CGMF & FREYA Verification in Monte Carlo Code RMC

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Abstract. Monte Carlo simulation has become a crucial method internationally for simulating neutron multiplicity counting devices. This method requires sampling of fission neutron multiplicities, energies, and directions, making accurate simulation of fission events highly important. To meet this demand, the Fission Reaction Event Yield Algorithm (FREYA) and the Cascading Gamma-ray Multiplicity with Fission (CGMF) models have been integrated into RMC. These models can simulate individual fission events, preserving momentum, energy, and angular momentum, and then emit correlated particles. In addition to simulating fission neutrons, CGMF and FREYA models have been employed to compute fission photons, laying the foundation for subsequent photon multiplicity counting. Simultaneously, neutron multiplicity counting has been calculated using CGMF and FREYA, and point model equations have been used to invert Pu material, yielding favorable results.

1 Introduction

The standard neutron multiplicity counting model does not simulate each fission process in detail but independently samples from distributions to generate average quantities. The standard model is invoked by using method=3 data=3 shift=1 on the FMULT card to generate realistic fission multiplicities, as opposed to the default MCNP options that only preserve the average value $\bar{v}$. This is further detailed in the MCNP manual [1]. In induced fission, the average neutron multiplicity $\bar{v}$ is obtained from the chosen nuclear data library. The multiplicity distribution is chosen by sampling a Gaussian distribution to preserve $\bar{v}$ without sampling negative numbers of neutrons. Spontaneous fission multiplicity is derived from measured data referenced in the MCNP manual. Neutron energies use Watt spectra parameters from the data library for induced fission or from the manual for spontaneous fission, which were generated by the Madland–Nix model [2]. All properties are independently sampled, meaning there are no neutron angular correlations, and all neutrons are emitted isotropically. The standard model in the RSICC release of MCNP6.2 is utilized, and this approach is consistent with the current use in RMC.

CGMF and FREYA simulate fission events, including the fission process and fission fragments. The latest version of MCNP integrates both models into RMC. This study provides a brief introduction to CGMF and FREYA, integrating them into RMC and comparing the

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neutron and photon multiplicities for different fission isotopes using FREYA and CGMF. Additionally, differences in neutron multiplicity counting between the standard model, CGMF, and FREYA are compared. The study also includes the inversion of Pu material using a point model, resulting in favorable outcomes.

2 CGMF & FREYA

2.1 CGMF

The CGMF code implements the Hauser-Feshbach statistical nuclear reaction model to follow the de-excitation of fission fragments by successive emissions of prompt neutrons and γ rays. The Monte Carlo technique is used to facilitate the analysis of complex distributions and correlations among the prompt fission observables. Nuclear structure and reaction input data from the RIPL3 library are used to describe fission fragment properties and decay probabilities. Characteristics of prompt fission neutrons, prompt fission γ rays, and independent fission yields can be studied consistently. Correlations in energy, angle and multiplicity among the emitted neutrons and γ rays can be easily analyzed as a function of the emitting fragments. In its current version, In its current version, CGMF is limited to the spontaneous fission of ^{238,240,242,244}Pu and ^{252,254}Cf, as well as to the neutron-induced fission reactions from thermal up to 20 MeV on $^{233,234,235,238U,\ 237}$Np, and ^{239,241}Pu isotopes [3].

2.2 FREYA

FREYA (Fission Reaction Event Yield Algorithm) is a fission event generator which models complete fission events. As such, it automatically includes fluctuations as well as correlations between observables, resulting from conservation of energy and momentum. The purpose of this paper is to present the main differences between FREYA versions 1.0 and 2.0.2: additional fissionable isotopes, angular momentum conservation, Giant Dipole Resonance form factor for the statistical emission of photons, improved treatment of fission photon emission using RIPL database, and dependence on the incident neutron direction. FREYA 2.0.2 has been integrated into the LLNL Fission Library 2.0.2, which has itself been integrated into MCNP6.2, TRIPOLI-4.10, and can be called from Geant4.10. The number of fission reactions that FREYA 2.0.2 implements has increased, it can currently handle spontaneous fissions of ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{244}Cm and ^{252}Cf. In addition to spontaneous fission, FREYA treats neutron-induced fission of ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu up to En = 20 MeV, and is sensitive to the direction of the incident neutron [4].

