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Simulation of Neutron and Gamma Ray Emission from Fission and Photofission

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1 Introduction

This paper describes a general-purpose and extensible software library to accurately simulate neutron and gamma-ray distributions from fission reactions (spontaneous, neutron induced and photon induced). This was originally motivated as a tool for detailed statistical studies of fission chains in multiplying media.

This library provides an event-by-event list of neutrons and gamma rays for a specific fission reaction and is intended to be used in conjunction with a Monte Carlo transport code. The parent code provides the reaction cross-section information, whereas this library samples the neutron and gamma multiplicity and energy distributions. This library is data-driven and incorporates all available multiplicity measurements found in the literature. Empirical models are employed whenever multiplicity data are not available.

Essentially no data are available for the correlations between the neutrons and gammas, so this model samples these distributions independently. By default, this model effectively scales the multiplicity data to match the average multiplicity value ($\bar{\nu}$) found in external evaluated data libraries. At present the gammas and neutrons are emitted isotropically. The data and empirical models are described in detail in the following subsections.

This model has been incorporated into Geant4 and has been submitted for inclusion in future versions of MCNPX. The standalone version of the software library can be downloaded from `http://nuclear.llnl.gov/simulation`.

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2 Spontaneous fission and neutron-induced fission

2.1 Neutron number distribution

Based on reasonable assumptions about the distribution of excitation energy among fission fragments, Terrell [1] showed that the probability P_ν of observing ν neutrons from fission can be approximated by a Gaussian-like distribution

$$\sum_{n=0}^{\nu} P_n = \frac{1}{2\pi} \int_{-\infty}^{\frac{\nu-\bar{\nu}+\frac{1}{2}+b}{\sigma}} e^{-\frac{t^2}{2}dt} \tag{1}$$

where $\bar{\nu}$ is the average number of neutrons, σ (set to 1.079) is the width of the distribution, and b is a small correction factor ($b < 0.01$) that ensures that the discrete probability distribution has the correct average $\bar{\nu}$. This model is used when no explicit multiplicity data are available.

Neutron-induced fission data

Zucker and Holden [3] measured the neutron multiplicity distributions for ^{235}U, ^{238}U, and ^{239}Pu (see Tables 1-3), as a function of the incident neutron energy E_n from zero through ten MeV in increments of one MeV. Fig. 1 shows the neutron number distribution for induced fission of ^{235}U. Gwin, Spencer and Ingle [4] measured the distribution at thermal energies for ^{235}U. In addition, there are many measurements of $\bar{\nu}$, the average number of emitted neutrons, for many isotopes. Since there are multiple methods for parameterizing the multiplicity data and renormalizing the overall distributions to agree with the specific measured values of $\bar{\nu}$, we provide four options for generating neutron multiplicity distributions. These options are selected by the internal variable `nudist`, default=3.

E_n	ν=0	1	2	3	4	5	6	7	$\bar{\nu}$
0	.0317223	.1717071	.3361991	.3039695	.1269459	.0266793	.0026322	.0001449	2.4140000
1	.0237898	.1555525	.3216515	.3150433	.1444732	.0356013	.0034339	.0004546	2.5236700
2	.0183989	.1384891	.3062123	.3217566	.1628673	.0455972	.0055694	.0011093	2.6368200
3	.0141460	.1194839	.2883075	.3266568	.1836014	.0569113	.0089426	.0019504	2.7623400
4	.0115208	.1032624	.2716849	.3283426	.2021206	.0674456	.0128924	.0027307	2.8738400
5	.0078498	.0802010	.2456595	.3308175	.2291646	.0836912	.0187016	.0039148	3.0386999
6	.0046272	.0563321	.2132296	.3290407	.2599806	.1045974	.0265604	.0056322	3.2316099
7	.0024659	.0360957	.1788634	.3210507	.2892537	.1282576	.0360887	.0079244	3.4272800
8	.0012702	.0216090	.1472227	.3083032	.3123950	.1522540	.0462449	.0107009	3.6041900
9	.0007288	.0134879	.1231200	.2949390	.3258251	.1731879	.0551737	.0135376	3.7395900
10	.0004373	.0080115	.1002329	.2779283	.3342611	.1966100	.0650090	.0175099	3.8749800

Table 1: Neutron number distribution for induced fission in ^{235}U.

The first option (`nudist=0`) uses a fit to the Zucker and Holden data [3] by Valentine [5, 6]. Valentine expressed the P_ν's (for $\nu = 0, ..., 8$) as 5th order polynomials in E_n, the incident neutron energy. These functions $P_\nu(E_n)$ are used to sample the neutron multiplicity for E_n in the range 0 to 10 MeV. When E_n is greater than 10 MeV, E_n=10 MeV is used to generate P_ν.

In addition to using the Zucker and Holden data above for incident neutron energies E_n above 1 MeV, the second option (`nudist=1`) also uses the Gwin, Spencer and Ingle data [4] for ^{235}U at thermal energies (0 MeV) to generate $P_\nu(E_n)$ polynomials. As in the first option, when E_n is greater than 10 MeV, E_n=10 MeV is used to generate P_ν.

The third option (`nudist=2`) implements an alternative polynomial fit from Valentine [6] of P_ν as a function of $\bar{\nu}$ instead of E_n. When a neutron induces a fission, the algorithm converts the incident neutron

E_n	ν=0	1	2	3	4	5	6	7	8	$\bar{\nu}$
0	.0396484	.2529541	.2939544	.2644470	.1111758	.0312261	.0059347	.0005436	.0001158	2.2753781
1	.0299076	.2043215	.2995886	.2914889	.1301480	.0363119	.0073638	.0006947	.0001751	2.4305631
2	.0226651	.1624020	.2957263	.3119098	.1528786	.0434233	.0097473	.0009318	.0003159	2.5857481
3	.0170253	.1272992	.2840540	.3260192	.1779579	.0526575	.0130997	.0013467	.0005405	2.7409331
4	.0124932	.0984797	.2661875	.3344938	.2040116	.0640468	.0173837	.0020308	.0008730	2.8961181
5	.0088167	.0751744	.2436570	.3379711	.2297901	.0775971	.0225619	.0030689	.0013626	3.0513031
6	.0058736	.0565985	.2179252	.3368863	.2541575	.0933127	.0286200	.0045431	.0031316	3.2064881
7	.0035997	.0420460	.1904095	.3314575	.2760413	.1112075	.0355683	.0065387	.0031316	3.3616731
8	.0019495	.0309087	.1625055	.3217392	.2943792	.1313074	.0434347	.0091474	.0046284	3.5168581
9	.0008767	.0226587	.1356058	.3076919	.3080816	.1536446	.0522549	.0124682	.0067176	3.6720432
10	.0003271	.0168184	.1111114	.2892434	.3160166	.1782484	.0620617	.0166066	.0095665	3.8272281

Table 2: Neutron number distribution for induced fission in ^{238}U.

E_n	ν=0	1	2	3	4	5	6	7	8	$\bar{\nu}$
0	.0108826	.0994916	.2748898	.3269196	.2046061	.0726834	.0097282	.0006301	.0001685	2.8760000
1	.0084842	.0790030	.2536175	.3289870	.2328111	.0800161	.0155581	.0011760	.0003469	3.0088800
2	.0062555	.0611921	.2265608	.3260637	.2588354	.0956070	.0224705	.0025946	.0005205	3.1628300
3	.0045860	.0477879	.1983002	.3184667	.2792811	.1158950	.0301128	.0048471	.0007233	3.3167800
4	.0032908	.0374390	.1704196	.3071862	.2948565	.1392594	.0386738	.0078701	.0010046	3.4707300
5	.0022750	.0291416	.1437645	.2928006	.3063902	.1641647	.0484343	.0116151	.0014149	3.6246800
6	.0014893	.0222369	.1190439	.2756297	.3144908	.1892897	.0597353	.0160828	.0029917	3.7786300
7	.0009061	.0163528	.0968110	.2558524	.3194566	.2134888	.0729739	.0213339	.0020017	3.9325800
8	.0004647	.0113283	.0775201	.2335926	.3213289	.2356614	.0886183	.0274895	.0039531	4.0865300
9	.0002800	.0071460	.0615577	.2089810	.3200121	.2545846	.1072344	.0347255	.0054786	4.2404900
10	.0002064	.0038856	.0492548	.1822078	.3154159	.2687282	.1295143	.0432654	.0075217	4.3944400

Table 3: Neutron number distribution for induced fission in ^{239}Pu.

energy E_n into $\bar{\nu}$ using conversion tables (typically ENDF/EDNL), generates the P_ν distributions for that value of $\bar{\nu}$, and then samples the P_ν distributions to determine ν. Following a suggestion of Frehaut [7], the least-square fits to the ^{235}U data are used for both ^{235}U and ^{233}U neutron induced fission, the fits to ^{238}U are used for ^{232}U, ^{234}U, ^{236}U and ^{238}U, while the fits to ^{239}Pu are used for ^{239}Pu and ^{241}Pu. Data come from Zucker and Holden. For ^{235}U, data comes from Zucker and Holden for E_n greater than 1 MeV, and Gwin, Spencer and Ingle for 0 MeV. The fits are only used when $\bar{\nu}$ is in the range of the $\bar{\nu}$'s for the tabulated data. Otherwise, Terrell's approximation is used.

