 finished in    3 Belos Block GMRES iterations.
```

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```
Calculating angular fluxes
Run complete
Cleaning up
            ...finished running Omnibus in 14.5 seconds
Running Omnibus postprocessing
Loading HDF5 file...
WARNING: Failed to build 'm' axis (via <bound method DataAxis.from_group of <class
↪'omnibus.data.axis.DataAxis'>>) for 'angular_flux' of '/denovo': "Unable to open␣
↪object (object 'mesh_m' doesn't exist)"
INFO: Loaded Omnibus output data from 'btest.out.h5', problem name 'Simple SWORD source-
↪detector problem', created on 2020MAR11 22:38 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'btest.out.h5', problem name 'Simple SWORD source-
↪detector problem', created on 2020MAR11 22:38 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Writing Denovo visualization file...
INFO: Wrote Denovo visualization file to btest.denovo.xmf
            ...finished writing Denovo visualization file
Building RST summary...
INFO: Wrote summary file to btest.rst
            ...finished building RST summary
```

A.2.5.3 Process results

```
from omnibus.formats.output import load
dnv = load("btest.out.h5")['denovo'].extract()
```

```
Loading HDF5 file...
WARNING: Failed to build 'm' axis (via <bound method DataAxis.from_group of <class
↪'omnibus.data.axis.DataAxis'>>) for 'angular_flux' of '/denovo': "Unable to open␣
↪object (object 'mesh_m' doesn't exist)"
INFO: Loaded Omnibus output data from 'btest.out.h5', problem name 'Simple SWORD source-
↪detector problem', created on 2020MAR11 22:38 using SCALE version 6.3.pre-b10 (branch
↪'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```

Uncollided flux

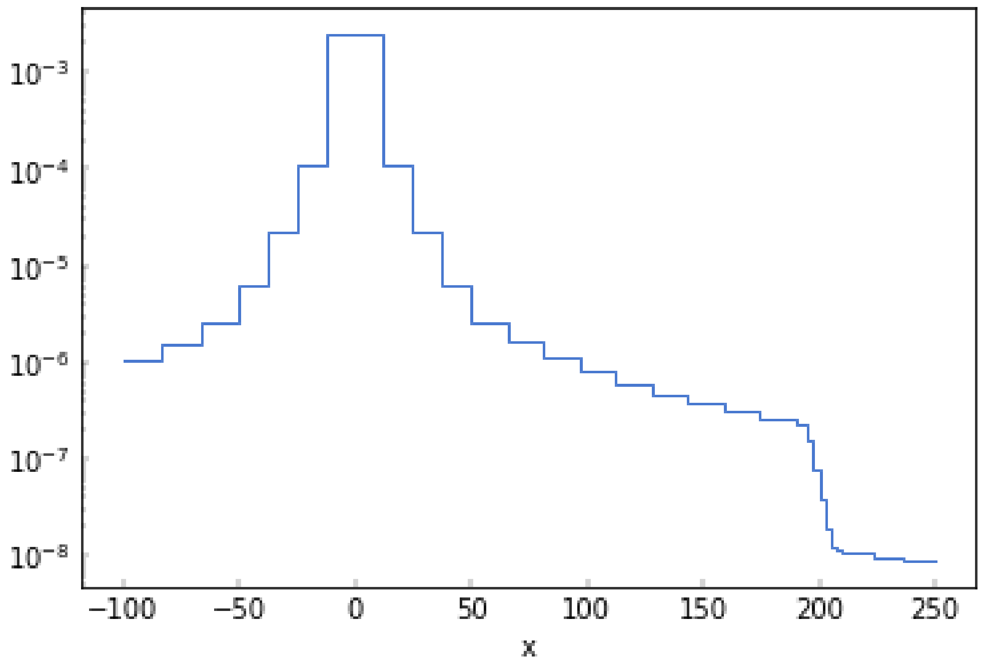
A good first step in analysis is to verify the source term: in this case, checking that it is nonzero only in the highest group. The `xs` command slices the data with the group index for a single group, or with a Python `slice` object to get a range of groups. (`a[slice(1,None)]` is equivalent to `a[1:]`.)

```
import numpy as np

uncflux = dnv['uncflux']
print(np.count_nonzero(uncflux.xs(g=0)))
print(np.count_nonzero(uncflux.xs_by_index(g=slice(1,None))))
```

```
13392
0
```

A lineout plot along $y = z = 0$ for the source group clearly shows the attenuation through the detector at $x = 200$.

```
from omnibus.data import plot

plots = plot(uncflux.xs(y=0.0, z=0.0, g=0), logy=True);
plots['ax'].set_ylabel('');
```



The "scalar flux" is the zeroth angular moment of the angular flux:

$$\phi = \int_{4\pi} \psi(\vec{x}, \vec{\Omega}) \mathrm{d}\Omega$$

It is effectively a measure of particle density, and is used in calculating reaction rates.

The following command extracts the data at the origin. Since the only remaining data axis is energy, the `plot` function will render a step plot of the group-average fluxes.

Flux

```
import matplotlib.pyplot as plt

flux = dnv['flux']
origin_spectrum = flux.xs(x=0, y=0, z=0)

plots = plot(origin_spectrum, logy=True)
ax = plots['ax']
```

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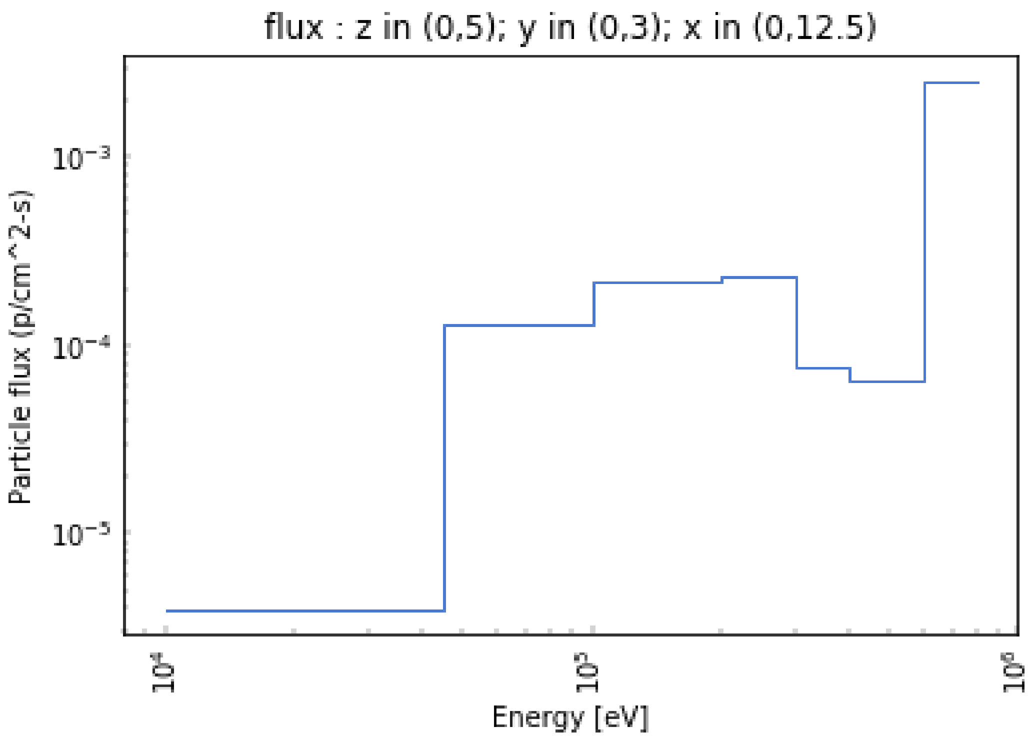
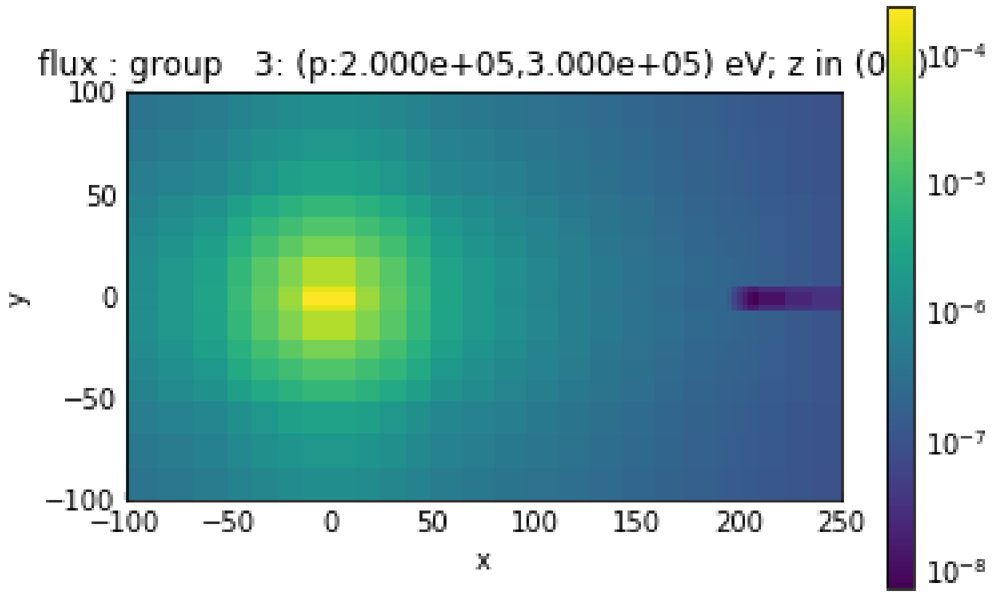
```
# Rotate the X tick labels
plt.setp(ax.get_xticklabels(), rotation=90);
ax.set_title(ax.get_ylabel())
ax.set_ylabel("Particle flux (p/cm^2-s)");
```



The next command accesses the flux at group index 3 (not 3 eV!) at z = 0. With the resulting x-y data, the plotter renders a pseudocolor plot. Specifying a special value for `norm` renders the colors on a logarithmic scale.

```
from matplotlib.colors import LogNorm

plot(flux.xs(z=0., g=3), norm=LogNorm());
```



Net current

The `current` field is the “net current”, the first moment of the angular flux:

$$\vec{J} = \int_{4\pi} \vec{\Omega}\psi(\vec{x},\vec{\Omega})\mathrm{d}\Omega\,.$$

It is stored as an energy, space, and direction-dependent field; the `data` attribute is the pointer to the HDF5 data.

The current describes the net flow rate of particles traveling through a point in space. The following command print the dimensionality of the current:

```
current = dnv['current']
print(", ".join("{}={}".format(d,s)
      for (d,s) in zip(current.dims, current.shape)))
```

```
g=7, z=24, y=18, x=31, dir=3
```

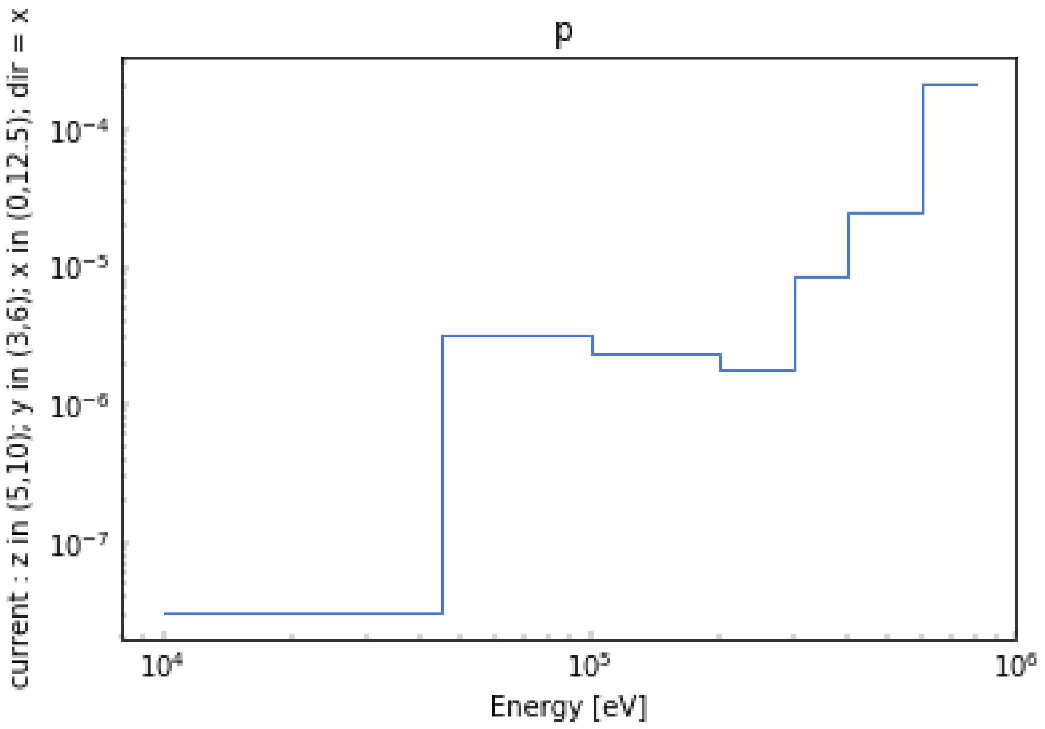
The following command takes a slice at the energy group for photons at 1e5 eV, at the XYZ coordinates of $(7, 3, 5)$. The resulting vector is the current along the (x, y, z) directions.

```
sliced = current.xs(x=7.0, y=3.0, z=5.0, g=('p', 1e5))
print(sliced.mesh('dir'))
sliced
```

```
['x' 'y' 'z']
```

Other slices are of course possible. This command plots the multigroup net current at a particular point:

```
plot(current.xs(x=7.0, y=3.0, z=5.0, dir='x'), logy=True);
```



The full angle-dependent particle flux can be approximated by using the angular moments. This is the P_N approximation.

$$\psi(\vec{x}, \vec{\Omega}) \approx \frac{1}{4\pi}(\phi(\vec{x}) + 3\vec{\Omega} \cdot \vec{J}(\vec{x}))$$

However, a much more accurate representation of the angular flux can be obtained directly from Denovo.

Angular flux

The full S_N flux can be saved by setting `angular_flux true` inside the `[DENOVO][OUTPUT]` block. This option requires careful consideration due to the disk space requirements: for an S_{16} quadrature set, it will be 288 times as large as the scalar flux.

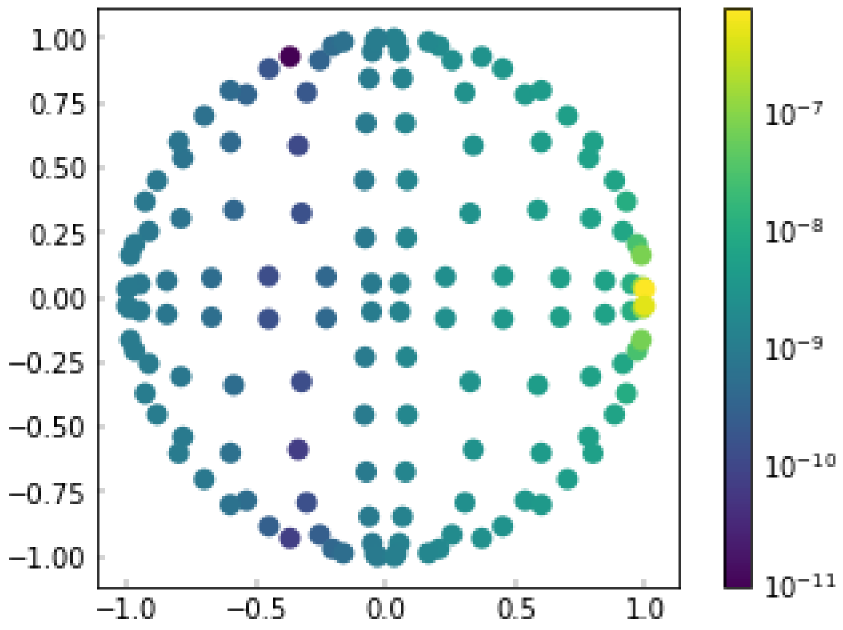
```
# Extract the angle-dependent flux averaged over a single spatial point in one energy␣
↪group
flux = dnv['angular_flux']
angle_flux = flux.xs(g=('p', 7e5), x=200.0, y=1.5 , z=2.5)
angle_flux
```

```
angles = dnv.quadrature_angles.extract()
angles
```

These tools can perform a wide range of functions. For example, numpy logical expressions can determine all the angle indices in the $+z$ direction, and matplotlib can then create a scatter plot of the angluar fluxes projected into the xy plane.

```
z_slice = angles.data[:,2] > 0

plt.scatter(angles[z_slice,0], angles[z_slice,1],
            c=np.abs(angle_flux.data[z_slice]),
            norm=LogNorm(), cmap='viridis', edgecolor='none')
plt.axis('square');
plt.colorbar();
```



A.2.6 EXNIHILO MESH INPUT DEFINITION

These small problems are used in the Denovo unit tests. The output files should be saved to `Geometria/mesh/rect/test/data`.

```
# Set up plotting
%matplotlib inline
from exnihilotools.matplotlib import screen_style
screen_style()
```

A.2.6.1 Problem A

This is a 3D problem with a volume source.

```
from omnibus.mesh import Mesh
from omnibus.formats.meshmodel import MeshModelFile
import numpy as np

mesh = Mesh(x=np.arange(21), y=np.arange(16), z=np.arange(11))
problem = MeshModelFile.from_mesh(mesh)
```

If the mesh axes were irregular, then a snippet of code like the following could be used to ‘slice’ the matids more easily. In order to select a view of the data to assign matids, we have to use standard python `slice` objects or integers.

```
from omnibus.data import simplify_logical_slice

x_centers = problem['matids'].axis('x').centers
def x_slice(xmin, xmax):
    return simplify_logical_slice((x_centers >= xmin) & (x_centers <= xmax))
print(x_slice(3,10))
```

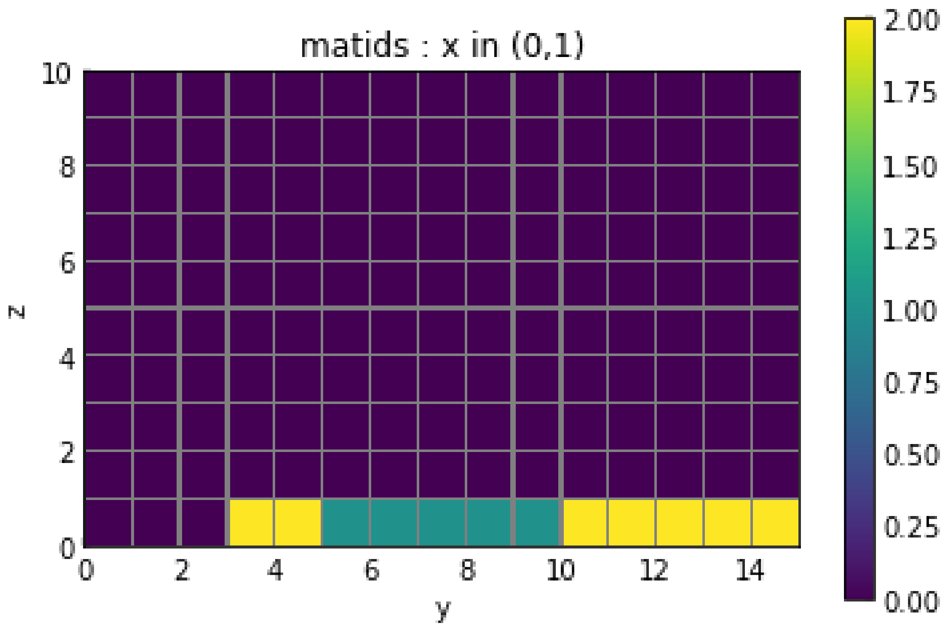
```
slice(3, 10, None)
```

The xs_by_index method selects subsets of the mesh, either multiple elements or a single element, along multiple axes. The following chunks of code are used to assign materials and a source definition.

```
from omnibus.data import plot

matids = problem['matids']
zmats = matids.xs_by_index(z=slice(1,))
zmats.xs_by_index(y=slice(5, 15)).data[:] = 1
zmats.xs_by_index(x=slice(0,15), y=slice(10,15)).data[:] = 2
zmats.xs_by_index(y=slice(3,5)).data[:] = 2

plot(matids.xs(x=0.5), edgecolor='gray', linewidth=0.25);
```



```
src = problem['volsrc']
spectra = src['spectra']

num_groups = 3
spectra.resize(2, num_groups)
spectra.get_spectrum(0)[:] = [0.6, 0.3, 0.1]
spectra.get_spectrum(1)[:] = [0.4, 0.2, 0.4]

srcids = src['ids']
```

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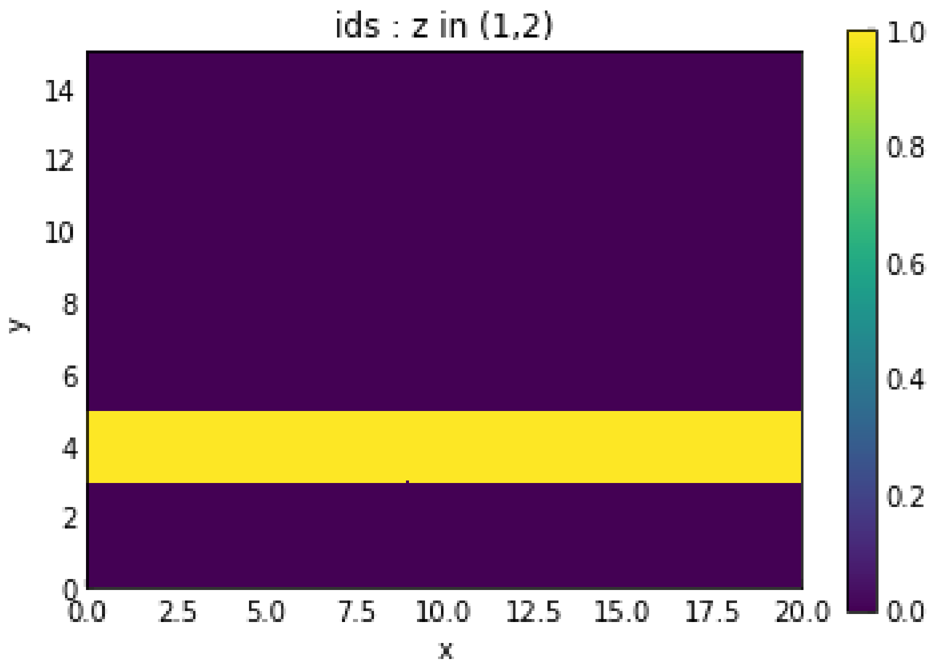
```
srcids.xs_by_index(y=slice(3,5), z=slice(1,9)).data[:] = 1
plot(srcids.xs(z=1.0));
```

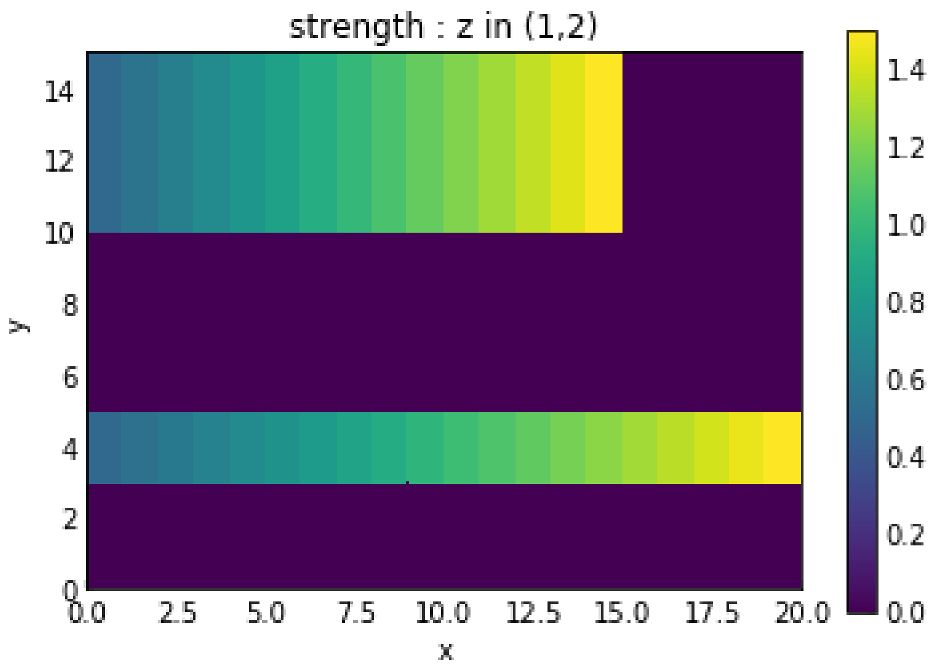


```
strength = src['strength']

q0 = np.linspace(0.5, 1.5, 15)
q1 = np.linspace(0.5, 1.5, 20)

strength.xs_by_index(x=slice(0,15), y=slice(10,15), z=slice(1,10)).data[:] = q0
strength.xs_by_index(y=slice(3,5), z=slice(1,10)).data[:] = q1

plot(strength.xs(z=1.0));
```



Now that the problem is constructed, it can be written to disk for later use in Omnibus:

```
import h5py
from omnibus.data import dump_root

with h5py.File("simple-3d.h5", 'w') as f:
    dump_root(problem, f)
```

```
INFO: Omitting empty point source
```

A.2.6.2 Problem B

This 2D problem is constructed similarly to the previous one.