3 Methods

By deducing the process of neutron emission from the source event through multiplication before being detected, we obtained the neutron multiplicity distribution after detection and multiplicity counting. Additionally, we derived the first three moments of the neutron multiplicity distribution. Within these factorial moments are the unknown parameters required to determine the fission rate, multiplication factor, and the ratio of (α, n) neutrons to spontaneously fission neutrons for the sample [5][6]. The derived equations are expressed as follows in Eq. 1.

$$\begin{aligned} S &= F\varepsilon M_L v_{s1}(1+\alpha) \\ D &= \frac{F\varepsilon^2 f_d M_L^2}{2}\left[v_{s2} + \left(\frac{M_L - 1}{v_{i1-1}}\right) v_{s1}(1+\alpha) v_{i2}\right] \\ T &= \frac{F\varepsilon^3 f_t M_L^3}{6}\left\{ \begin{array}{c} v_{s3} + \left(\frac{M_L-1}{v_{i1}-1}\right)[3v_{s2}v_{i2} + v_{s1}(1+\alpha)v_{i3}] + \\ 3\left(\frac{M_L-1}{v_{i1}-1}\right)^2 v_{s1}(1+\alpha)v_{i2}^2 \end{array} \right\} \end{aligned} \tag{1}$$

In Eq. 1, F denotes the spontaneous fission rate, ε represents the neutron detection efficiency, M_L is the leakage multiplication factor, α signifies the ratio of the neutron emission rate from (α, n) reactions to the spontaneous fission neutron emission rate, f_d stands for the double-gate fraction, and f_t denotes the triple-gate fraction, reflecting the proportion of the gate width G over the entire decay time. v_{ij} is the induced fission neutron multiplicity jth moment, and v_{sj} is the jth moment of the multiplicity of spontaneous fission neutrons. By solving the system of three equations, the three unknowns F, M_L, and α can be determined, and the mass of fissionable material can be calculated through F.

In the above Eq. 1, there are three variables related to the system: the fission rate of the sample F, the ratio of (α, n) neutrons to spontaneously fissioned neutrons α, and the leakage multiplication factor M_L. In the solving process, the usual approach is to first eliminate the fission rate and neutron ratio by simultaneously solving the three equations, resulting in a cubic equation in terms of the leakage multiplication factor by Eq. 2.

$$a + bM_L + cM_L^2 + M_L^3 = 0 \tag{2}$$

The parameters a, b, and c can be solved using S, D, T and the related nuclear data. The expressions for parameters a, b, and c are given by Eq. 3.

$$\left\{ \begin{aligned} a &= \frac{-6Tv_{sf2}\left(v_{if1}-1\right)}{\varepsilon^2 f_t S\left(v_{sf2}v_{if3} - v_{sf3}v_{if2}\right)} \\ b &= \frac{2D\left[v_{sf3}\left(v_{if1}-1\right) - 3v_{sf2}v_{if2}\right]}{\varepsilon f_d S\left(v_{sf2}v_{i3} - v_{sf3}v_{i2}\right)} \\ c &= \frac{6Dv_{sf2}v_{if2}}{\varepsilon f_d S\left(v_{sf2}v_{if3} - v_{sf3}v_{if2}\right)} - 1 \end{aligned} \right. \tag{3}$$

Subsequently, the roots of the cubic equation can be computed using Eq. 2 and Eq. 3, yielding the value of M_L. The equivalent ^{240}Pu spontaneous fission rate F and the α parameter for the sample can be calculated by Eq. 4.