The fourth option, which is the default (`nudist=3`), is similar to the third option except that the P_ν distributions are not functions of $\bar{\nu}$, but are left intact as multiplicity distributions for the data listed in Gwin, Spencer and Ingle, and for the data listed in Zucker and Holden. The multiplicity distribution P_ν from which the number of neutrons will be sampled is selected based on the value of $\bar{\nu}$ for a given induced fission event. For instance, if $\mathrm{P}_\nu(1MeV)$ has $\bar{\nu} = 2.4$, $\mathrm{P}_\nu(2MeV)$ has $\bar{\nu} = 2.6$, and $\bar{\nu}$ is 2.45 at the energy of the incident fission-inducing neutron (this value $\bar{\nu}$ comes typically from cross-section data libraries such and ENDF/ENDL), the probability of sampling the number of neutrons ν from $\mathrm{P}_\nu(1MeV)$ and $\mathrm{P}_\nu(2MeV)$ will be 75% and 25%, respectively. This technique is only used when $\bar{\nu}$ is in the range of the $\bar{\nu}$'s for the tabulated data. Otherwise, Terrell's approximation is used. This last way of computing ν has several advantages: first, the data as listed in the original papers is used exactly, as opposed to approximated by low-ordered polynomials least-square fitting the original data. Second, the data from the Gwin, Spencer and Ingle paper, and the data from the Zucker and Holden paper is entered as-is as a table in the code, and can easily be checked and maintained if necessary by the application developer. Third the method provides a simple and statistically correct mechanism of sampling the data tables. The fission module behaves in this

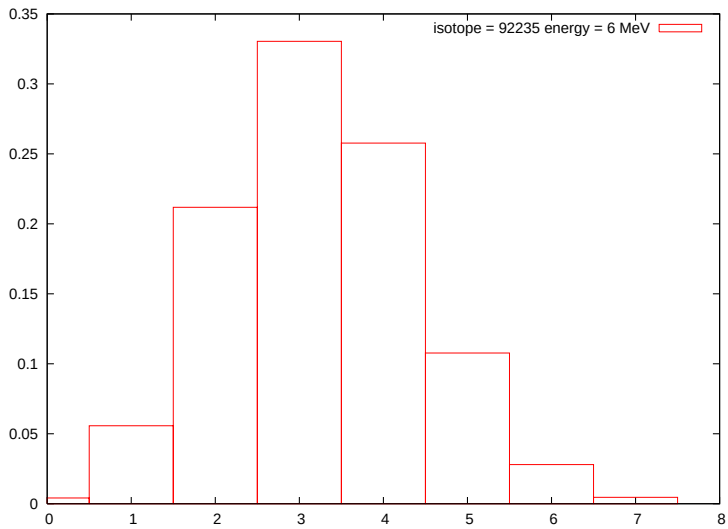

Figure 1: Induced fission in ^{235}U, incident neutron energy = 6MeV

manner when the 'nudist' option is set to 3, which is also the default behavior.

Spontaneous fission data

Table 4 summarizes the spontaneous fission neutron number distributions for several isotopes, along with their references [8, 9, 10, 11, 12, 13]. For ^{252}Cf, the fission module can be set to use either the measurements by Spencer [14] (`ndist=0`), which is the default, or Boldeman [15] (`ndist=1`). For ^{246}Cm, ^{248}Cm, ^{246}Cf, ^{250}Cf, ^{254}Cf, ^{257}Fm and ^{252}No, the Watt parameters are not available, so even though the number of spontaneous fission neutrons could be sampled, no energy could be attributed to them, and the fission library module thus fails for these 7 nuclides.

isotope	ν=0	1	2	3	4	5	6	7	8	9
^{238}U [8]	.0481677	.2485215	.4253044	.2284094	.0423438	.0072533	0	0	0	0
^{236}Pu [9]	.0802878	.2126177	.3773740	.2345049	.0750387	.0201770	0	0	0	0
^{238}Pu [9]	.0562929	.2106764	.3797428	.2224395	.1046818	.0261665	0	0	0	0
^{240}Pu [8]	.0631852	.2319644	.3333230	.2528207	.0986461	.0180199	.0020406	0	0	0
^{242}Pu [8]	.0679423	.2293159	.3341228	.2475507	.0996922	.0182398	.0031364	0	0	0
^{242}Cm [8]	.0212550	.1467407	.3267531	.3268277	.1375090	.0373815	.0025912	.0007551	.0001867	0
^{244}Cm [8]	.0150050	.1161725	.2998427	.3331614	.1837748	.0429780	.0087914	.0002744	0	0
^{246}Cm [10]	.0152182	.0762769	.2627039	.3449236	.2180653	.0755895	.0072227	0	0	0
^{248}Cm [10]	.0067352	.0596495	.2205536	.3509030	.2543767	.0893555	.0167386	.0016888	0	0
^{246}Cf [11]	.0005084	.1135987	.2345989	.2742853	.2208697	.1259660	.0301731	0	0	0
^{250}Cf [12]	.0038191	.0365432	.1673371	.2945302	.2982732	.1451396	.0472215	.0040174	.0031188	0
^{252}Cf [14]	.00211	.02467	.12290	.27144	.30763	.18770	.06770	.01406	.00167	.0001
^{252}Cf [15]	.00209	.02621	.12620	.27520	.30180	.18460	.06680	.01500	.00210	0
^{254}Cf [12]	.0001979	.0190236	.1126406	.2638883	.3183439	.1941768	.0745282	.0150039	.0021968	0
^{257}Fm [12]	.0205736	.0520335	.1172580	.1997003	.2627898	.2007776	.1061661	.0333033	.0073979	0
^{252}No [13]	.0569148	.0576845	.0924873	.1437439	.1832482	.1831510	.1455905	.0962973	.0382048	.0026776

Table 4: Neutron number distributions for spontaneous fission, along with their references.

If no full multiplicity distribution data exists, the fission module uses Terrell [1]'s approximation with $\bar{\nu}$

from Ensslin [16]. The measured values from Ensslin are listed in Table 5.

isotope	$\bar{\nu}$	a [MeV^{-1}]	b [MeV^{-1}]	isotope	$\bar{\nu}$	a [MeV^{-1}]	b [MeV^{-1}]
^{232}Th	2.14	1.25	4.0	^{239}Pu	2.16	1.12963	3.80269
^{232}U	1.71	1.12082	3.72278	^{240}Pu	2.156	1.25797	4.68927
^{233}U	1.76	1.16986	4.03210	^{241}Pu	2.25	1.18698	4.15150
^{234}U	1.81	1.29661	4.92449	^{242}Pu	2.145	1.22078	4.36668
^{235}U	1.86	1.29080	4.85231	^{241}Am	3.22	1.07179	3.46195
^{236}U	1.91	1.36024	5.35746	^{242}Cm	2.54	1.12695	3.89176
^{238}U	2.01	1.54245	6.81057	^{244}Cm	2.72	1.10801	3.72033
^{237}Np	2.05	1.19985	4.24147	^{249}Bk	3.40	1.12198	3.79405
^{238}Pu	2.21	1.17948	4.16933	^{252}Cf	3.757	0.847458	1.03419

Table 5: Average number of neutrons per fission and Watt parameters for spontaneous fission [16].

2.2 Neutron energy distribution

All of the fission spectra in the Evaluated Nuclear Data Library, ENDL [17] are defined by a simple analytical function, a Watt spectrum defined as

$$W(a,b,E') = Ce^{-aE'} sinh(\sqrt{bE'}) \tag{2}$$

where $C = \sqrt{\pi \frac{b}{4a}} \frac{e^{\frac{b}{4a}}}{a}$, and E' is the secondary neutron energy. The coefficients a and b vary weakly from one isotope to another.

For spontaneous fission, the parameters a and b are taken from Ensslin [16] and are listed in Table 5. For spontaneous fission of ^{236}Pu, there is no data for the Watt fission spectrum. We made the assumption that ^{236}Pu has the same Watt fission spectrum as ^{237}Np since they have approximately the same $\bar{\nu}$ (2.07 versus 2.05). We think this is a good approximation since Cullen [19] showed that the Watt fission spectra for neutron-induced fissions can very well be approximated with the single parameter a by setting b equal to 1.0, instead of the 2 parameters a and b. Since there is only 1 parameter characterizing a Watt spectrum, Watt spectra with identical $\bar{\nu}$'s must have the same value for that parameter a (that is because the integral of the spectrum with respect to the energy gives $\bar{\nu}$, within a normalization factor). If we assume that Watt spectra can be approximated by a single parameter a for spontaneous fissions as well (which we verified and seems to be a valid assumption), there can only be a single Watt spectrum for a given spontaneous fission $\bar{\nu}$. We thus concluded that the Watt spectrum for ^{236}Pu should be close to the Watt spectrum for ^{237}Np and used the Watt parameters of ^{237}Np for ^{236}Pu. The Watt spectrum is used for all isotopes except ^{252}Cf, for which a special treatment summarized by Valentine [6] is applied. The neutron spectrum for ^{252}Cf is sampled from the Mannhart [21] corrected Maxwellian distribution, the Madland and Nix [22] or the Watt fission spectra from Froehner [23]. These options are selected by the internal variable `neng=0(default),1,2` respectively. The Mannhart distribution is used by default.

For neutron-induced fission, the coefficients a and b in Eq. 2 not only vary weakly from one isotope to another, but they also vary weakly with the incident neutron energy E. The fission module follows TART [18, 19]'s implementation by setting the coefficient b equal to 1.0, and using the following functional form for the coefficient $a(E)$:

$$a(E) = a_0 + a_1 E + a_2 E^2 \tag{3}$$

where E is the incident neutron energy.