```
from omnibus.mesh import Mesh2D

# Make the mesh
mesh = Mesh2D(x=np.arange(21), y=np.arange(16))
problem = MeshModelFile.from_mesh(mesh)

# Assign data directly: note that the axes are ordered
# in reverse, so slice indices must also be reversed
matids = problem['matids'].data
assert problem['matids'].dims == ['y', 'x']
matids[5:15,:] = 1
matids[10:15,0:15] = 2
matids[3:5,:] = 2

src = problem['volsrc']
spectra = src['spectra']
```

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```
spectra.resize(2, 3)
spectra.get_spectrum(0)[:] = [0.6, 0.3, 0.1]
spectra.get_spectrum(1)[:] = [0.4, 0.2, 0.4]

srcids = src['ids'].data
srcids[3:5,:] = 1

strength = src['strength'].data

q0 = np.linspace(0.5, 1.5, 15)
q1 = np.linspace(0.5, 1.5, 20)

strength[10:15,0:15] = q0
strength[3:5,:]      = q1

with h5py.File("simple-2d.h5", 'w') as f:
    dump_root(problem, f)
```

```
INFO: Omitting empty point source
```

A.2.6.3 Problem C

This 3D problem includes mix tables and does not specify a source definition.

```
import matplotlib.pyplot as plt
from omnibus.formats.meshmodel import MixTable


mesh = Mesh(x=np.arange(17), y=np.arange(9), z=np.arange(9))
problem = MeshModelFile.from_mesh(mesh)

matids = problem['matids'].data

# Note that dimensions are z/y/x
matids[:] = 0
matids[:6,2:6,4:13] = 2 # mixture
matids[3:5,3:5,5:12] = 1 # pure

(fig, ax) = plt.subplots()
ax.pcolormesh(mesh.x, mesh.y, matids[4,:,:], edgecolor=(.5,.5,.5))
ax.set_aspect(1.0);

# Build a mix table
mix_table = np.array([[1.0, 0.0],
                      [0.0, 1.0],
                      [0.5, 0.5]])
problem['mixtable'] = MixTable.from_table(mix_table)

# Print the COO representation it made
print(problem['mixtable'].data)
```

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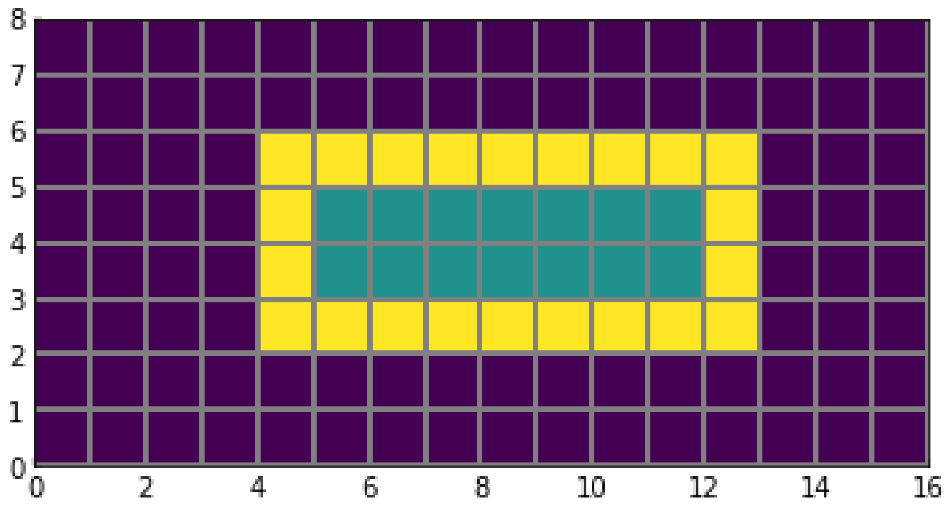
```
# Save to disk
with h5py.File("mixed-3d.h5", 'w') as f:
    dump_root(problem, f)
```

```
INFO: Omitting empty volume source
INFO: Omitting empty point source
```

```
[(0, 0, 1. ) (1, 1, 1. ) (2, 0, 0.5) (2, 1, 0.5)]
```



A.2.6.4 Uniform source and material

```
mesh = Mesh(x=np.arange(10, dtype='f8'),
            y=np.arange(10, dtype='f8'),
            z=np.arange(10, dtype='f8'))
problem = MeshModelFile.from_mesh(mesh)

matids = problem['matids'].data
matids[:] = 0

# Define source spectra
src = problem['volsrc']
spectra = src['spectra']
spectra.resize(1,1)
spectra.get_spectrum(0)[:] = [1.0]

# Assign IDs and source strengths
srcids = src['ids'].data
srcids[:] = 0
strength = src['strength'].data
strength[:] = 1.0

# Save to disk
with h5py.File("uniform-3d.h5", 'w') as f:
    dump_root(problem, f)
```

```
INFO: Omitting empty point source
```

A.2.6.5 Both point and volume sources

The input file constructed here will contain both volume and point sources.

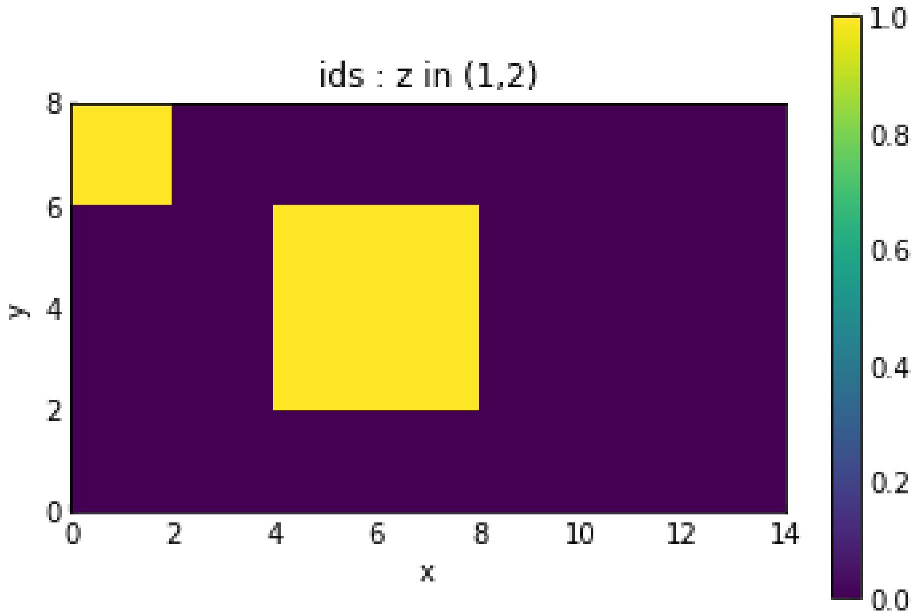
```
mesh = Mesh(x=np.arange(15, dtype='f8'),
            y=np.arange(9, dtype='f8'),
            z=np.arange(5, dtype='f8'))
problem = MeshModelFile.from_mesh(mesh)

# Add volume sources
src = problem['volsrc']
spectra = src['spectra']

num_groups = 3
spectra.resize(4, num_groups)
spectra.get_spectrum(0)[:] = [0.6, 0.3, 0.1]
spectra.get_spectrum(1)[:] = [0.4, 0.2, 0.4]
spectra.get_spectrum(2)[:] = [0.3, 0.5, 0.2]
spectra.get_spectrum(3)[:] = [1.0, 0.0, 0.0]

srcids = src['ids'].data
srcids[:3,6:8,0:2] = 1
srcids[:,2:6,4:8] = 1

plot(src['ids'].xs(z=1.0));
```



Next, set varying strengths in the different cells.

```
strength = src['strength'].data
strength[:3,6:8,0:2].flat = np.linspace(0.1, 1.1, 3*2*2)
```

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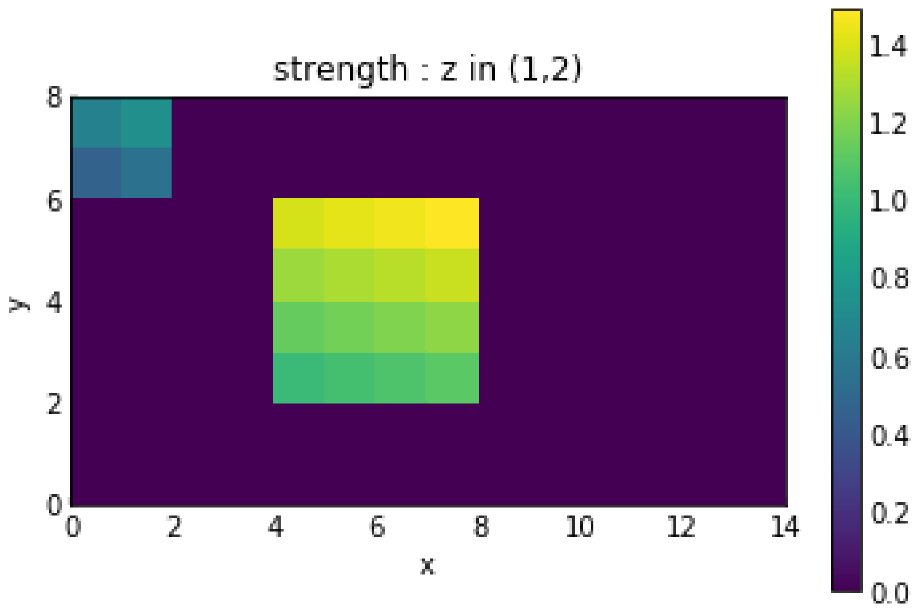
```
strength[:,2:6,4:8].flat  = np.linspace(0.5, 2.5, 4*4*4)

plot(src['strength'].xs(z=1.0));
```



Finally, add the point sources and write the problem to disk.

```
# Add point sources
pointsrc = problem['ptsrc']

# Points are in X,Y,Z and use the same spectra as the volume source
pointsrc.resize(2, spectra.num_groups)
pointsrc.set_point(0, (10.5, 5.5, 0.5), 3.45, spectra.get_spectrum(2))
pointsrc.set_point(1, (13.5, 7.5, 3.5), 2.34, spectra.get_spectrum(3))

with h5py.File("points.h5", 'w') as f:
    dump_root(problem, f)
```

A.3 MULTIGROUP DATA EXPLORATION

These examples show how to use Exnihilo's Python bindings (page 2) to extract and visualize multigroup and other Denovo-related data.

A.3.1 CROSS SECTION GENERATION

This example demonstrates generating and visualizing multigroup cross sections using the Exnihilo python interface.

```
# Set up example
%matplotlib inline
%load_ext wurlitzer
from exnihilotools.matplotlib import screen_style
screen_style()
```

A.3.1.1 SCALE XSProc generation

We provide an interface to SCALE's modern cross section processing routines. The input can be specified either as a SCALE composition block or an Exnihilo `Composition` object. The cross section library name can be a path to a SCALE library or one of the library aliases given in the SCALE `FileNameAliases.txt` which lives in the SCALE installation.

```
from nemesis import cmake_config, Std_DB, make_view, make_const_view

db = Std_DB.from_dict({
    'Pn_order'    : 3,
    'xs_library' : "test-8grp",
    'downscatter': False})
```

```
from robus import (Composition, NEUTRON, TOTAL, SCATTERING, FISSION,
                   Nuclide_Metadata as NMD)
import transcore

NMD.load_SCL()
builder = transcore.XS_Builder_Fulcrum(db)

# Add a 'void' composition for matid=0
builder.add(0, Composition())

# Add a composition from number densities
water = Composition(300.0,
        [1001, 1002, 8016, 8017],
        [6.6728e-02, 7.6745e-06,  3.3287e-02, 1.2680e-05])
builder.add(2, water)

# Run the cross section processing and get the cross sections
builder.build()
mats = builder.get_materials()
```

```
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
>>> Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
>>> Retained 4 of 449 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
```

A.3.1.2 1-D Cross section visualization

The cross sections can be viewed through `numpy` wrappers. (No data copying is being done here.)

```
bounds = builder.group_bounds.group_bounds(NEUTRON)
water_xs = mats.get_material(2)
```

We can plot the reaction rates:

```
import numpy as np

sigma = np.asarray(water_xs.sigma)
```

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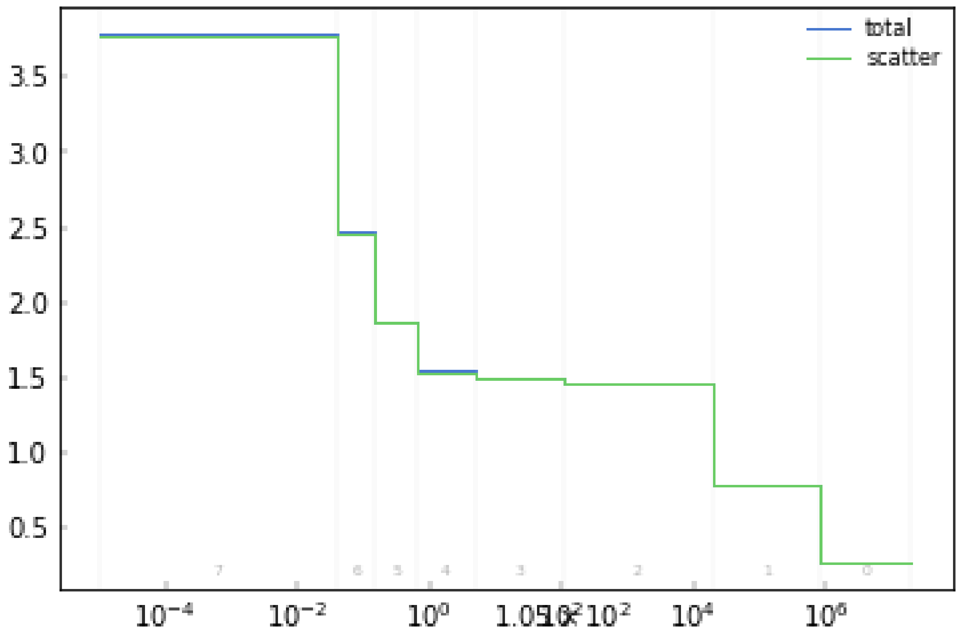
```
sigma_s = np.asarray(water_xs.sigma_x(SCATTERING))
#sigma_f = np.asarray(water_xs.sigma_x(FISSION))
```

```
import matplotlib.pyplot as plt
from matplotlib.colors import Normalize, LogNorm
from exnihilotools.matplotlib.artists import plot_multigroup
from exnihilotools.matplotlib.axes import grid_groups, annotate_groups

(fig, ax) = plt.subplots(subplot_kw=dict(xscale='log'))
plot_multigroup(ax, bounds, sigma, label='total')
plot_multigroup(ax, bounds, sigma_s, label='scatter')
ax.legend()
grid_groups(ax, bounds)
annotate_groups(ax, bounds);
```



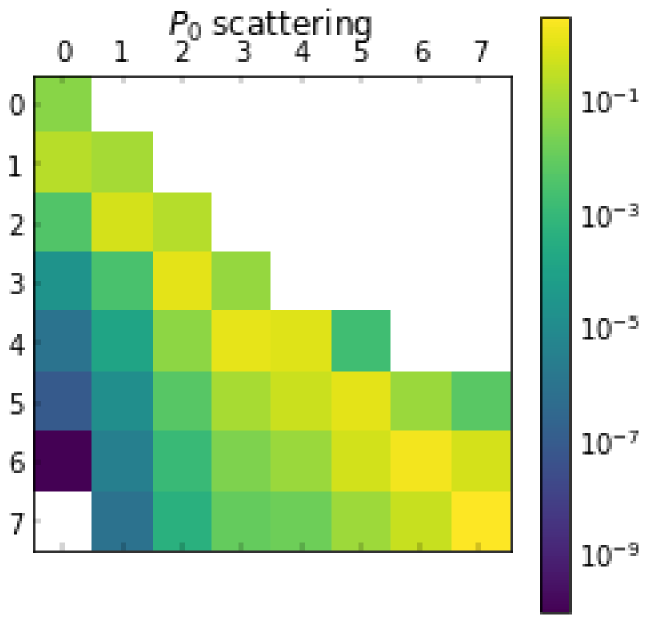
A.3.1.3 Scattering matrix visualization

The scattering matrix with all the requested angular moments (g, g', l) can be pulled directly from the cross section container. In this example, there are 4 moments since we requested P_3 scattering.

```
scat = water_xs.scatter_matrix
scat.shape
```

```
(8, 8, 4)
```

```
plt.matshow(scat[:,:,0], cmap='viridis', norm=LogNorm())
plt.title("$P_0$ scattering")
plt.colorbar();
```



```
scat[3,3,:]
```

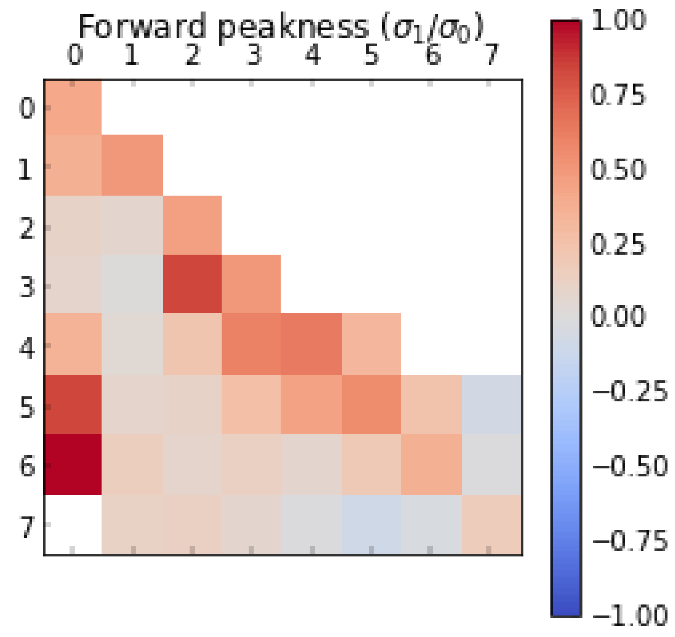
```
array([0.06847651, 0.03386217, 0.01825174, 0.00616768])
```

A scattering cross section that's perfectly forward-peaked

$$\sigma_s(\mu) = \delta(\mu - 1)$$

will have $\sigma_0 = \sigma_1 = \sigma_2 = ...$

```
plt.matshow(scat[:,:,1] / np.ma.masked_equal(scat[:,:,0], 0.0), cmap='rb_linear',␣
↪norm=Normalize(-1,1))
plt.title(r"Forward peakness ($\sigma_1 / \sigma_0$)")
plt.colorbar();
```

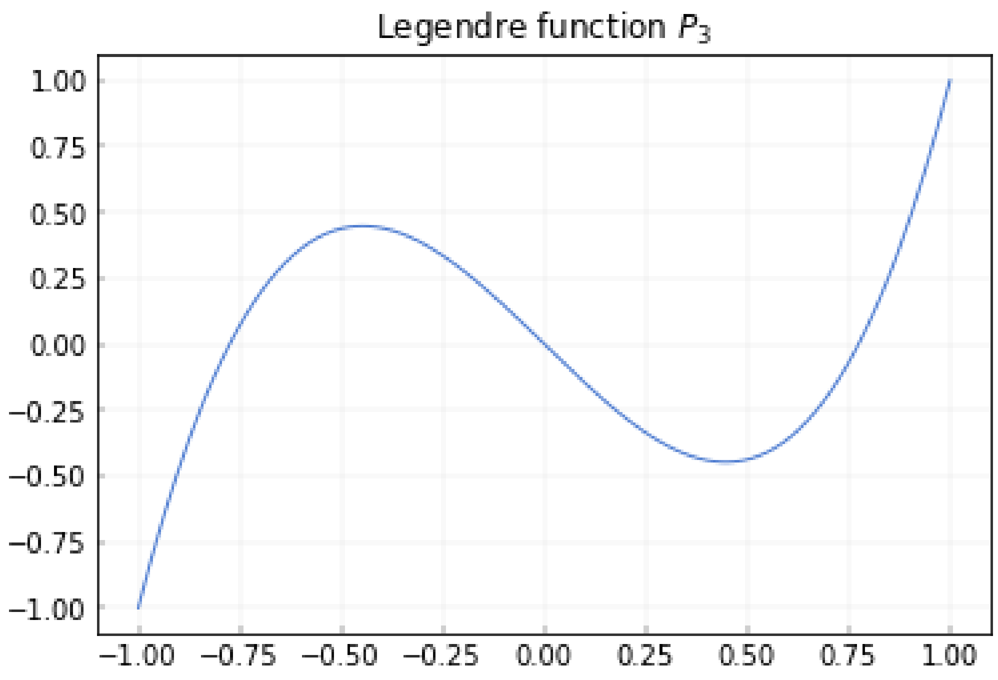


Legendre coefficents

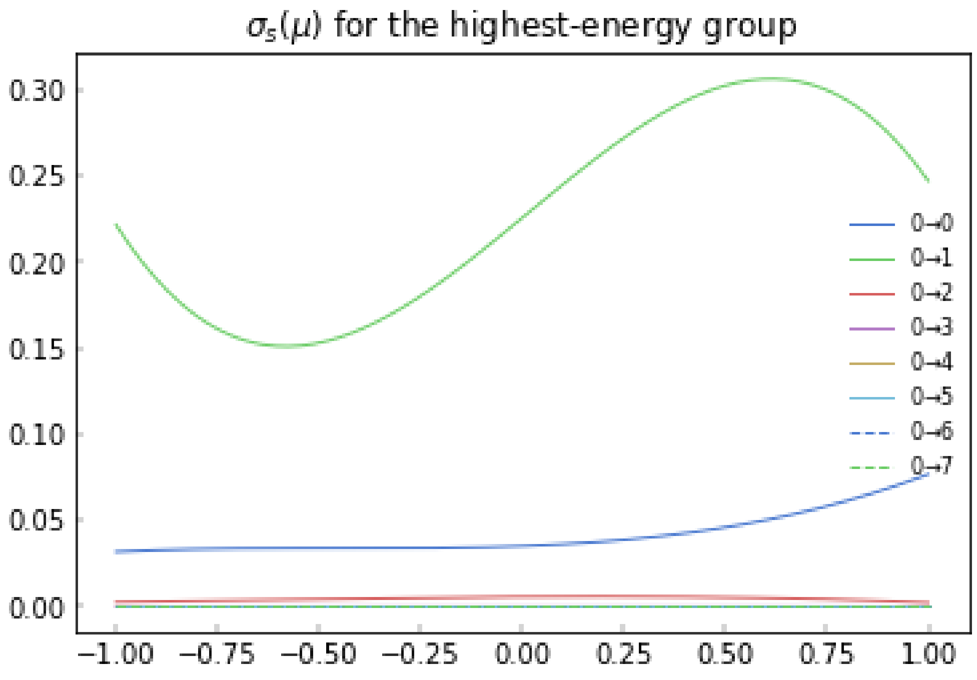
The numpy package has a function for evaluating a Legendre series at a series of points. This allows us to easily visualize the reconstructed scattering as a function of angle.

```
from numpy.polynomial.legendre import legval
x = np.linspace(-1, 1, 128)

def plot_legendre(ax, coeffs, norm=False, **kwargs):
    if norm:
        coeffs = coeffs / coeffs[0]
    ax.plot(x, legval(x, coeffs), **kwargs)
    #ax.set_ylim(-1, 1)
    ax.grid()
    return ax
```

```
(fig, ax) = plt.subplots()
plot_legendre(ax, [0,0,0,1]);
ax.set_title("Legendre function $P_3$");
```



```
g = 0
(fig, ax) = plt.subplots() # subplot_kw=dict(yscale='log'))

# Loop through all the outscatter groups for the highest-energy xs
for gp in range(8):
    plot_legendre(ax, scat[gp, g, :], label=r'${:d} \to {:d}$'.format(g,gp))
ax.legend();
ax.set_title(r'$\sigma_s(\mu)$ for the highest-energy group');
```



A.3.2 INFINITE-MEDIUM CRITICALITY SEARCH

Simple linear algebra can solve for the k_{eff} of an infinite homogeneous medium given multigroup cross sections. This advanced example ties together some low-level Exnihilo utilities (in Robus and Transcore) with python packages `numpy` and `scipy`.

This example's objective is to determine a critical homogeneous mixture of 5%-enriched UO_2 and water. The final result will be a composition that can then be used for unit testing.

```
# Set up example
%matplotlib inline
%load_ext wurlitzer
from exnihilotools.matplotlib import screen_style
screen_style()
```

A.3.2.1 Construct compositions

There are some utility functions in Exnihilo that build UO_2 compositions and can calculate mixtures.

```
from robus import (Composition, Comp_Mixer, NEUTRON, TOTAL, SCATTERING, FISSION, NU_
↪FISSION,
                   Nuclide_Metadata as NMD)

NMD.load_SCL()

temperature = 300.0
density = 10.257
enrichment_pcwt = 5.0
uo2 = Comp_Mixer.get_enriched_uo2(temperature, density, enrichment_pcwt)

density = 1.0
h2o = Composition(temperature, density, [1001, 8016],
            [0.11191539275728472, 0.8880846072427153]);
```

```
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
```

```
MIX_DENSITY = 2.0 # Irrelevant for infinite medium
def mix(fuel, mod, frac_fuel):
    return Comp_Mixer.mix(MIX_DENSITY, fuel, mod, frac_fuel, Comp_Mixer.MIX_BY_WEIGHT)

mixture = mix(uo2, h2o, frac_fuel=0.5)
mixture._asdict()
```

```
{'name': '',
 'matid': 3,
 'temperature': 300.0,
 'density': 2.0,
 'fissionable': True,
 'depletable': True,
 'zaid': array([ 1001,  8016, 92234, 92235, 92236, 92238], dtype=uint32),
 'wtfrac': array([5.59576964e-02, 5.03307698e-01, 1.96126900e-04, 2.20367303e-02,
       1.01368959e-04, 4.18400380e-01])}
```

A.3.2.2 Calculating k of a composition

The multigroup approximation allows k-effective of a homogeneous composition to be calculated straightforwardly by explicitly constructing a matrix whose largest eigenvalue is k. The first step of this process is to use SCALE's XSProc code via the `XS_Builder_Fulcrum` class to collapse an eight-group test library into a homogeneous set of cross sections, which are then converted into native `numpy` arrays.