$$\left\{ \begin{aligned} F &= \frac{\frac{2D}{\varepsilon f_d} - \frac{M_L(M_L-1)v_{if2}S}{v_{if1}-1}}{\varepsilon M_L^2 v_{sf2}} \\ \alpha &= \frac{S}{F\varepsilon v_{sf1}M_L} - 1 \end{aligned} \right. \tag{4}$$

Firstly, the parameters f_d and f_t are derived. Calculate the neutron decay time constant τ, and then, through the computations using Eq. 5, f_d and f_t can be obtained.

$$\left\{ \begin{aligned} f_{\mathrm{d}} &= e^{-P/\tau}\left(1 - e^{-G/\tau}\right) \\ f_{\mathrm{t}} &= f_{\mathrm{d}}^2 \end{aligned} \right. \tag{5}$$

Using the double coincidence gate ratio method, while keeping the pre-delay time constant, two different gate widths are selected. The double counting rates are calculated for each gate width, and the comparison of these two double counting rates yields the corresponding the Eq. 6.

$$\frac{R_1}{R_2} = \frac{1 - e^{-G1/\tau}}{1 - e^{-G2/\tau}} \tag{6}$$

Where R_1 and R_2 are the double counting rates calculated for gate widths G_1 and G_2, respectively, and τ is the decay time. If G_2=2G_1, the decay time τ can be further simplified. The further simplified formula is given in Eq. 7.

$$\tau = \frac{-G_1}{\ln\left(\frac{R_2}{R_1} - 1\right)} \tag{7}$$

The calculation of ε is expressed as follows in Eq. 8 [7].

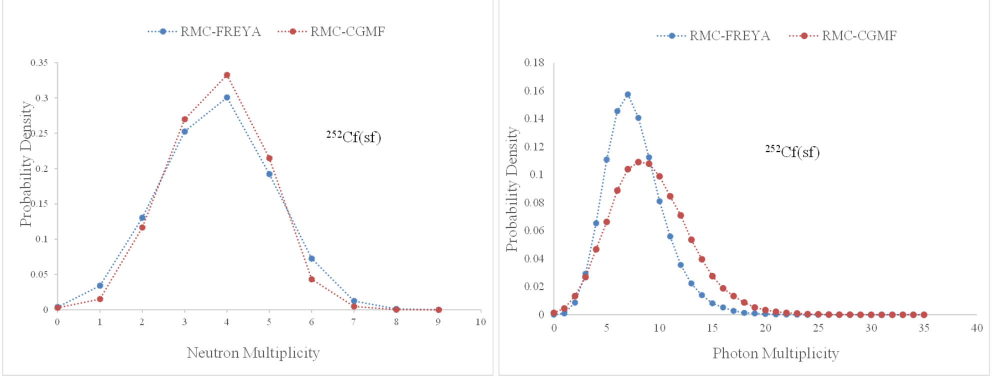
$$\varepsilon = \frac{S}{Y} \tag{8}$$

Where S is the singles counting rate, and Y is the source strength. The calibration of detection efficiency is commonly performed using a ^{252}Cf point source.

This work, based on the neutron multiplicity counting functionality of the Monte Carlo program RMC [8][9], analyzed the HLNC2 device.

