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Using the MCNP6.2 Correlated Fission Multiplicity Models, CGMF and FREYA

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INTRODUCTION

The culmination of a multi-year, collaborative effort by researchers at Los Alamos National Laboratory (LANL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL) and the University of Michigan, led to the delivery of two new correlated fission multiplicity models available within the latest release of [1]MCNP® version 6.2 [1]. The needs within the nuclear nonproliferation community, particularly in simulating and predicting the neutron and gamma-ray signatures of special nuclear materials (SNM), provided the motivation for this major collaborative effort. From LANL, the CGMF code [2] has been implemented as an upgrade to the original Cascading Gamma-ray Multiplicity (CGM) code [3]. Additionally, the LLNL Fission Library [4] has been upgraded from the original implementation released in prior versions of MCNP6/X to include the LBNL/LLNL Fission Reaction Event Yield Algorithm (FREYA) code [5]. Both new codes are capable of simulating fission events with correlated neutron and gamma-ray emissions.

Due to the release of these new models within MCNP6.2, the purpose of this paper is to describe the differences between these new models and existing capabilities, demonstrate their use in the context of simulation inputs and outputs, and to discuss some of the ongoing work directed toward the next generation of these features.

BACKGROUND

The latest release of MCNP6.2 not only includes the two new correlated fission multiplicity models, CGMF and FREYA, but it also includes fission multiplicity options dating back to many of the previous releases, including MCNP6.1.1 [6]. Briefly, starting with the default and most basic fission multiplicity treatments in MCNP while building up to the newest fission models, the various prompt fission secondary neutron and gamma-ray treatments are reviewed in the following sections.

[1]MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Los Alamos National Security, LLC, manager and operator of Los Alamos National Laboratory. Any third party use of such registered marks should be properly attributed to Los Alamos National Security, LLC, including the use of the designation as appropriate. For the purposes of visual clarity, the registered trademark symbol is assumed for all references to MCNP within the remainder of this paper.

Bounded Integer Sampling

By default in MCNP, the well-known bounded integer sampling scheme is employed to simulate secondary neutrons emitted from fission reactions. Essentially, given the average number of neutrons emitted in fission, $\bar{\nu}$, when a fission event occurs the number of neutrons emitted is either the largest integer number below $\bar{\nu}$ or one integer larger, where the probabilities of selecting these two integers are chosen to preserve the expected value of $\bar{\nu}$. By preserving the expected number of fission neutrons, the expected values of flux, reactions rates, k_{eff}, etc. are unbiased, but if the objective is to analyze the event-by-event nature of these reactions (e.g. simulation of neutron multiplicity counters) the microscopic behavior of the fission reaction is needed.

Neutron Multiplicity Sampling with `FMULT`

In the release of MCNP6, the capabilities in both MCNP5 and MCNPX were merged leading to the expansion of the `FMULT` input card specifically meant to give users the ability to select various fission multiplicity treatments. On this card, many options exist in order to specify both spontaneous and neutron-induced fission neutron multiplicity distributions, $P(\nu_n)$. In the case that the suggested sampling algorithm or data in the literature is desired (e.g. in Ref. [7]), the `METHOD`, `DATA` and `SHIFT` keywords on the `FMULT` card can be used.

While the `FMULT` input card does offer flexibility in simulating spontaneous and neutron-induced prompt fission neutron multiplicities, it is limited in its use in applications where the possibility of fission neutron angular and energy correlations have a negligible impact, and where fission gamma rays are unimportant or not measured.

LLNL Fission Library

In order to address a few of the standard `FMULT` deficiencies, the LLNL Fission Library was implemented in the MCNPX code and included in the recent releases of MCNP6. Within this version of the LLNL Fission Library, the neutron multiplicity distributions were taken from the literature (similar to the `FMULT` data) while the neutron energy spectra are based on the analytical Watt spectrum evaluations which differ for the major actinides within the ENDF/B-VII.1 nuclear data library, released with MCNP.

With the LLNL Fission Library, one of the primary issues in the FMULT treatment was addressed: the inclusion of gamma-ray multiplicity emission for fission events. Using the FMULT METHOD=5 input card turns on the LLNL Fission Library. For spontaneous and neutron-induced fission (as well as photofission, not discussed here), the gamma-ray multiplicity is included when running a neutron and photon problem. Note that prior to the inclusion of the LLNL Fission Library, all photons produced from all neutron reaction channels were sampled prior to the selection of the neutron reaction, meaning that gamma rays could not be correlated with specific neutron reactions actually taking place in the simulation.