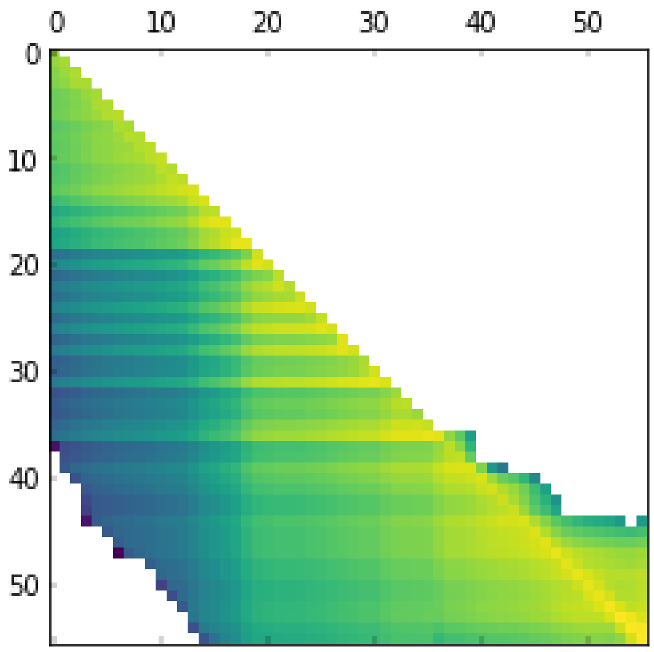
```
from nemesis import Std_DB, make_view, make_const_view
import transcore
import numpy as np

# Set up the builder
db = Std_DB.from_dict({
    'Pn_order'    : 0,
    'xs_library' : "v7-56",
    'downscatter': False})
builder = transcore.XS_Builder_Fulcrum(db)
builder.add(0, mixture)

# Generate and retrieve cross sections
builder.build()
bounds = builder.group_bounds.group_bounds(NEUTRON)
mats = builder.get_materials()
mixture_xs = mats.get_material(0)

# Extract cross sections as native Python objects
sigma_t = np.asarray(mixture_xs.sigma)
sigma_s = np.asarray(mixture_xs.scatter_matrix)[:,:,0] # P0 moments of scattering matrix
nu_sigma_f = np.asarray(mixture_xs.sigma_x(NU_FISSION))
chi = np.asarray(mixture_xs.chi)
```

```
>>> Loading AMPX library at '/usr/local/scale/data/scale.rev04.xn56v7.1'
>>> Retained 6 of 457 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
```

```
from exnihilotools.matplotlib.artists import plot_multigroup
from exnihilotools.matplotlib.axes import grid_groups, annotate_groups
```

Here is the scattering matrix:

```
import matplotlib.pyplot as plt
from matplotlib.colors import LogNorm
plt.matshow(sigma_s, norm=LogNorm());
```



The multigroup neutron balance equation (with fission and no extraneous source) is:

$$\Sigma_{t,g}\phi_g = \sum_{g'=0}^{G-1} \Sigma_{s,g'\to g}\phi_{g'} + \frac{1}{k}\chi_g \sum_{g'=0}^{G-1} \nu\Sigma_{f,g'}\phi_{g'} \,,$$

which can be written as the linear algebra equation

$$T\Phi = S\,\Phi + \frac{1}{k}\chi f^T \Phi \,,$$

where $f^T\Phi$ is the fission source strength density (a scalar), S is the scattering matrix, and T is diag(Σ_t).

Simple manipulations yield an explicit eigenvalue equation

$$k\Phi = (T - S)^{-1}\chi f^T \Phi \,.$$

The following code constructs the right-hand-side matrix and solves for its eigenvalues:

```
t_minus_s = (np.diag(sigma_t) - sigma_s)
chi_nusig = np.outer(chi, nu_sigma_f)
final_matrix = np.matmul(np.linalg.inv(t_minus_s), chi_nusig)
(all_k, all_phi) = np.linalg.eig(final_matrix)
```

```
def max_eigenvalue(all_k, all_phi):
    # Find k-eff
    k_idx = np.argmax(all_k)
    k = all_k[k_idx].real
    # Get the corresponding eigenvector and make sure it's positive
    phi = all_phi[:,k_idx].real
    if np.min(phi) < 0 and np.max(phi) <= 0:
        phi *= -1
```

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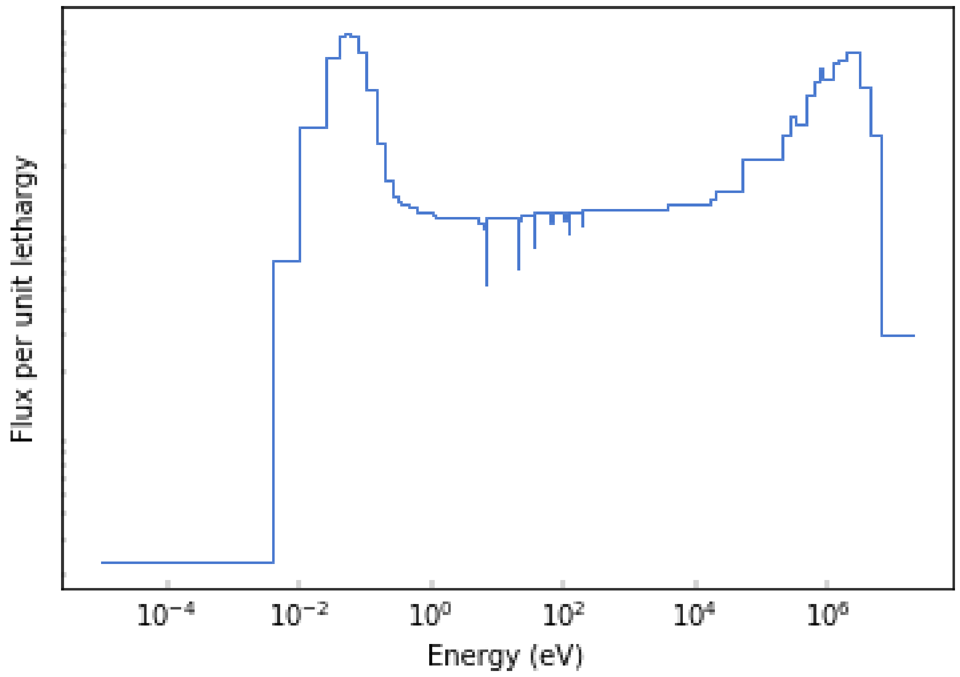
```
    return (k, phi)

(k, phi) = max_eigenvalue(all_k, all_phi)
```

```
print("K-eff is", k)
```

```
K-eff is 1.3696586943136313
```

```
delta_lethargy = -np.diff(np.log(bounds))
(fig, ax) = plt.subplots(subplot_kw=dict(xscale='log', yscale='log'))
plot_multigroup(ax, bounds, phi / delta_lethargy)
ax.set_xlabel('Energy (eV)')
ax.set_ylabel('Flux per unit lethargy')
ax.set_yticks([])
ax.set_yticklabels([]);
```



A.3.2.3 Finding criticality

The above process successfully calculates the eigenvalue (k_{eff}) and eigenvector (flux spectrum) given a single scalar, the fuel fraction. It is condensed below into a single function `calc_k`, which is the workhorse of a function `calc_reactivity` that gives the reactivity,

$$\rho = \frac{k-1}{k},$$

as a function of the fuel fraction. Solving for the single root $\rho = 0$ is therefore solving for the critical fuel fraction.

Using an 8-group test library instead of the 56-group library above substantially reduces the calculation time.

```
db = Std_DB.from_dict({
    'Pn_order'    : 0,
    'xs_library' : "test-8grp",
    'downscatter': False})

def calc_k(frac_fuel):
    mixture = mix(uo2, h2o, frac_fuel=frac_fuel)
    builder = transcore.XS_Builder_Fulcrum(db)
    builder.add(0, mixture)

    # Generate and retrieve cross sections
    builder.build()
    bounds = builder.group_bounds.group_bounds(NEUTRON)
    mats = builder.get_materials()
    mixture_xs = mats.get_material(0)

    # Get cross sections as numpy objects
    sigma_t = np.asarray(mixture_xs.sigma)
    sigma_s = np.asarray(mixture_xs.scatter_matrix)[:,:,0] # P0 moments of scattering␣
↪matrix
    nu_sigma_f = np.asarray(mixture_xs.sigma_x(NU_FISSION))
    chi = np.asarray(mixture_xs.chi)

    # Construct fission-transport matrix
    t_minus_s = (np.diag(sigma_t) - sigma_s)
    chi_nusig = np.outer(chi, nu_sigma_f)
    final_matrix = np.matmul(np.linalg.inv(t_minus_s), chi_nusig)

    # Calculate eigenvalue and eigenvector
    (all_k, all_phi) = np.linalg.eig(final_matrix)
    return max_eigenvalue(all_k, all_phi)
```

```
def calc_reactivity(frac_fuel):
    if frac_fuel <= 0:
        k = 0
        rho = -np.inf
    elif frac_fuel >= 1:
        k = rho = np.inf
    else:
        assert not np.isnan(frac_fuel)
        (k, _) = calc_k(frac_fuel)
        rho = (k - 1.0) / k
    print("{frac_fuel:f} fuel -> k={k:.5f} (rho={rho:g})".format(**locals()))
    return rho
```

Finally, we use the optimization toolkit from scipy to find the root, giving our final answer.

```
from scipy.optimize import root_scalar

result = root_scalar(calc_reactivity, method='brentq', bracket=(0,1), x0=0.5, rtol=1e-4)
print(result)
frac_fuel = result.root
```

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```
print("Final fuel fraction:", frac_fuel)
```

```
0.000000 fuel -> k=0.00000 (rho=-inf)
1.000000 fuel -> k=inf (rho=inf)
0.500000 fuel -> k=1.47630 (rho=0.322633)
```

```
>>> Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
>>> Retained 6 of 449 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
>>> Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
>>> Retained 6 of 449 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
```

```
0.250000 fuel -> k=1.03433 (rho=0.0331943)
0.125000 fuel -> k=0.64392 (rho=-0.552994)
0.242922 fuel -> k=1.01642 (rho=0.016158)
```

```
>>> Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
>>> Retained 6 of 449 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
>>> Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
>>> Retained 6 of 449 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
>>> Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
>>> Retained 6 of 449 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
```

```
0.236399 fuel -> k=0.99956 (rho=-0.000440535)
0.236572 fuel -> k=1.00000 (rho=1.41172e-06)
0.236560 fuel -> k=0.99997 (rho=-3.22038e-05)
      converged: True
           flag: 'converged'
 function_calls: 9
     iterations: 8
           root: 0.23657180483813495
Final fuel fraction: 0.23657180483813495
```

```
>>> Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
>>> Retained 6 of 449 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
>>> Loading AMPX library at '/usr/local/scale/data/test8g_v7.1'
>>> Retained 6 of 449 nuclides on the master AMPX library
>>> Running XSProc on 1 cells
```

The final answer, the critical fuel mixture, is thus:

```
mix(uo2, h2o, frac_fuel=frac_fuel)._asdict()
```

```
{'name': '',
 'matid': 11,
 'temperature': 300.0,
 'density': 2.0,
 'fissionable': True,
 'depletable': True,
 'zaid': array([ 1001,  8016, 92234, 92235, 92236, 92238], dtype=uint32),
 'wtfrac': array([8.54393663e-02, 7.06029871e-01, 9.27961893e-05, 1.04265381e-02,
        4.79620753e-05, 1.97963466e-01])}
```

A.4 SHIFT

A.4.1 DEBUGGING GEOMETRY PROBLEMS IN SHIFT

It is not unusual to make an error when constructing a geometry model. This example gives a few useful procedures for tracking down geometry errors.

```
# Set up example environment
import os
from exnihilotools.matplotlib import screen_style
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
%matplotlib inline
screen_style()
```

A.4.1.1 Construct compositions via the SCL

Since this test geometry is a Geometria XML input, it doesn't natively support composition definitions. Here is one of the many ways to define compositions: loading them using the `robus` Python wrappers from the SCALE standard composition library, and then writing them to an HDF5 file which is then specified in the Omnibus input.

```
from robus import (Composition, load_scl_compositions, load_hdf5_compositions, save_hdf5_
↪compositions)

# Load the compositions into a dictionary (the method returns a vector of Composition␣
↪objects)
scl_comps = dict((c.name, c) for c in load_scl_compositions())
# Display a couple of them in alphabetical order
print(sorted(scl_comps.keys())[:5])
```

```
['al2o3', 'b4c', 'balsa', 'benzene', 'beo']
```

```
# Pick a few compositions
export_comps = [scl_comps[k] for k in ["dry-air", "ss304", "water"]]
# Dump them to an HDF5 file
save_hdf5_compositions(os.path.join(SOURCE_DIR, "data", "buggy.comp.h5"), export_comps)
```

A.4.1.2 Run Shift through Omnibus

With a pre-constructed (but broken) geometry file, an Omnibus input file, and the set of compositions just generated, Omnibus can be run to see what happens.

```
%cat {SOURCE_DIR}/data/buggy.omn
!omnibus-run {SOURCE_DIR}/data/buggy.omn
```

```
[PROBLEM]
name "Buggy geometry"
mode forward

[MODEL=gg]
input "buggy.gg.omn"

[COMP]
! Note: this file should be generated automatically by the example
input "buggy.comp.h5"

[PHYSICS=ce]
ce_lib "ce_v7.1_endf"

[SOURCE=separable beam_point]
[SOURCE][SHAPE=point]
point -3 -2 0
[SOURCE][ANGLE=mono]
dir 1 0 0
[SOURCE][ENERGY=mono]
energy 14e6
particle_type n

[TALLY]
[.][DIAGNOSTIC=debug_history]
! [..][DIAGNOSTIC=history]
[..][MESH global_mesh]
reactions flux
x -4 7i 4
y -4 7i 4
z -4 7i 4

[SHIFT]
np 100

[RUN=serial]
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/buggy.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
Generating Geometria XML input file from .gg.omn...
INFO: Starting Geometria preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/buggy.gg.omn
```

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```
            ...finished loading problem db from Omnibus ASCII file
INFO: Writing Geometria input ParameterList to buggy.gg.xml
            ...finished generating Geometria XML input file from .gg.omn
INFO: Set default for 'fissionable_only' to 'False' in '/source/beam_point'
INFO: Set default for 'mode' to 'n' in '/physics/ce'
INFO: Set default for 'xs_cache' to 'tot' in '/physics/ce'
INFO: Set default for 'xs_accel' to 'True' in '/physics/ce'
INFO: Set default for 'fission_neutrons' to 'True' in '/physics/ce/fission'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'decomposition' to '{'_type': 'none'}' in '/shift'
INFO: Set default for 'verbosity' to 'low' in '/shift/transporter'
INFO: Set default for 'method' to 'roulette' in '/shift/vr'
INFO: Writing Omnibus input ParameterList to buggy.inp.xml
INFO: Writing preprocessed file to buggy.pp.json
INFO: Writing processed ASCII input to 'buggy.inp.omn'
INFO: Launching Omnibus driver on 1 cores
Running Omnibus...
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
 ↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
 ↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
 ↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
 ↪sclib
INFO: Loading compositions from /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
 ↪example/data/buggy.comp.h5
INFO: Creating default boundary mesh from (-4 -4 -4) to (4 4 4) for GG geometry
Building physics 'ce'
INFO: Loading CE library /usr/local/scale/hpcdata/ce_v7.1_endf.h5
WARNING: The following nuclide IDs were remapped due to missing neutron data
WARNING: Remapped 2 nuclide IDs: 6012->6000, 6013->6000
WARNING: The following neutron cross sections were set to zero: 8018
INFO: Corrected thermal xs balance: 1.2e-05% error in h-1 @ 293.6K
Building tallies
Building sources
Building Shift solver internals
Building Shift sources
Initializing Shift solver
Building Shift tallies
Running Shift transport calculation
ERROR: Geometry error in particle 0:0: In universe 'global': Failed to move from left␣
 ↪(local volume #0) across left.s (local surface #1) at local point {0.5,-2,0} along {1,
 ↪0,0}: possible neighbors are {left (#0), fill (#2)}, possible nearby volumes are {left␣
 ↪(#0), right (#1), fill (#2), EXTERIOR (#3)}
ERROR: Geometry error in particle 0:1: In universe 'global': Failed to move from left␣
 ↪(local volume #0) across left.s (local surface #1) at local point {0.5,-2,0} along {1,
 ↪0,0}: possible neighbors are {left (#0), fill (#2)}, possible nearby volumes are {left␣
 ↪(#0), right (#1), fill (#2), EXTERIOR (#3)}
FATAL ERROR: Input validation failed:
FATAL ERROR: Lost too many particles (2) locally
```

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```
FATAL ERROR: ^^^ at /rnsdhpc/code/src/scale/Exnihilo/packages/Shift/mc_transport/inst_gg_
↪sce/../DR_Source_Transporter.t.hh:374
Cleaning up
            ...failed while running Omnibus after 2.0 seconds
INFO: Omnibus run failed; printing log since the last successful status message
INFO:
*************************      OMNIBUS ERROR LOG       *************************
::: Cleaning up
*************************        END ERROR LOG         *************************

FATAL ERROR: An unexpected error occurred. Please check the log file at omnibus_2020-03-
↪11-223747.log for more details.
FATAL ERROR: Command '/rnsdhpc/code/build/Exnihilo-examples/Exnihilo/packages/Omnibus/
↪driver/omnibus buggy.inp.xml' returned non-zero exit status 1.
```

A.4.1.3 Understanding the error message

Oops! Too many particles encountered geometry errors, so the problem aborted. The first thing to do is to try to understand the error message.

```
!!! Geometry error in particle 0:0: In universe 'global': Could not find the volume
connecting volume 0 (left) across surface 2 (right.s) at local point 0.5 -2 0 along
{1 0 0}: neighbors are {0, 2}, bounding volumes are {0, 1, 2, 3}
 ^^^ at {0.5 -2 0} along {1 0 0}
```

The first thing to note is the particle identification: `3:15` means the 16th history on the 4th Shift thread being run. Since Omnibus error messages use C indexing, `0:0` means the very first particle to be transported on the only instance of Shift.

Shift indicated a problem with the geometry as opposed to the CE data or physics options that were set. Since this problem uses GG as the geometry model, the error message also provides contextual details of how the error occurred, which can be compared to the provided geometry:

```
%cat {SOURCE_DIR}/data/buggy.gg.omn
```

```
[GEOMETRY]
global "global"

[UNIVERSE=general global]
interior -outer

[UNIVERSE][SHAPE=sphere outer]
radius 4

! Overlapping left and right spheres
[UNIVERSE][SHAPE=sphere left]
radius 1.5
origin -1 -2 0
[UNIVERSE][SHAPE=sphere right]
radius 1.5
origin  1 -2 0
```

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```
! Cell definitions
[UNIVERSE][CELL left]
comp water
shapes -left
[UNIVERSE][CELL right]
comp ss304
shapes -right
[UNIVERSE][CELL fill]
comp "dry-air"
shapes +left +right -outer
```

The message says it's a problem connecting the cell named "left" with the surface named "right.s" (which we can guess is the spherical surface created by the "right" sphere shape). It shows the point in space and direction of travel; and if this error had happened inside of a daughter universe (such as an assembly in a reactor), the positions both in local space and global problem space would be presented.

The other information about neighbors and bounding volumes is not immediately useful because it only provides internal IDs for those cells rather than names that you the user input. However, the Omnibus Python front end tools can help translate thse cell IDs. (Note that since the GG input file does not provide a mapping between composition names and internal IDs, an explicit `compositions` argument must be passed to the `load_gg` call.)

```
from omnibus.raytrace.load import load_gg
model = load_gg(os.path.join(SOURCE_DIR, "data", "buggy.gg.omn"),
                compositions=load_hdf5_compositions(os.path.join(SOURCE_DIR, "data",
↪"buggy.comp.h5")))
```

```
Generating Geometria XML input file from .gg.omn...
            ...finished generating Geometria XML input file from .gg.omn
```

The resulting model contains the geometry, compositions, and (for some geometry/model types) other data such as tallies. In this case, the only concern is the geometry. The generic "describe" function will print a detailed description of the geometry's structure.

```
print(model.geometry.describe())
```

```
****************************************
GG Geometry Description
****************************************

Source file: ``buggy.gg.xml``

Geometry construction/tracking tolerances and options:

 - Length scale: 1 cm

 - Surface elision: 1e-08

 - Surface simplification: 1e-08 cm
```

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```
 - Shape enclosure: 1e-08

 - Bounding box expansion: 1e-07

 - Almost-lost particle bump: 1e-08 cm

 - Fast geometry shortcuts are enabled.

Note that volumes are described in [Reverse Polish Notation]
(https://en.wikipedia.org/wiki/Reverse_Polish_notation), where
'~' is the negation operator, '&' is the intersection/and
operator, and '|' is the union/or operator.

************************************************
global: General universe
************************************************
:# Cells:      4 (offset = 0)
:# Surfaces:   3 (offset = 0)
:Bounding box: ``{-4 -4 -4 to 4 4 4}``

Volumes (local indexing):

======= ======== ================================================
ID      Name     Surface logic
======= ======== ================================================
0       left     1 ~
1       right    2 ~
2       fill     0 ~ 1 & 2 &
3       EXTERIOR 0
======= ======== ================================================

Surfaces:

======= ======= ================================================
ID      Name    Description
======= ======= ================================================
0       outer.s Sphere: r=4
1       left.s  Sphere: r=1.5 at -1 -2 0
2       right.s Sphere: r=1.5 at 1 -2 0
======= ======= ================================================

Material fills:

======= ========================= =========================
Cell ID Name                      Fill
======= ========================= =========================
0       left                      matid 2
1       right                     matid 1
2       fill                      matid 0
3       EXTERIOR                  EXTERIOR
======= ========================= =========================
```

From this diagnostic description, it is clear that the only “neighbor” for volume 0 (`left`) is volume 2 (`fill`), but the failed particle tries to cross a surface `right.s`. In other words, the left and right cells are not connected but the particle crosses the “right” sphere while inside the left. We examine the input and notice that the two spheres overlap. Excluding the right sphere from the left one (or separating the spheres or reducing their size) will fix the problem.

A.4.1.4 Post-mortem analysis of problem run

For more sinister cases in which the error only occurs after some other sequence of events, or for geometry types that don’t provide as much useful debugging information as GG, another diagnostic tool may prove useful: the history tally.

Fortunately, the input already has a `debug_history` diagnostic although if it did not, it could be simply added and the problem run again to get the same error, since Shift is reproducible on the same number of processors when domain replicated.

The `debug_history` option keeps a rolling list of all particle events on all processors, and if the particle dies because of an error (usually a geometry error), an HDF5 file will be written with that particle’s history. Otherwise, or for successfully transported particles, no history will be output. Thus, for histories where no error occurs, the performance impact of the diagnostic will be minimal: no I/O is occurring, and little to no data is even being allocated.

The erroneous history files are saved to files named `debug_history-pNNNN.h5`, where `NNNN` is the process that failed (in this case just zero). The easiest and clearest way to visualize the output is with the convenience function `to_frame` that returns the data as a Pandas dataframe.

```python
from omnibus.formats.debug_history import load as load_debug_history

hist_file = load_debug_history("./debug_history-p0.h5")
hist_file['histories'].to_frame()
```

```
Loading HDF5 file...
INFO: Loaded DebugHistoryDiagGroup data from './debug_history-p0.h5'
            ...finished loading HDF5 file
```

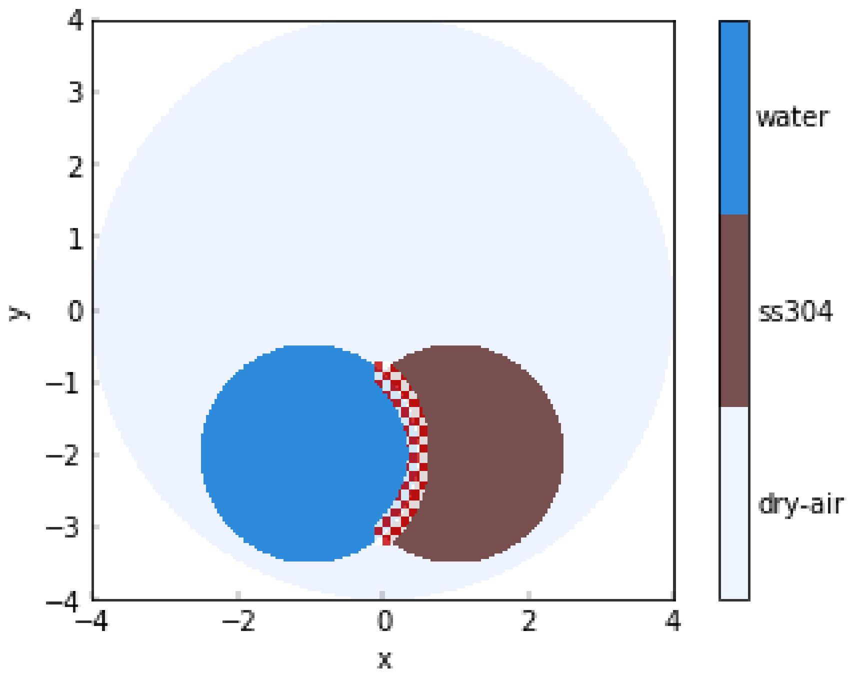
A.4.1.5 2D raytracing through Python

Visualizing the erroneous part of the geometry is also an extremely useful tool. By default, the ray tracer enables error checking.