The coefficients a_0, a_1 and a_2 in Eq. 3 are listed in Table 6 for 40 isotopes. The fission module does not support neutron-induced fission for isotopes other than the ones in the table. The fissioning isotope and incident neutron energy determine the value of the coefficient a in Eq. 2, and the energy E' of the secondary neutron emitted is sampled using the Los Alamos' Monte Carlo sampler attributed to Mal Kalos [20].

isotope	a_2 [MeV^{-3}]	a_1 [MeV^{-2}]	a_0 [MeV^{-1}]	isotope	a_2 [MeV^{-3}]	a_1 [MeV^{-2}]	a_0 [MeV^{-1}]
^{231}Th	6.00949e-05	-0.00836695	0.950939	^{239}Pu	8.50642e-05	-0.0101099	0.887305
^{232}Th	6.54348e-05	-0.00886574	0.955404	^{240}Pu	9.10537e-05	-0.0105303	0.889439
^{233}Th	7.08174e-05	-0.00922676	0.950088	^{241}Pu	9.43014e-05	-0.0107134	0.882632
^{233}Pa	6.35839e-05	-0.00863646	0.924584	^{242}Pu	0.000102656	-0.0113155	0.891617
^{232}U	2.12325e-05	-0.00827743	0.918556	^{243}Pu	0.000106118	-0.0114972	0.885182
^{233}U	6.21336e-05	-0.00845652	0.914717	^{241}Am	9.08474e-05	-0.0104296	0.871943
^{234}U	6.81386e-05	-0.00899142	0.921955	^{242}Am	9.35633e-05	-0.0105612	0.86393
^{235}U	7.32627e-05	-0.00936909	0.920108	^{243}Am	0.00010194	-0.0111574	0.873153
^{236}U	8.06505e-05	-0.00995417	0.92789	^{242}Cm	9.19501e-05	-0.0104229	0.858682
^{237}U	8.33208e-05	-0.0101073	0.917692	^{243}Cm	9.42992e-05	-0.0105099	0.849104
^{238}U	8.96945e-05	-0.0106491	0.925496	^{244}Cm	0.000102747	-0.0111371	0.860434
^{239}U	9.44608e-05	-0.010894	0.917796	^{245}Cm	0.000105025	-0.0112139	0.851102
^{240}U	0.000101396	-0.0115098	0.929395	^{246}Cm	0.00011413	-0.0118692	0.862838
^{235}Np	6.8111e-05	-0.00891619	0.900048	^{247}Cm	0.000115164	-0.0118554	0.851307
^{236}Np	7.21126e-05	-0.00920179	0.895723	^{248}Cm	0.000127169	-0.0127033	0.868624
^{237}Np	7.82371e-05	-0.00967051	0.899575	^{249}Bk	0.000124195	-0.0124047	0.848974
^{238}Np	8.27256e-05	-0.00999353	0.897462	^{249}Cf	0.000112616	-0.0115135	0.819709
^{236}Pu	0.000131389	-0.0080106	0.891084	^{250}Cf	0.000123637	-0.012287	0.835392
^{237}Pu	7.29458e-05	-0.00922415	0.880996	^{251}Cf	0.000122724	-0.0121678	0.82257
^{238}Pu	8.02384e-05	-0.00978291	0.888964	^{252}Cf	0.000133892	-0.0129268	0.837123

Table 6: Values of the a_0, a_1 and a_2 coefficients in Eq. 3 for the neutron induced fission Watt spectrum.

The Watt spectrum for ^{235}U and an incident neutron energy of 6 MeV is shown in Fig. 2.

Neutron energy conservation

The user can choose from three different methods of handling the correlations between neutron energies in a single fission event. These methods are selected by the internal variable `correlation` (default=0).

0. `correlation=0.` (default) Neutron energies are all sampled independently, so there is no explicit energy conservation.

1. `correlation=1.` A total event energy constraint is imposed in the following way. Beck et al. [24] calculated the average total fission neutron lab kinetic energy as a function of incoming neutron energy E_n for the following 3 isotopes based on the Los Alamos Madland-Nix model [25]:

$$\begin{aligned} < E^{tot}_{neutron} > &= 4.838 + 0.3004 E_n \quad {}^{235}\mathrm{U} \\ < E^{tot}_{neutron} > &= 4.558 + 0.3070 E_n \quad {}^{238}\mathrm{U} \\ < E^{tot}_{neutron} > &= 6.128 + 0.3428 E_n \quad {}^{239}\mathrm{Pu} \end{aligned} \tag{4}$$

The fission module uses these average values of the kinetic energies as the mean total neutron energy available to the emission of neutrons. For each fission reaction, the number of neutrons N is sampled from the number multiplicity distributions in Sec. 2.1, the total fission neutron energy $E^{tot}_{neutron}$ is sampled from a normal distribution of mean $< E^{tot}_{neutron} >$ and of standard deviation equal to $< E^{tot}_{neutron} > /4$. This normal distribution is truncated at 10 keV to avoid very low total prompt fission

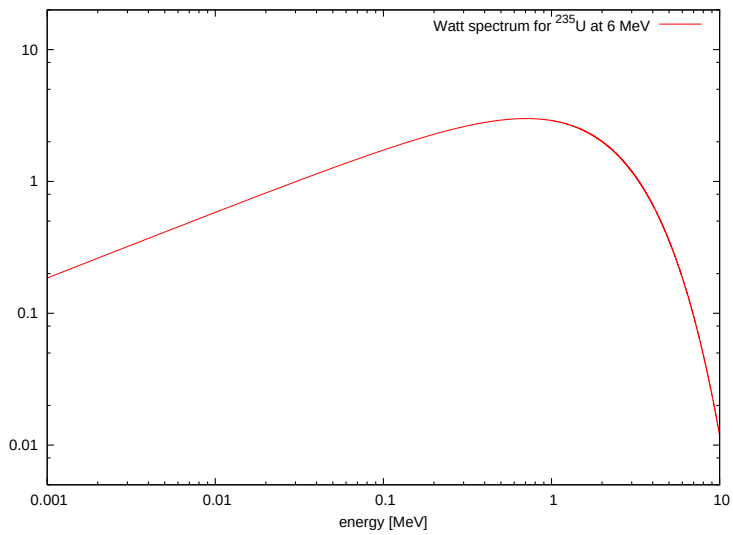

Figure 2: Watt spectrum for ^{235}U and an incident neutron energy of 6 MeV.

neutron energies. The Watt spectrum is then sampled N times to get the energy of these N neutrons. The sampled neutron energies are then rescaled in such a way that the sum of their energies is equal to $E^{tot}_{neutron}$. One of the limitations of this second approach is that it works only for induced fission and for the following 3 isotopes: ^{235}U, ^{238}U and ^{239}Pu.

2. `correlation=2`. A total event energy constraint is imposed by a method different than that of option 1 above. In 2008, Vogt [26] extended the above Beck et al. [24] method to all actinides, major and minor, in the Evaluated Nuclear Data Library 2008 release, ENDL2008, using data from ENDL2008 and ENDL99. In this extension, the average outgoing prompt gamma energy and prompt neutron energy are expressed by a quadratic expression of the form

$$< E^{tot}_{n/p}(E_n) >= c_{n/p} + b_{n/p}E_n + a_{n/p}E_n^2 \tag{5}$$

where the 3 coefficients are actinide-dependent and the subscripts n and p stand for prompt fission neutrons and gamma-rays. The coefficients of this quadratic form for prompt fission neutrons are given for 73 actinides in table 7. However, because the Watt spectrum is only available for the 40 isotopes listed in table 6, the fission module is limited to these 40 for neutron-induced fission.

Actinide	c_n (MeV)	b_n	a_n (MeV^{-1})	Actinide	c_n (MeV)	b_n	a_n (MeV^{-1})
^{225}Ac	3.478	0.1937	-0.001317	^{239}Pu	6.092	0.3707	-0.002495
^{226}Ac	3.635	0.1231	0.004442	^{240}Pu	5.906	0.2477	0.008608
^{227}Ac	3.396	0.1888	-0.000144	^{241}Pu	6.161	0.2356	0.009310
^{227}Th	4.275	0.1225	0.006569	^{242}Pu	5.926	0.2192	0.008356
^{228}Th	3.787	0.2181	0.003449	^{243}Pu	5.781	0.4692	0.005751
^{229}Th	4.216	0.1339	0.006267	^{244}Pu	5.655	0.2557	0.008807
^{230}Th	3.847	0.1422	0.007380	^{246}Pu	5.145	0.3155	0.007922
^{231}Th	4.095	0.1196	0.006487	^{240}Am	7.150	0.3473	0.002294
^{232}Th	3.401	0.3465	-0.000431	^{241}Am	6.957	0.4243	-0.004504
^{233}Th	3.736	0.2566	0.000663	^{242}Am	7.150	0.3473	0.002294
^{234}Th	3.387	0.2290	0.003476	^{243}Am	7.422	0.3523	-0.002387
^{229}Pa	4.605	0.1744	0.005433	^{244}Am	6.543	0.3837	0.0
^{230}Pa	4.720	0.1879	0.005562	^{240}Cm	7.525	0.2786	0.011040
^{231}Pa	4.524	0.1726	0.006436	^{241}Cm	7.699	0.3648	0.007316
^{232}Pa	4.699	0.1683	0.006763	^{242}Cm	7.701	0.2683	0.011400
^{233}Pa	4.076	0.3671	0.000639	^{243}Cm	8.104	0.2363	0.005492
^{230}U	4.977	0.1832	0.006792	^{244}Cm	7.103	0.2061	0.010830
^{231}U	5.196	0.2127	0.005808	^{245}Cm	7.984	0.2279	0.005426
^{232}U	6.082	0.2782	0.003243	^{246}Cm	6.939	0.2245	0.009390
^{233}U	5.141	0.2540	0.002915	^{247}Cm	8.216	0.3896	0.008595
^{234}U	4.728	0.2339	0.002704	^{248}Cm	7.295	0.2499	0.013550
^{235}U	4.864	0.3114	-0.001424	^{249}Cm	7.124	0.3777	0.008907
^{236}U	4.505	0.2969	0.004555	^{250}Cm	6.973	0.4062	0.006831
^{237}U	4.999	0.2680	0.001783	^{245}Bk	8.210	0.3643	0.009615
^{238}U	4.509	0.3574	-0.004351	^{246}Bk	8.274	0.4764	0.005445
^{239}U	4.580	0.3647	0.004266	^{247}Bk	7.831	0.4266	0.008129
^{240}U	4.561	0.3596	0.000273	^{248}Bk	8.145	0.4796	0.006656
^{241}U	4.268	0.3998	0.002821	^{249}Bk	7.519	0.4021	0.010130
^{234}Np	5.880	0.2311	0.007642	^{250}Bk	7.879	0.4204	0.008308
^{235}Np	5.576	0.2484	0.007751	^{246}Cf	8.900	0.4323	0.009000
^{236}Np	5.080	0.2446	0.008116	^{248}Cf	8.661	0.3877	0.010700
^{237}Np	5.330	0.2768	0.005819	^{249}Cf	9.428	0.4746	0.007067
^{238}Np	5.214	0.2650	0.007559	^{250}Cf	8.226	0.4980	0.007397
^{239}Np	5.416	0.2489	0.004159	^{251}Cf	9.407	0.4454	0.010790
^{236}Pu	6.112	0.2240	0.009279	^{252}Cf	8.627	0.5190	0.007184
^{237}Pu	6.177	0.2599	0.006790	^{253}Cf	8.449	0.2396	0.018650
^{238}Pu	6.087	0.2189	0.008211				