In the following two sections discussing FREYA and CGMF, the issues with missing event-by-event energy, angular and particle correlations are resolved with the explicit Monte Carlo modeling of the fission process. Note that if the LLNL Fission Library cannot perform the calculation for some isotope in an MCNP simulation, then the default FMULT parameters and algorithms are used to simulate the neutron multiplicity of that particular event.

FREYA

In the latest released of MCNP6.2, the newest fission event generators are considered to be significant improvements over the simple neutron and gamma-ray multiplicity treatments discussed previously. One of the two new fission event generators is the FREYA code. This code is implemented through the LLNL Fission Library version 2.0.1 and can be accessed in an MCNP6.2 calculation with the FMULT METHOD=6 input card. It is important to note that FREYA is currently under active development, therefore the isotopes for which FREYA can simulate prompt fission neutron and gamma-ray emissions is just a subset of the total number of isotopes that the LLNL Fission Library can currently handle.

Currently, the FREYA code can handle the spontaneous fission of ^{238}U, ^{238,240,242}Pu, ^{244}Cm and ^{252}Cf, and the neutron-induced fission (up to 20 MeV incident neutron energy) of ^{233,235,238}U and ^{239,241}Pu. When one of these events takes place, the FREYA code samples for the initial conditions of the fully accelerated fission fragments and then uses a Monte Carlo Weisskopf approach to simulate the de-excitation of the fission fragments. This de-excitation process is simulated by emitting neutrons only at first until the residual excitation energy in the fission fragment falls below a particular threshold. Then, after all neutrons have been emitted, the simulation concludes by emitting the gamma rays from the remainder of the residual energy. These simulated neutrons and gamma rays are then put into the MCNP secondary particle bank and tracked through the problem as usual, using the fission event location, time and weight, and the FREYA simulated energy and direction for these secondary particles.

In the MCNP6.2 implementation, if a fissioning isotope is selected for which FREYA cannot perform the simulation, the LLNL Fission Library default options will perform the simulation.

CGMF

The second of the two new fission event generators included in MCNP6.2 is an upgrade to the LANL CGM code capability, the CGMF code (CGM+Fission). To access this option, the FMULT METHOD=7 input card is needed. However, this option only enables the neutron and gamma-ray multiplicity modeling from fission events. In order to model secondary multiplicities from all nonelastic and fission reactions, the 9^{th} entry on the PHYS:N card should be set to 2, turning on the CGM option. When CGM is enabled, the CGMF code is used for all fission reactions by default. Note that in the previous release of MCNP6.1.1, the LLNL Fission Library was used as the default for all fission reactions when CGM was enabled, but this is not the case in the release of MCNP6.2.

For all intents and purposes, the initial fission fragment conditions are sampled in CGMF from the same yield data that are used in FREYA. Therefore, the primary difference between these models comes from the nuclear physics theory. CGMF performs the simulations of the decay of the excited fission fragments using the Hauser-Feshbach statistical theory of nuclear reactions, where competition between the neutron and gamma-ray emission at each step of the simulation is one of the primary differences between the CGMF and FREYA codes. As a result of this difference in the selection of nuclear fission theory and due to the algorithms chosen in its implementation, CGMF suffers from a significant increase in computational cost compared to FREYA with orders of magnitude differences expected in simulation times using the two models.

Similar to FREYA, CGMF is limited to the simulation of the spontaneous fission of ^{240,242}Pu and ^{252}Cf, and the neutron-induced fission of ^{235,238}U and ^{239}Pu. Therefore, if an isotope is selected in the MCNP6.2 simulation for which CGMF cannot handle, the default LLNL Fission Library is used to produce the secondary neutron and gamma rays.

NUMERICAL RESULTS

All of the following MCNP6.2 numerical results have been computed using the list-mode or PTRAC output format. Using mcnptools [8], now distributed with MCNP6.2, parsing the PTRAC output is straightforward to obtain many quantities of interest.