```python
from omnibus.raytrace.colors import ColorMap
from omnibus.raytrace.imager import Imager

colors = ColorMap.from_compositions(model.compositions)
imager = Imager.from_extents(model.geometry, z=0.0, max_pixels=512)
imager.names = [c.name for c in model.compositions]
imager.colors = colors
imager.plot();
```

```
WARNING: Geometry errors were encountered
```



Note the checkered white and red area in the plot indicating the erroneous boundary. The actual exception messages (describing in detail the geometry errors) are printed to the terminal rather than this notebook. However, the error message (similar to the one seen during transport) is visible by disabling error checking on the plotter:

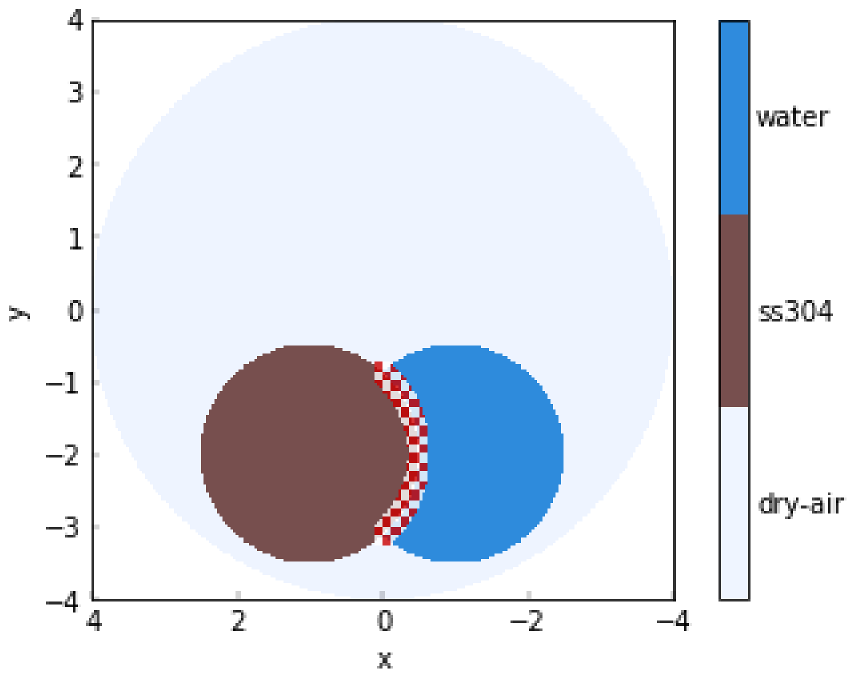
```
imager.check_errors = False
try:
    imager.plot()
except RuntimeError as e:
    print("Oops!", e)
```

```
Oops! In universe 'global': Failed to move from left (local volume #0) across left.s␣
↪(local surface #1) at local point {0.000945598,-0.882813,0} along {1,0,0}: possible␣
↪neighbors are {left (#0), fill (#2)}, possible nearby volumes are {left (#0), right (
↪#1), fill (#2), EXTERIOR (#3)}
 ^^^ at {0.0009455978442431196,-0.882812500000009,0} along {1,0,0}
```

More information on the error can be gleaned by seeing how the geometry appears when tracing rays in the opposite direction. To do that, a second Imager is constructed with a `basis` vector opposite from the default $(1, 0, 0)$:

```
imager = Imager(model.geometry, (4,-4,0), (-4,4,0), basis=(-1,0,0), max_pixels=512)
imager.names = [c.name for c in model.compositions]
imager.colors = colors
imager.plot();
```

```
WARNING: Geometry errors were encountered
```



Again the plot shows the erroneous region. Since the basis vector is reversed, so is the *x* axis. Note that comparing to the previous plot shows that the overlap between the two circles appears to be a different material depending on the particle's direction of travel.

A.4.1.6 Detailed geometry debugging

One final tool for finding and debugging geometry errors is the `GG_Debugger` class. (For MCNP geometries, use `Lava_Debugger`.) Since these tools by default use the C cout/cerr pipes to print, the wurlitzer[23] tool is needed to redirect terminal output to this notebook.

```
%load_ext wurlitzer
from geometria import GG_Debugger
ggd = GG_Debugger(model.geometry)
```

We can print detailed information about a particle track through the geometry, including the universes and surface names. If an error occurs, the detail particle state is printed.

```
try:
    ggd.print_track((-4,-2,0), (1,0,0))
except RuntimeError as e:
    print("Caught error:", e)
```

```
Caught error: In universe 'global': Failed to move from left (local volume #0) across␣
↪left.s (local surface #1) at local point {0.5,-2,0} along {1,0,0}: possible neighbors␣
↪are {left (#0), fill (#2)}, possible nearby volumes are {left (#0), right (#1), fill (
↪#2), EXTERIOR (#3)}
 ^^^ at {0.5,-2,0} along {1,0,0}
```

[23] https://github.com/minrk/wurlitzer

```
Tracking from -4 -2 0 along 1 0 0
                    POS        CUR_CELL       CUR_SURF   NEXT_DIST        UNIV           ␣
↪       LOCAL_POS  VOLID SURF_IDX NEXT_IDX
...moved distance 0.535898384862246 to enter geometry
{-3.4641,    -2,     0}            fill        outer.s      0.9641      global{  -3.4641,␣
↪    -2,      0}      2        0        1
{   -2.5,    -2,     0}            left         left.s           3      global{     -2.5,␣
↪    -2,      0}      0        0        0
!!! In universe 'global': Failed to move from left (local volume #0) across left.s␣
↪(local surface #1) at local point {0.5,-2,0} along {1,0,0}: possible neighbors are
↪{left (#0), fill (#2)}, possible nearby volumes are {left (#0), right (#1), fill (#2),␣
↪EXTERIOR (#3)}
 ^^^ at {0.5,-2,0} along {1,0,0}
Failed during surface crossing:
                          POSITION                   DIRECTION                POLARIZATION
Global: {     0.5,     -2,      0}{       1,      0,      0}{       0,     -1,      0}
Local:  {     0.5,     -2,      0}{       1,      0,      0}{       0,     -1,      0}
In cell left (0), matid=2, crossing surface left.s (1)
==================== ======= ==============
UNIVERSE             VOL ID  CELL LABEL
==================== ======= ==============
global               0       left
==================== ======= ==============

Current volume state for volume ID = 0:
  Surface IDs: 1
  Senses:     {-}
  Current and next surface index: 0 -> 0
```

A.4.2 SHIFT DEPLETION WITH MOVABLE CONTROL RODS

This example demonstrates how to run and post-process a Shift depletion run using an MCNP model with movable elements.

```
# Set up example environment
import os
from exnihilotools.matplotlib import screen_style
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
%matplotlib inline
screen_style()
```

A.4.2.1 Previsualization

Before running the problem, it is useful to render the input geometry for verification. Note that the different fuel regions (all initially the same composition, but with unique material IDs) are automatically assigned slightly different shades of red by the `ColorMap`'s constructor.

```
from omnibus.raytrace.load import load_mcnp
from omnibus.raytrace.colors import ColorMap
from omnibus.raytrace.imager import Imager

model = load_mcnp(os.path.join(SOURCE_DIR, "data", "movable.mcnp"))
```

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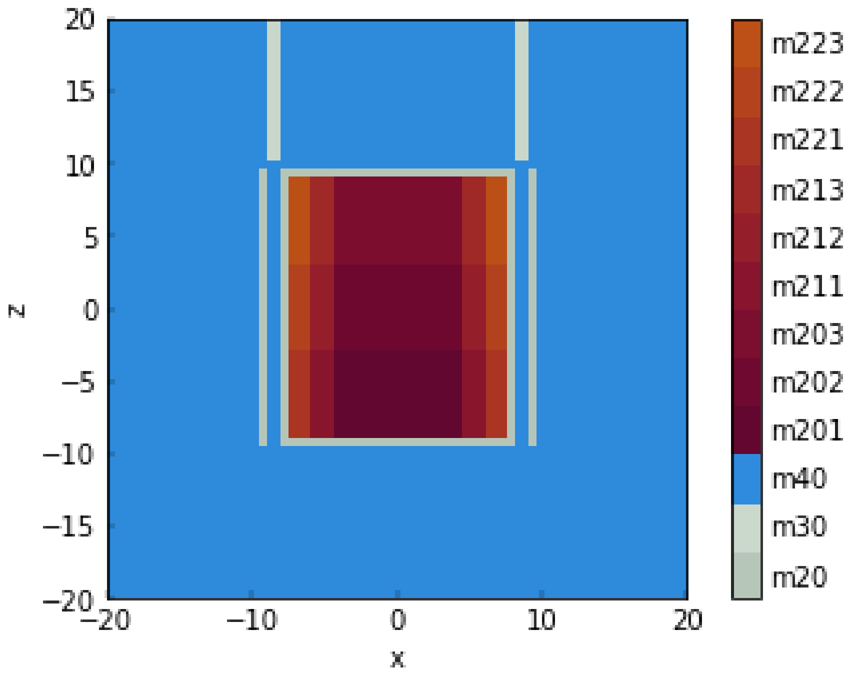
```
colors = ColorMap.from_compositions(model.compositions)
colors[colors.unassigned] = 'Set3'
imager = Imager(model.geometry,
                lower=(-20, 0, -20),
                upper=(20, 0, 20),
                basis=(1, 0, 0),
                max_pixels=1024)
imager.names = [c.name for c in model.compositions]
imager.colors = colors
imager.plot();
```

```
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file in 2.8 seconds
```



The model's composition data can be used to plot number densities in the reactor. The first step in such a visualization is extracting number densities and their corresponding nuclide IDs from the model's compositions. Note that `zaid` returns a view (which for efficiency we translate into a `numpy` array), whereas `calc_nd` returns a vector that is automatically translated to a native python object.

```
import numpy as np

def calc_number_densities(comp):
    return dict(zip(np.asarray(comp.zaid).tolist(), comp.calc_nd()))

def calc_mass_densities(comp):
    zaid = np.asarray(comp.zaid)
    wt   = np.asarray(comp.get_wt_fractions()) * comp.density
    return dict(zip(zaid.tolist(), wt.tolist()))
```

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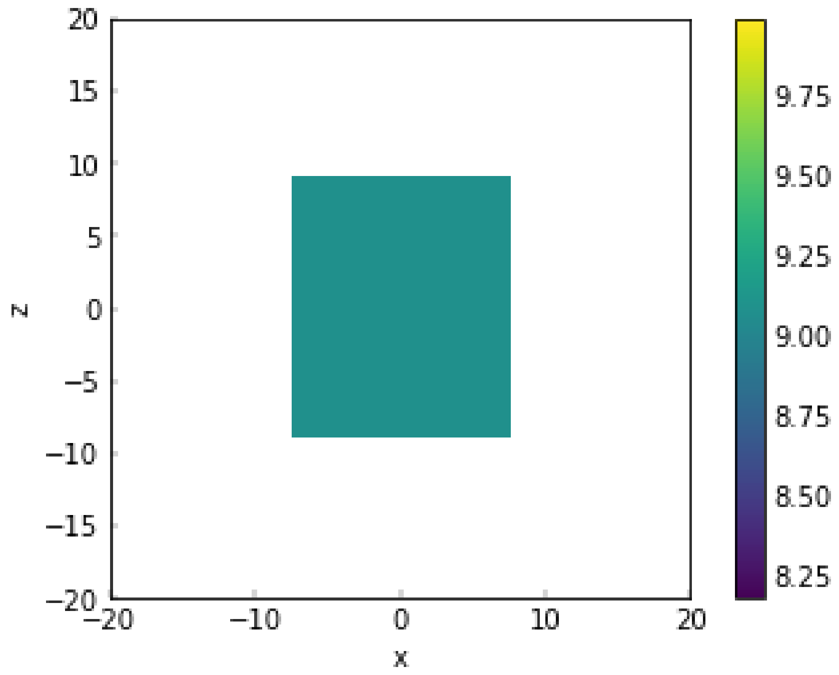
```
densities = [calc_mass_densities(c) for c in model.compositions]
densities[10]
```

```
{1001: 0.06633015932148201,
 8016: 0.5422080954790859,
 92235: 9.085977478992715,
 92238: 0.6606715344205284}
```

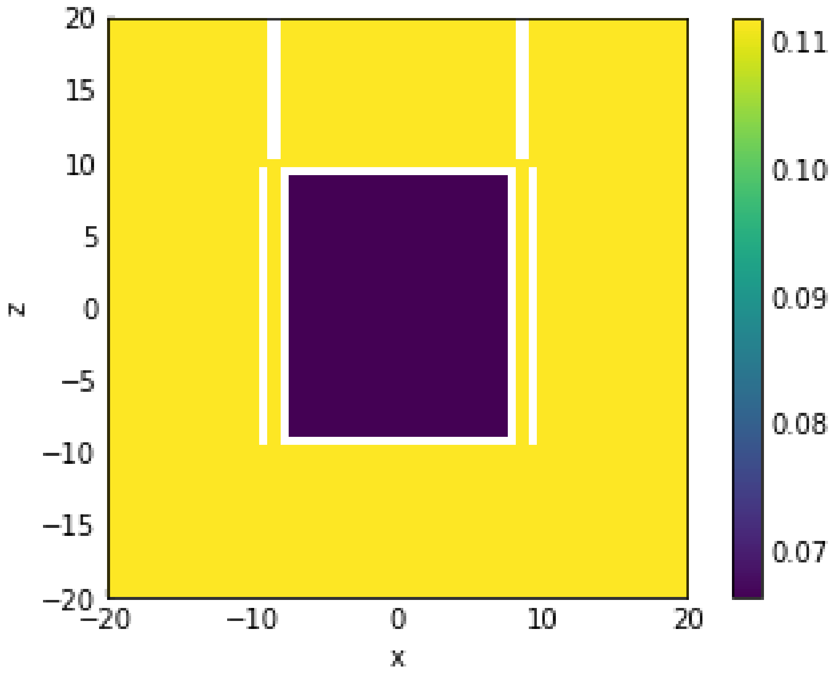
The next step is to extract a particular nuclide's densities for every pixel's matid in the raytrace's view. This requires a Numpy array of values for each matid. Using `np.nan` instead of 0.0 means the value will be hidden rather than rendered as a zero-value, making it more obvious which parts of the problem have trace nuclides as opposed to none of the nuclide. The `pcolor` method of the Imager will render an image where the value of each pixel is calculated from the index in the `pcolor` argument vector corresponding to the material ID at that pixel.

```
def get_dens(zaid):
    return np.array([d.get(zaid, np.nan) for d in densities])

u235 = get_dens(92235)
assert u235[10] == densities[10][92235]
assert np.isnan(u235[0])

imager.pcolor(u235);
```



Here is the mass density plot for hydrogen:

```
imager.pcolor(get_dens(1001));
```



With a little code, it is possible to automate the rendering of *all* the nuclides in the problem:

```
from matplotlib.colors import LogNorm
from matplotlib.offsetbox import AnchoredText
import matplotlib.pyplot as plt
from omnibus.db.validator import to_nuclide

zaids = set()
for d in densities:
    zaids.update(d.keys())

zaid_to_nuclide = to_nuclide.zaid_to_pretty_nuclide
norm = LogNorm(vmin=0.05, vmax=10.0)

nr = int(np.ceil(np.sqrt(len(zaids))))
fig, axes = plt.subplots(nr, nr, figsize=(9,9))

ijax_iter = np.ndenumerate(axes)
for (zaid, ((i,j), ax)) in zip(sorted(zaids), ijax_iter):
    show_colorbar = (i == 0 and j == 0)

    # Plot the actual densities
    imager.pcolor(get_dens(zaid), ax=ax, colorbar=show_colorbar, norm=norm)

    # Add a nice inset title
    at = AnchoredText(zaid_to_nuclide(zaid),
                      prop=dict(size=8), frameon=True,
                      loc=2)
```

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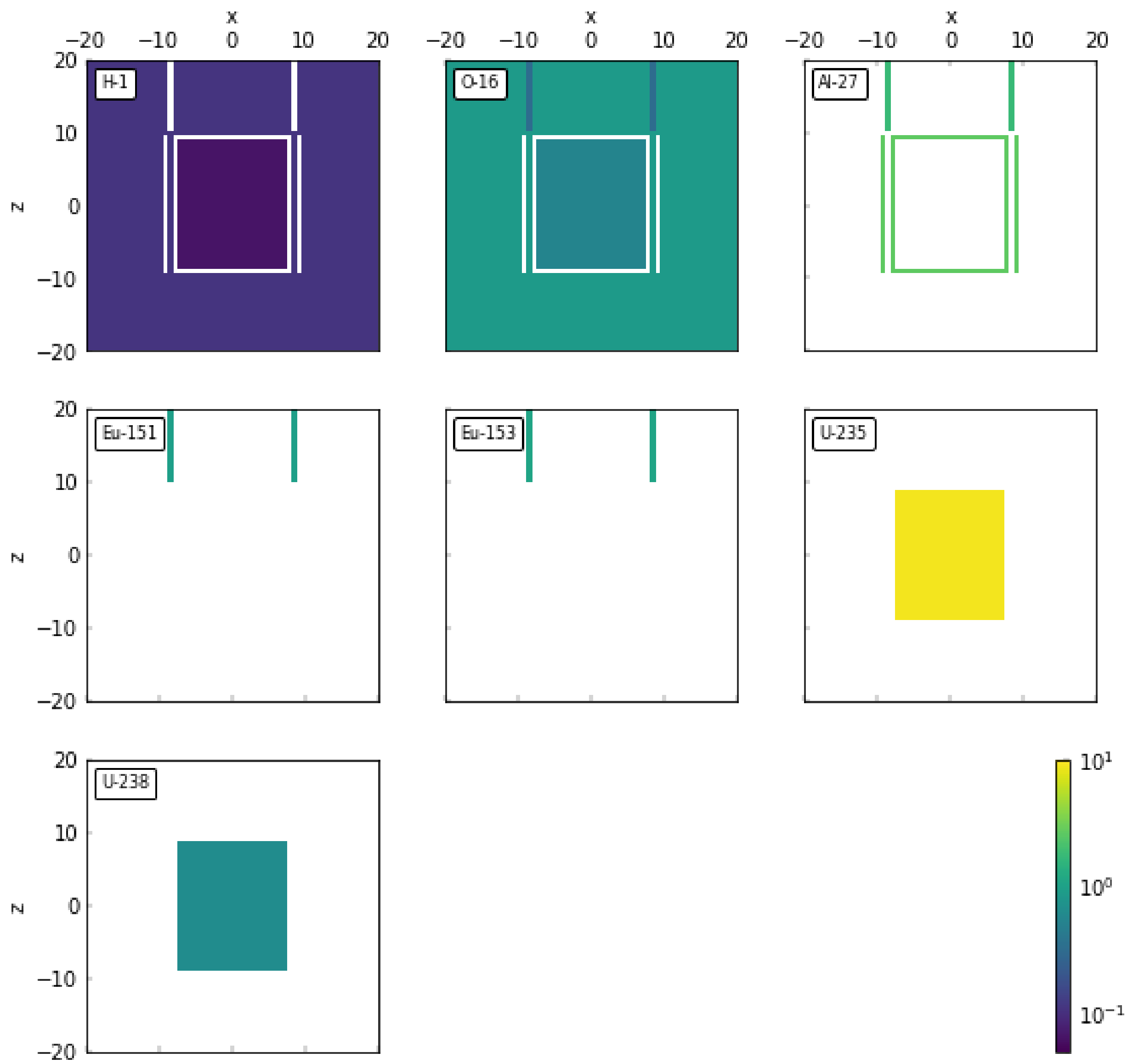
```
    at.patch.set_boxstyle("round,pad=0.,rounding_size=0.2")
    ax.add_artist(at)

    # Hide tick labels if it's not the outermost plot on the upper left
    if i == 0:
        ax.xaxis.set_label_position('top')
        ax.xaxis.set_ticks_position('top')
    else:
        ax.set_xlabel("")
        ax.set_xticklabels([])

    if j != 0:
        ax.set_ylabel("")
        ax.set_yticklabels([])

# Clear remaining axes
for ((i,j), ax) in ijax_iter:
    fig.delaxes(ax)
```

```
/usr/local/anaconda3/envs/exnihilo/lib/python3.7/site-packages/matplotlib/colors.
↪py:1028: RuntimeWarning: invalid value encountered in less_equal
  mask |= resdat <= 0
```



A.4.2.2 Execute Omnibus

The following Omnibus depletion input transports on this model with four kcode solves, using alternating burn/decay steps. Before the first step, the control rod is moved downward by 10 cm; the next time step it is moved upward by 5 cm.

```
%cat {SOURCE_DIR}/data/movable.omn
!omnibus-run {SOURCE_DIR}/data/movable.omn
```

```
[PROBLEM]
name "Depletion problem with moving control rod"
mode kcode

[MODEL=mcnp]
input "movable.mcnp"
```

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```
extents -100 100 -100 100 -100 100

[MODEL][MOVABLE=surfaces control_rod]
surfaces 1  2

[DEPLETION]
deplete_cells 201 202 203
              211 212 213
              221 222 223
tracking_set "addnux1"  ! TRITON "addnux" set
tracking_nuclides na-23 ! additional nuclides to track
! Decay steps
burn_length : decay_length : power : num_burn_steps : num_decay_steps
    1.0         1.0          0.005         1             1
    1.5         0.7          0.005         1             1
! Write cross sections to HDF5
write_xs true
! Reduce accuracy but reduce run time
predictor_substeps 1
renormalization_method boss

[DEPLETION][MOVE control_rod]
! movement for each time step: -20 is fully inserted, 0 is fully out
delta    -10.0 5.0

[PHYSICS=ce]
ce_lib ce_v71
mode n

[SOURCE=separable fission]
[SOURCE][SHAPE=box]
box -3.25 3.25 -3.25 3.25 -9.0 9.0

[SHIFT]

[.][KCODE]
num_histories_per_cycle 1000
num_cycles 20
num_inactive_cycles 5

[TALLY]
[.][CYLMESH globalcyl]
reactions flux nu_fission
r     0 4.33012702 6.12372436 7.5 9.5 12 20 50
theta 0 3i 1.0
z     -20 -15 -9 5i 9 15 20

[..][CELL fuel]
reactions flux nu_fission
cells 201 202 203
      211 212 213
      221 222 223
```

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```
nbins 1e7 39ilog 1e-3

[RUN=mpi]
np 4
INFO: Starting Omnibus preprocessor, omnibus version 6.3.pre-b10 (branch 'omnibus-doc'
↪#98d73c8e on 2020MAR11)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/movable.omn
            ...finished loading problem db from Omnibus ASCII file
Loading problem db from Python file...
            ...finished loading problem db from Python file
INFO: Set default for 'mpiexec_args' to '['-np', '4']' in '/run'
Generating MCNP runtpe file...
            ...finished generating MCNP runtpe file
INFO: Set default for 'energy' to '{'_type': 'watt'}' in '/source/fission'
INFO: Defaulting Watt spectrum to U-235
INFO: Set default for 'angle' to '{'_type': 'isotropic'}' in '/source/fission'
INFO: Set default for 'fissionable_only' to 'True' in '/source/fission'
INFO: Set default for 'xs_cache' to 'totfisnu' in '/physics/ce'
INFO: Set default for 'xs_accel' to 'True' in '/physics/ce'
INFO: Set default for 'fission_neutrons' to 'False' in '/physics/ce/fission'
INFO: Set default for 'load_scl' to 'True' in '/comp'
INFO: Set default for 'decomposition' to '{'_type': 'none'}' in '/shift'
INFO: Set default for 'verbosity' to 'none' in '/shift/transporter'
INFO: Set default for 'method' to 'roulette' in '/shift/vr'
INFO: Writing Omnibus input ParameterList to movable.inp.xml
INFO: Writing preprocessed file to movable.pp.json
INFO: Writing processed ASCII input to 'movable.inp.omn'
INFO: Launching Omnibus driver on 4 cores
Running Omnibus...
WARNING: The Exnihilo software revision (r540) used to generate the input file differs␣
↪from this version being used to run it (r539).
WARNING: This could cause internal consistency checks to unexpectedly fail, and it could␣
↪even lead to unexpected database value changes.
WARNING: Please check your output very carefully after this run to make sure the␣
↪interpreted values match your input values.
Building model
INFO: Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
INFO: Loading compositions from MCNP input
INFO: Creating default boundary mesh from (-100 -100 -100) to (100 100 100) for MCNP␣
↪geometry
Building physics 'ce'
INFO: Loading CE library /usr/local/scale/hpcdata/ce_v7.1_endf.h5
INFO: Corrected thermal xs balance: 1.2e-05% error in h-1 @ 293.6K
Building tallies
Building sources
Building Shift solver internals
Building Shift sources
Initializing Shift solver
Building depletion solver internals
```

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```
INFO: Using the default VESTA group structure in the depletion tally
Building depletion material data
INFO: Loading ORIGEN library /usr/local/scale/data/origen_library/pwr.rev03.orglib
INFO: Loading fission yield library /usr/local/scale/data/origen_data/origen.rev05.yields.
↪data
INFO: Loading JEFF multigroup library /usr/local/scale/data/origen.rev01.jeff252g
Loading depletion cross sections
INFO: Total initial heavy-metal mass in system: 0.0310027 MT
Building Shift tallies
Solving depletion step 0 from 0 days to 1 days at 0.005 MW
INFO: Moving control_rod by -10 cm
Running Shift transport calculation
Beginning inactive cycles
INFO: Completed 5 inactive cycles
Beginning active cycles
INFO: Completed 15 active cycles
Collapsing cross sections
Writing tally results
Solving depletion step 1 from 1 days to 2 days at 0 MW
INFO: Deleted delayed fission data because the CE data lacks a delayed fission spectrum:␣
↪cm-243 @ 293K, am-242m @ 293K
Running Shift transport calculation
Beginning inactive cycles
INFO: Completed 5 inactive cycles
Beginning active cycles
INFO: Completed 15 active cycles
Collapsing cross sections
Writing tally results
Solving depletion step 2 from 2 days to 3.5 days at 0.005 MW
INFO: Moving control_rod by 5 cm
Running Shift transport calculation
Beginning inactive cycles
INFO: Completed 5 inactive cycles
Beginning active cycles
INFO: Completed 15 active cycles
Collapsing cross sections
Writing tally results
Solving depletion step 3 from 3.5 days to 4.2 days at 0 MW
Running Shift transport calculation
Beginning inactive cycles
INFO: Completed 5 inactive cycles
Beginning active cycles
INFO: Completed 15 active cycles
Collapsing cross sections
Writing tally results
Running Shift transport calculation
Beginning inactive cycles
INFO: Completed 5 inactive cycles
Beginning active cycles
INFO: Completed 15 active cycles
Collapsing cross sections
Writing tally results
```

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```
WARNING: The first and second halves of the active cycles have statistically different (3.
↪75514 sigma) Shannon entropy
Run complete
Cleaning up
            ...finished running Omnibus in 11.2 seconds
Running Omnibus postprocessing
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'movable.out.h5', problem name 'Depletion problem␣
↪with moving control rod', created on 2020MAR11 22:38 using SCALE version 6.3.pre-b10␣
↪(branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'movable.out.h5', problem name 'Depletion problem␣
↪with moving control rod', created on 2020MAR11 22:38 using SCALE version 6.3.pre-b10␣
↪(branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
Plotting k-effective and related diagnostics...
/rnsdhpc/code/build/Exnihilo-examples/Exnihilo/packages/Omnibus/python/omnibus/formats/
↪tally/field.py:308: FutureWarning: Using a non-tuple sequence for multidimensional␣
↪indexing is deprecated; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future␣
↪this will be interpreted as an array index, `arr[np.array(seq)]`, which will result␣
↪either in an error or a different result.
  mom = data[slc]
INFO: Saved k-eff plot to movable.keff.pdf
            ...finished plotting k-effective and related diagnostics in 1.4 seconds
Writing cell tally results to CSV files...
INFO: Wrote cell tally 'fuel' to movable.fuel.t0.csv
INFO: Wrote cell tally 'fuel' to movable.fuel.t1.csv
INFO: Wrote cell tally 'fuel' to movable.fuel.t2.csv
INFO: Wrote cell tally 'fuel' to movable.fuel.t3.csv
INFO: Wrote cell tally 'fuel' to movable.fuel.t4.csv
            ...finished writing cell tally results to CSV files
Writing mesh tally visualization file...
            ...finished writing mesh tally visualization file
Writing depletion number densities...
INFO: Not creating number density CSV file because it would be too large (expected size␣
↪1289 kB exceeds user-given size 4000000); set the 'csv_max' parameter or use Python␣
↪tools
            ...finished writing depletion number densities
Writing depletion cross sections...
Writing cross sections to CSV...
            ...finished writing cross sections to CSV
INFO: Wrote depletion cross sections to movable.xs.csv
            ...finished writing depletion cross sections
Building RST summary...
INFO: Wrote summary file to movable.rst
            ...finished building RST summary
```

The output file produced includes all the data from the run: debug information, system information, log messages, etc.

