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Correlated Fission Multiplicity Model Verification Efforts in MCNP6

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INTRODUCTION

The need for a predictive capability in the detection of special nuclear materials (SNM) has led to the introduction of new correlated fission multiplicity models into [1]MCNP® 6 [1]. From LANL, the CGMF code [2] has been implemented as an upgrade to the original Cascading Gamma-ray Multiplicity code, CGM [3], with the additional capability to handle neutron-induced and spontaneous fission events with correlated neutron and photon emissions. Additionally, the LLNL Fission Library has been upgraded from the original implementation released in prior versions of MCNP6 to include the Fission Reaction Event Yield Algorithm (FREYA) code [4] also capable of simulating fission events with correlated neutron and photon emissions.

In preparation for the release of the MCNP6.2 code, it is necessary to verify that the new fission event generators are performing as expected. To this end, it is assumed that the fission event generators released by the respective developers has already undergone verification testing with respect to the nuclear fission theory for which they are based upon as well as compared against some applicable experimental measurements. Therefore, from the perspective of the MCNP user and developer community, it is necessary to ensure that the results from the released version of the fission event generators are being captured properly in the integrated version within the next release of MCNP6.2.

For the remainder of this paper, we first briefly discuss some background on the new fission event generators, CGMF and FREYA. Second, the strategy for verifying the implementation of the fission event generators into MCNP6.2 is introduced and discussed. Third, the initial numerical verification results are shown with some discussion on what was discovered in previous versions of MCNP6 which warranted an improvement to the secondary neutron-photon emission physics algorithm. Finally, we summarize the numerical results and draw conclusions on the initial verification efforts with a look forward to the needed MCNP fission event model validation efforts.

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BACKGROUND

In the next release of MCNP, version 6.2, two upgraded fission event generators will be included. Previously, in the most recent version of MCNP6.1.1 [5], two low-energy neutron-photon multiplicity packages were released: the LLNL Fission Library [6] and the Cascading Gamma-ray Multiplicity (CGM) code from LANL [3]. The released version of the LLNL Fission Library, version 1.8, included neutron and photon multiplicity distributions, but did not include any correlations between emitted particles by default. Likewise, the released version of the CGM code handles a variety of reactions, but does not include emitted particles or photons from fission reactions. The newest versions of these event generators, to be included in the MCNP6.2 release, are significantly improved over their predecessors by addressing some of these immediate deficiencies mentioned above.

Secondary Particle Event Generators

The LANL CGMF code can be described as a superset of the original CGM code with the new capability of handling fission reactions. Simply, CGM models the statistical nature of emitted particles from compound nuclei with excitation energy. The CGMF code adds the fission process to this capability by sampling from a joint probability distribution of the mass (A), charge (Z) and total kinetic energy (TKE) yields to obtain the initial conditions of the excited fission fragments prior to particle emission. From these two fission fragments, the original CGM portion of the code base performs event-by-event simulations of the decay of the excited fragments using the Hauser-Feshbach statistical theory of nuclear reactions [2].

Alternatively, the FREYA code now implemented in MCNP6 through the LLNL Fission Library package is similar to the CGMF code in that it acts as an event generator for neutron-induced and spontaneous fission events. While the initial conditions for the fission fragments (A, Z, TKE yields, etc.) are very similar, the primary difference in methodology between the two event generator codes is that FREYA uses a Monte Carlo Weisskopf approach while CGMF uses a Monte Carlo Hauser-Feshbach approach. This difference in methodology manifests itself in both the calculated results and the overall computation cost of the models [7], where some evidence of the numerical differences can be seen in the results to follow.

