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Author(s): Wilcox, Trevor
McKinney, Gregg W.
Kawano, Toshihiko

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MCNP6 Gets Correlated with CGM 3.4

T. A. Wilcox, G. W. McKinney, and T. Kawano

Los Alamos National Laboratory, Bikini Atoll Rd. P.O. Box 1663, MS-C921, Los Alamos, NM 87545
 wilcox@lanl.gov, gwm@lanl.gov, kawano@lanl.gov

INTRODUCTION

Version 3.4 of the Cascading Gamma-ray Multiplicity (CGM) code has been integrated into version 6 of the Monte Carlo radiation transport code MCNP. The current release is MCNP6 which is the merger of MCNPX 2.7.0 and MCNP5. MCNP6 [1] is a general purpose Monte Carlo radiation transport code that can transport 34 different particles and heavy ions. CGM was originally integrated into MCNPX 2.7.0 as an undocumented feature, but was never released to the public. With the integration of CGM into MCNP6 the code now has the capability of producing correlated secondary particle/gamma emissions [2] and should be available in future release of MCNP. Before the integration of CGM, MCNP only used libraries that contain the total multiplicity but not the multiplicity distribution or the correlations. Lacking this information requires the code to use integer sampling to determine the multiplicity. In the example of thermal neutron capture on Cl-35, presented in the results section, MCNP does integer sampling. The means MCNP would produce one gamma 17% of the time and two gammas 82% giving a mean multiplicity of 1.83. Using CGM, MCNP can now produce a spectrum of multiplicities.

DESCRIPTION OF ACTUAL WORK

For neutron interactions MCNP determines the reaction and calculates the excitation energy and passes the isotope atomic number, mass number, and excitation energy to CGM through an interface routine (CGM_INTERFACE). The excitation energy is calculated as follows

$$E_x = \frac{A_1}{A_1 + m_1} Elab_1 - \frac{A_2}{A_2 + m_2} Elab_2 - \frac{A_3}{A_3 + m_3} Elab_3 + Q \quad (1)$$

where

$Elab_1$ = Incident particle energy in lab system

$Elab_2$ = First secondary particle energy in lab system

$Elab_3$ = Second secondary particle energy in lab system

A_1 = Target nucleus mass

A_2 = Residual nucleus mass after emission of first secondary particle

A_3 = Residual nucleus mass after emission of second secondary particle

m_1 = Incident particle mass

m_2 = First secondary particle mass

m_3 = Second secondary particle mass

Q = Reaction Q value

CGM then creates a distribution of spin and parity states and statistically samples the de-excitation levels to produce the correlated secondary gammas. The energies and the production probabilities of these gamma-rays are calculated by a combination of the gamma-ray strength function and the level density of the nucleus based on the statistical Hauser-Feshbach theory [3]. The gamma energies are passed back to CGM_INTERFACE and are emitted isotropically. CGM does calculate the angular emission of the gammas, but this is currently not implemented in MCNP6. CGM requires two data files, KCKSYST.DAT and RIPL-3.DAT, to calculate the gammas. The data file KCKSYST.DAT contains the level density systematic, and RIPL-3.DAT (Reference Input Parameter Library) contains data pertaining to branching ratios, spins, parities, discrete level schemes, etc. [4]. If the model-physics feature is turned on for a particular isotope, CGM is not called. The LLNL library [5] LLNLGAM is called by default to process fission reactions and produce prompt fission neutrons and gammas. CGM is invoked by setting the 8th entry on the PHYS:n card to 2.

RESULTS

Two test cases will be presented to highlight gamma multiplicity. Both cases are thermal neutrons incident on a small sphere of Cl-35 and Ni-61. The first-collision-only treatment was used to force all source particles to collide in the sphere and all progeny to escape without

further interaction [1]. This treatment allows for the current tally to only record prompt gammas created from the initial neutron interaction.

The resulting gamma spectrum for neutron capture on Cl-35 is shown in Figure 1. The blue dashed line is the spectrum generated using the ACE (A Compact ENDF, ACE here refers to ENDF/B VII.0 neutron and proton libraries and ENDF/B VI.0 photon libraries with new Thompson scattering form factors) libraries and the solid black line is the spectrum from CGM.

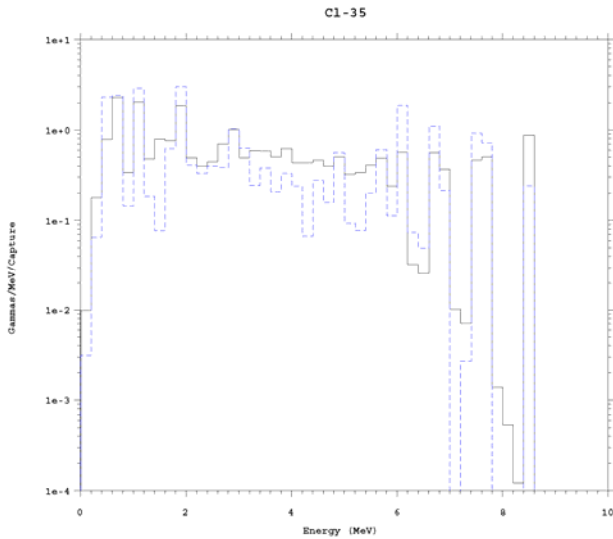


Fig. 1. Prompt gamma spectrum for thermal neutrons on Cl-35

The multiplicity plots were created using a pulse-height special tally feature (FT PHL). The F8 tally with the FT PHL option uses an F1 tally (second entry on the ft8) in combination with energy bins. The energy bins denote the multiplicity bins. It should be noted that collisions that produce no gammas are not recorded using this method. One could take the tally data from the output file and add in the zero gamma data (print table 160) to create a multiplicity plot that includes the zero gamma multiplicity. Using a F1 tally in the FT8 PHL option is currently a fatal error and requires the MCNP6 “fatal” option on execution.

```
f11:p 1
f8:p 1
ft8 PHL 1 11 1 0
e8 0 0.5 1.5 2.5 3.5 4.5 5.5 6.5 7.5 8.5 9.5 10.5
```

