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The DIORAMA Neutron Emitter

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1 Introduction

Emission of neutrons in a given event is modeled by the `DioramaEmitterNeutron` object, a subclass of the abstract `DioramaEmitterModule` object. The `GenerateEmission` method of this object is the entry point for generation of a neutron population for a given event. Shown in table 1, this method requires a number of parameters to be defined in the event definition.

2 The Neutron Emission

The neutron emission within DIORAMA feeds a deterministic propagator model and is specified as a neutron count distribution g_n that is differential in neutron energy E_n :

$$g_n(E_n) = \frac{dN_n}{dE_n} \quad (1)$$

where dN_n is the number of neutrons emitted with energy between E_n and $E_n + dE_n$. Further, one may define a cumulative neutron count distribution $G_n(E)$ as the definite integral of g_n from $E_n = 0$ to $E_n = E$, and G_n converges to the total number of neutrons emitted in the event as E goes to infinity.

For scenarios typically handled within DIORAMA, neutron count distributions are specified in tabular form with discrete data points. Therefore, the DIORAMA neutron emission is treated as a one-dimensional, discretely-binned neutron count distribution. Bin contents $g_{n,i}$ in the i^{th} energy bin of this neutron count histogram are given by:

Table 1: Description of all event definition parameters required by the neutron source model.

Parameter name	Min.	Max.	Unit	Description
yield	0.0	1e10	kT	Total device yield
neutron_yield_fraction	0.0	1.0		Fraction of the total yield that should be emitted as neutron energy
neutron_spectrum_type				The type of output emission to generate (fission, thermonuclear, monoenergetic)
neutron_energy	1.E-9	1.E4	MeV	If using a monoenergetic spectrum, this will specify the energy
neutron_emission_interpolation_type				For tabular emission distributions, respective values of <i>linear</i> and <i>monotonic_spline</i> select linear or spline interpolation of the CDF

$$\begin{aligned}
g_{n,i} &= \frac{1}{\Delta E_i} \int_{E_{n,i}}^{E_{n,i+1}} dE g_n(E) \\
&= \frac{1}{\Delta E_i} (G(E_{n,i+1}) - G(E_{n,i}))
\end{aligned}$$

where $E_{n,i}$ and $E_{n,i+1}$ respectively represent the lower and upper neutron energy limits for the i^{th} energy bin. Unless otherwise stated, binning of the neutron count distribution should be assumed to be contiguous.

For a given event in which neutrons are emitted, a DioramaEmission object is generated, which includes the above-mentioned binned neutron count distribution along with various pieces of meta data. The neutron count distribution is generated according to one of the available neutron emission models described below. The emission model for the event is selected using the `neutron_spectrum_type` input parameter for the emitter.

3 The mono-energetic neutron source

Primarily for low-level validation of the neutron propagator and sensor models, the neutron emitter supports a mono-energetic neutron feature. This emission type is enabled by setting the `neutron_spectrum_type` input parameter to `monoenergetic`. In this case, the `neutron_energy` input parameter must also be given as the desired value of the energy in units of MeV.

Since the emission is handled in a discretely-binned distribution, some precision is lost in the mono-energetic emission. The total number of neutrons emitted is calculated as the ratio of the neutron yield (in units of energy) to the true mono-energetic neutron energy. This

number of neutrons is then placed in the energy bin containing the mono-energetic neutron energy and normalized by the bin width. At this point, the mono-energetic emission might be better described as a uniform distribution between the energy limits of the bin, since this is how it will be treated by the propagator. This aliasing results in a deviation of the emitted neutron yield from the requested neutron yield when the mono-energetic energy differs from the mean energy of the bin.

4 The tabular neutron source

A tabular neutron source is selected by choosing any available option for the `neutron_spectrum_type` other than `monoenergetic`. At present, this includes a `thermonuclear` and `fission` spectrum type. Tabular data for neutron count distributions are taken from an Oak Ridge National Laboratory technical report titled “Production and Testing of the DNA Few-Group Neutron-Gamma Cross-Section Library” [1, table 5.A].

Tabulated neutron emission probabilities are published as integrated emission probabilities over a series of discrete and contiguous neutron energy bins. This data is best described as the integral of the cumulative neutron emission probability distribution over a set of discrete bins. Therefore, this data is best treated as input for an emission cumulative probability distribution (CDF) from which an energy-differential probability distribution (PDF) is derived.