Secondary Particles from Fission

The average values for the neutron and gamma-ray number and energy listed in Table 1 have been generated using the default MCNP6.2 behavior (bounded integer sampling), the `FMULT` method using Lestone's data [7], the LLNL Fission Library, FREYA and CGMF. While the results from the n(1.0273 MeV)+^{239}Pu fission reaction is shown here, many other fission reactions have been compared in the same way.

Model	$\bar{\nu}_n$	$\bar{\chi}_n$	$\bar{\nu}_\gamma$	$\bar{\chi}_\gamma$
Default	3.0126(1)	2.139(1)	*	*
FMULT	3.012(1)	2.137(1)	*	*
LLNL	3.014(1)	2.036(1)	7.307(3)	0.8985(3)
FREYA	3.012(1)	2.153(1)	6.876(2)	1.0098(4)
CGMF	3.048(1)	2.033(1)	7.905(3)	0.9293(3)

Table 1. The average multiplicity, $\bar{\nu}$, and energy, $\bar{\chi}$, in MeV of secondary neutrons and gamma rays for several MCNP6.2 options for the n(1.0273 MeV)+^{239}Pu fission reaction. Note the parenthesis indicate the standard deviation and * indicates that fission-specific gamma rays are not available in the simulation.

In Figure 1, both the neutron multiplicity probability density, $P(\nu_n)$, and the average gamma-ray multiplicity, $\bar{\nu}_\gamma$ are shown as a function of the neutron multiplicity number. From these results it is obvious to see that the bounded integer sampling scheme compared to the `FMULT` method preserves the average neutron multiplicity (see $\bar{\nu}_n$ in Table 1) as expected. The negative slope of the average gamma-ray multiplicity as a function of neutron multiplicity is an interesting result that is predicted by both FREYA and CGMF. The LLNL Fission Library fission gamma-ray production is independent of the neutron production shown by the flat slope of the dashed blue line. While the simulation of the fission-specific gamma-rays varies significantly between the MCNP6.2 options, the neutron-neutron angular correlations predicted by FREYA and CGMF may be just as important in identifying SNM in real-world applications.

Correlated Proton Recoils in a Detector Array

Experimental work that would be interesting to use in the validation of the correlated fission multiplicity models generally include arrays of detectors used for coincidence counting. One example of this type of experiment is the NEUANCE detector array [9] setup at LANL. In Figure 2, a simplified MCNP model includes 21 stilbene detectors arranged in a cylindrical array. At the very center of this basic model is a small ^{252}Cf source. This source

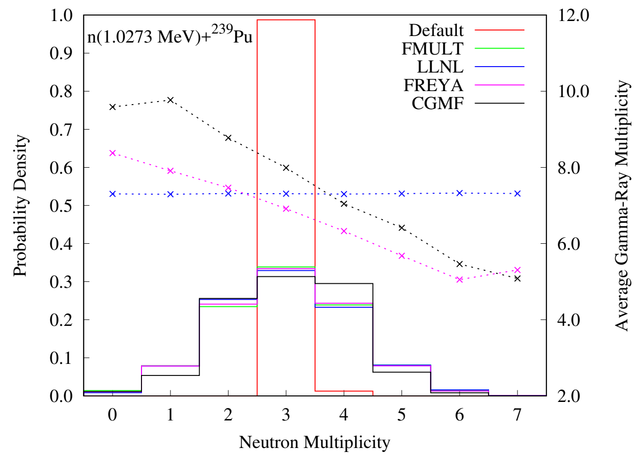

Fig. 1. The prompt fission neutron multiplicity distribution, $P(\nu_n)$ (solid histogram, left axis), and the average gamma-ray multiplicity, $\bar{\nu}_\gamma$ (dashed line, right axis), as a function of the neutron multiplicity.

was simulated in MCNP6.2 while tabulating list-mode data with CGMF as the spontaneous fission event generator. In the list-mode output, the position and the energy of recoiled protons within each stilbene detector is recorded. On an event-by-event basis, in Figure 3 the CGMF predicted neutron-neutron angular correlations are compared against the proton recoil angular correlations observed in the detectors with and without an energy cutoff of 300 keV. Note that no corrections regarding specific detector responses have been made during the analysis of this data.