4 Numerical Results

4.1 Distributions Comparsion

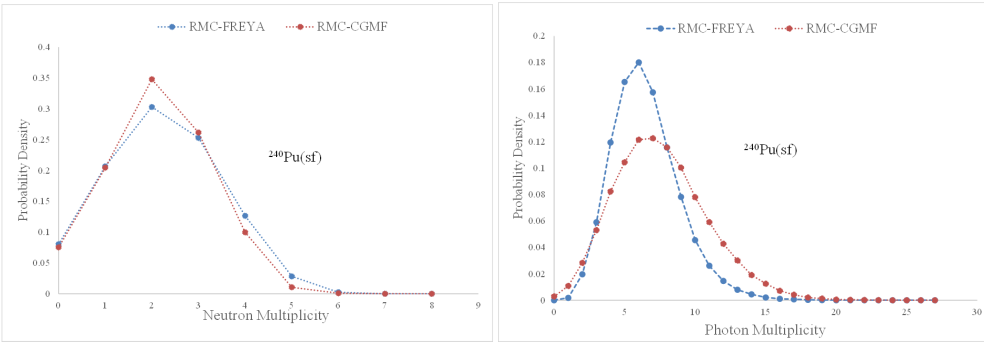


(a) Neutron Multiplicity (b) Photon Multiplicity

Figure 1: The neutron and photon multiplicity distributions of spontaneous fission of ^{252}Cf

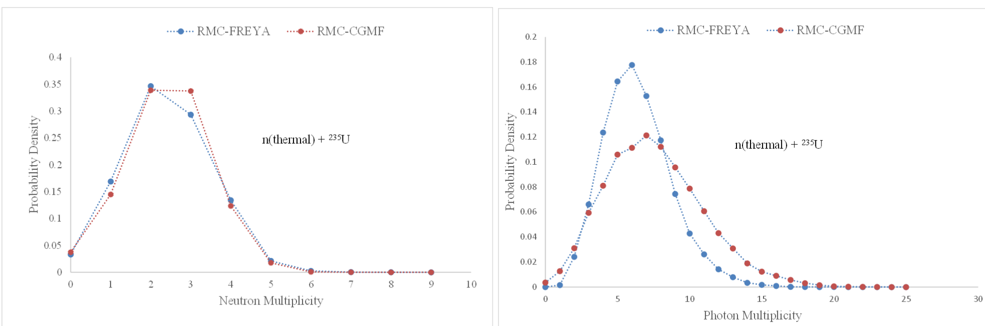
First, utilize RMC-FREYA and RMC-CGMF to compute the multiplicity distributions of spontaneous fission neutrons and photons in ^{252}Cf, as shown in Figure 1.

Next, use RMC-FREYA and RMC-CGMF to compute the multiplicity distributions of spontaneous fission neutrons and photons in ^{240}Pu, as shown in Figure 2.



(a) Neutron Multiplicity (b) Photon Multiplicity

Figure 2: The neutron and photon multiplicity distributions of spontaneous fission of ^{240}Pu



(a) Neutron Multiplicity (b) Photon Multiplicity

Figure 3: The neutron and photon multiplicity distributions of neutron-induced fission of n(thermal)+^{235}U

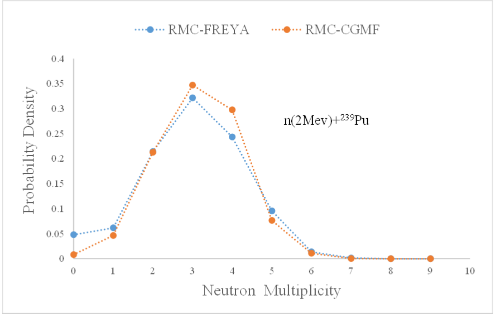
Then, utilize RMC-FREYA and RMC-CGMF to compute the multiplicity distributions of thermal neutron-induced fission neutrons and photons in ^{235}U, as shown in Figure 3.

Last, using RMC-FREYA and RMC-CGMF to calculate the multiplicity distributions of 2MeV neutron-induced fission neutrons and photons in ^{239}Pu, as shown in Figure 4.

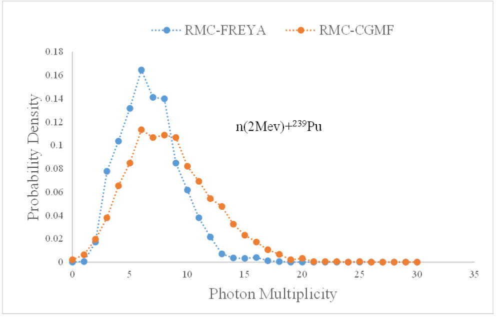
From Table 1, it can be seen that the neutron multiplicity distributions calculated using RMC-CGMF and RMC-FREYA match well, but there is a significant difference in the photon multiplicity distributions.