4.1 From tabular data to neutron emission

Tabular neutron emission data is used to generate a probability distribution that defines the shape of the emission spectra; so overall normalization of input tabular neutron data is ignored. The probability distribution dP/dE_n is defined as follows:

$$\frac{dP}{dE_n} = \frac{1}{N_n} \frac{dN_n}{dE_n} \quad (2)$$

where N_n represents the total number of neutrons emitted in the event.

The total number of neutrons N_n is derived from integral parameters taken from the event parameterization as well as from the tabulated neutron spectrum. The product of the total yield Y and neutron yield fraction $f_{neutron}$ define the total energy of the emitted neutron population for a given event:

$$Y f_{neutron} = \int_0^\infty dE_n \frac{dN_n}{dE_n} E_n \quad (3)$$

The two parameters on the left-hand side represent integral characteristics of the emitted neutron population that are provided as input for the modeled event. The right-hand side of the equation represents an integral property of the neutron population defined by the shape of the energy spectrum.

The right-hand side of equation 3 can be rewritten in terms of a mean neutron energy $\bar{E}_n$ as follows:

$$\int_0^\infty dE_n \frac{dN_n}{dE_n} E_n = N_n \bar{E}_n \quad (4)$$

where:

$$\bar{E}_n = \frac{1}{N_n} \int_0^\infty dE_n \frac{dN_n}{dE_n} E_n = \int_0^\infty dE_n \frac{dP}{dE_n} E_n \quad (5)$$

Combining equations 3 and 4, one arrives at a formula for the integrated neutron count N_n in terms of input parameters and the mean energy of the tabulated distribution:

$$N_n = \frac{Y f_{neutron}}{\bar{E}_n} \quad (6)$$

In short, the above formula states that the mean number of electrons generated in the event is equal to the ratio of the total energy of the emitted neutron population and the mean energy of the neutron energy distribution, a somewhat obvious formulation that may not warrant such a detailed derivation.

As discussed below, the mean neutron energy $\bar{E}_n$ is calculated and cached once for each loaded neutron source data table. The mean energy is used along with neutron yield event parameters to determine an integrated mean neutron count for the event. The probability density function dP/dE_n is calculated on an energy axis defined within the DIORAMA emission request object. Binning of the emission request energy axis typically deviates from that of the input tabular data; so an interpolation algorithm is used to redistribute the tabulated probability onto the emission request energy axis. It is noted that the mean energy of the tabulated distribution is always calculated using the binning specified in the input tabular data.

4.2 Probability distributions and mean energy from tabular data

Tabular neutron emission data is managed with the DIORAMA table manager object `NeutronSourceTable`. Upon initialization, the table manager is provided a table of neutron count probabilities and energy bin limits. As discussed above, tabulated neutron emission probabilities are published as energy-integrated probabilities over discrete neutron energy bins. As such, these tabulated values can be viewed as CDF increments, and a true CDF at each bin edge can be derived by cumulatively summing the tabulated CDF increments, and assuming a CDF value of zero at the leading bin edge. To yield a properly normalized probability distribution over the neutron energy range covered by the tabular data, the last CDF data point should be unity, and an overall normalization of the CDF graph is applied, if necessary, to ensure this characteristic.

$$CDF_i = \sum_0^i \delta CDF_N$$

and where $CDF_0 = 0$ and i and N represent bin indices. The mean neutron energy for the population is defined as:

$$\bar{E}_{neutron} = \sum_i \delta \text{CDF}_i E_i$$

where E represents the geometric center of the PDF bin with dimensions of neutron energy. It is noted that the choice of geometric center is most appropriate for cases of slow, roughly linear variations of the PDF with kinetic energy. In cases in which the PDF is exponential or follows a power law, this choice may not be appropriate.

Subject to the above described inputs, the neutron emitter object provides a neutron source spectrum $\frac{dN_n}{dE}$ differential in energy with units of the ratio of the number of neutrons per bin and the bin width (i.e., neutrons / MeV). Since binning of the neutron population PDF does not in general match binning of the emission spectrum, an interpolation of the source CDF is used to partition the emission spectrum with arbitrary dispersion. Using this algorithm, the content of each source spectrum bin is calculated as:

$$\frac{dN}{dE}_i = \frac{N_n}{\Delta E_i} \times (\text{CDF}(E_{upper,i}) - \text{CDF}(E_{lower,i}))$$

where ΔE , E_{lower} , and E_{upper} represent the width, lower, and upper limit of each bin of the emission spectrum.