Also from Figure 3, the amount of crosstalk between detectors can be crudely estimated by studying the shapes

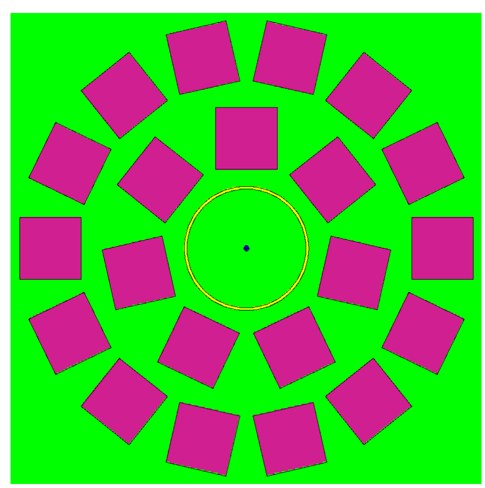

Fig. 2. A mocked-up model of NEUANCE, an array of stilbene detectors (in magenta), with a ^{252}Cf spontaneous fission source at the center.

of these curves. In magenta, the neutron-neutron angular correlations predicted by CGMF are shown. From the same MCNP6.2 simulation, in blue and red are the proton recoil angular correlations with and without proton recoil energy cutoff above 300 keV, respectively. With the energy cutoff, the agreement between the source and the recoiled protons is slightly improved, but significant crosstalk can still be observed in the forward direction, $cos(\theta) \approx 1$.

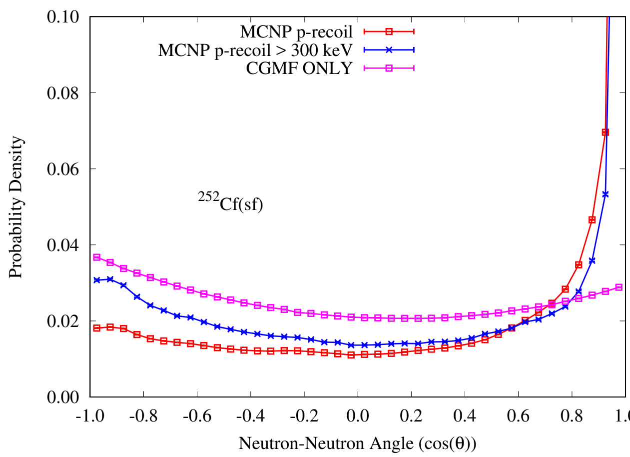

Fig. 3. The neutron-neutron angular correlations observed in the detector array simulation using CGMF. Lines labeled "MCNP p-recoil" correspond to observed proton recoils in the detectors and "CGMF ONLY" corresponds to the observed spontaneous fission neutron source directions.

The next step in comparing the simulated data to real measured data is to model the detectors as realistically as possible to simulate all aspects of the detector response. To this end, the DRiFT tool [10], distributed with MCNP6.2, will be used to analyze the MCNP output to build the appropriate detector responses for comparison to experimental data.

SUMMARY AND CONCLUSIONS

Two new correlated fission multiplicity models, FREYA and CGMF, are now included and available in MCNP6.2. While some of the observables from these models can differ due to the subtle differences of their approach to the Monte Carlo simulation of neutron and gamma-ray emission from excited fission fragments, these new features provide users with the ability to simulate an entire new class of experiments with MCNP6.2. Other multiplicity methods, primarily employed for neutron multiplicity emission from fission, have been discussed in this paper alongside the newest multiplicity models to help guide the user in which models best suit their use in various applications. A couple of simple simulation examples have provided numerical evidence of some of the new nuclear fission physics features and their predictions.

The next steps in understanding these new models is to apply them to real-world experimental configurations and perform a detailed analysis of the difference between the measurements and predictions. This could include setting up a detailed MCNP6.2 model of an experiment, like NEUANCE, running the simulation with multiple neutron and gamma-ray multiplicity models, collecting the list-mode results and then processing the results through a proper detector response function, like DRiFT, to obtain simulated results which can be directly compared to experimentally processed results. With the new FREYA and CGMF models available within MCNP6.2 and the post-processing capabilities in mcnptools and DRiFT, now distributed as utility programs with MCNP6.2, a new pathway is now available to make this type of effort tractable. And as part of a continuation of this nuclear nonproliferation collaboration, one of the primary goals is to provide this kind of detailed validation of the new simulation tools and capabilities in order to deliver the next generation of correlated multiplicity simulation capabilities to MCNP6 users.

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