Table 7: Coefficients of Eq. 5 for the energy-dependent average outgoing prompt fission neutron energy.

2.3 Gamma-ray number distribution

The fission module uses Brunson [27]'s double Poisson model for the spontaneous fission gamma ray multiplicity of ^{252}Cf (see Fig. 3).

$$\Pi(G) = 0.682\frac{7.20^G e^{-7.20}}{G!} + 0.318\frac{10.71^G e^{-10.72}}{G!} \tag{6}$$

where G is the gamma ray multiplicity.

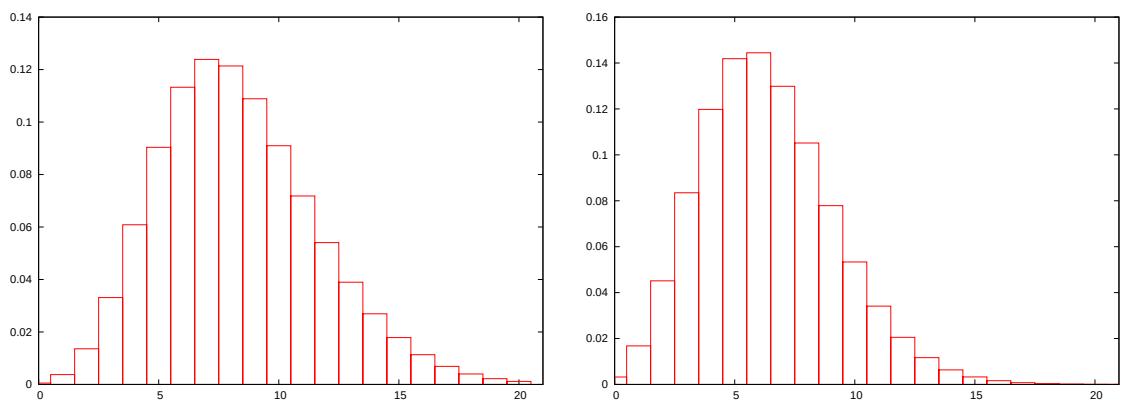

Figure 3: Gamma-ray multiplicity for spontaneous fission of ^{252}Cf (left) and ^{238}U (right).

The prompt gamma ray multiplicity ranges from 0 to 20 gama rays per fission with an average of 8.32 gamma rays per fission. This model is a fit to experimental data measured by Brunson himself.

For other isotopes, there is no data available for the multiplicity of prompt gamma rays. Valentine [28] used an approximation that was adopted by the fission module. The probability of emitting G fission gamma rays obeys the negative binomial distribution:

$$\Pi(G) = \begin{pmatrix} \alpha + G - 1 \\ G \end{pmatrix} p^G (1-p)^G \tag{7}$$

where the parameter p can be written as $p = \frac{\alpha}{\alpha+\bar{G}}$, α is approximately 26 and $\bar{G}$ is the average number of gamma rays per fission. $\bar{G}$ is approximated by

$$\bar{G} = \frac{E_t(\bar{\nu}, Z, A)}{\bar{E}} \tag{8}$$

where

$$E_t(\bar{\nu}, Z, A) = (2.51(\pm 0.01) - 1.13 \cdot 10^{-5}(\pm 7.2 \cdot 10^{-8}) Z^2 \sqrt{A})\bar{\nu} + 4.0 \tag{9}$$

is the total prompt gamma ray energy, $\bar{\nu}$ is the average number of prompt neutrons, and

$$\bar{E} = -1.33(\pm 0.05) + 119.6(\pm 2.5)\frac{Z^{\frac{1}{3}}}{A} \tag{10}$$

is the average prompt gamma ray energy. The multiplicity distribution for the spontaneous fission of ^{238}U is shown in Fig. 3.

These multiplicity distributions are only estimates and are not measured data. The fission module uses this model for estimating the number of prompt fission gamma rays emitted by both spontaneous and thermal-neutron induced fissions, and also by higher-energy neutron induced fissions. Note that the energy dependence of the gamma multiplicity for neutron induced fission enters through the parameter $\bar{\nu}$, which is calculated by the parent transport code for the specified isotope.

2.4 Gamma-ray energy distribution

The only measured energy spectra for fission gamma rays are from the spontaneous fission of ^{252}Cf and from thermal-neutron-induced fission of ^{235}U. Both spectra are similar [29]. Instead of using either spectra directly, we use the following mathematical representation:

$$N(E) = \begin{cases} 38.13(E-0.085)e^{1.648E} & E < 0.3 \text{ MeV} \\ 26.8e^{-2.30E} & 0.3 < E < 1.0 \text{ MeV} \\ 8.0e^{-1.10E} & 1.0 < E < 8.0 \text{ MeV} \end{cases} \tag{11}$$

which is shown in Fig. 4. This analytic expression comes from Valentine's [6] and is a fit to the ^{235}U measurements of Maienschein [30, 31] (which are more precise than the ^{252}Cf measurements).

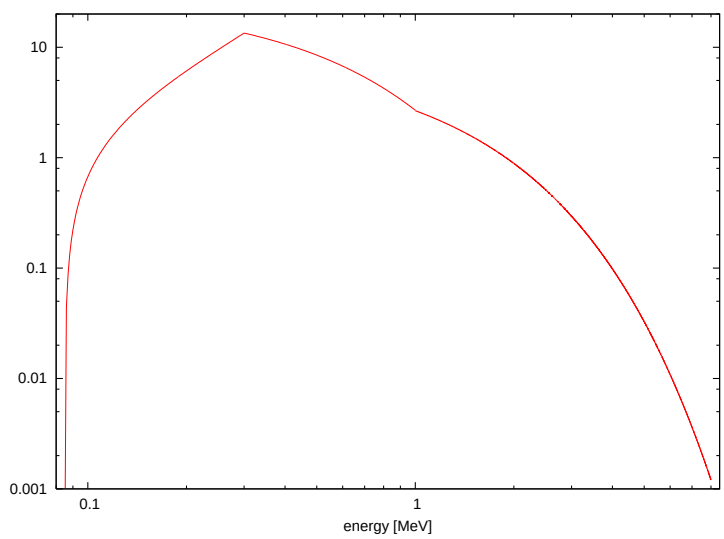

Figure 4: Fission gamma-ray spectrum from fit to ^{235}U measurements.

Gamma-ray energy conservation

The user can choose from three different methods of handling the correlations between gamma-ray energies in a single fission event. The average prompt gamma-ray energy differs significantly between the second and third method given below. This difference is explained in detail in Vogt [26]. The available methods are the same as for neutrons and are selected by the internal variable `correlation` (default=0):

0. `correlation=0.` (default) Gamma-ray energies are all sampled independently from the spectrum shown in Fig. 4, so there is no explicit energy conservation.

1. `correlation=1.` A total event energy constraint is imposed in the following way. Beck et al. [24] computed the average total fission gamma-ray energy to be:

$$\begin{aligned} <E_\gamma^{tot}> &= 6.600 + 0.0777E_n && ^{235}\text{U} \\ <E_\gamma^{tot}> &= 6.680 + 0.1239E_n && ^{238}\text{U} \\ <E_\gamma^{tot}> &= 6.741 + 0.1165E_n - 0.0017E_n^2 && ^{239}\text{Pu} \end{aligned} \tag{12}$$

For each fission reaction, the number G of prompt fission gammas is sampled from the number multiplicity distributions in Sec. 2.3 using Eqs. 7 through 10, where Eq. 9 giving the total fission gamma-ray energy E_t is replaced by Eq. 12. The gamma-ray spectrum shown in Fig. 4 is then sampled G times to obtain the preliminary energies of the G prompt fission gamma-rays. The total fission gamma-ray energy E_γ^{tot} is sampled from a normal distribution of mean $< E_\gamma^{tot} >$ and standard deviation $< E_\gamma^{tot} > /8$, where $< E_\gamma^{tot} >$ is given by Eq. 12. This normal distribution is truncated at 100 keV to avoid the very low probability region of the prompt fission gamma-ray spectrum shown in Fig. 4. The preliminary prompt fission gamma-ray energies are then rescaled in such a way that the sum of their energies equals E_γ^{tot}. This energy conservation method as well as the one below can give rise to a prompt fission gamma-ray energy spectrum that is different from the one in Fig. 4. One of the limitations of this second approach is that it works only for induced fission and for the following 3 isotopes: ^{235}U, ^{238}U and ^{239}Pu.