4.3 Interpolation of the CDF

The neutron energy PDF is taken as the derivative of the CDF; so one must be careful in defining the CDF interpolation algorithm to avoid unphysical or unrealistic artifacts in the resulting PDF. For example, the PDF should always be non-negative; so the CDF should be monotonically increasing with neutron energy. The simplest and most robust interpolation technique is a first order polynomial (i.e., linear) interpolation between bin edges. This technique is simple to implement, absolutely preserves monotonicity of the discrete CDF data points, and will not produce ringing or spurious spikes in the interpolating function. However, the derivative of a first-order linear interpolating function for the CDF is not continuous, leading to undesirable discrete steps in the resulting PDF.

Cubic spline interpolation is a commonly-used algorithm which can provide a continuous first derivative. However, compared to the often-used natural cubic spline, additional constraints to the spline parameters must be applied to assure monotonicity and minimal oscillations. Required constraints for such a spline are given in [3] along with a relatively simple iterative technique to generate a monotonic cubic spline. A more sophisticated formalism is derived in [7] making use of a global minimization of an stress or energy metric. This formalism is intended to yield a smoother interpolating function. However, it is more complex and not as robust as that given in [3]; so the former algorithm is adopted for the present application.

Both linear and monotonic cubic spline interpolation of the tabular neutron emission CDF are supported in DIORAMA, and the choice of interpolation algorithm is selected event by event by setting the `neutron_emission_interpolation_type` event parameter. Possible values are `linear` and `monotonic_spline`. Linear interpolation is supported using the GNU scientific library (GSL) spline interface [2]. For monotonic spline support, the Fritsch and Carlson algorithm has been implemented in C++ within the Open Porous Media (OPM)

Table 2: Reproduction of neutron source distributions taken from [6]. Units for tabular data are interpreted as dimensionless probability of neutron emission.

Upper bin edge (MeV)	Thermonuclear	Fission
15.0	7.06E-2	1.568E-4
12.2	2.56E-2	8.932E-4
10.0	1.41E-2	3.480E-3
8.19	1.47E-2	1.392E-2
6.36	1.80E-2	3.457E-2
4.97	1.70E-2	3.507E-2
4.07	2.60E-2	1.072E-1
3.01	1.90E-2	8.898E-2
2.46	5.00E-3	2.323E-2
2.35	2.80E-2	1.203E-2
1.83	6.20E-2	2.181E-1
1.11	8.50E-2	1.983E-1
0.55	1.02E-1	1.403E-1
0.110	3.65E-1	1.550E-2
0.0335	1.22E-1	0.
0.000583	2.40E-2	0.
0.000101	2.00E-3	0.
0.0000290	0.0	0.
SUM	1.00	1.00

project [5]. As opposed to adding a dependency on the relatively large `OPM` library, the source and header files for the monotonic interpolator have been added to the `DIORAMA` math package.

4.4 Summary of available tabular neutron data

Tabular data for neutron PDFs are taken from an Oak Ridge National Laboratory technical report titled “Production and Testing of the DNA Few-Group Neutron-Gamma Cross-Section Library” [1, table 5.A] and two references therein from which fission and thermonuclear neutron spectra were derived [4, table 2][6, table 2]. The Bartine report references a set of neutron and gamma source disitributions “commonly used in defense-related calculations”, and the source distributions are reproduced in tables 3, 4, and 2. Reference [1] includes three distributions but only those referred to as *thermonuclear* and *fission* are included in `DIORAMA` to define neutron source definitions. To use these neutron emission distributions, the `neutron_spectrum_type` parameter in the event definition should be set to one of the following: `ORNL-TM4464_fission`, `ORNL-TM4464_thermonuclear`, `ORNL-TM4840_fission`, `ORNL-TM4840_thermonuclear`, or `ORNL-TM4841_fission`.

Treatment of the tabulated data is summarized in figures 1, 2, 3, 5, and 4. In all figures, the upper panel represents the tabulated CDF along with the linear and monotonic spline

Table 3: Reproduction of neutron source distributions commonly used for defense-related calculations taken from [1]. Only the distributions denoted thermonuclear and fission are used in DIORAMA. Units for the tabular data are given as “neutrons / source neutron” and are interpreted as dimensionless neutron emission probability.