4.2 Neutron Multiplicity Countings Comparsion

The High Level Neutron Coincidence Counter (HLNCC) was developed by Los Alamos National Laboratory (LANL) in 1979 for the measurement of mass in large quantities of plutonium materials. A new upgraded version of the HLNCC has been designed and fabricated called HLNC2. The detector still contains 18 ^{3}He tubes, but in a cylindrical polyethylene body [6]. HLNC2 experimental setup was selected to test and validate the developed functionality [10]. The schematic diagram of RMC modeling is shown in the Figure 5.



(a) Neutron Multiplicity



(b) Photon Multiplicity

Figure 4: The neutron and photon multiplicity distributions of neutron-induced fission of n(2MeV)+^{239}Pu

Table 1: Average and covariance of the neutron and Photon multiplicities for the nuclides ^{252}Cf, ^{240}Pu, ^{235}U and ^{239}Pu calculated with FREYA AND CGMF

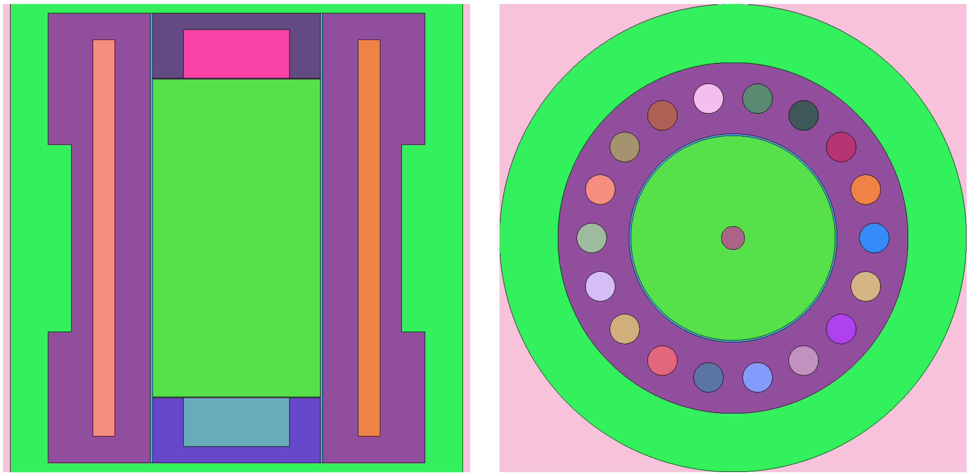
	RMC-FREYA	
Isotope	Average Neutron Multiplicity ($\bar{\upsilon}$)	Average Photon Multiplicity ($\bar{\mu}$)
^{252}Cf	3.7488	7.6959
^{240}Pu	2.2329	6.4920
^{235}U	2.4018	6.3955
^{239}Pu	3.0004	6.7592
	RMC-CGMF	
Isotope	Average Neutron Multiplicity ($\bar{\upsilon}$)	Average Photon Multiplicity ($\bar{\mu}$)
^{252}Cf	3.7559	9.1576
^{240}Pu	2.1409	7.5627
^{235}U	2.4207	7.5621
^{239}Pu	3.1546	8.4557

Place the ^{252}Cf source at the center of the sample chamber to calculate first-order, second-order, and third-order neutron multiplicity count rates. According to the Eq. 8, the calculated detection efficiency ε is 0.1692. Besides, according to the Eq. 6, the calculated neutron decay time is 38.52 μs.