```
from omnibus.formats.output import load
output = load("movable.out.h5")
output
```

```
Loading HDF5 file...
INFO: Loaded Omnibus output data from 'movable.out.h5', problem name 'Depletion problem␣
↪with moving control rod', created on 2020MAR11 22:38 using SCALE version 6.3.pre-b10␣
↪(branch 'omnibus-doc' #17579cc6 on 2020MAR10)
            ...finished loading HDF5 file
```

For example, the compositions can be extracted and printed (only a subset is shown here, for brevity):

```
output['comp']['compositions'].tolist()[1:3]
```

```
[{'matid': 1,
  'name': 'm20',
  'temperature': 293.59433519120626,
  'density': 2.688233813164135,
  'fissionable': False,
  'depletable': False,
  'zaid': array([13027], dtype=uint32),
  'wtfrac': array([1.])},
 {'matid': 2,
  'name': 'm30',
  'temperature': 293.59433519120626,
  'density': 4.180967304626936,
  'fissionable': False,
  'depletable': False,
  'zaid': array([ 8016, 13027, 63151, 63153], dtype=uint32),
  'wtfrac': array([0.0784097 , 0.42199784, 0.23721664, 0.26237582])}]
```

The following block of code extracts all the output groups that correspond to an Omnibus run sequence, and then sorts them by their execution order (the `index` accessor).

```
memory = [(name, block['peak_memory'].data['global'])
          for (name, block) in output.items() if 'peak_memory' in block]
memory.sort(key=(lambda n_pm: output[n_pm[0]].index))
memory
```

```
[('system', 223484),
 ('model', 315388),
 ('comp', 315552),
 ('physics-ce', 780108),
 ('tally', 1669588),
 ('source', 781292),
 ('depletion', 1668844),
 ('shift', 1821808)]
```

The ‘tally’ memory usage is higher than the ‘source’ usage due to an internal implementation detail. (The tallies are initialized before the source but saved after the depletion tallies have been created.)

A.4.2.3 Visualize tally results

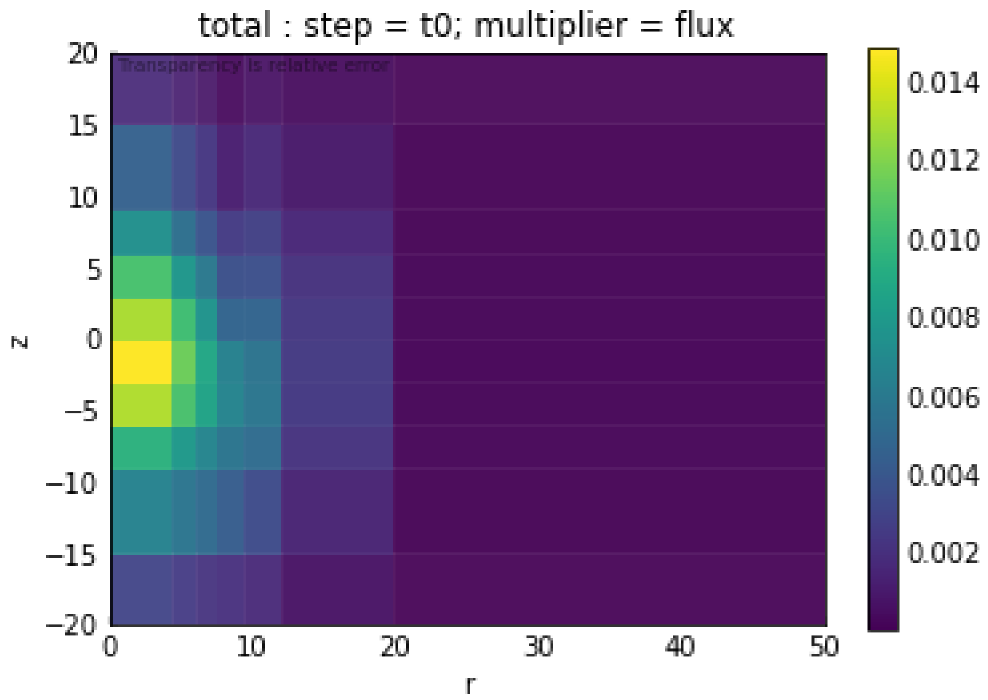
```
tallies = output['tally']
cyltal = tallies['globalcyl']
assert cyltal is tallies.globalcyl
cyltal = cyltal.extract()
cyltal
```

The `num_histories` field is the number of active histories per depletion step. The `total` field contains energy-integrated tallies:

```
cyltal = cyltal.total
cyltal
```

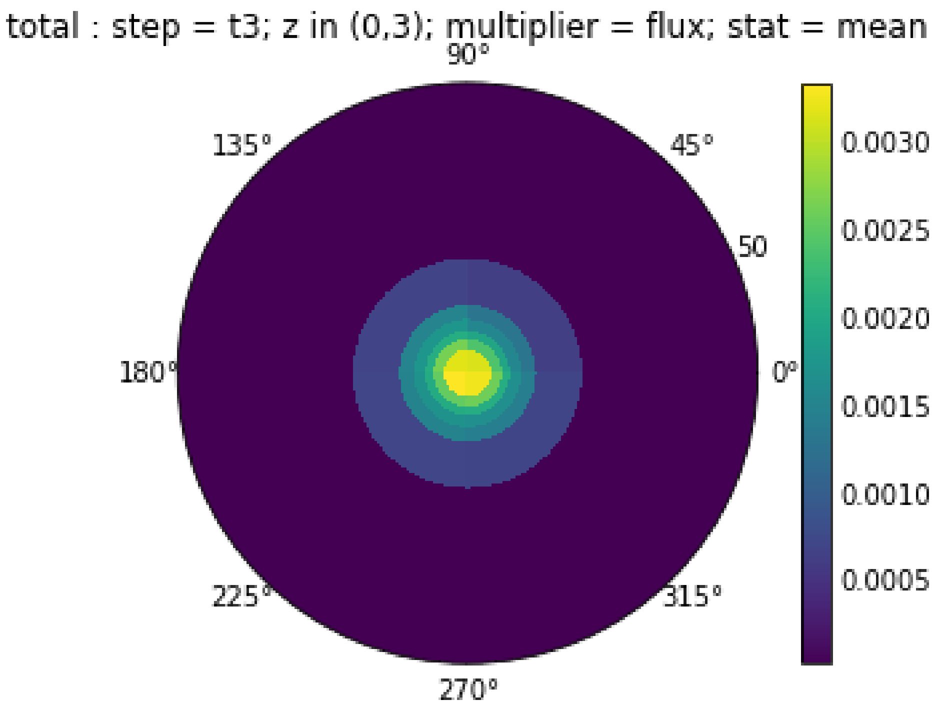
The tallies can be "sliced" along any of the axes at any of the values. The following code plots the tally estimate of the scalar flux at the initial time step, integrated over all the theta bins.

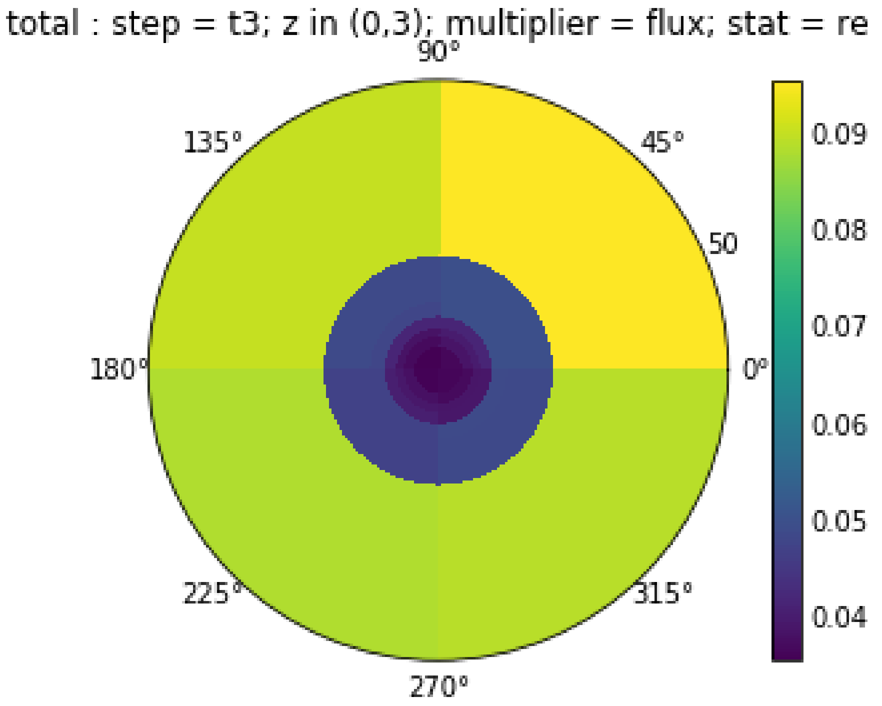
```
from omnibus.data import plot
plot(cyltal.xs(step='t0', multiplier='flux').sum('theta'));
```



A slice along the `z` axis, instead of an integral over the polar axis, yields a polar pseudocolor plot.

```
flux = cyltal.xs(step='t3', multiplier='flux', z=0.0)
plot(flux.mean)
plot(flux.re);
```



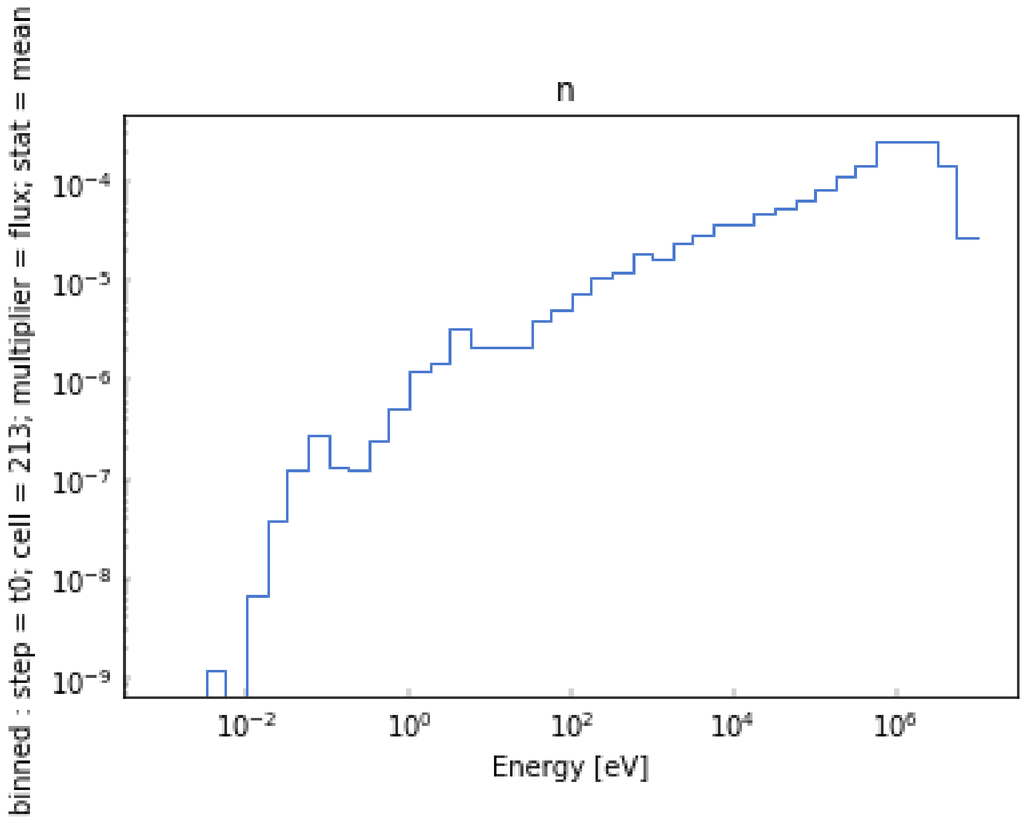


Cell tallies can also be plotted:

```
celltal = tallies['fuel'].extract()
binned_tally = celltal['binned']
print(binned_tally.mesh('cell'))
binned_tally
```

```
['201' '202' '203' '211' '212' '213' '221' '222' '223']
```

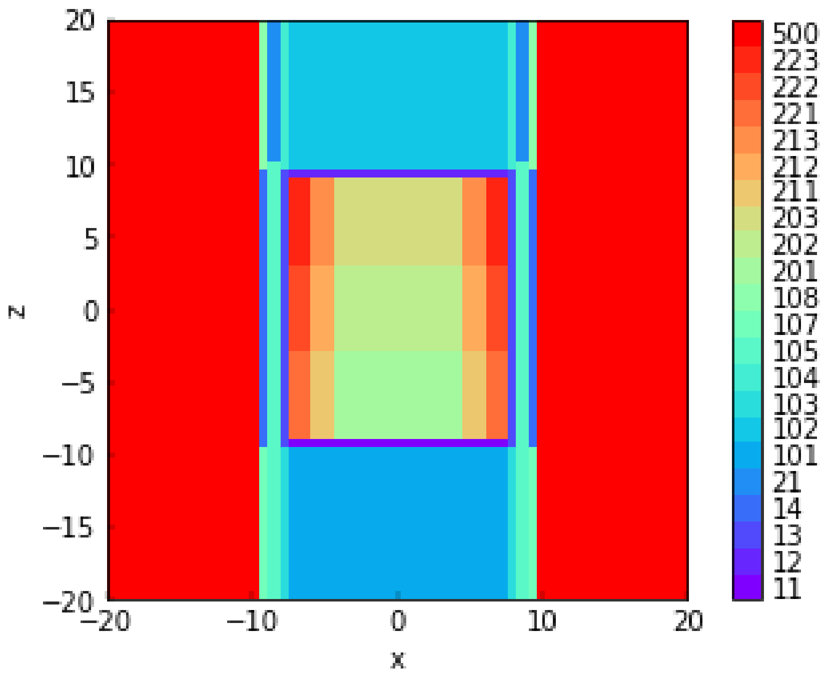
```
plot(binned_tally.xs(step='t0', multiplier='flux', stat='mean', cell='213'),
     logy=True);
```



From the spectrum, this is clearly a fast reactor.

In conjunction with the Imager, cell tally results can actually be rendered onto the geometry with a ray trace. Here is a slice of the cells in the geometry at $y = 0$:

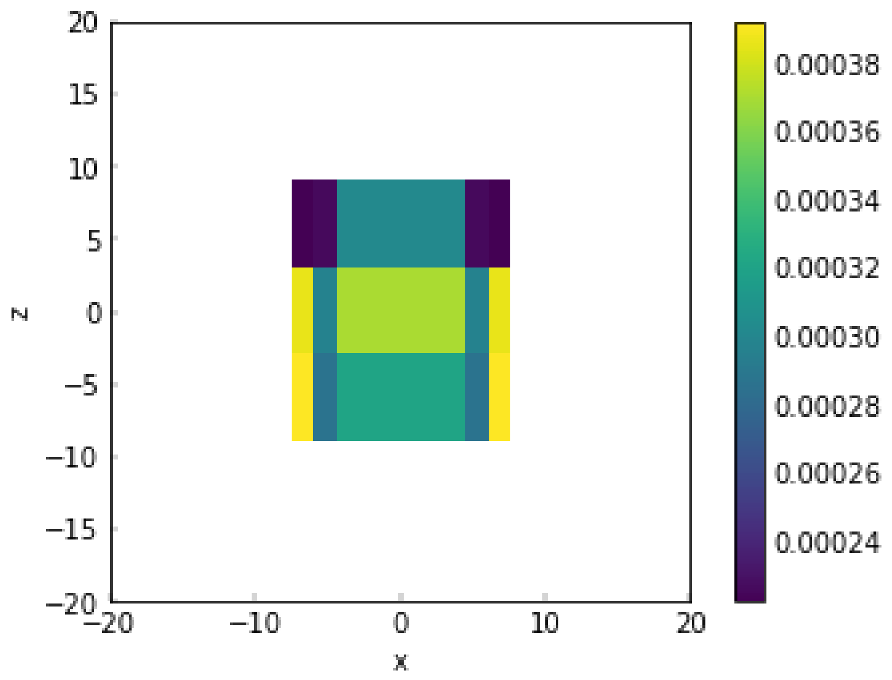
```
imager = Imager(model.geometry,
                lower=(-20, 0, -20),
                upper=(20, 0, 20),
                basis=(1, 0, 0),
                max_pixels=1024,
                trace='cell')
imager.plot();
```



Plotting the reaction rates in each cell requires one-dimensional data (one value per cell), so here are the energy-integrated fluxes at one particular time step.

```
cell_production = celltal.total.xs(step='t3', stat='mean', multiplier='nu_fission')
print(cell_production.selection)
print("Active dimensions:", cell_production.dims)
imager.pcolor(cell_production.data, labels=cell_production.mesh('cell'));
```

```
step = t3; multiplier = nu_fission; stat = mean
Active dimensions: ['cell']
```



A.4.2.4 Visualize depletion results

Additional processing and visualization can be peformed from the number densities and one-group cross sections in the depletion output.

```
# Reduce number of output rows to keep the documentation small
import pandas as pd
pd.options.display.max_rows = 15

depl = output['depletion']
depl
```

The number density is a function of step, cell, and ZAID. Note that to support restart capability, the "zaid" axis has duplicate entries in it, since ORIGEN tracks some nuclides multiple times. A built-in `collapse_nuclides` function consolidates these nuclides. Calling this function on a field will pull the entire dataset from disk and return a new field with the collapsed nuclides. This is going to be memory-, disk-, and CPU-intensive, so it is not a bad idea to slice the data first to reduce the amount of work that has to be done if the entire result is not needed.

```
num_dens = depl.num_dens
num_dens
```

```
num_dens = num_dens.collapse_nuclides()
num_dens
```

Note that the `data` entry of the initial `num_dens` points to an on-disk HDF5 object, whereas after collapsing nuclides the data is an in-memory Numpy array.

```
# Convert xenon densities to a Pandas dataframe
xe_dens = num_dens.xs(zaid=to_nuclide('xe-135')).to_series().unstack('cell')
xe_dens
```

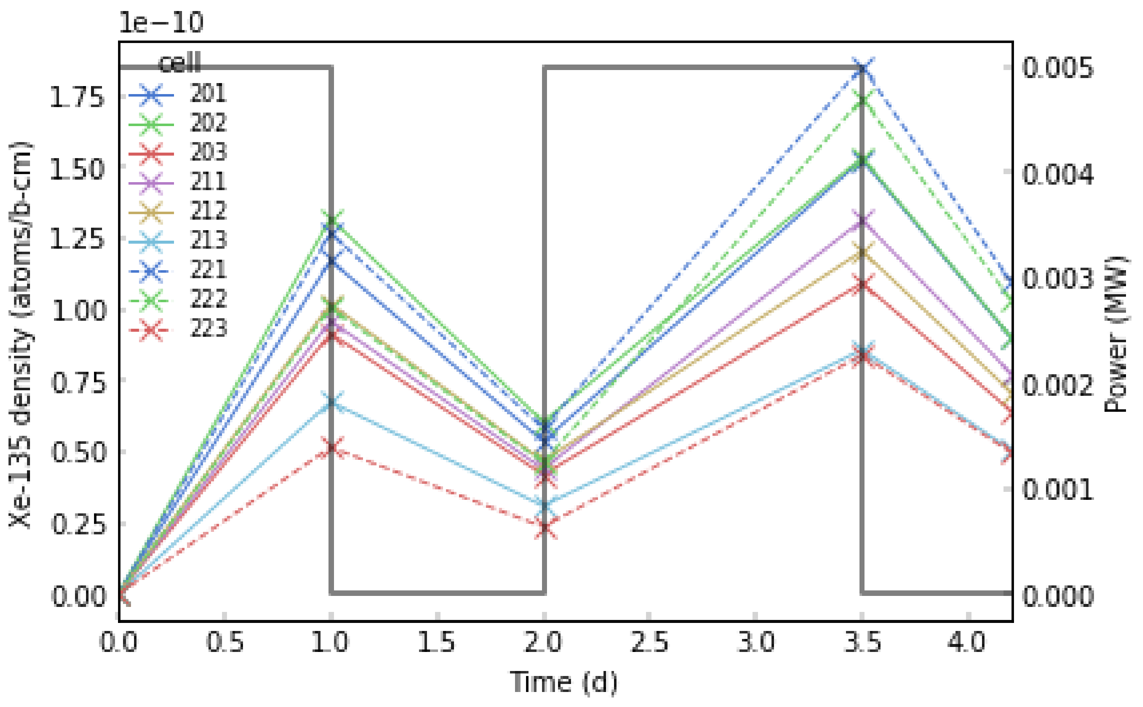
```
/rnsdhpc/code/build/Exnihilo-examples/Exnihilo/packages/Omnibus/python/omnibus/data/field.
↪py:692: FutureWarning: the 'labels' keyword is deprecated, use 'codes' instead
  index = pd.MultiIndex(levels=levels, labels=labels, names=names)
```

```
# Change indexing from labels to actual simulated time
simtime = depl.simtime.extract()
xe_dens.index = simtime.data

# Plot number densities in each cell
ax = xe_dens.plot(marker='x')
ax.set_ylabel("Xe-135 density ({})".format(num_dens.units))
ax.set_xlabel("Time ({})".format(simtime.units))

# Plot power
power = depl.totpower.extract()
ax2 = ax.twinx()
ax2.plot(simtime.data, power.data, drawstyle='steps-post', linewidth=2, color=(0,0,0,.5))
ax2.set_ylabel("Power ({})".format(power.units))
```

```
Text(0, 0.5, 'Power (MW)')
```



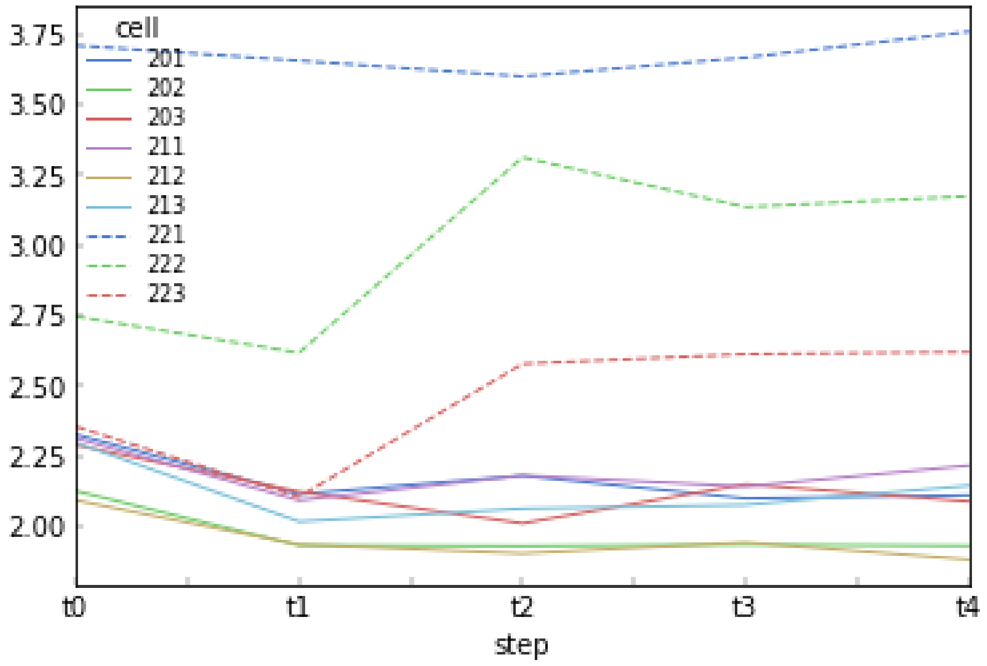
The collapsed cross sections are stored in a single array that holds (ZAID,MT) pairs (since not all nuclides have all reaction types). Because the `omnibus.data.Field` class is built for only regular multi-dimensional data (no ragged edges), it can be easier to process this field using the Pandas package. The `to_series` function converts a field into a Pandas series. The `zaid_mt` axis gets expanded into two different “levels” in a `pandas.MultiIndex` object.