VERIFICATION STRATEGY

With any new feature in MCNP6, after a need has been demonstrated, the primary goal of developers is to ensure that it is working as it is expected. In the case of these fission event generators, it is assumed that they are verified against the theory that they represent (i.e. Hauser-Feshbach). If this is the case, it is sufficient to verify these new features by comparing the results from the event generator codes in a standalone-mode to them integrated within MCNP6. The quantities we wish to model correctly through these event generators include:

- Averages
  - Multiplicity: $\bar{\nu}_n$ and $\bar{\nu}_\gamma$
  - Energy: $\bar{\chi}_n$ and $\bar{\chi}_\gamma$
- Distributions
  - Multiplicity: $P(\nu_n)$ and $P(\nu_\gamma)$
  - Energy: $\chi_n(E)$ and $\chi_\gamma(E)$
- Correlations
  - Multiplicity: $P(\nu_n, \nu_\gamma)$
  - Angular: $n(\vec{\Omega}) \cdot n(\vec{\Omega})$

The first obvious quantities to compare between models are the average quantities such as the first moment of the neutron and photon multiplicity distributions, $\bar{\nu}_n$ and $\bar{\nu}_\gamma$, respectively, and the first moment of the neutron and photon energy spectrum, $\bar{\chi}_n$ and $\bar{\chi}_\gamma$, respectively. The multiplicity distributions, $P(\nu_n)$ and $P(\nu_\gamma)$, and the energy distributions, $\chi_n(E)$ and $\chi_\gamma(E)$, are the natural choices for the next quantities in need of comparison to demonstrate the integration of the event generators has been verified. An unexpected large difference in any of these quantities could indicate a significant deficiency in the integrated versus standalone codes while any small differences will be difficult to distinguish if errors truly exist or if they are due to statistical fluctuations. While the numerical results for these average and distribution quantities are briefly discussed in this paper, it is important to mention these types of comparisons have been done previously [8].

To truly verify that the event generators have been integrated properly, it is necessary to look at the event-by-event results from these models. For example, the multiplicities and energies from these models may be easily verified with some standard tallies in MCNP6, but proving the neutron-neutron angular correlations are handled properly within MCNP6 would require analysis of the list-mode output. The following numerical results and discussion will address the verification of the correlated quantities listed above: the multiplicity correlations in $P(\nu_n, \nu_\gamma)$ and the neutron-neutron angular correlations, $n(\vec{\Omega}) \cdot n(\vec{\Omega})$, observed on an event-by-event basis.

NUMERICAL RESULTS

All of the following MCNP6 numerical results have been computed using the PTRAC output from a very simplified model where only the secondary particles are observed. Therefore, the integrated code results correspond directly to the CGMF or FREYA standalone results. While it is interesting to compare the observable values between each fission event generator model, but the immediate goal is to verify the integrated codes are performing as they are expected. Each simulation, either with MCNP6 or with the standalone codes, includes approximately 1E6 fission events.

Average Quantities

The average values listed in Table 1 are all generally in agreement taking the statistical fluctuations into account. With more fission event histories, the average values should approach each other (columns two and three) with the only source of discrepancy coming from the statistical fluctuations. If there are any issues with the integrated event generators, they would be very difficult to determine from this comparison of the average values.

Quantity	Standalone	MCNP
FREYA		
$\bar{\nu}_N$	3.7505(12)	3.7507(12)
$\bar{\nu}_\gamma$	6.8756(30)	6.8814(30)
$\bar{\chi}_n$	2.2278(10)	2.2302(10)
$\bar{\chi}_\gamma$	0.7098(2)	0.7105(2)
CGMF		
$\bar{\nu}_N$	3.8798(13)	3.8818(13)
$\bar{\nu}_\gamma$	8.6813(33)	8.6780(33)
$\bar{\chi}_n$	2.0974(8)	2.0983(8)
$\bar{\chi}_\gamma$	0.8132(3)	0.8131(3)

Table 1. The average multiplicity and energy of the secondary neutrons and photons for each code for the spontaneous fission of ^{252}Cf. Note the values in parenthesis indicate the standard deviation of the computed mean in the final one or two decimal places.

Distributions

Again comparing the integrated code results to the standalone code results, the calculated energy spectra of photons from ^{252}Cf spontaneous fission reactions are shown in Fig. 1. The differences between the standalone and integrated codes in MCNP are only due to the statistical fluctuations in the calculated spectra. However, if there exist any problems with the integrated event generators, it would be nearly impossible to identify it from these calculated energy spectra.