2. `correlation=2`. A total event energy constraint is imposed by a method based on Vogt [26]. This option is very similar to the one above, but instead of using Eq. 12 to determine both the number G of prompt fission gammas and the average outgoing prompt gamma energy $< E_\gamma^{tot} >$, this method uses Eq. 5, where the 3 coefficients are given in table 8. As with the previous option, the total energy $< E_\gamma^{tot} >$ is used to build a normal distribution, which is sampled to obtain the total fission gamma-ray energy E_γ^{tot} available to all G prompt fission gamma-rays. The rescaling of the G preliminary prompt fission gamma-ray energies is identical to the method above. This option applies to all major and minor actinides, but since there is data for just a few few actinides in ENDL, most actinides use a generic set of coefficients.

Actinide	c_p (MeV)	b_p	a_p (MeV^{-1})
^{232}U*	7.256	0.0255	0.000182
^{235}U	7.284	0.2295	-0.00474
^{238}U	6.658	0.01607	-1.22e-7
^{239}Pu	6.857	0.4249	-0.009878
^{252}Cf	6.44186	0.01831	0.
generic	6.95	0.01693	7.238e-8

Table 8: Coefficients of Eq. 5 for the energy-dependent average outgoing prompt fission photon energy. (*) ^{232}U coefficients are used for ^{233}U, ^{234}U, ^{236}U, ^{237}U, ^{240}U and ^{241}U.

3 Photofission

3.1 Photonuclear physics

A photonuclear interaction begins with the absorption of a photon by a nucleus, leaving the nucleus in an excited state. The nucleus then undergoes multiple de-excitation processes emitting secondary particles and possibly undergoing fission. There are two main mechanisms for photon absorption in a nucleus: through the giant dipole resonance (relevant for photon energies in the range 12-16 MeV) and quasi-deutron absorption (relevant if photon energy < 150 MeV).

The giant dipole resonance can be viewed as an electromagnetic wave (photon) inducing an electric dipole-like vibrational resonance of the nucleus as a whole, which results in a collective excitation of the nucleus. The giant dipole resonance occurs with highest probability when the wavelength of the photon is comparable to the size of the nucleus. This typically occurs for photon energies in the range of 12 to 16 MeV and has a resonance width of a few MeV. For energies above 16 MeV, photons are mostly absorbed through the quasi-deuteron absorption process. Here the incident photon interacts with the dipole moment of a correlated neutron-proton pair inside the target nucleus.

Once the photon has been absorbed by the nucleus, single or multiple particle emission can occur. For energies below 150 MeV, a combination of gamma-rays, neutrons, protons, deuterons, tritons, helium-3 particles, alphas and fission fragments can be emitted. The threshold for the production of a given secondary particle is governed by the separation energy of that particle, which is typically a few MeV up to 10's of MeV. Most of these particles are emitted via pre-equilibrium and equilibrium mechanisms.

Pre-equilibrium emission occurs when a particle within the nucleus receives a large amount of energy from the absorption mechanism and escapes the binding force of the nucleus after at least one, but very few, interactions with other particles. This process occurs on a fast time scale compared to equilibrium emission.

Equilibrium emission can be viewed as particle evaporation. This process typically occurs after the available energy has been distributed among the nucleons. In the classical sense, particles boil out of the nucleus as they penetrate the nuclear potential barrier. For heavy elements, evaporation neutrons are emitted preferentially (versus charged particles, such as protons, deuterons, alphas, etc.) as they are not subject to the Coulomb barrier. After these initial emissions, the nucleus will be left in an excited state, and will relax to the ground state by the emission of one or more gamma-rays.

Fission is often modeled as a form of evaporation, and it occurs at roughly the same time scale (i.e. it competes with equilibrium emission but occurs after pre-equilibrium emission), however it is a completely separate kind of process. Fission is viewed as a mostly adiabatic distortion of a highly deformed nucleus. The fission process results in two fragments. For each parent nucleus, there is a relatively broad distribution of possible daughter fragment combinations. Each daughter nucleus can then undergo further decay.

3.2 Photonuclear data

In the mid 1990's a research coordination project was formed under the auspices of the International Atomic Energy Agency (IAEA) to collect all relevant experimental photonuclear data and to release a library of evaluated data files covering major isotopes of importance to structural, shielding, activation analysis, fission, and transmutation applications [32]. The two main goals were:

1. Review and choose the highest quality photonuclear data available at that time, taking from the Korean Atomic Energy Institute (KAERI), the Japanese Atomic Energy Institute (JENDL), a collaboration between IPPE/Obninsk and CDFE/Moscow (BOFOD, Russia), the Chinese Nuclear Data Center (CNDC) and the Los Alamos National Laboratory (LANL) libraries;

2. Develop new evaluations for important nuclei not covered by other libraries.

As part of this coordinated effort, the LANL Nuclear Theory and Applications group (T-2) produced a series of photonuclear evaluations for the Accelerator Production of Tritium (APT) project. These were released in 1999 as the LANL150u nuclear data library [33].

The complete IAEA photonuclear library was released in 2000 [34], which itself contained all of the LANL150u library. Later, the US nuclear data program produced a new photonuclear data library as part of ENDF/B-VII.0, which was released in 2006 [35]. There is substantial overlap between evaluations among these libraries: the ENDF/B-VII.0 photonuclear data was taken almost entirely from the IAEA Photonuclear Library, with only 24 isotopes added/improved. The actinides that were improved for ENDF/B-VII.0 now contain prompt and delayed fission neutron spectra. In addition, ^{240}Pu and ^{241}Am were added to ENDF/B-VII.0.

3.3 Emission of particles from photofission

Because of the lack of data as much as the lack of usable theoretical model for photofission, the photofission library used here is mainly based on neutron-induced data. This model assumes that nuclei will usually fission the same way, independently of the particle that excited them, whether it be a neutron or photon, as long as the excitation levels are the same. Based on that assumption, the model only needs to know the excited level of the nucleus. With this model in mind, the library can determine the multiplicity distributions of the neutrons and gammas emitted by photofission from their neutron-induced fission counterparts. The energy spectra of the neutrons and gammas emitted by photofission are determined similarly.

Limitations of the photofission model

The photofission model requires knowledge of the neutron separation energies and of the Watt spectra of the fissioning nuclei. Because the Watt spectra are only available for 40 isotopes in table 6 and out of these 40, the neutron separation energy for ^{241}U could not be found in the litterature, the photofission library only works for the 39 isotopes listed in table 9.

Neutron number distribution

The number ν of prompt neutrons emitted per photofission is sampled from a prompt fission neutron multiplicity distribution. Similarly to the case of neutron-induced fission, the neutron multiplicity distribution for photofission can be obtained four ways, depending on the option selected via the internal variable `nudist` (default=3). It can be obtained from the Zucker and Holden data [3] (`nudist=0`), from that data along with the Gwin, Spencer and Ingle data [4] (`nudist=1`), or from the two other methods (`nudist=2,3`) described in Sec. 2.1.

For the first two methods (`nudist=0,1`), the neutron multiplicity distribution depends on the incident neutron energy. Neutron multiplicity distributions are widely available for neutron-induced fissions, as we have seen in Sec. 2.1, but not so for photofission. To be able to use the neutron-induced multiplicity distributions for the photofission reaction, we will reduce the energy of the incident photon by the neutron separation energy of the neutron in the nucleus to account for the extra energy that an incident neutron brings in as it is captured by a nucleus. If the resulting "neutron-equivalent" energy happens to be negative — which happens rarely — the model constrains this neutron-equivalent energy to be 0. This is an important constraint as a nucleus could fission by a photon of lower energy than the neutron separation energy for that nucleus. Given the lack of data in this energy regime, we assume in this case that the fission is induced by a thermal neutron. Once this adjustment is made to the neutron-equivalent energy, we consider in this model that the nucleus is in the same excited state as the one that would have been brought there by a neutron inducing fission, and thus the nucleus would fission the same way.

One important point is the nucleus that is used for photofission. In a neutron-induced fission reaction, a nucleus captures a neutron before fissioning. Thus the number of neutrons in the nucleus increases by 1 for a very short time before fissioning. In a photofission on the contrary, the number of neutrons remains the same. Consequently, in order to use neutron-induced fission data (such as the prompt fission multiplicity distribution) to handle photofission, one has to use the neutron-induced fission data for an isotope that has one less neutron: Z(A-1). The following example illustrates this point. Let's consider a 10 MeV photon on a ^{236}U nucleus. If the ^{236}U nucleus photofissions, the model assumes that this photofission can as well be represented by a neutron-induced fission, that is by a x MeV neutron on a ^{235}U nucleus, because the ^{235}U nucleus first captures the neutron and becomes an excited ^{236}U nucleus. The energy x of the neutron inducing fission is the incident photon energy reduced by the neutron separation energy S_n, that is 10 MeV - 6.5448 MeV, or 3.4552 MeV. In conclusion, the model will use the data for a 3.4552 MeV neutron inducing fission in a ^{235}U nucleus to emulate the 10 MeV photon photofissioning the ^{236}U nucleus.