```
# Print a table of cross sections, with step/zaid/mt as rows
xs = depl['xs'].to_series().unstack('cell')
xs
```

```
/rnsdhpc/code/build/Exnihilo-examples/Exnihilo/packages/Omnibus/python/omnibus/data/field.
↪py:652: FutureWarning: .labels was deprecated in version 0.24.0. Use .codes instead.
  lab[:] = list(zip(*mi.labels))
```

```
# Tabulate just the fission cross sections
_.xs(18, level='mt')
```

```
# View U-235 cross sections as a function of time in each of the different cells
_.xs(92235, level='zaid').plot();
```



A.4.3 CUSTOM COMPOSITIONS IN OMNIBUS

The Omnibus `[COMP][MATERIAL]` block is convenient for defining small numbers of compositions with few nuclides, but it can be tedious to use for more complex inputs, and especially tedious if the compositions are already defined in another input model. This example demonstrates how to extract compositions from an existing SCALE input and use them in an Omnibus problem with a Geometria-based geometry.

```
# Set up example environment
import os
from exnihilotools.matplotlib import screen_style
SOURCE_DIR = os.environ.get("SOURCE_DIR", ".")
%matplotlib inline
```

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```
%load_ext wurlitzer
screen_style()
```

A.4.3.1 Load existing compositions

Loading the SCALE model provides access to both the geometry definition *and* the compositions. The `_asdict` method of a composition object allows it to be rendered as a native Python dictionary for easy perusal.

```
from omnibus.raytrace.load import load_scale
scale_model = load_scale(os.path.join(SOURCE_DIR, "data", "godiva-keno.inp"))
comps = [c._asdict() for c in scale_model.compositions]
comps
```

```
>>> Using SCALE geometry from 'csas6' sequence.
>>> Loading SCALE Standard Composition Library from /usr/local/scale/data/scale.rev40.
↪sclib
```

```
[{'name': 'void',
  'matid': 0,
  'temperature': 1e-07,
  'density': 0.0,
  'fissionable': False,
  'depletable': False,
  'zaid': array([], dtype=uint32),
  'wtfrac': array([], dtype=float64)},
 {'name': 'media 1',
  'matid': 1,
  'temperature': 293.0,
  'density': 18.739884256874777,
  'fissionable': True,
  'depletable': True,
  'zaid': array([92234, 92235, 92238], dtype=uint32),
  'wtfrac': array([0.01019995, 0.93709968, 0.05270038])}]
```

A.4.3.2 Exporting compositions

The compositions can be immediately saved to disk if they do not need modification:

```
from robus import save_hdf5_compositions
save_hdf5_compositions("godiva_keno.comp.h5", scale_model.compositions)
```

Changing the names and ordering of the compositions demonstrate some of the capabilities of the Python representation of the compositions. Writing Python objects to HDF5 requires the Omnibus format wrappers (usually seen when processing existing Omnibus output files).

```
import h5py
from omnibus.data import dump_root
from omnibus.formats.comp import Compositions, CompBlock

```

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```
# Create a compositions object with modified properties
comps[1]['name'] = 'uranium'
comps = [comps[1], comps[0]]

# TODO: this may not be necessary for Omnibus, but it currently is necessary for␣
↪raytracing
for matid, c in enumerate(comps):
    c['matid'] = matid

export_comps = Compositions.from_list(comps)
export_comp_block = CompBlock(data={'compositions': export_comps})
with h5py.File(os.path.join(SOURCE_DIR, "data", "godiva-gg.comps.h5"), 'w') as f:
    dump_root(export_comp_block, f)
```

A.4.3.3 Using compositions with GG

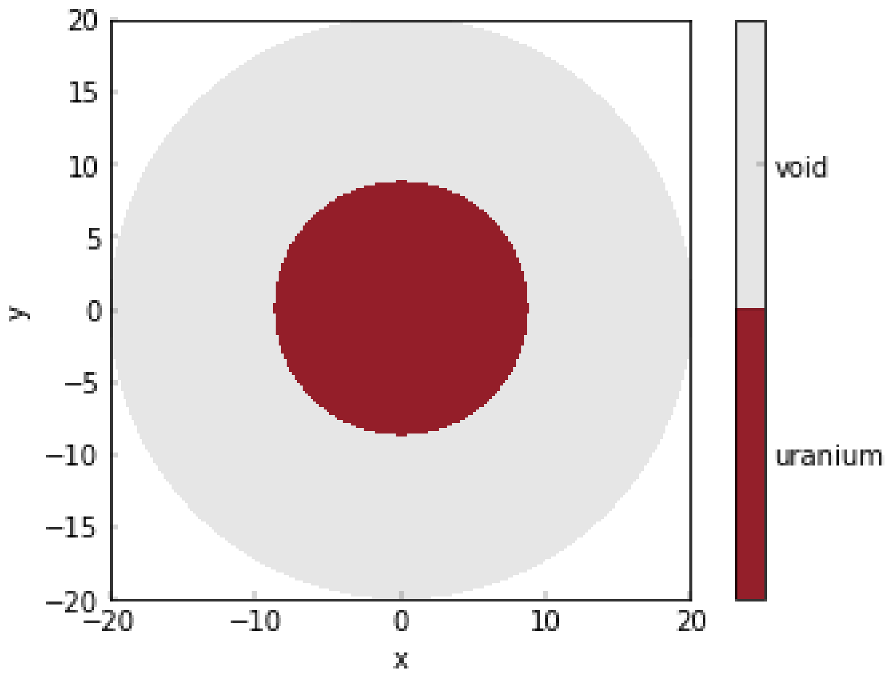
Now that updated compositions have been computed, they can be loaded as part of the Geometria model for raytracing. Although this example uses compositions loaded directly from a SCALE model, it is also possible to directly use compositions loaded from an existing Omnibus HDF5 output file, in which case `export_comps` here would be replaced by `output_file['comp']['compositions']`.

```
from omnibus.raytrace.load import load_gg
model = load_gg(os.path.join(SOURCE_DIR, "data", "godiva.gg.omn"),
                compositions=export_comps)
```

```
Generating Geometria XML input file from .gg.omn...
INFO: Starting Geometria preprocessor, omnibus version 6.3.pre-b11 (branch 'comp-example
↪' #4d164aa1 on 2020APR14)
Loading problem db from Omnibus ASCII file...
Loading Omnibus input file at /rnsdhpc/code/src/scale/Exnihilo/packages/Omnibus/driver/
↪example/data/godiva.gg.omn
            ...finished loading problem db from Omnibus ASCII file
INFO: Writing Geometria input ParameterList to godiva.gg.xml
            ...finished generating Geometria XML input file from .gg.omn
```

```
from omnibus.raytrace.colors import ColorMap
from omnibus.raytrace.imager import Imager

colors = ColorMap.from_compositions(model.compositions)
imager = Imager.from_extents(model.geometry, z=0.0)
imager.names = [c.name for c in model.compositions]
imager.colors = colors
imager.plot();
```



A.5 CE DATA

A.5.1 INTERACTING WITH CE CROSS SECTION DATA

This example demonstrates some basic tools for interacting with AMPX-processed continuous energy cross sections.

```
# Set up example
%matplotlib inline
from exnihilotools.matplotlib import screen_style, grid
screen_style()
```

Providing various options to the `Library` loader, such as disabling the loading of kinematics data, will reduce data load times and memory consumption. Printing the database after loading shows the defaults for other options not provided in the input database.

```
from nemesis import cmake_config, Std_DB, make_view, make_const_view
from robus import Library
from omnibus.db.validator import mt_to_str, to_mt, to_nuclide
from omnibus.scale import ce_file_resolver

db = Std_DB.from_dict({
    'ce_lib_path': ce_file_resolver.resolve("ce_v7.1_endf"),
    'gamma_production': False,
    'kinematics': False,
    'reactions': [to_mt(k) for k in """N_TOTAL N_ELASTIC N_FISSION N_ABSORPTION
                                       N_N_X1 N_N_XC N_GAMMA N_NU N_SAB""".split()],
    'broaden_db': {
        'kinematics': False,
    }
```

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```
    })
library = Library(db)
print(db)
```

```
/rnsdhpc/code/install/Exnihilo/python/omnibus/__init__.py:93: UserWarning: Version␣
↪mismatch between 'exnihilotools' and 'omnibus' packages: 6.3.pre-b10 (branch 'omnibus-
↪doc' #98d73c8e on 2020MAR11) (at /rnsdhpc/code/build/Exnihilo-examples/Exnihilo/
↪packages/Nemesis/python/exnihilotools/__init__.py) is not the same as 6.3.pre-b10␣
↪(branch 'fix-origen-install' #b3af8ef1 on 2020MAR06) (at /rnsdhpc/code/install/Exnihilo/
↪python/omnibus/__init__.py); This is probably because of a PYTHONPATH error and may␣
↪cause unexpected failures on import
  UserWarning)
```

```
############################################################
Path: /std_db

Database for std_db has:
         2 integer entries
         5 double entries
         9 bool entries
         1 string entries
         7 vector<int> entries
         0 vector<double> entries
         0 vector<string> entries
         0 vector<bool>   entries
         1 nested database entries

============================================================
Entries in                                      std_db database
============================================================
integer entries
------------------------------------------------------------
                 sizeof_data_float                         4
               sizeof_energy_float                         8

double entries
------------------------------------------------------------
                          ethermal                        10
                      n_energy_max                    2e+07
                      n_energy_min                    1e-05
                      p_energy_max                  2.5e+07
                      p_energy_min                    10000

bool entries
------------------------------------------------------------
                 collision_moments                         0
                     collision_pdf                         0
           collision_probabilities                         0
                              dbrc                         1
                  gamma_production                         0
                        kinematics                         0
```

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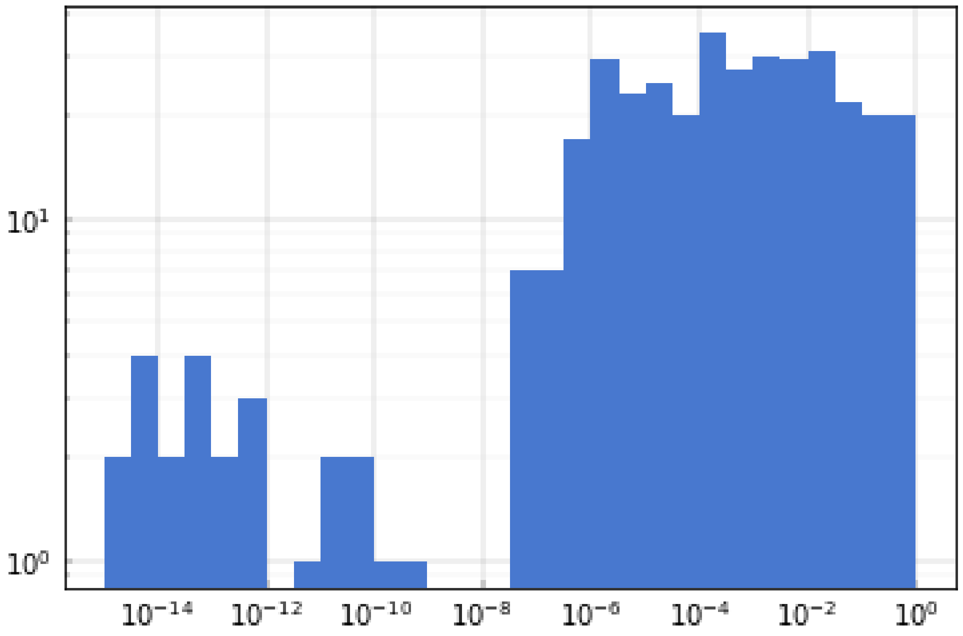
```
                    missing_as_zero                        0
                 probability_tables                        1
                    unionize_energy                        0

string entries
------------------------------------------------------------
                        ce_lib_path/usr/local/scale/hpcdata/ce_v7.1_endf.h5

vector<int> entries                   (number of elements)
------------------------------------------------------------
                        omit_zaid_n                        0
                        omit_zaid_p                        0
                        orig_zaid_n                        0
                        orig_zaid_p                        0
                          reactions                        9
                        subs_zaid_n                        0
                        subs_zaid_p                        0

############################################################
Path: /std_db/broaden_db

Database for broaden_db has:
         0 integer entries
         1 double entries
         2 bool entries
         0 string entries
         0 vector<int> entries
         0 vector<double> entries
         0 vector<string> entries
         0 vector<bool>   entries
         0 nested database entries

============================================================
Entries in                                broaden_db database
============================================================
double entries
------------------------------------------------------------
                    temperature_tol                        4

bool entries
------------------------------------------------------------
                         kinematics                        0
                             legacy                        0

############################################################
############################################################
```

A.5.1.1 Analyze energy grid spacing

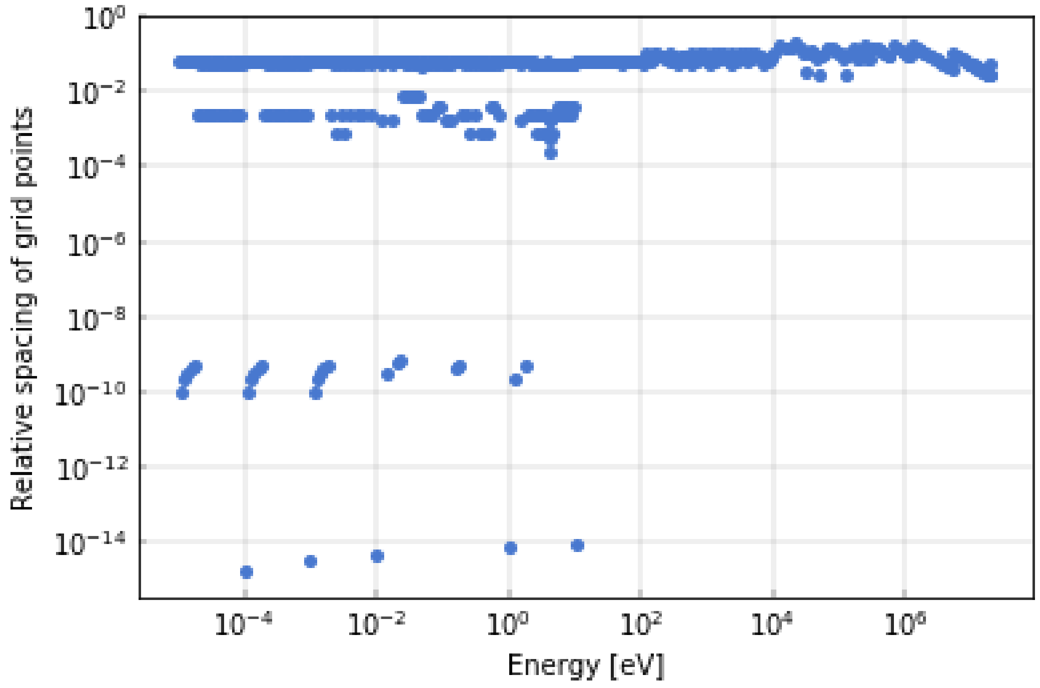
How are the energy grid points distributed for water-bound hydrogen? The Exnihilo python bindings can extract any property of the physics data and manipulate it natively in Python. Here, the ubiquitous Numpy package's powerful math utilities are used to plot a distribution of the relative spacing of the energy grid points.

```
import numpy as np
import matplotlib.pyplot as plt

def centers(x):
    return (x[:-1] + x[1:]) * 0.5

nucl = library.load_nuclide_n(1001, 293)
rxn = nucl.get_reaction(to_mt("N_TOTAL"))
energy = np.asarray(rxn.energy)

delta_e = np.diff(energy)
energy_mid = centers(energy)
relative_delta_e = delta_e

(fig, ax) = plt.subplots(subplot_kw=dict(xscale='log', yscale='log'))
ax.hist(relative_delta_e, bins=np.logspace(-15,0,31));
grid(ax, 'both')
```



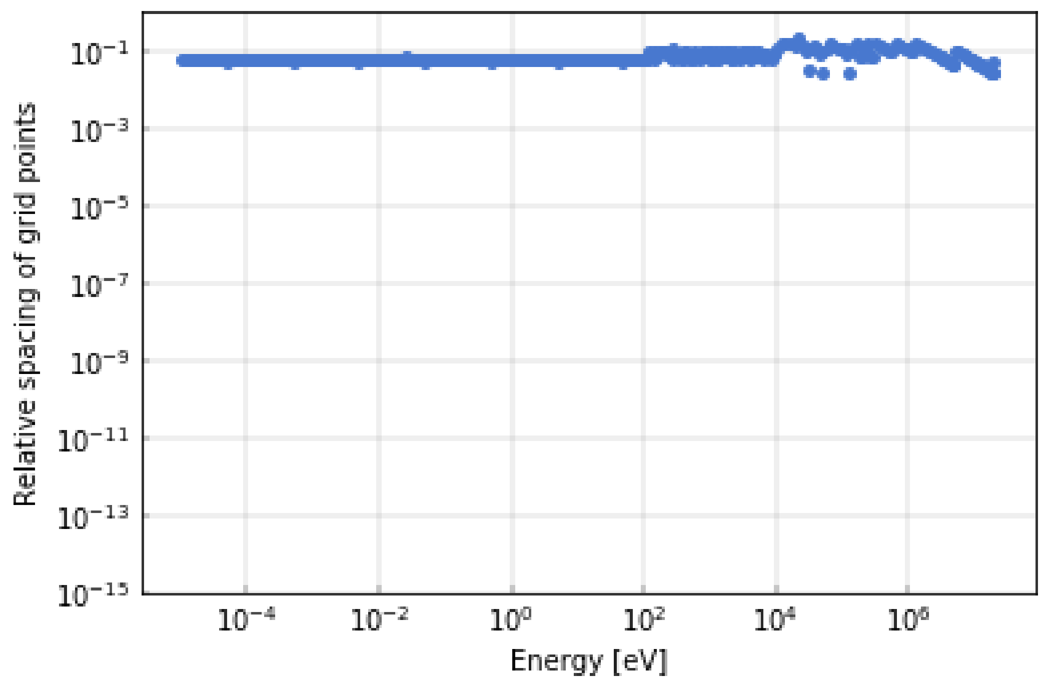
Plotting as a function of energy reveals that the thermal range has lots of micro-sized points, likely a result of AMPX processing of the thermal scattering.

```
def plot_rel_spacing(energy_mid, delta_e):
    (fig, ax) = plt.subplots(subplot_kw=dict(xscale='log', yscale='log'))
    ax.plot(energy_mid, delta_e/energy_mid, linestyle='none', marker='.')
    ax.set_xlabel("Energy [eV]")
    ax.set_ylabel("Relative spacing of grid points")
    grid(ax, which='major')
    return ax

plot_rel_spacing(energy_mid, delta_e);
```



Comparing against free-gas hydrogen confirms that the artifacts are related to the bound cross section treatment:

```
nucl = library.load_nuclide_n(8001001, 293)
rxn = nucl.get_reaction(to_mt("N_TOTAL"))
energy = np.asarray(rxn.energy)

ax = plot_rel_spacing(centers(energy), np.diff(energy))
ax.set_ylim(1e-15, 1);
```



A.5.1.2 Resonance broadening

This example shows how Doppler broadening affects the cross sections of a large iron resonance. The `broaden_db` option passed to the `Library` above enables run-time broadening of cross sections, even if not previously generated for the CE library being used.

```
zaid = to_nuclide('Fe-56')
print("Nuclide ID: ", zaid)
rxn_mt = to_mt("N_TOTAL")
print("Reaction MT:", mt_to_str(rxn_mt))

# Pre-load temperatures, including interpolated at midpoint
temperatures = sorted(set(library.get_temperatures(zaid)) | {420, 750, 900, 1800})
library.load_nuclide_n(zaid, temperatures)

nuclides = [library.load_nuclide_n(zaid, t) for t in temperatures]
print("Loaded temperatures: " + ", ".join(str(nucl.temperature) for nucl in nuclides))
```

```
Nuclide ID:  26056
Reaction MT: 1=N_TOTAL
Loaded temperatures: 293.0, 420.0, 565.0, 600.0, 750.0, 900.0, 1200.0, 1800.0, 2000.0,␣
↪2400.0
```

Plot an overall view of the cross sections:

```
nucl = nuclides[0]
rxn = nucl.get_reaction(rxn_mt)

def get_desc(nucl, rxn):
    return "{:s} at {:.1f} for MT {:s}".format(
```

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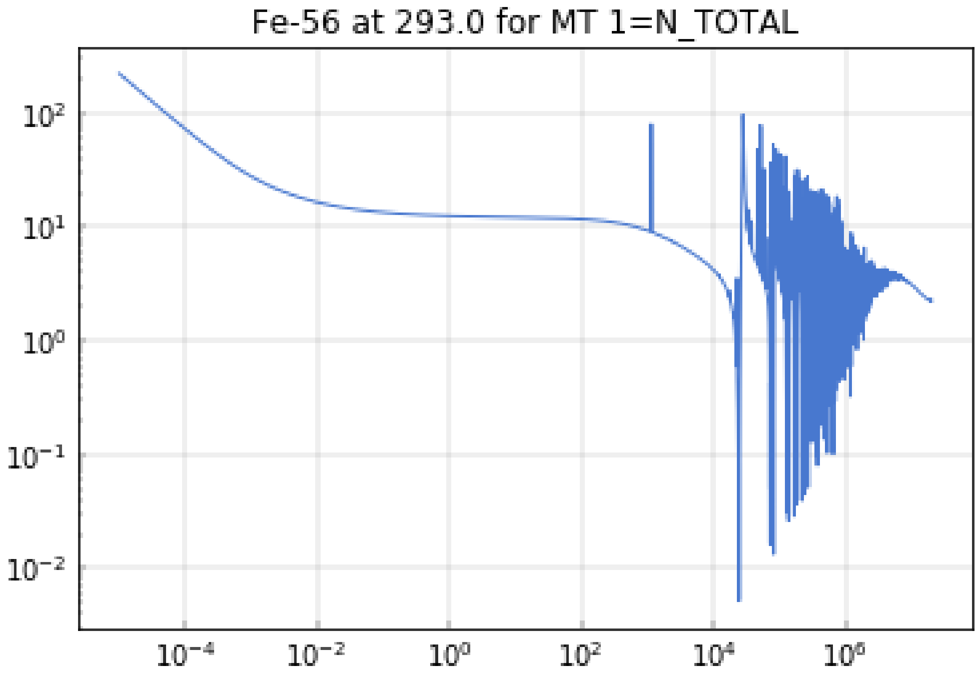
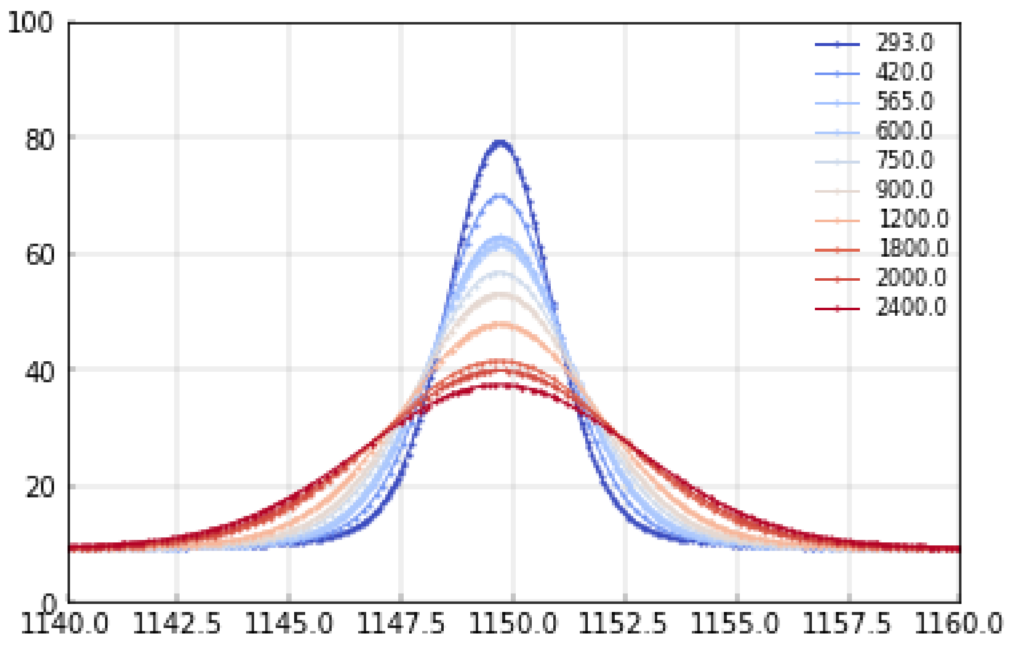
```
        to_nuclide.zaid_to_pretty_nuclide(nucl.zaid),
        nucl.temperature,
        to_mt.to_str(rxn.mt))

(fig, ax) = plt.subplots()
ax.loglog(rxn.energy, rxn.xs, '-')
ax.set_title(get_desc(nucl, rxn))
grid(ax)
```



A close-up visualization of the lowest-energy resonance shows how the cross sections vary as a function of temperature:

```
from matplotlib.cm import get_cmap
from matplotlib.colors import LogNorm
cmap = get_cmap('coolwarm')
norm = LogNorm(vmin=nuclides[0].temperature, vmax=nuclides[-1].temperature)

(fig, ax) = plt.subplots()
ax.set_xlim(1140, 1160)
ax.set_ylim(0, 100)
for nucl in nuclides:
    rxn = nucl.get_reaction(rxn_mt)
    plt.plot(rxn.energy, rxn.xs,'-o',
             markeredgecolor="none", markersize=2,
             label="{:.1f}".format(nucl.temperature),
             color=cmap(norm(nucl.temperature)))
ax.legend(loc="upper right")
grid(ax)
```



The values at the cross sections at the peaks of these resonances can be found using Numpy:

```
for nucl in nuclides:
    rxn = nucl.get_reaction(rxn_mt)
    e = np.asarray(rxn.energy)
    xs = np.asarray(rxn.xs)
    erange = (e > 1100) & (e < 1200)
    max_local_index = np.argmax(xs[erange])
    max_index = np.where(erange)[0][max_local_index]
    print("For {:s} at {:7.1f}, resonance peaks at index {:d} "
          "(E = {:.3f} eV) with sigma = {:.1f} cm^-1".format(
            to_nuclide.zaid_to_pretty_nuclide(nucl.zaid),
            nucl.temperature, max_index, e[max_index], xs[max_index]))
```

```
For Fe-56 at   293.0, resonance peaks at index 613 (E = 1149.700 eV) with sigma = 79.4␣
↪cm^-1
For Fe-56 at   420.0, resonance peaks at index 436 (E = 1149.748 eV) with sigma = 70.0␣
↪cm^-1
For Fe-56 at   565.0, resonance peaks at index 612 (E = 1149.700 eV) with sigma = 62.9␣
↪cm^-1
For Fe-56 at   600.0, resonance peaks at index 612 (E = 1149.700 eV) with sigma = 61.6␣
↪cm^-1
For Fe-56 at   750.0, resonance peaks at index 436 (E = 1149.748 eV) with sigma = 56.8␣
↪cm^-1
For Fe-56 at   900.0, resonance peaks at index 606 (E = 1149.700 eV) with sigma = 53.2␣
↪cm^-1
For Fe-56 at  1200.0, resonance peaks at index 606 (E = 1149.700 eV) with sigma = 47.9␣
↪cm^-1
For Fe-56 at  1800.0, resonance peaks at index 436 (E = 1149.748 eV) with sigma = 41.6␣
↪cm^-1
For Fe-56 at  2000.0, resonance peaks at index 614 (E = 1149.597 eV) with sigma = 39.9␣
↪cm^-1
```

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```
For Fe-56 at  2400.0, resonance peaks at index 617 (E = 1149.597 eV) with sigma = 37.5␣
↪cm^-1
```

A.5.1.3 Cross section interpolation

The Python methods in this notebook directly access the underlying Shift C++ data using Numpy arrays, with no copying, enabling high performance (speed of C rather than Python) operations on large data sets. This example demonstrates the performance of interpolating the hydrogen cross section onto a 100k-point energy grid.