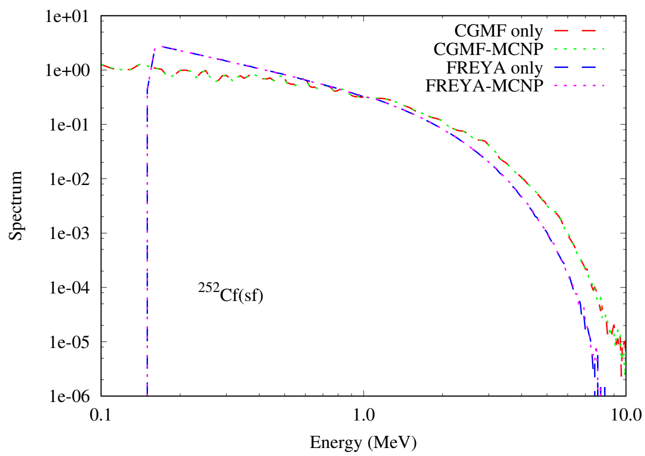

Fig. 1. The photon spectra of the ^{252}Cf spontaneous fission reaction calculated using MCNP6, FREYA and CGMF.

There is clearly a very big difference between FREYA and CGMF in the average photon multiplicity and energy in Table 1 as well as the energy distribution in Fig. 1. This discrepancy is primarily due to a difference in the low-energy cut-off value for photons used in the models which is generally a parameter used to tune the models to replicate experiments measuring secondary photons from fission. With the final released version of MCNP6.2 a final verification and validation document will be included and this difference in observables will be discussed in far more detail.

Neutron and Photon Correlations

While all of the previous numerical results were calculated from list-mode data, they represent simple quantities that can in fact be calculated using standard tallies in MCNP6. To be certain that the event generators have been implemented correctly, it was decided that the multiplicity and angular correlations need to be studied and compared between standalone and integrated codes. In the process of studying the list-mode data from MCNP6, through the PTRAC option, a minor bug was discovered in the neutron-induced fission physics algorithm within MCNP6. Basically, when using the fission event generators for neutron-induced fission events, within the `COLIDN` routine in the MCNP6 source code, if zero neutrons were emitted in a fission event then the history would incorrectly exit prior to putting any fission photons from the event generators into the secondary particle bank.

Since this bug has been fixed for the next release of MCNP6.2, secondary fission photons coming from the

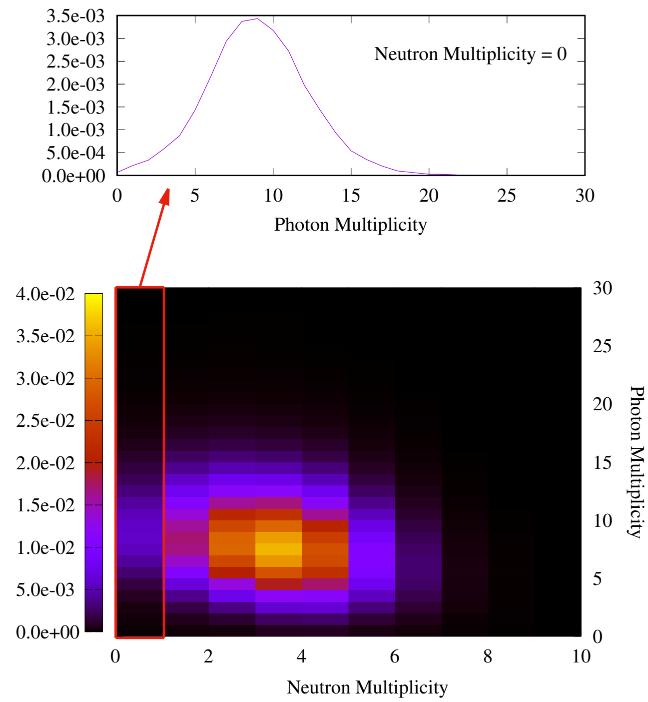

Fig. 2. On bottom is the neutron-photon multiplicity matrix calculated from the MCNP PTRAC data using the integrated CGMF for n(1.0273 MeV)+^{239}Pu fission reactions. Note a clear trend can be seen that neutron multiplicity increases for decreasing photon multiplicity. On top is the photon multiplicity when zero neutrons are emitted in a fission event.

event generators are now tracked when zero neutrons are emitted in a neutron-induced fission event. In Fig. 2, with the fixed fission physics algorithm, the photon multiplicity distribution is shown as a function of neutron multiplicity. Because the probability of having zero neutrons emitted in a n(1.0273 MeV)+^{239}Pu fission reaction is very small ($<3\%$), these missing photons were not detected in the verification tests using the average or distribution quantities discussed above.