From the summary table in the output file, CGM produced 2.6 gammas per capture and ACE produced 2.7 gammas per capture. The gamma multiplicity is shown in Figure 2. For ACE, 100% of the collisions produced gammas with a gamma multiplicity of one 17% of the time and two 82% of the time, giving a mean value of

1.83. For CGM approximately 32% of the collisions were elastic scatter, producing no gammas. The other 68% of the collisions produced a mean value of 2.6 gammas.

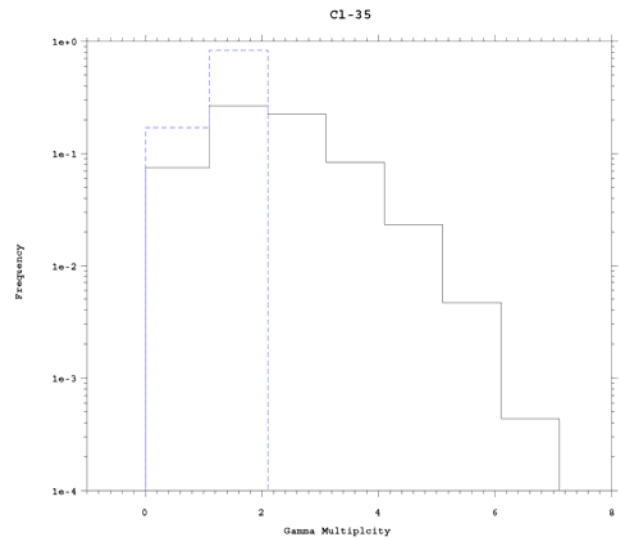


Fig. 2. CGM and ACE gamma multiplicities for thermal neutrons on Cl-35

The CGM and ACE prompt gamma spectra for thermal neutrons on Ni-61 are shown in Figure 3. ACE produced 3.32 gammas per capture and CGM produced 2.86 gammas per capture. The gamma multiplicity for CGM and ACE can be seen in Figure 4. For CGM approximately 81% of the collisions were elastic scatter, producing no gammas. The other 19% of the collisions produced a mean value of 3.57 gammas. For ACE 20% of the collisions produce no gammas and 80% create one gamma.

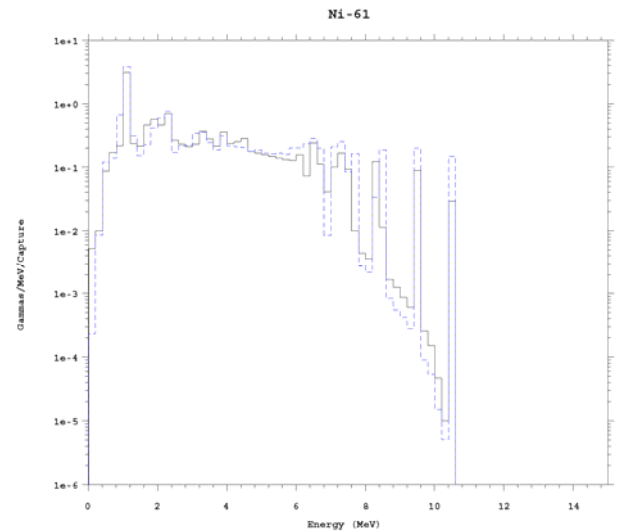


Fig. 3. Prompt gamma spectrum for thermal neutrons on Ni-61

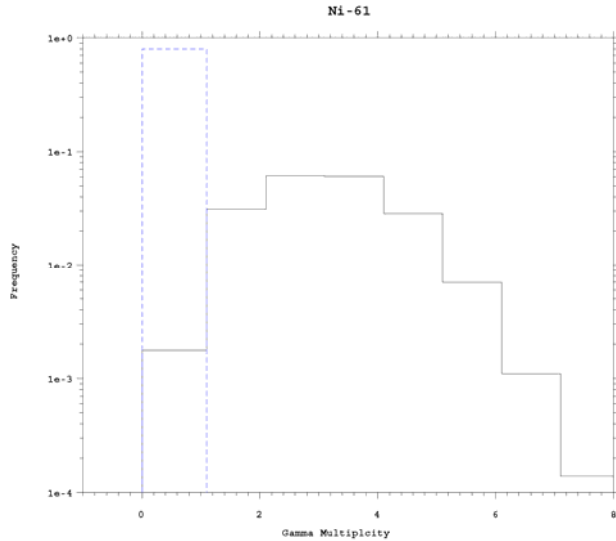


Fig. 4. CGM and ACE gamma multiplicities for thermal neutrons on Ni-61

CONCLUSION

The use of CGM has several advantages over the use of ACE data libraries in MCNP6; 1) it has correlated gamma production and 2) it produces a distribution of gamma multiplicities per interaction, whereas ACE produces an average between two integer multiplicities 3) it is a theoretical model that may predict experimentally unmeasured physical quantities that may not be in experimental based data libraries. CGM conserves energy and angular momentum internally to CGM; however, angular emission information is not currently sent back to MCNP6. Future work will include the integration of correlated neutrons from CGM. Also, the reaction type will be passed to CGM to set the spin and parity for a particular reaction when possible.

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