```
nucl = library.load_nuclide_n(1001, 600.0)
rxn = nucl.get_reaction(1)
print("Reaction: MT {:s} from {:s} at {:.1f}K".format(
        to_mt.to_str(rxn.mt),
        to_nuclide.zaid_to_pretty_nuclide(nucl.zaid),
        nucl.temperature,))

from physica import calc_micro_xs
interp_energy = np.logspace(-3, 6, 100000)
interp_xs = np.zeros_like(interp_energy, dtype='float32')
print("Interpolation time:")
%timeit calc_micro_xs(rxn, make_const_view(interp_energy), make_view(interp_xs))
```

```
Reaction: MT 1=N_TOTAL from H-1 at 600.0K
Interpolation time:
1.24 ms ? 19.5 ?s per loop (mean ? std. dev. of 7 runs, 1000 loops each)
```

A.5.1.4 Find nonlinear interpolation schemes

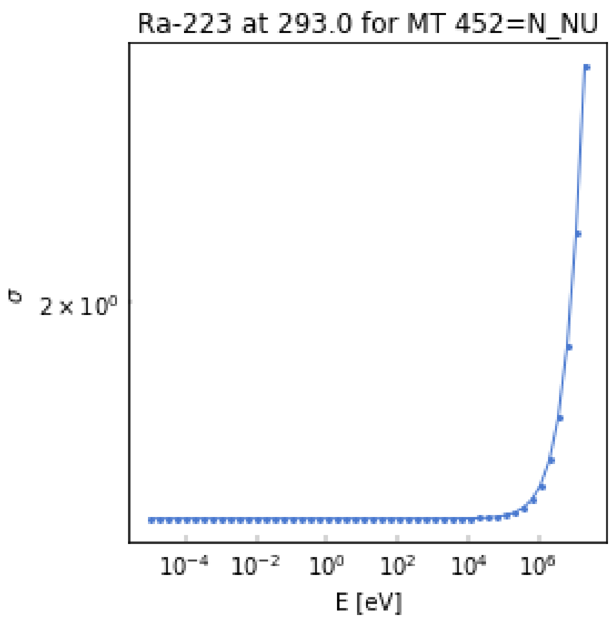
Most of the SCALE cross sections use linear-linear interpolation. To check whether any nonlinear interpolation is used at all, one can loop through all reactions in all nuclides. To reduce load time, gamma production data and kinematics (collision) data are ignored.

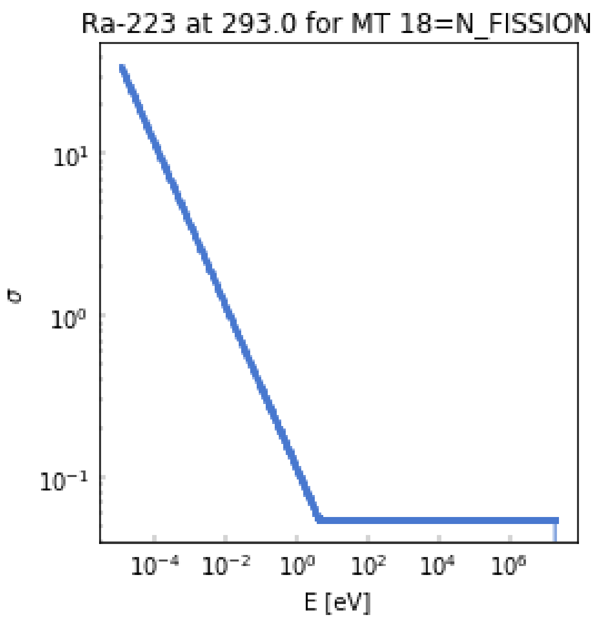
```
from robus import NEUTRON

library = Library(Std_DB.from_dict({
    'ce_lib_path': ce_file_resolver.resolve("ce_v71"),
    'gamma_production': False,
    'kinematics': False,
    'probability_tables': False
}))

for zaid in library.get_zaids(NEUTRON):
    temperature = 300.
    nucl = library.load_nuclide_n(zaid, temperature)
    for mt in nucl.get_mts():
        rxn = nucl.get_reaction(mt)
        if rxn.find_interpolation(0) != 2:
            print(zaid, mt)
```

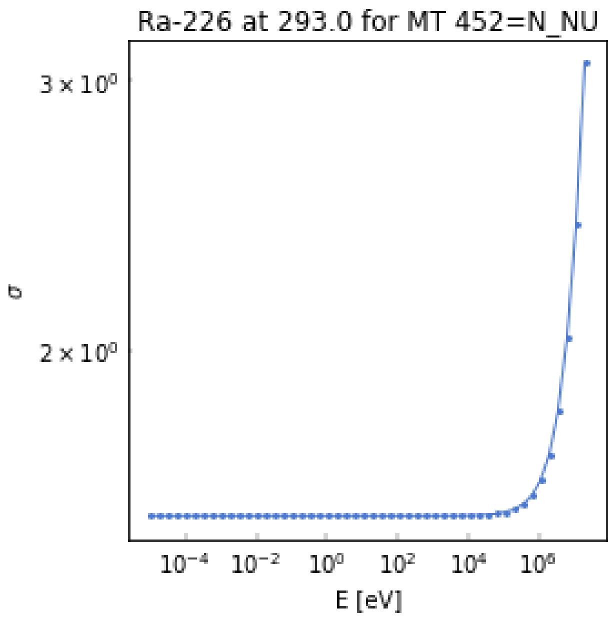
```
88223 452
88226 452
```

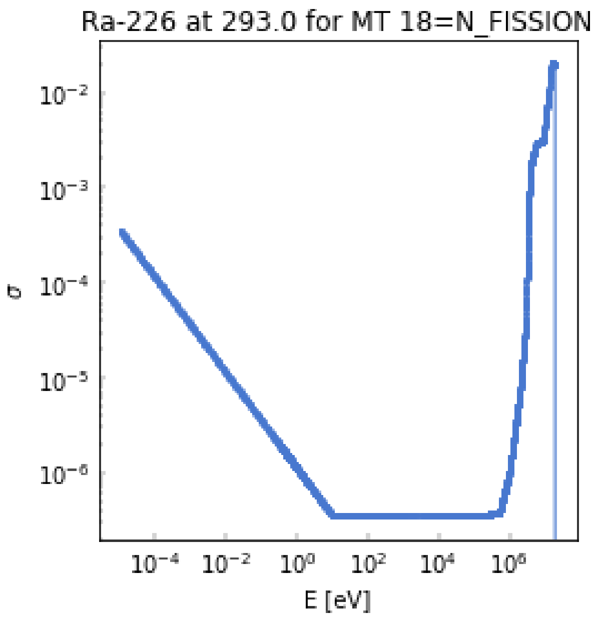
The two nonlinear interpolations are for nu (average neutron yield per fission) in two isotopes of radium!

```python
(fig, axes) = plt.subplots(2, 2, figsize=(8,8))

for (i, zaid) in enumerate([88223, 88226]):
    nucl = library.load_nuclide_n(zaid, 293)
    for (j, mt) in enumerate([452, 18]):
        ax = axes[i, j]
        rxn = nucl.get_reaction(mt)
        ax.loglog(rxn.energy, rxn.xs, '-o',
                  markeredgecolor="none", markersize=3)
        ax.set_title(get_desc(nucl, rxn))
        ax.set_xlabel("E [eV]")
        ax.set_ylabel("$\sigma$")
plt.tight_layout()
```









It is exceedingly odd that Radium has fission and production reactions, and that its fission reaction has that obviously nonphysical shape. This has the smell of bad ENDF data.

A.5.1.5 Debug errors during broadening

During testing of a new feature, Shift developers discovered that the highest few energy grid points in Fe-56 were being broadened strangely, producing large relative errors. Additionally, broadening of MT=5 failed. This section shows some of the steps taken to debug the failure.

```
db = Std_DB.from_dict({
    'ce_lib_path': ce_file_resolver.resolve("ce_v71"),
    'gamma_production': False,
    'kinematics': False,
```

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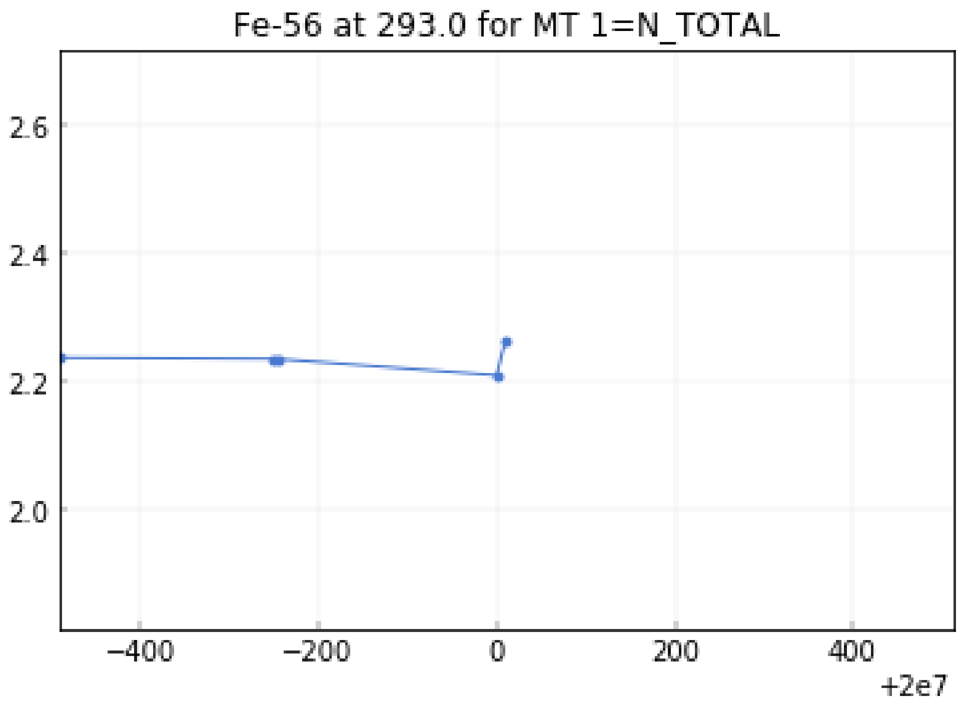
```
    })
library = Library(db)
nucl = library.load_nuclide_n(26056, 300.0)
rxn = nucl.get_reaction(1)
```

The cross sections for the highest energies are plotted here:

```
(fig, ax) = plt.subplots()
ax.plot(rxn.energy, rxn.xs,'-o',
        markeredgecolor="none", markersize=4,)

(energy, xs) = (np.asarray(v) for v in (rxn.energy, rxn.xs))
ax.set_xlim(energy[-5], 2 * energy[-1] - energy[-5])
ax.set_ylim(.8 * xs[-1], 1.2 * xs[-1])
ax.set_title(get_desc(nucl, rxn))
ax.grid();
```



```
print("Final energy points:", energy[-5:])
```

```
Final energy points: [19999508.63125662 19999749.43095107 19999754.31487379 20000000.
 20000010.        ]
```

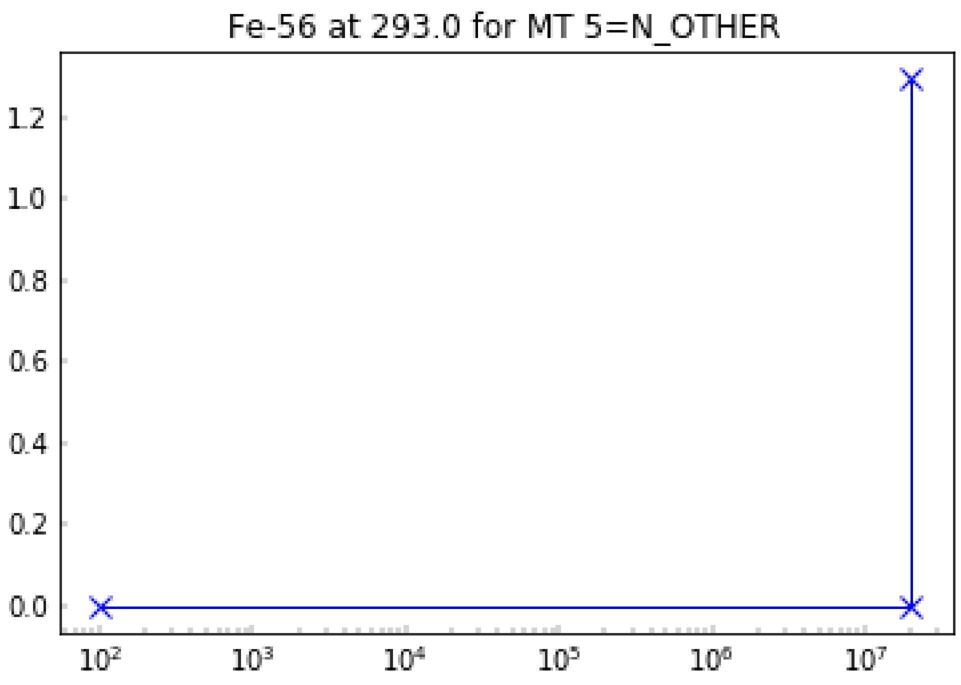
Note that the discontinous point at the end of the cross section is above the maximum requested energy, indicating an error in the CE data processing.

Next let’s look at MT 5, which was crashing because it had fewer than ~6 energy grid points.

```
rxn = nucl.get_reaction(5)
print("Energy:", np.asarray(rxn.energy))
print("XS:     ", np.asarray(rxn.xs))

(fig, ax) = plt.subplots()
ax.semilogx(rxn.energy, rxn.xs, 'b-x')
ax.set_title(get_desc(nucl, rxn));
```

```
Energy: [1.00000002e+02 2.00000000e+07 2.00000100e+07]
XS:     [0.         0.         1.29554]
```



This AMPX internal-use implementation MT is also clearly nonphysical.

A.5.2 UNRESOLVED RESONANCE REGION DATA

Shift uses AMPX-generated probability table data to evaluate particle cross sections in the unresolved resonance region (URR), where at a single “energy” a particle may encounter a range of cross sections.

```
from nemesis import Std_DB, make_view, make_const_view
from robus import Library, data_path
from physica import calc_micro_xs
from omnibus.db.validator import mt_to_str, to_mt, to_nuclide
from omnibus.scale import ce_file_resolver

import numpy as np
import matplotlib.pyplot as plt
from matplotlib.cm import get_cmap
from matplotlib.colors import Normalize, LogNorm

%matplotlib inline
```

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```
from exnihilotools.matplotlib import screen_style
screen_style()
```

```
/rnsdhpc/code/install/Exnihilo/python/omnibus/__init__.py:93: UserWarning: Version␣
↪mismatch between 'exnihilotools' and 'omnibus' packages: 6.3.pre-b10 (branch 'omnibus-
↪doc' #98d73c8e on 2020MAR11) (at /rnsdhpc/code/build/Exnihilo-examples/Exnihilo/
↪packages/Nemesis/python/exnihilotools/__init__.py) is not the same as 6.3.pre-b10␣
↪(branch 'fix-origen-install' #b3af8ef1 on 2020MAR06) (at /rnsdhpc/code/install/Exnihilo/
↪python/omnibus/__init__.py); This is probably because of a PYTHONPATH error and may␣
↪cause unexpected failures on import
  UserWarning)
```

```
def which_ptables(nucl):
    ptable_mts = []
    for mt in nucl.get_mts():
        rxn = nucl.get_reaction(mt)
        if rxn.has_ptable:
            ptable_mts.append(mt)
    return ptable_mts

def extract_ptable(nucl, mt):
    assert nucl.has_reaction(mt)
    rxn = nucl.get_reaction(mt)
    assert rxn.has_ptable
    ptable = rxn.ptable
    energy = np.asarray(ptable.energy)
    # Make a table out of the multiband cross sections at each energy
    xs_elastic = np.array([ptable.xs(ei) for ei in range(len(energy))])
    return (energy, xs_elastic)

def plot_ptable_and_mean(nucl, mt):
    (energy, ptable) = extract_ptable(nucl, mt)
    # Extract reported mean values from no-ptable energy grid
    rxn = nucl.get_reaction(mt)
    noptab_energy = np.asarray(rxn.energy)
    noptab_xs = np.asarray(rxn.xs)

    # Calculate the mean of the ptable bands (OK since equiprobable)
    ptab_mean = np.mean(ptable, axis=1)

    cmap = get_cmap('srj_rainbow')
    norm = Normalize(vmin=0, vmax=ptable.shape[1])

    (fig, ax) = plt.subplots(figsize=(8,4))
    for band in range(ptable.shape[1]):
        ax.loglog(energy, ptable[:,band],'-o',
                  color=cmap(norm(band)),
                 markeredgecolor="none", markersize=2,)

    ax.plot(energy, ptab_mean, 'k-', linewidth=2)
    ax.plot(noptab_energy, noptab_xs, 'r--', linewidth=2)
```

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```
    ax.grid()
    ax.grid(axis='x', which='minor')
    ax.set_axisbelow(True)
    ax.set_xlim(.7 * energy[0], 1.4 * energy[-1])
    ax.set_ylim(.5 * np.min(ptable), 2 * np.max(ptable));
```

```
db = Std_DB.from_dict({
    'ce_lib_path': data_path("ce_v71"),
    })
library = Library(db)
```

A.5.2.1 Tungsten

```
nucl = library.load_nuclide_n(74186, 300)
library.flush_warnings()
print("Reactions with probability table data:",
       ", ".join(mt_to_str(mt) for mt in which_ptables(nucl)))
```

```
Reactions with probability table data: 1=N_TOTAL, 2=N_ELASTIC, 102=N_GAMMA
```

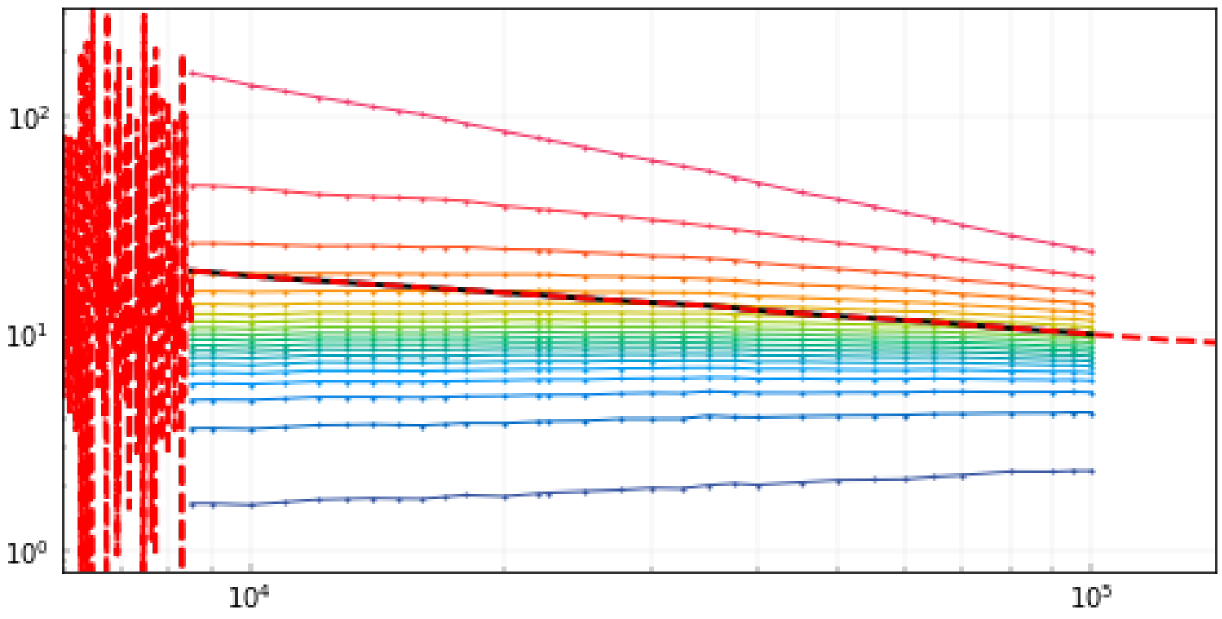
Print the energy points, as well as the table shape (energy points, cross section bands)

```
(energy, ptable) = extract_ptable(nucl, to_mt("N_TOTAL"))
print(energy)
print(ptable.shape)
```

```
[  8500.    9000.   10000.   11000.   12000.   13000.   14000.   15000.   16000.
  17000.   18000.   20000.   22000.   22500.   25000.   27500.   30000.   32500.
  35000.   37500.   40000.   45000.   50000.   55000.   60000.   65000.   70000.
  80000.   90000.   95000.  100000.]
(31, 20)
```

Plot the total cross section at each of the cross section bands and compare it to the mean cross section value. Since the probability table bands at each cross section are discrete and equiprobable, the “mean” cross section provided by the library should equal the mean value across bands:

```
plot_ptable_and_mean(nucl, mt=1)
```



A.5.2.2 Uranium 235

The MT=1 (total neutron cross section) probability table data stored in AMPX data is defined as the sum of the other probability table reactions, even if other non-probability-table reactions are present. In other words, for every energy point *i* and every probability band *b*:

$$\sigma_{\mathrm{t},i,b} = \sum_{x \in \{\mathrm{e,f,g}\}} \sigma_{x,i,b}$$

```
nucl = library.load_nuclide_n(92235, 300)
library.flush_warnings()
print("Reactions with probability table data:",
       ", ".join(mt_to_str(mt) for mt in which_ptables(nucl)))

xs = {}
for k in "total elastic fission gamma".split():
    (energy, ptab_xs) = extract_ptable(nucl, to_mt("N_" + k.upper()))
    xs[k[0]] = ptab_xs

delta = xs['t'] - xs['e'] - xs['f'] - xs['g']
rel_err = np.abs(delta / xs['t'])
print("Maximum relative error:", np.max(np.abs(delta / xs['t'])))
```

```
Reactions with probability table data: 1=N_TOTAL, 2=N_ELASTIC, 18=N_FISSION, 102=N_GAMMA
Maximum relative error: 8.809924e-08
```

The error (on the order of single-precision floating point epsilon) confirms this is the case.

A.5.3 FISSION SPECTRUM SAMPLING

When sampling the energy of a daughter neutron from a fission event, Shift chooses between prompt and delayed spectra. What do these distributions look like? Is the data consistent?