The neutron-neutron angular correlation calculations make up the final verification test used in the present work to prove the fission event generators have been integrated into MCNP6 properly. In both Figures 3 and 4, the neutron-neutron angular correlations observed in these fission event generator models are shown for both n(1.0273 MeV)+^{239}Pu neutron-induced and ^{252}Cf spontaneous fission reactions, respectively. As with all of the comparisons between standalone and integrated fission event generator results, the neutron-neutron angular correlations are in great agreement with each other. However, to serve as a reminder, these quantities are not readily available from MCNP6 in any standard output or tallies; they can only

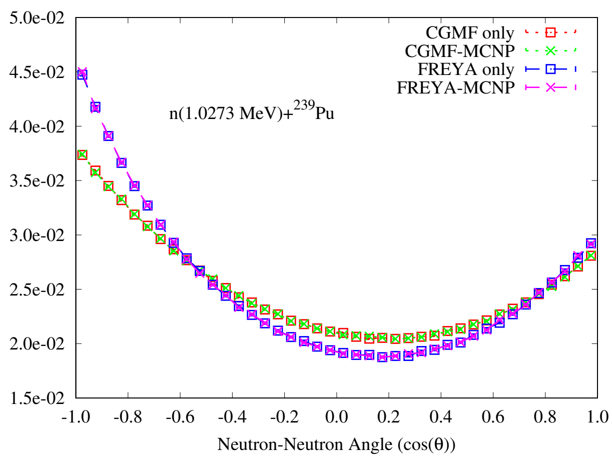

Fig. 3. The neutron-neutron angular correlations for the n(1.0273 MeV)+^{239}Pu reaction calculated using MCNP6, FREYA and CGMF.

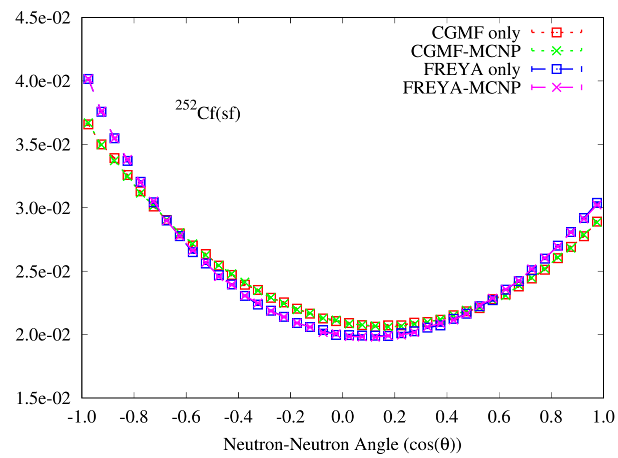

Fig. 4. The neutron-neutron angular correlations for the ^{252}Cf spontaneous fission reaction calculated using MCNP6, FREYA and CGMF.

be computed by analyzing the list-mode data through the MCNP PTRAC option.

CONCLUSIONS

At the present time, the new and updated fission event generators included in MCNP6.2 have been verified to be functioning properly through a variety of detailed tests. This work represents the amount of effort necessary to perform this verification such that a complicated fission event generator, like FREYA or CGMF, is integrated into MCNP6 properly. Ultimately, with the knowledge that MCNP6 is making use of these models appropriately, we can now begin to validate the models against benchmarked experiments. Some benchmarks, including criticality and subcriticality experiments interested in multiplication and bulk counting rates, are easy to model and understand but are likely insensitive to the detailed nature of these models. It will take some new measurements with coincidence detection capabilities to be able to stress the physics within each of these fission event generator models. Once the models are validated and it is understand where the models can truly be predictive, then we can study what SNM observables can be characterized for nonproliferation applications.

ACKNOWLEDGMENTS

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