Upper bin edge (MeV)	Thermonuclear	Fission
19.6	0.0	0.0
16.9	0.0	0.0
14.9	1.89E-2	0.0
14.2	9.34E-3	0.0
13.8	2.66E-2	0.0
12.8	1.67E-2	0.0
12.2	1.69E-2	0.0
11.1	1.24E-2	0.0
10.0	7.48E-3	3.84E-3
9.0	6.82E-3	3.50E-3
8.2	6.78E-3	5.39E-3
7.4	1.03E-2	7.35E-3
6.4	1.81E-2	1.84E-2
5.0	3.62E-3	3.25E-3
4.7	1.24E-2	8.47E-3
4.1	2.60E-2	5.50E-2
3.0	2.37E-2	3.24E-2
2.4	3.75E-3	1.06E-2
2.3	2.56E-2	9.72E-2
1.8	6.44E-2	1.47E-1
1.1	8.85E-2	2.16E-1
5.5E-01	9.14E-2	1.50E-1
1.6E-01	1.16E-2	1.93E-2
1.1E-01	1.11E-1	1.21E-1
5.2E-02	5.40E-2	5.73E-2
2.5E-02	5.68E-3	6.00E-3
2.2E-02	9.26E-2	2.40E-2
1.0E-02	1.16E-1	1.44E-2
3.4E-03	7.38E-2	0.0
1.2E-03	2.32E-2	0.0
5.8E-04	2.03E-2	0.0
1.0E-04	1.90E-3	0.0
2.9E-05	0.0	0.0
1.1E-05	0.0	0.0
3.1E-06	0.0	0.0
1.1E-06	0.0	0.0
4.1E-07	0.0	0.0
1.0E-11		
SUM	1.00	1.00

Table 4: Reproduction of the neutron source distribution taken from [4]. Units are interpreted as dimensionless emission probability of neutron emission.

Upper bin edge (MeV)	Fission
10.	7.342E-3
8.18	1.274E-2
6.36	1.832E-2
4.96	1.177E-2
4.06	5.481E-2
3.01	2.871E-2
2.46	5.743E-3
2.35	1.060E-1
1.83	1.468E-1
1.11	2.159E-1
0.55	1.693E-1
0.111	2.227E-1
0.00335	0.0
SUM	1.00

interpolations. Although differences between interpolation algorithms appear small in these semi-logarithmic plots, they are far more apparent in the lower two panels which show the resulting PDF from linear interpolation (middle panel) and spline interpolation (lower panel).

In both of the linear and spline panels, “tabulated” PDF data is represented for comparison as a filled, blue histogram and is produced by taking the ratio of the tabulated CDF increments and the discrete neutron energy bin widths. These reference histograms are best described as the mean PDF for each energy bin. The “tabulated” PDF is overlaid with interpolations with 100 (red) and 1000 (blue) logarithmically spaced neutron energy bins. As expected, linear interpolation of the CDF yields PDF that are very similar to the “tabulated” mean PDF, including discontinuities at table bin edges. With 100 bins, there is some aliasing apparent at table bin edges. However, this is significantly reduced in the 1000-bin scenario. For the spline interpolation, smoothing of the PDF is very reasonable in energy regions where the tabulated CDF changes in a rather controlled way (e.g., neutron energy range from less than 10^{-4} MeV up to 10^{-2} MeV for the *thermonuclear* distribution. However, abrupt changes in the tabular CDF lead to ringing in the PDF when using spline interpolation. This ringing can create artificial enhancement and suppression of neutron flux at certain energies that can skew simulation results. Ringing in the *TM4840 thermonuclear* distribution is fairly limited. However, this is not the case for the *TM4840 fission* emission distribution where the tabular data includes more pronounced discrete steps. For simplicity, one might considered strictly using linear interpolation to avoid oscillations in the neutron emission PDF.

Since the mean neutron energy is taken directly from the tabulated PDF/CDF data, any difference between the tabulated and interpolated distributions will yield an error in the emitted neutron yield. For the specific case of linear interpolation of the *TM4840 thermonu-*

clear distribution with 100 bins, this deviation in yield was found to be 0.17%. It should be reasonably negligible for 1000-bin linear interpolations. Although not specifically evaluated, one might expect this error to be large for spline interpolation due to the more dramatic ringing of the interpolated PDF when compared to the mean PDF.

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Figure 1: Summary of treatment of the tabulated ORNL/TM-4464 thermonuclear PDF within the DIORAMA neutron emitter module.

Figure 2: Summary of treatment of the tabulated ORNL/TM-4464 fission PDF within the DIORAMA neutron emitter module.

Figure 3: Summary of treatment of the tabulated ORNL/TM-4840 thermonuclear PDF within the DIORAMA neutron emitter module.

Figure 4: Summary of treatment of the tabulated ORNL/TM-4840 fission PDF within the DIORAMA neutron emitter module.

Figure 5: Summary of treatment of the tabulated ORNL/TM-4841 fission PDF within the DIORAMA neutron emitter module.