```
from nemesis import Std_DB, make_view, make_const_view
from robus import Library, data_path
from physica import calc_micro_xs
from omnibus.db.validator import mt_to_str, to_mt
import matplotlib.pyplot as plt
import numpy as np

%matplotlib inline
from exnihilotools.matplotlib import screen_style
screen_style()
```

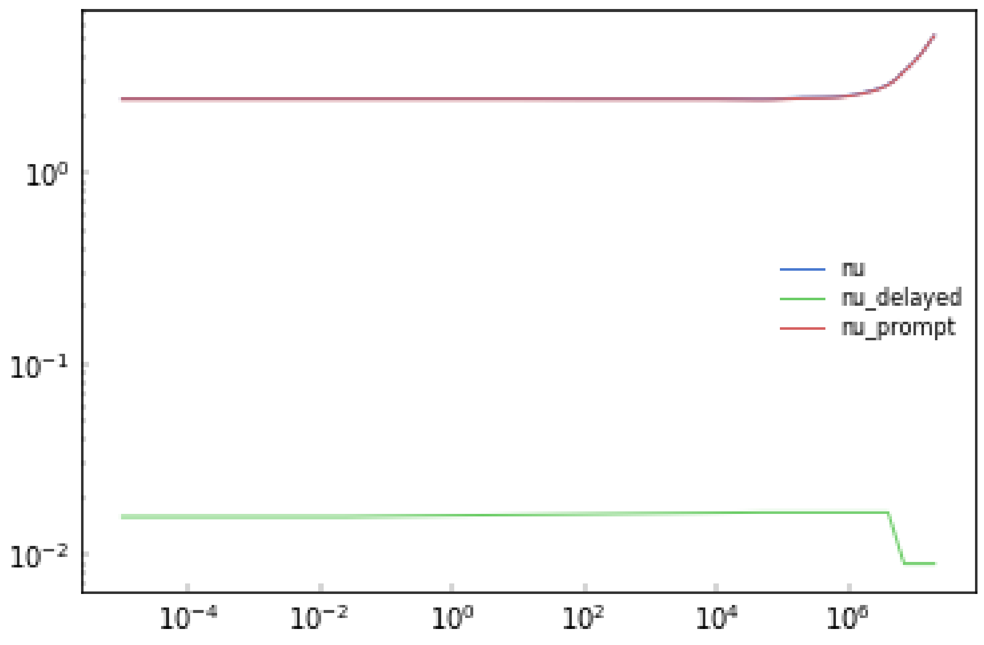
```
/rnsdhpc/code/install/Exnihilo/python/omnibus/__init__.py:93: UserWarning: Version␣
↪mismatch between 'exnihilotools' and 'omnibus' packages: 6.3.pre-b10 (branch 'omnibus-
↪doc' #98d73c8e on 2020MAR11) (at /rnsdhpc/code/build/Exnihilo-examples/Exnihilo/
↪packages/Nemesis/python/exnihilotools/__init__.py) is not the same as 6.3.pre-b10␣
↪(branch 'fix-origen-install' #b3af8ef1 on 2020MAR06) (at /rnsdhpc/code/install/Exnihilo/
↪python/omnibus/__init__.py); This is probably because of a PYTHONPATH error and may␣
↪cause unexpected failures on import
  UserWarning)
```

```
library = Library(Std_DB.from_dict({
   'ce_lib_path': data_path("ce_v71"),
   'gamma_production': True,
}))
```

```
nucl = library.load_nuclide_n(92235, 300.)
```

```
reactions = dict([(v.lower(), nucl.get_reaction(to_mt('N_' + v)))
                  for v in ("NU", "NU_DELAYED", "NU_PROMPT")])
```

```
for (k, rxn) in reactions.items():
    plt.loglog(rxn.energy, rxn.xs, label=k)
plt.legend(loc='best');
```



Do the reactions share an energy grid?

```
print({k: len(reactions[k].energy) for k in sorted(reactions)})
print(np.allclose(reactions['nu'].energy, reactions['nu_prompt'].energy))
```

```
{'nu': 79, 'nu_delayed': 6, 'nu_prompt': 79}
True
```

Do the reactions balance? Since the ‘delayed’ component is on a separate energy grid, it must be interpolated.

```
rxn = reactions['nu_delayed']
egrid = np.array(reactions['nu'].energy)
interp_delayed = np.empty(egrid.shape, dtype='f4')
calc_micro_xs(rxn, make_const_view(egrid), make_view(interp_delayed))

xs_total = np.array(reactions['nu'].xs)
xs_prompt = np.array(reactions['nu_prompt'].xs)
xs_delayed = np.array(interp_delayed)
print(np.allclose(xs_total, xs_prompt + xs_delayed))
```

```
True
```

A.5.3.1 Examine fission-related reactions

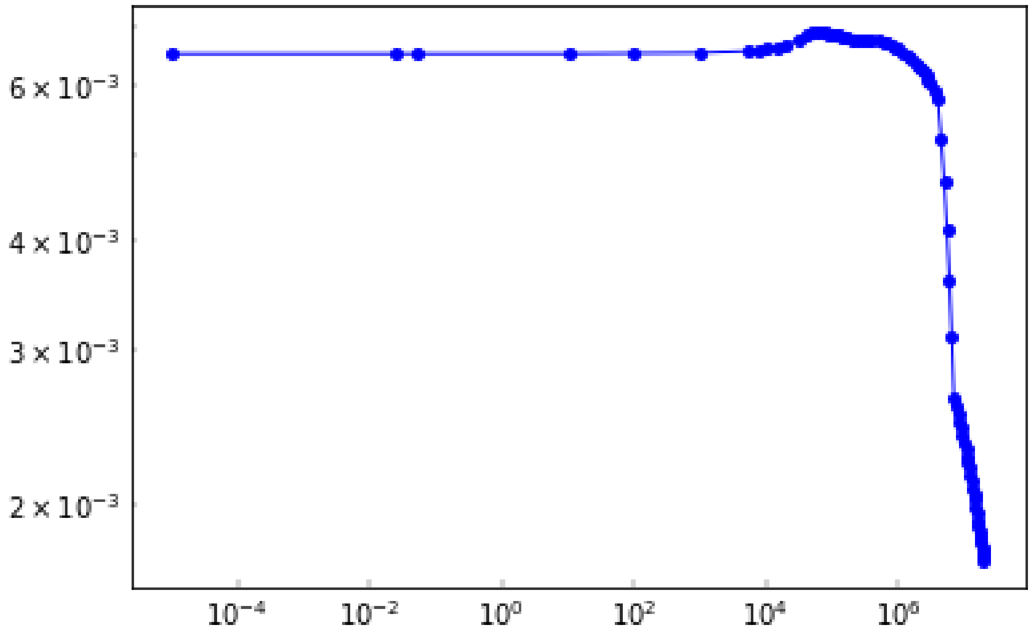
Which of the reactions have kinematics data?

```
fission_mts = set([18,19,20,21,38] + list(range(450, 461)))
fission_mts &= set(nucl.get_mts())
for mt in sorted(fission_mts):
    rxn = nucl.get_reaction(mt)
    print(mt_to_str(mt), "has collision" if rxn.has_collision else "")
```

```
18=N_FISSION has collision
452=N_NU
455=N_NU_DELAYED has collision
456=N_NU_PROMPT
459=N_FISS_YIELD
```

Examine the fission spectrum:

```
rxn = nucl.get_reaction(459)
plt.loglog(rxn.energy, rxn.xs, '.b-');
```



A.5.4 KERMA DATA SPLICING THROUGH AMPX

Shift supports reading AMPX multigroup files into its CE transport routines for use in reaction rates etc. Note that when splicing AMPX data through the python interface, it is necessary to load the `build_library` function from `physica` rather than calling the `Library` constructor.

```
from nemesis import Std_DB
from robus import Library, data_path
from physica import build_library
from omnibus.db.validator import mt_to_str, to_mt

import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
from exnihilotools.matplotlib import plot_multigroup, screen_style, grid
screen_style()

library = build_library(Std_DB.from_dict({
'ce_lib_path': data_path("ce_v71"),
'gamma_production': False,
```

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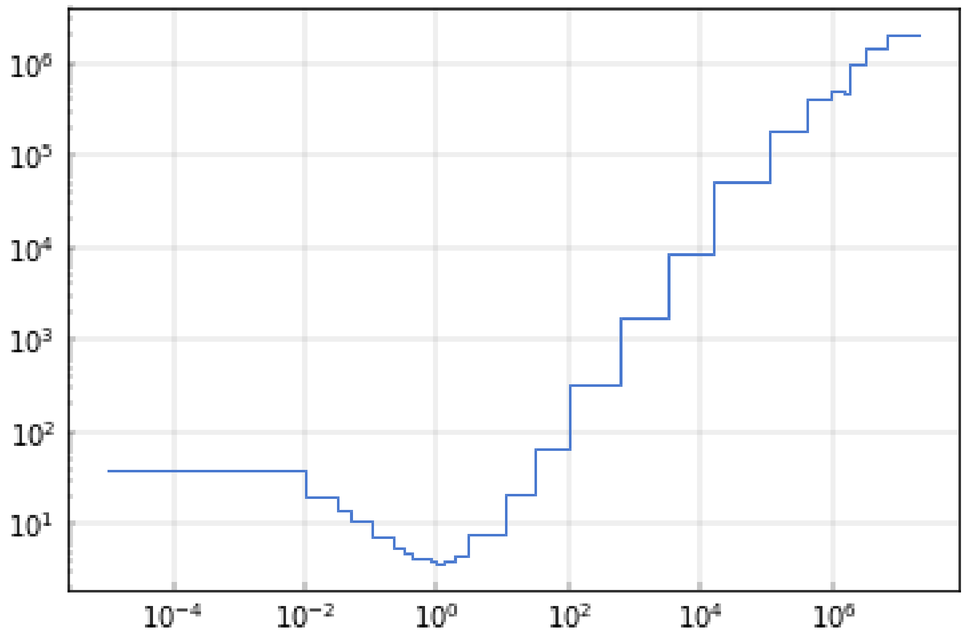
```
'splice_ampx_db': {
   'reactions': [to_mt(k) for k in "N_KERMA P_KERMA".split()],
   'xs_library': "/usr/local/scale/kerma/scale.rev11.xn27g19v7",
   'orig_zaid_p': [4000],
   'subs_zaid_p': [4009],
   },
}))
```

```
/rnsdhpc/code/install/Exnihilo/python/omnibus/__init__.py:93: UserWarning: Version␣
↪mismatch between 'exnihilotools' and 'omnibus' packages: 6.3.pre-b10 (branch 'omnibus-
↪doc' #98d73c8e on 2020MAR11) (at /rnsdhpc/code/build/Exnihilo-examples/Exnihilo/
↪packages/Nemesis/python/exnihilotools/__init__.py) is not the same as 6.3.pre-b10␣
↪(branch 'fix-origen-install' #b3af8ef1 on 2020MAR06) (at /rnsdhpc/code/install/Exnihilo/
↪python/omnibus/__init__.py); This is probably because of a PYTHONPATH error and may␣
↪cause unexpected failures on import
  UserWarning)
```

With the the KERMA data loaded, it can now be plotted:

```
nucl = library.load_nuclide_n(4009, 300.)
rxn = nucl.get_reaction(to_mt('N_KERMA'))
xs = np.asarray(rxn.xs)
assert xs[-1] == xs[-2]
plt.loglog(rxn.energy, xs, drawstyle='steps-post')
grid(plt.gca());
```



```
nucl = library.load_nuclide_p(4000)
library.flush_warnings()
rxn = nucl.get_reaction(to_mt('P_KERMA'))
```

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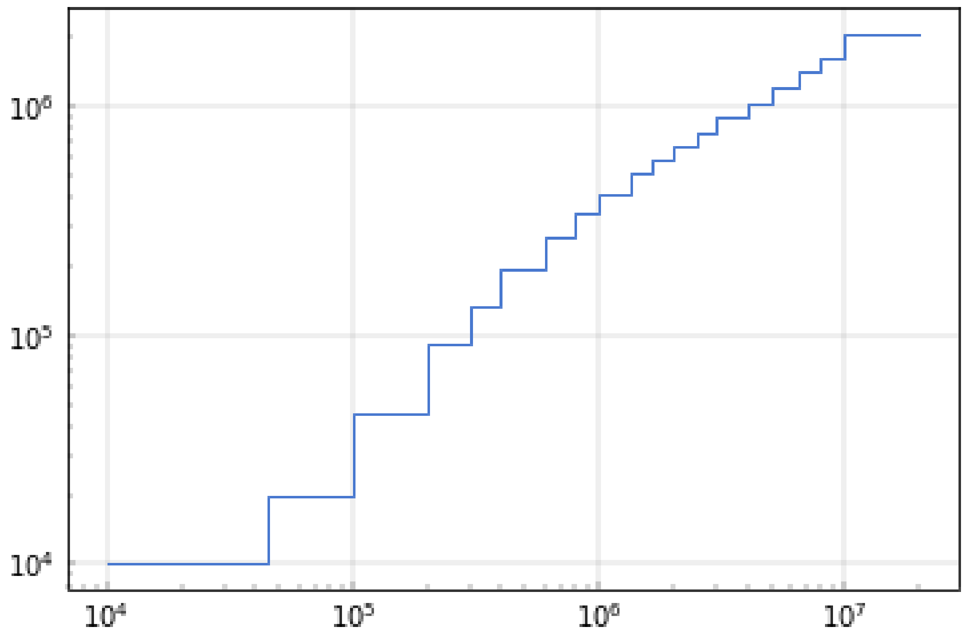
```
xs = np.asarray(rxn.xs)
assert xs[-1] == xs[-2]
plt.loglog(rxn.energy, xs, drawstyle='steps-post')
grid(plt.gca());
```



A.6 SUPPLEMENTAL

A.6.1 USING THE H5SH TOOL

To enter the `h5sh` shell, just run `h5sh HDF5_FILE`. Here is an example of what it looks like:

```
$ h5sh kcode_sce.out.h5
kcode_sce.out.h5:/> l
comp        Group (6 items)
metadata    Group (8 items)
model       Group (4 items)
physics-ce Group (5 items)
response    Group (2 items)
shift       Group (5 items)
source      Group (3 items)
system      Group (4 items)
tally       Group (9 items)
kcode_sce.out.h5:/> cd physics-ce
kcode_sce.out.h5:/physics-ce> prompt "> "
db log mixtures peak_memory timers
> ls
db log mixtures peak_memory timers
> dump log
/physics-ce/log :  scalar |S435
>>> Creating default boundary mesh from (-5 -5 -5) to (5 5 5) for RTK Core
```

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```
geometry
>>> Loading CE library /usr/local/scale/hpcdata/ce_v7.0_endf.h5
*** The following nuclide IDs were remapped due to missing neutron data
*** Remapped 1 nuclide IDs: 6012->6000
>>> Corrected total xs in probability table data: u-234 @ 293K, u-234 @
565K, u-234 @ 300K, u-235 @ 293K, u-235 @ 565K, u-235 @ 300K, u-238 @ 293K,
u-238 @ 565K, u-238 @ 300K

> cd ../tally
> ls
cyl description fission_site kcode medium mytally peak_memory timers xs
> cd mytally
> ls
description max_encountered_bins mesh_stat mesh_x mesh_y mesh_z multiplier_descs␣
↪multiplier_names normalization num_histories total volumes
> ls -l
description          Dataset (S: scalar)
max_encountered_bins Dataset (L: scalar)
mesh_stat            Dataset (O: 2)
mesh_x               Dataset (d: 11)
mesh_y               Dataset (d: 11)
mesh_z               Dataset (d: 11)
multiplier_descs     Dataset (O: 2)
multiplier_names     Dataset (O: 2)
normalization        Dataset (d: scalar)
num_histories        Dataset (d: scalar)
total                Dataset (d: 10x10x10x2x2)
volumes              Dataset (d: 10x10x10)
> attr
type=mesh
> dump mesh_x
/tally/mytally/mesh_x :  11 float64
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
> dump -o tally.txt total
> cd ../kcode/keff
cd: /tally/kcode/keff is not a group
> cd ../kcode/
> ls
entropy entropy_crossover_cycle entropy_mesh keff keff_estimators
mesh_cycle mesh_moment mesh_stat moments statistics_pass
> print keff
h5sh: print: command not found
> help
Available commands:
attr     - Print attributes of the current group
cd       - Change the current HDF5 group
dump     - Print the contents of a dataset
exit     - Exit h5sh
filename - Print the name of the file being examined
help     - List available commands
l        - Alias for 'ls -l'
ls       - List items in the current group
```

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```
prompt   - Get or change the terminal prompt
pwd      - Print the path to the current HDF5 group
> dump keff
/tally/kcode/keff :  2 float64
Attributes: {'DIMENSION_LABELS': array([b'stat'], dtype=object)}
Chunked: (2,)
[  1.00356147e+00   1.52605295e-05]
> exit
```

A.6.2 RUNNING OMNIBUS THROUGH PYTHON

Because the Omnibus front end is simply a Python script, it is possible to drive it through another Python script. For example, the shell command

```
$ omnibus-run nyoka.omn
```

can be written as the following python script:

```python
from omnibus.scripts.omnibus_run import run

run(["nyoka.omn"])
```

The first argument to `run` takes a list, because multiple files can be passed to the input just like with the scripted front end. An additional and very useful feature is that a python *function* can also be passed to modify the database, just like a Python script can be passed through the command line:

```python
from omnibus.scripts.omnibus_run import run

def change_name(db):
    db['problem']['name'] = "Something else"

run(["nyoka.omn", change_name])
```

This opens up exciting possibilities of automating scaling studies and parameter studies. To this end, a helper class is available that can drive multiple Omnibus executions with variable parameters. Here is an example that modifies an Omnibus input `base-input.omn`, loops over different numbers of compute cores and particles per cores, saves the output to subdirectories inside `weak-scaling/ppc`*nnnnnn*`-np`*nnnn*, and then extracts a few different timers and transport diagnostics and writes them to `weak-scaling/results.json`.

```python
from omnibus.scripts.omnibus_run import MultiRun

class ScalingRun(MultiRun):
    inp = "base-input.omn"
    fmt = "ppc{ppc:06d}-np{cores:04d}".format
    basedir = "weak-scaling"

    timers = {
        'init_time': ("shift", "shift::sensitivity::Processor.initialize"),
        'transport_time': ("shift", "shift::DR_Source_Transporter.solve"),
        'rebalance_time': ("shift", "shift::Fission_Sourcer.complete"),
        'comm_time': ("shift",
```

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```
            "shift::sensitivity::Processor.communicate_tallies"),
        'total_time': ("shift", "shift::KCode_Solver.solve"),
        }

    db_entries = {
        'comm_iters': ('SHIFT','DIAGNOSTICS','sensitivity_comm_iters'),
        'memory':     ('SHIFT','MEMORY','VmHWM'),
        'particles':  ('SHIFT','DIAGNOSTICS','particles_transported'),
        }

    def update(self, db, cores, ppc):
        db['run'] = {
                '_type': "pbs",
                'ppn': ppn,
                'nodes': 1,
                'walltime': "2:00:00",
                'when_email' : "", # never
                'name': self.fmt(**locals()) + "-shift",
                }

        # Set number of particles per core per cycle
        db['shift']['kcode']['npk'] = ppc * cores

def main():
    with ScalingRun() as run:
        # Scale up to 8 cores
        for cores in [1,2,4,8]:
            # Vary particles per core
            for ppc in [10,100,1000]:
                run(cores=cores, ppc=ppc)

main()
```

The resulting JSON file looks something like this:

```json
{"comm_time":[ 0.0601811408996582, 0.06244254112243652,
    0.06316995620727539, 0.09857296943664551, 0.1872391700744629,
    0.5450944900512695, 0.1900339126586914, 0.4031996726989746,
    0.3892052173614502, 0.2579929828643799, 0.6250407695770264,
    1.1602895259857178 ],
"cores":[ 1, 1, 1, 2, 2, 2, 4, 4, 4, 8, 8, 8 ],
"memory":[ 769736, 878304, 1939864, 807824, 916060, 1967500, 816452,
    925144, 1983192, 815940, 925492, 1998944 ],
"ppc":[ 10, 100, 1000, 10, 100, 1000, 10, 100, 1000, 10, 100, 1000 ],
}
```

which can be plotted or analyzed easily using Pandas:

```python
import json
import pandas as pd

with open("weak-scaling-twogroups/results.json") as f:
```

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```python
    results = pd.DataFrame.from_dict(json.load(f))
results.index = pd.MultiIndex.from_arrays([
    results.pop('cores'), results.pop('ppc')])
results.sort_index(inplace=True)
results['comm_time'].unstack('cores').plot()
```

To use this functionality, the user must subclass the *MultiRun* class and provide:

- a base input filename (“box.omn” in the attached example),
- a formatter for the name of the subdirectories for each file to run (using the new Python-style keyword formatting),
- the root directory of the output files (under which the subdirs will be created, as well as the ‘results.json’ summary)
- a database of timer names to be recorded from each run,
- a database of DB entries to be recorded from each run, and
- an *update* method that modifies the problem input based on the keyword arguments specified. (The first two arguments of this function must be `self` for the class and `db` for the problem database.)

The class is then instantiated as a context manager and called with the keyword arguments specified in the *update* method.

```python
with WeakScalingRun() as run:
    for ppn in range(1,32+1):
        run(instance=0, nodes=1, ppn=ppn)
```

It will record all the keywords, the timers, and the DB entries into a JSON file, and will reuse existing output if it is there. If the program aborts from a keyboard interrupt or a failed run, then the context manager will still output all the results it has gathered.

Appendix B. FILE FORMAT SPECIFICATIONS

Appendix B. FILE FORMAT SPECIFICATIONS

Omnibus uses multiple file formats for input (e.g., geometry definitions and material properties) and output (e.g., Denovo flux HDF5 files).

B.1 DENOVO OUTPUT SPECIFICATION

Denovo uses parallel HDF5 to write multiple sets of data that correspond to its interpreted input and the solution output. Since it supports both 2D and 3D problem definitions, the mesh cell–based dimensions will change depending on the problem type. Additionally, depending on the problem input parameters, some of the fields may be absent. Notably, if the P_N order is zero, then the solution is isotropic, and no `current` field will be output.

Note: Since Denovo uses column-major ordering for meshes, 'x' is always the fastest varying axis. Thus the HDF5 (row-major) dimensions for cells will be (Z,Y,X) or (Y,X).

Tip: Denovo uses the HDF5 Dimension Scale API[24] to write dimension labels to its output. If you review these (e.g. with `h5dump -A file`) you can be sure of the significance of the different dimensions.

B.1.1 ROOT LEVEL DESCRIPTION

Datasets:

Name	Type	Dims	Description
mesh_x	double	X + 1	Mesh edges along the x axis.
mesh_y	double	Y + 1	Mesh edges along the y axis.
mesh_z	double	Z + 1	Mesh edges along the z axis.
group_bounds_n	double	NN+1	Neutron group boundaries, or empty if no neutron groups are being solved.
group_bounds_p	double	NG+1	Photon group boundaries, or empty if no photon groups are being solved.
flux	double	G,Z,Y,X	Scalar fluxes for each group in each mesh cell.
source	double	G,Z,Y,X	Volumetric source term if an isotropic fixed source was used.
uncflux	double	G,Z,Y,X	Uncollided flux if used.
current	double	G,Z,Y,X,3	Currents (first scalar flux moment).
block	u short	Z,Y,X	KBA block index for each cell.
matids	int	Z,Y,X	Global mixture ID.
mixtable	COO	M	Global mix table.

Groups:

Name	Description
metadata	Metadata about the problem, system, and Exnihilo version used to create the output file.

[24] https://www.hdfgroup.org/HDF5/doc/HL/RM_H5DS.html

All quantities follow the standard nuclear engineering practice of being averaged over space and integrated in energy and angle.

The mix table stores mixture IDs as rows, and it stores composition IDs/pure matids as columns. For parallel problems, the mix table is essentially the concatenation of all the domain-local mix tables, but with pure materials placed in the beginning rows of the table. Thus, the mix table may have duplicate rows if run in parallel.

B.2 HDF5 MESH MODEL SPECIFICATION

Denovo accepts an explicit problem model definition via an HDF5 input file. Since it supports both 2D and 3D problem definitions, the mesh cell–based dimensions will change depending on the problem type.

Note: Since Denovo uses column-major ordering for meshes, ‘x’ is always the fastest-varying axis. Thus the HDF5 (row-major) dimensions for cells will be (Z,Y,X) or (Y,X).

B.2.1 ROOT LEVEL DESCRIPTION

Datasets:

Name	Type	Dims	Description
mesh_x	double	X + 1	Mesh edges along the x axis.
mesh_y	double	Y + 1	Mesh edges along the y axis.
mesh_z	double	Z + 1	Mesh edges along the z axis. (For a 2D problem, this field should not be present.)
matids	int	Z,Y,X	Material IDs in each mesh cell. (For a 2D problem, dimensions are Y,X.)
mixtable	COO	M,P	Sparse matrix representation: M is the number of mixtures, P the number of “pure” materials (original problem matids)
source		G,Z,Y,X	Optional volumetric source definition.

The mix table is stored in Coordinate matrix format, a structure of (‘row’, ‘col’, ‘val’) elements with types (int, int, double), respectively. These datasets are written consistently with the Denovo Output Specification (page B–3) output specification so that it can be used as a restart file.

Groups:

Name	Description
volsrc	Optional cell-based volume source definitions.
ptsrc	Optional point source definitions. Only applicable to 3D.
metadata	Optional metadata about the version of Omnibus used to generate the input file.

B.2.2 VOLSRC GROUP DESCRIPTION

Datasets:

Name	Type	Dims	Description
ids	int	Z,Y,X	Spectrum IDs in each mesh cell.
strength	double	Z,Y,X	Source strength in each cell.
spectra	double	S,G	The row index (zero-based) in the table is the spectrum ID; the row itself is a normalized spectrum for all G groups.

B.2.3 PTSRC GROUP DESCRIPTION

Datasets:

Name	Type	Dims	Description
mesh_point	double	P,3	Point source locations. Each row is a separate point.
strength	double	P	Point source strengths.
spectra	double	P,G	Normalized spectra. Each row is the normalized spectrum for all G groups corresponding to the point at that row index.

B.3 RTK XML INPUT SPECIFICATION

The RTK XML geometry input specification will be documented once the format is finalized.

B.4 XS XML INPUT SPECIFICATION

The XML cross section input specification will be documented once the format is finalized.