For the next two methods (`nudist=2,3`), the average number $\bar{\nu}_{photofission}$ of prompt photofission neutrons must be provided by the parent code. These two methods proved to be very useful as new photonuclear data libraries such as ENDF/B-VII contain that quantity as a function of the incident photon energy for a good number of isotopes (see Sec. 3.2). Based on the ZA of the nucleus and on the value of $\bar{\nu}_{photofission}$, the full photofission multiplicity distribution for nucleus ZA is built from the neutron-induced fission multiplicity distributions data (as in Sec. 2.1) for a nucleus with one less neutron Z(A-1) and setting $\bar{\nu} = \bar{\nu}_{photofission}$. For instance, for photofission on ^{240}Pu with $\bar{\nu}_{photofission} = 2.5$, the model uses the multiplicity distributions from neutron-induced fission on ^{239}Pu with $\bar{\nu} = 2.5$. This model assumes that a nucleus ZA incurring photofission with as average $\bar{\nu}_{photofission}$ fission neutrons is in the same excited state and fissions the same way as a nucleus Z(A-1) incurring neutron-induced fission with an average $\bar{\nu}$ neutrons, as long as $\bar{\nu}$ equals $\bar{\nu}_{photofission}$. The number ν of prompt neutrons emitted per photofission is finally sampled from the full photofission multiplicity distribution.

Neutron energy distribution

The energy distribution of the neutrons emitted by photofission of a nucleus ZA is assumed to be the Watt spectrum described in Sec. 2.2. The parameters a and b in Eq. 2 are taken from table 6 for a nucleus of one less neutron, i.e. Z(A-1). While $b = 1$, a depends on the incident neutron energy via Eq. 3. The incident neutron energy E in Eq. 3 is however replaced by a neutron equivalent energy, which is equal to the energy of the incident photon minus the neutron separation energy in nucleus ZA.

Because the Watt spectrum is only available for the 40 isotopes listed in Table 6 and there were no

isotope	S_n	isotope	S_n	isotope	S_n
^{232}Th	6.4381	^{237}Np	6.580	^{244}Am	5.3637
^{233}Th	4.78635	^{238}Np	5.48809	^{243}Cm	5.6933
^{234}Th	6.189	^{239}Np	6.2168	^{244}Cm	6.8007
^{234}Pa	5.217	^{237}Pu	5.8775	^{245}Cm	5.5198
^{233}U	5.760	^{238}Pu	7.0005	^{246}Cm	6.4580
^{234}U	6.8437	^{239}Pu	5.6465	^{247}Cm	5.156
^{235}U	5.29784	^{240}Pu	6.5335	^{248}Cm	6.213
^{236}U	6.5448	^{241}Pu	5.24160	^{249}Cm	4.7135
^{237}U	5.125	^{242}Pu	6.3094	^{250}Bk	4.970
^{238}U	6.1520	^{243}Pu	5.034	^{250}Cf	6.6247
^{239}U	4.80626	^{244}Pu	6.021	^{251}Cf	5.109
^{240}U	5.933	^{242}Am	5.53757	^{252}Cf	6.172
^{236}Np	5.730	^{243}Am	6.3670	^{253}Cf	4.806

Table 9: Isotopes available for photofission, along with their neutron separation energies S_n in MeV.

neutron separation energies available in Ref. [36] for ^{241}U, the photofission library only works for the 39 isotopes listed in Table 9.

The same neutron energy conservation methods as the ones presented in Sec. 2.2 are available to photofission. The prompt fission neutron energies can either be sampled independently, or be constrained by one of two energy conservation principles. In the latter two cases, the energy E_n of the incident neutron in Eqs. 4 and 5 is replaced by the neutron-equivalent incident photon energy. The first energy constraint method works only for the following 3 isotopes incurring photofission: ^{236}U, ^{239}U and ^{240}Pu, while the second one works for the 39 isotopes listed in table 9.

Gamma-ray number distribution

The number of gamma-rays emitted at each photofission is sampled from the same negative binomial as for neutron-induced fissions, see Eq. 7. To compute $\bar{G}$, the photofission model uses Z protons and A-1 nucleons instead of Z protons and A nucleons — to account for the additional neutron that is first captured in a neutron-induced fission — and if needed the neutron-equivalent energy of the photon inducing photofission instead of the incident neutron energy.

Gamma-ray energy distribution

The energies of the gamma-rays emitted by photofission are sampled the same way as neutron-induced fission and is explained in Sec. 2.4. They can be sampled three different ways, either independently or bound by one of two constraints on the total energy available to all prompt fission gamm-rays energy using either Eqs. 12 or 5. For last 2 methods using the energy bounds, the energy E_n of incident neutron is replaced by the neutron-equivalent energy of the photon inducing photofission. In case of the first method binding the total energy available to all prompt fission gamma-rays, this method works only for the following 3 isotopes incurring photofission: ^{236}U, ^{239}U and ^{240}Pu.

Advantages of the photofission model

The fission library enables the user to simulate the photofission process exactly, and therefore enables co-incidence counting of photofission neutrons and gammas for instance. This is different from the default settings of MCNPX for instance, where secondary particles emitted by photonuclear interactions are only correct on average over a large number of interactions, because the numbers of secondary particles, as well as their energies and directions are averaged over all possible photonuclear interactions.

4 User manual

This section describes how to use this software library to accurately simulate neutron and gamma-ray emission from individual fission reactions. The library is already compiled into the Monte Carlo transport codes MCNPX [37] and Geant4 [38, 39]. Section 4.2 describes how to run this library with MCNPX. Section 4.3 describes how to run this library with Geant4. Section 4.4 describes the fission library programmers interface. The standalone version of the software library can be downloaded from `http://nuclear.llnl.gov/simulation`.

4.1 Limitations of the fission library

The range of neutron energies for which induced fission neutron multiplicity data are available in the literature spans the range from 0 to 10 MeV, to which corresponds a range of $\bar{\nu}$ values. The sampling of number of neutrons per fission is based on either the incident neutron energy or the $\bar{\nu}$ corresponding to that energy (depending on the option selected in *setnudist*).

When sampling is based on $\bar{\nu}$ (the default), and the $\bar{\nu}$ is in the range for which we have multiplicity data from the literature, that data is used. Outside that range, the Terrell approximation is used.

If the user selects the option to sample based on energy, and the energy is within the range for which we have multiplicity data from the literature, that data is used. If the energy is above 10 MeV, then the 10 MeV data is used. As this will be inaccurate as the energy becomes much higher than 10 MeV, the user should select sampling based on $\bar{\nu}$ in this case. The same considerations apply for photofission.

In the case of spontaneous fission, data is only available for the following isotopes: ^{232}Th, ^{232}U, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242}Cm, ^{244}Cm, ^{249}Bk, and ^{252}Cf. The Monte-Carlo codes MCNPX and Geant4 do not emit any particles if a different spontaneous fission isotope is specified.

4.2 MCNPX

The spontaneous fission, neutron-induced fission and photon-induced fission physics models are all available in the "beta" version since MCNPX v27c and will appear in the next public RSICC release. The original version of MCNPX had an analog and discrete treatment for neutron emission from fission. Activating our physics module replaces the neutron emission with the model described in this document. This model includes more data and more empirical models than the original version and other features described in this document.

The original version of MCNPX did not have an analog and discrete treatment for photon emission. Previously photons from fission were included in a total average photonuclear photon count. So it was impossible to have an accurate event-by-event model of photon emission from fission. Our library solved this problem by separating out the photons from the fission process and treating them in a discrete fashion. This took much careful work in cooperation with the MCNPX developers. Activating our physics module therefore activates this separate treatment of the fission process as well as provides the features described in this document.

Neutron-induced and spontaneous fission model

To enable sampling of neutrons and gamma-rays using this fission library set the 6th entry *fism* of the PHYS:N card to value=5, e.g.:

```
phys:n 100 0 0 -1 -1 5
```

Note that currently *fism=5* is the only MCNPX setting for which gamma-rays are sampled in analog mode for fission reactions.

Spontaneous fission reactions are activated when definition card *sdef* is set to *sf*:

```
sdef par=sf
```

In the case of spontaneous fissions, only the isotopes listed above in section 4.1 have data in the fission library. For other spontaneous fission isotopes, no neutrons, nor gamma-rays are emitted.

Photon-induced fission model

To enable the analog production of photons and neutrons from photofission reactions, the 7th entry *illnlphfis* of the PHYS:P card should be set to 1:

```
phys:p 3j -1 2j 1
```

When this flag is set, photofission secondaries are sampled only when a photofission event occurs, and are not sampled when other photonuclear reactions occur.

This is different from the default behavior (*illnlphfis=0*), where photons undergoing photonuclear interactions produce an average number of secondary particles each having a sampled energy/angle though not necessarily from the same photonuclear reaction. The number of secondary particles, as well as their energies and directions are averaged over all possible photonuclear interactions (including photofission). While this default setting is obvisouly not correct microscopically, and we cannot use it to do coincidence counting of photofission neutrons/gammas for instance, it is however correct on average over a large number of interactions.

It is important to note that the 4th entry *ispn* of the PHYS:P card should be set to -1 to enable analog photonuclear collision sampling. If this is not enabled, the photofission library will not be enabled either.

Regarding the data libraries, the physics module needs the ENDF/B-VII photonuclear data library *endf7u*, which is currently only available in beta version from the MCNPX website. Lines have to be appended to the file *xsdir* for MCNPX to access this photonuclear data library. These lines are also available from the MCNPX website. Both *xsdir* and the data library *endf7u* must be in the directory pointed to by the variable *DATAPATH*.

Photofission is only available for the 39 isotopes listed in Table 9. Regardless of the option chosen in the 7th entry of the PHYS:P card, delayed neutrons and gammas from photofission can be turned on and off independently via a different card.