Pu with the same mass as in the literature was selected for calculation. PuO_2 is a cylinder with a height of 20 cm and a radius of 5 cm, and its density is 2.5 g/cm^3. The calculated mass of ^{240}Pu that can be obtained is 695.04 g. The chosen pre-delay time is 4.5 μs, and the gate width is 64 μs. Firstly, calculate the second and third order gate fractions based on pre-delay time and gate width. The calculated second-order gate fraction and third-order gate fraction are as follows according to the Eq. 9:

$$\begin{cases} f_{\mathrm{d}} = 0.7228 \\ f_{\mathrm{t}} = 0.5195 \end{cases} \tag{9}$$

Next, neutron multiplicity counting was calculated using RMC and compared with the MCNP results in the literature [10], as shown in Table 2.



(a) Axial Schematic (b) Radial Schematic

Figure 5: RMC Modeling Schematic

Table 2: Neutron Multiplicity Countings Results(with the mass of 695.04 g of ^{240}Pu)

Multiplicity counting (counts/s)	MCNP	RMC	Relative error
singles	180800	179839	0.53%
doubles	26130	25678	1.73%
triples	4284	4181	2.41%

The neutron multiplicity count results computed using RMC-CGMF and RMC-FREYA are shown in Table 3 and Table 4 respectively.

Table 3: Neutron Multiplicity Countings Results(with the mass of 695.04 g of ^{240}Pu)

Multiplicity counting (counts/s)	MCNP	RMC-CGMF	Relative error
singles	180800	178330	1.37%
doubles	26130	24982	4.39%
triples	4284	3760	12.22%

It can be observed that after using FREYA and CGMF, the computed neutron multiplicity countings deviate significantly from those without employing the standard model at the third-order countings. This deviation is primarily due to inherent biases in the third-order countings itself. Additionally, the introduction of fission models leads to certain deviations in the neutron multiplicity distribution.

The final step involved using the point model equation set for the mass inversion of ^{240}Pu, and the settlement results are shown in the Table 5. It can be seen that the deviations of the ^{240}Pu mass computed using CGMF and FREYA from the standard mass are both within 5%, indicating the correctness of the computed results. More tests will be conducted later

Table 4: Neutron Multiplicity Countings Results(with the mass of 695.04 g of ^{240}Pu)

Multiplicity counting (counts/s)	MCNP	RMC-FREYA	Relative error
singles	180800	184658	-2.13%
doubles	26130	28147	-7.72%
triples	4284	4821	-12.53%

Table 5: Mass Calculation Results

Calculation Mode	^{240}Pu Mass (g)	Relative_error
RMC	716.58	3.10%
RMC-cgmf	728.92	4.87%
RMC-freya	691.76	-0.47%

to explore the reasons for the significant deviations in the computed results between RMC-FREYA and RMC-CGMF.

5 Conlusions

These new models simulate fission events to generate emitted particles used for nuclear material measurements. The detailed simulation of fission events incorporates many aspects of fission signatures that were previously ignored. The newly simulated correlations represent a significant advancement in Monte Carlo capabilities, but preserving the fundamental, well-known aggregate quantities is crucial.

This paper integrates the fission models FREYA and CGMF into RMC, comparing the fission neutron and photon multiplicity distributions for commonly used fission isotopes. Comparing RMC-CGMF with RMC-FREYA, the results show a closer agreement in the fission neutron multiplicity distribution than in the fission photon multiplicity distribution. Additionally, RMC-CGMF and RMC-FREYA were used to calculate the neutron multiplicity counting results for the HLNC2 experimental setup. Due to differences in the neutron multiplicity distribution between spontaneous fission of ^{240}Pu and induced fission of ^{239}Pu, the neutron multiplicity counting results differ significantly from those obtained using the standard model. However, the mass inversion results using a point model equation show smaller differences compared to the standard values.

In future work, neutron angular correlations and energy dependencies will be considered in the multiplicity counting devices. Research will also be conducted on fast neutron multiplicity counting and photon multiplicity counting.

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