Photofission example

In this example, we will consider a 12 MeV photon beam impinging on a ^{235}U ball. The photonuclear reaction cross-sections for ^{235}U are plotted in Fig. 5.

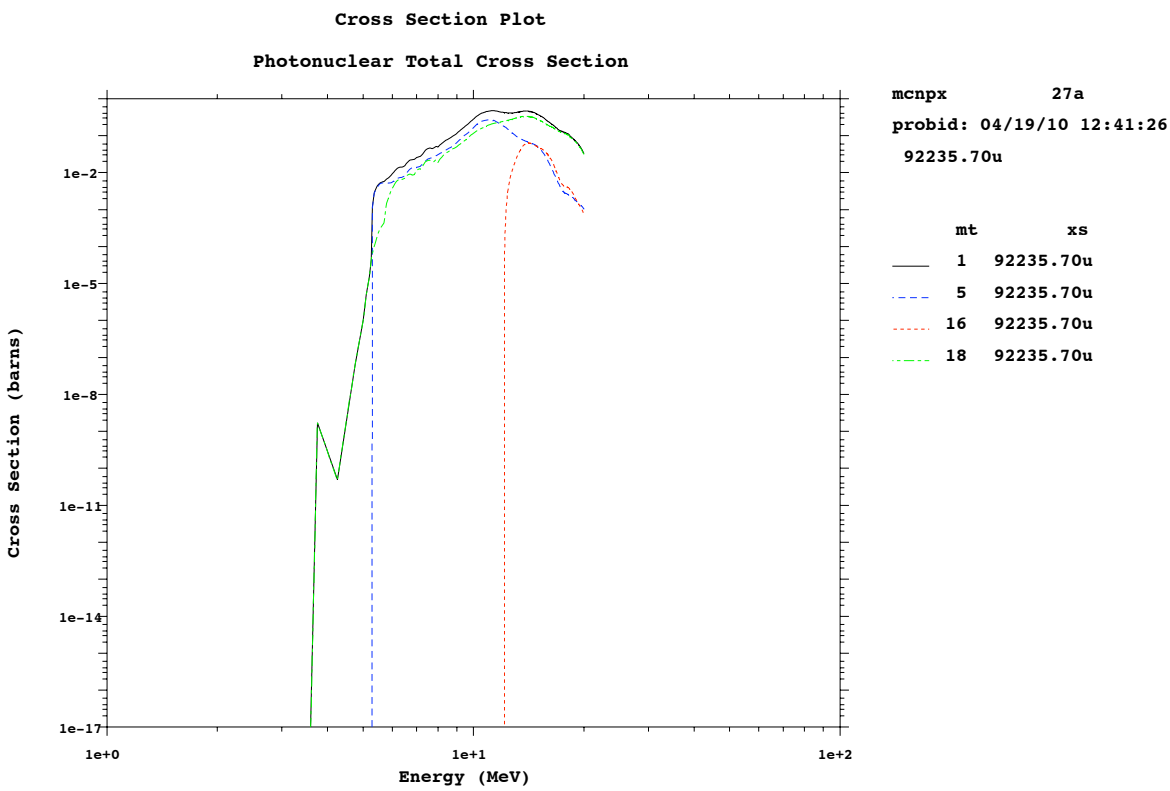

Figure 5: Photonuclear cross-sections for ^{235}U (taken from 92235.70u). Black curve is total, red curve is (γ,2n), green curve is photofission, blue is all other photonuclear reactions.

The MCNPX input deck that describes this example is given below:

```
12 MeV x-rays into U-235
1 1 -19.0 -1 imp:n=1
2 0 1 imp:n=0

1 so 1.0

mode n p
m1 92235 1 pnlib=.70u
PHYS:P j 1 j -1 2j 1 $ 0=ACE,1=LLNL
```

```
sdef par=p erg=12
LCA 7j -2
nps 1000000
f1:n 1
e1 1e-6 199log 12
f11:p 1
e11 1e-3 199log 12
ft11 tag 3
fu11 -1 0.00004 92000.00003 92235.00005 92000.00005 92235.00018 1e10
```

To switch from the default ACE MCNPX model to the LLNL photofission library, the 7th entry of the PHYS:P is set to 1 in the input deck. Note that the 4th entry of the PHYS:P card is set to -1 to turn on analog photonuclear particle production. We are interested here in the spectrum of prompt photofission gamma-rays emitted by ^{235}U. Figure 6 shows the energy distribution of the photofission gamma-rays for different MCNPX settings.

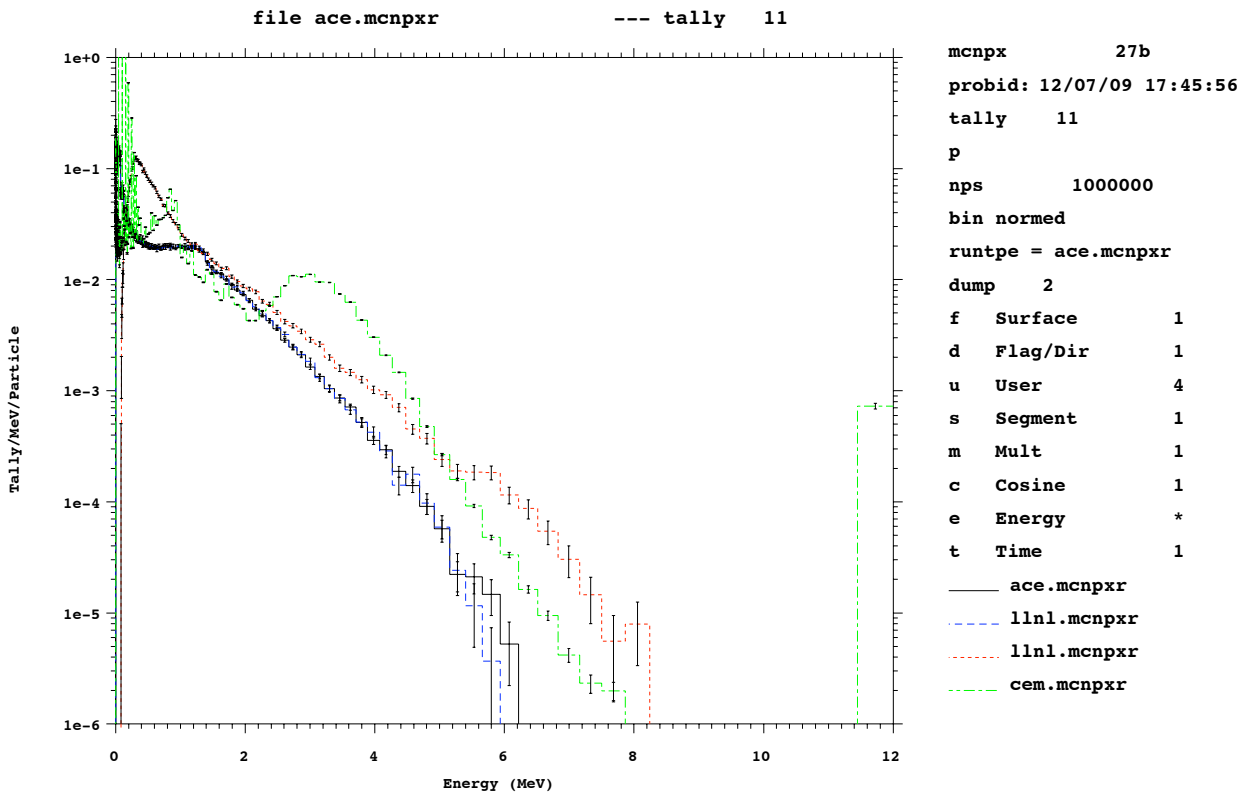

Figure 6: Energy spectrum of the photofission gamma-rays from a 12 MeV gamma-ray beam impinging on ^{235}U. The black, blue & red, and green curves were generated by MCNPX simulations with the ACE, LLNL, and CEM models, respectively.

The black curve was generated from a simulation with the ACE model, it shows the spectrum of all gamma-rays produced by photonuclear reactions with the ACE model. The default MCNPX ACE model produces prompt photofission neutrons but does not produce any prompt photofission gamma-rays, because there is no such data available in the photonuclear data libraries ENDF/B-VII.

The blue and red curves were generated from a simulation where the LLNL photofission library was turned on. The red curve is the spectrum of gamma-rays produced by photofission, while the blue one corresponds to gamma-rays produced by all other photonuclear reactions.

Finally, a last simulation was performed with the much slower CEM model, and the green curve shows the gamma-ray spectrum of all photonuclear reactions with this model.

4.3 Geant4

This physics module is now part of the Geant4 distribution as of release 4.9.0. Please refer to the Geant4 documentation for information on how to use this fission model. Instructions on how to add this library by hand in earlier versions are described below.

Limitations

The neutron-induced fission data available in G4NDL3.10 is very limited. At the time of this writing, there are only data files for seven isotopes of Uranium: ^{232}U, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{237}U and ^{238}U. The origin of the data has not been investigated. For other isotopes, induced fission will not emit any particles. This fission library does not have any spontaneous fission data for isotopes other than the ones listed in section 4.1. Photofission has not been implemented in Geant4.

Compilation

Please refer to the `geant` directory in the fission library source code distribution for a complete example and explicit instructions for compiling and linking the fission library with Geant4. Besides setting the usual environmental variables for Geant4, one also needs to set EXTRALIBS to -lFission before building the executable. The fission library libFission.a must be located in a directory specified in the link line. A good place for libFission.a is the directory $G4WORKDIR/tmp/$G4SYSTEM/exec_name The header file Fission.hh must be in the include directory.

Execution

The environment variable *NeutronHPCrossSections* must point to the G4NDL3.10 directory, where the induced fission cross-sections and data are located.

Description of c++ classes

For neutron induced fission, this model is intended to be used with the low energy neutron interaction data libraries with class *G4Fisslib* specified in the physics list as the *G4HadronFissionProccess* instead of class *G4NeutronHPFission*. Here is an example code snippet for registering this model in the physics list:

```
G4ProcessManager* pmanager = particle->GetProcessManager();
G4String particleName = particle->GetParticleName();

if (particleName == "gamma") {
  (...)
} else if (particleName == "neutron") {
  (...)
  // Fission library model
  G4HadronFissionProcess *theFissionProcess = new G4HadronFissionProcess();
  G4FissLib* theFissionModel = new G4FissLib;
  theFissionProcess->RegisterMe(theFissionModel);
  pmanager->AddDiscreteProcess(theFissionProcess);
  (...)
} else ...
```

The constructor of *G4FissLib* does two things. First it reads the necessary fission cross-section data in the file located in the directory specified by the environment variable *NeutronHPCrossSections*. It does this by initializing one object of class *G4NeutronHPChannel* per isotope present in the geometry. Second, it registers an instance of *G4FissionLibrary* for each isotope as the model for that reaction/channel. When Geant4 tracks a neutron to a reaction site and the fission library process is selected among all other process for neutron reactions, the method *G4FissLib::ApplyYourself* is called, and one of the fissionable isotopes present at the reaction site is selected. This method in turn calls *G4NeutronHPChannel::ApplyYourself* which calls *G4FissionLibrary::ApplyYourself*, where the induced neutrons and gamma-rays are emitted by sampling the fission library.

For spontaneous fission the user must provide classes *PrimaryGeneratorAction*, *MultipleSource*, *MultipleSourceMessenger*, *SingleSource*, *SponFissIsotope* to generate spontaneous fission neutrons and gammas. Examples of these classes can be downloaded from `http://nuclear.llnl.gov/simulation`. Spontaneous fissions are generated in the *PrimaryGeneratorAction* class. The spontaneous fission source needs to be described in terms of geometry, isotopic composition and fission strength. Once this information is given, the constructor creates as many spontaneous fission isotopes of class *SponFissIsotope* as specified, and adds them to the source of class *MultipleSource*. When Geant needs to generate particles, it calls the method *PrimaryGeneratorAction::GeneratePrimaries*, which first sets the time of the next fission based on the fission rates entered in the constructor, and then calls the method *MultipleSource::GeneratePrimaryVertex* which determines which one of the spontaneous fission isotopes will fission. This method in turn calls the method *SponFissIsotope::GeneratePrimaryVertex* for the chosen isotope. It is in this method that the neutrons and photons sampled from the fission library are added to the stack of secondary particles. Sources other than spontaneous fission isotopes can be added to the source of class *MultipleSource*. For instance, a background term emitting a large number of background gamma-rays can be added, as long as it derives from the class *SingleSource*. The intensity of that source would be set the same way as for the spontaneous fission isotope sources.

4.4 Fission library interface

The interface to the fission library consists of 23 C functions, each of which will be described below:

void genspfissevt_(int *isotope, double *time)

This function is called to trigger a spontaneous fission. Multiple neutrons and gamma-rays are generated and stored in a stack along with their energies, directions and emission times. The arguments of this function are

isotope: entered in the form ZA (e.g. 94239 for ^{239}Pu)
time: the time of the spontaneous fission

The generated neutrons and gamma-rays, along with their properties will be lost upon the next call to genspfissevt_, genfissevt_ or genphotofissevt_. Therefore, they must be retrieved immediately by the caller using the appropriate functions described below.

void genfissevt_(int *isotope, double *time, double *nubar, double *eng)

This function is called to trigger a neutron-induced fission. In addition to the arguments above, the fission inducing neutron is characterized by:

nubar: user-specified average number of neutrons emitted per fission (e.g. as tabulated in the cross-section libraries used by the particle transport code)
eng: energy of the neutron inducing fission

Either the average number $\bar{\nu}$ of neutrons emitted per fission or the energy *eng* of the fission inducing neutron will be used to determine the number of neutrons sampled, see function setnudist_ below. The number of gamma-rays sampled only depends on $\bar{\nu}$. Similarly to genspfissevt_, the generated neutrons and gamma-rays are lost upon subsequent calls to genspfissevt_, genfissevt_ or genphotofissevt_.

void genphotofissevt_(int *isotope, double *time, double *nubar, double *eng)

This function is called to trigger a photon-induced fission. In addition to the arguments specified in genfissevt_, the fission inducing neutron is characterized by:

nubar: user-specified average number of neutrons emitted per photofission (e.g. as tabulated in the photonuclear cross-section libraries used by the particle transport code)
eng: energy of the photon inducing fission

Either the average number $\bar{\nu}$ of neutrons emitted per photofission or the energy *eng* of the fission inducing photon will be used to determine the number of neutrons sampled, see function setnudist_ below. The number of gamma-rays sampled only depends on $\bar{\nu}$. Similarly to genspfissevt_, the generated neutrons and gamma-rays are lost upon subsequent calls to genspfissevt_, genfissevt_ or genphotofissevt_.

int getnnu_() and int getpnu_()

These functions return the numbers of fission neutrons and gamma-rays emitted in the fission reaction, or -1 if no number could be sampled in the fission library due to lack of data. The reader is referred to the physics reference manual to find the list of isotopes for which sampling will return positive numbers.

double getneng_(int *index) and double getpeng_(int *index)
double getnvel_(int *index) and double getpvel_(int *index)

These functions return the energies and velocities of the neutrons/gamma-rays.

double getndircosu_(int *index), double getndircosv_(int *index), double getndircosw_(int *index)

double getpdircosu_(int *index), double getpdircosv_(int *index), double getpdircosw_(int *index)

These 2 families of functions return the direction cosines of the velocity vector on the x, y and z axes for the fission neutrons and gamma-rays.

double getnage_(int *index) and double getpage_(int *index)

This functions returns the age of the fission neutron/gamma-ray, or -1 if index is out of range. The age returned might be different from the time specified in genfissevt_, genspfissevt_ and genphotofissevt_ for delayed neutrons and gamma-rays, see function setdelay_ below. Currently, delayed fission neutrons/gamma-rays are not implemented, so all fission products are emitted promptly.

void setdelay_(int *delay)

This function is called to enable delayed neutrons and gamma-rays. The argument *delay* is set to

0 (default)	for strictly prompt neutrons and photons
1 (n/a)	for prompt neutrons, prompt and delayed photons
2 (n/a)	for prompt and delayed neutrons, prompt photons
3 (n/a)	for prompt and delayed neutrons, prompt and delayed photons

Delayed neutrons and gamma-rays have not yet been implemented in the fission library. This setting has presently no effect on the age sampling. All neutrons and photons are currently emitted promptly (delay=0).

void setcorrel_(int *correlation)

This function is called to set the type of neutron/gamma-ray correlation. The argument *correlation* is set to

0 (default)	for no correlation between neutrons and photons
1	total fission neutron energy and total fission gamma-ray energy are sampled from normal distributions of means given in Beck et al. [24]. No correlation between the number of neutrons and the number of gamma-rays
2	total fission neutron energy and total fission gamma-ray energy are sampled from normal distributions of means given in Vogt [26]. No correlation between the number of neutrons and the number of gamma-rays
3 (n/a)	for number and energy correlation between neutrons and photons

void setnudist_(int *nudist)

This selects the data to be sampled for the neutron number distributions for neutron-induced fission. If there is no data available, then in all cases the Terrell approximation is used. The argument *nudist* can take 3 values:

0	Use the fit to the Zucker and Holden tabulated P_ν distributions as a function of energy for ^{235}U, ^{238}U and ^{239}Pu.
1	Use fits to the Zucker and Holden tabulated P_ν distribution as a function of energy for ^{238}U and ^{239}Pu, and a fit to the Zucker and Holden data as well as the Gwin, Spencer and Ingle data (at thermal energies) as a function of energy for ^{235}U.
2	Use the fit to the Zucker and Holden tabulated P_ν distributions as a function of $\bar{\nu}$. The ^{238}U fit is used for the ^{232}U, ^{234}U, ^{236}U and ^{238}U isotopes, the ^{235}U fit for ^{233}U and ^{235}U, the ^{239}Pu fit for ^{239}Pu and ^{241}Pu.
3 (default)	Use the discrete Zucker and Holden tabulated P_ν distributions and corresponding $\bar{\nu}$s. Sampling based on the incident neutron $\bar{\nu}$. The ^{238}U data tables are used for the ^{232}U, ^{234}U, ^{236}U and ^{238}U isotopes, the ^{235}U data for ^{233}U and ^{235}U, the ^{239}Pu data for ^{239}Pu and ^{241}Pu.

void setcf252_(int *ndist, int *neng)

This function is specific to the spontaneous fission of ^{252}Cf. It selects the data to be sampled for the neutron number and energy distributions and takes the following arguments:

ndist: Sample the number of neutrons
- 0 (default) from the tabulated data measured by Spencer
- 1 from Boldeman's data

neng: Sample the spontaneous fission neutron energy
- 0 (default) from Mannhart corrected Maxwellian spectrum
- 1 from Madland-Nix theoretical spectrum
- 2 from the Froehner Watt spectrum

void setrngf_(float (*funcptr) (void)) and void setrngd_(double (*funcptr) (void))

This function sets the random number generator to the user-defined one specified in the argument. If either setrngf_ or setrngd_ are not specified, the default system call srand48 is used. The arguments are random number generator functions that returns variables of type float and double respectively.

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