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Verification of the Pulse Height Tally in MCNP 5

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Abstract

Pulse height tallies are commonly used in Monte Carlo codes to predict detailed measured photon spectra for spectrometry purposes. The pulse height tally is unique among the various tallies in MCNP. Unlike flux or current talliers, which are calculated as soon as the particle exits or collides in the cell, the entire set of tracks for a history must be completed before the pulse height tally can be made. The objective of this work was to verify the pulse height tally and verify the new MCNP 5 variance reduction features with the pulse height tally.

In this paper, we give details to the analytic solution of the pulse height distribution using a modification to Shuttleworth's fictitious elements, report MCNP5 results for the pulse height tally, energy deposited, and current tallies for the problem.

Key words: analytic; benchmark; pulse height; detector; code verification

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1 Introduction

MCNP[1] is a Monte Carlo code used worldwide to model neutron, photon, and electron transport for many different applications. The objective of this work was to verify the pulse height tally in MCNP 5 for photon transport. The pulse height is defined to be the energy entering a cell minus the energy leaving that cell for the entire history for a single incident particle; that is, the total energy deposited in a cell including all progeny created by the initial single source particle. The amount of energy deposited in a cell is the pulse

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height for that history. The pulse height tally in MCNP is analogous to the pulse height seen in a radiation detector. A radiation detector would record the energy deposited by the incident source particle and all of its progeny as a single pulse. A full pulse height spectrum is created when the distribution of the energy deposited by all incident source particles is recorded.

The pulse height tally is unique among the various tallies in MCNP. Unlike other tallies which are calculated as soon as the particle exits or collides in the cell, the pulse height tally requires the entire set of tracks for a history must be completed. This requires detailed bookkeeping by a Monte Carlo code where variance reduction is used to reduce uncertainty in Monte Carlo results.

Verification of the computational algorithms in MCNP are required to satisfy the numerous software quality assurance requirements. One approach to code verification is to compare the calculated results produced by the code for a problem with a known analytic solution with its associated verification data[4]. One difficulty with this type of code verification is that even simple transport problems involve complex physical laws and are difficult to solve analytically. Usually the physics, data, and geometry have to be simplified simultaneously to obtain analytic solutions.

Shuttleworth[2] has cleverly devised a set of fictitious elements with greatly simplified physical interaction mechanisms for the verification of MCBEND[3], a British radiation transport code. His verification problems make use of the fictitious elements with a simple geometry that is continuous in space and discrete in energy and angle. Shuttleworth has included some analytic results for the pulse height tally, energy deposited, and flux using his unique set of elements. We use these fictitious elements to verify a few types of tallies in MCNP. In this work, we show the analytic solution to the pulse height distribution and report MCNP 5 results for the pulse height tally, energy deposited, and current tallies for the problem. Many other tallies can be analytically verified using these fictitious elements but are not done here.

2 Problem Definition

The verification problem defined by Shuttleworth consists of a cylinder made with three fictitious elements, each with the total macroscopic cross section of 1.0 cm^{-1}. The elements and their physical interaction mechanisms are defined as:

- Moron, atom fraction 0.2 At all energies, a collision with this nuclide absorbs the incident particle.

- Odium, atom fraction 0.3 At all energies, a collision with this nuclide produces one secondary particle that has half the energy of the incident particle. The secondary particle is not deflected.
- Kneeon, atom fraction 0.5 At all energies, a collision with this nuclide produces two secondary particles, each having one quarter of the energy of the incident particle. At, or above an incident energy of 1.0 MeV, one particle is scattered forwards and one particle is scattered through 90. Below 1.0 MeV, both particles are scattered forwards.

These three nuclides represent the photon physical interactions of photoelectric absorption (Moron), Compton scatter (Odium), and pair production (Kneeon).

The cylinder that makes up the problem is actually divided into an insensitive region followed by an active region. Each region is a cylinder of length ln(2) and radius ln(2), as shown in Figure 1. The source particles start on the cylinder axis at 0. The particles passing through the material are directed along the cylinder axis, and have an initial energy of 3.2 MeV. All particles are absorbed at 0.15 MeV or below. With this simplified problem, we can analytically determine the probability of each possible pulse height for 1, 2, or any combination of regions. The probabilities for axial and radial escape binned by energy, as well as the number of collisions that occurred in the cell are also easily calculated.

A pulse is generated by the energy deposited in either region by a single particle history. A distribution is accumulated with more and more incident source particles. Normalizing this distribution to the total number of source particles generates a probability for each amount of energy deposited. The pulse height tally, or F8 tally as it is referred to in MCNP, is unique among tallies in that it must follow the entire track of the particle before energy data can be recorded. MCNP sums this tally by adding any energy that enters the cell and subtracting any energy leaving the cell. This creates extra bookkeeping where variance reduction is used, changing the weight of a particle in mid-path.

3 The Analytic Solution

Given these simplified interaction mechanisms, the probabilities of all possible interactions can be analytically derived. The derivation begins with examining the probability of a single collision in a material between points a and b:

$$\int_b^a \exp(-\Sigma x)\Sigma dx = \exp[-\Sigma(b-a)] \tag{1}$$

where $\exp(-\Sigma x)$ is the probability of travelling a distance x without collision, and Σdx is the probability of having a collision in dx.

We can use Eqn. 1 to examine the case of two collisions at points a and b followed by an escape, as shown in Figure 2. We get the probability of escaping with one collision between points a and L as:

$$\begin{aligned} \int_L^a \exp\left[-\Sigma(b-a)\right]\exp\left[-\Sigma(L-b)\right]\Sigma db &= \Sigma\exp\left[-\Sigma(L-a)\right]\int_L^a db \\ &= \Sigma\exp\left[-\Sigma(L-a)\right](L-a) \end{aligned}$$

where $\exp[-\Sigma(b-a)]$ is the probability of no collision between a and b, Σdb is the probability of collision in db, and $\exp[-\Sigma(L-b)]$ is the probability of no collision after b.

Similarly, the probability of reaching point L with two collisions between 0 and L becomes:

$$\begin{aligned} \int_0^L \exp\left[-\Sigma a\right]\left[\Sigma\exp\left[-\Sigma(L-a)\right](L-a)\right]\Sigma da &= \Sigma^2\exp\left[-\Sigma L\right]\int_0^L (L-a)da \\ &= \Sigma^2\exp\left[-\Sigma L\right]\frac{L^2}{2} \end{aligned}$$

where $\exp[-\Sigma a]$ is the probability of no collision between *0* and a, and Σda is the probability of collision in da.

Figure 3 gives an example track in a single region. This track deposites 2.8 MeV in the cell. The pulse height of the example history for the two specific axial collisions and one specific radial collision with Σ=1 is:

$$\begin{aligned} P &= \frac{(0.5)(0.3)e^{-\ln 2}(\ln 2)^2}{2}\left[(0.2)(1-e^{-\ln 2})\right] \\ P &= 0.0018017 \end{aligned}$$

The probablities for all 110 possible tracks for a single region can be calculated using this procedure.

4 Generation and Comparison of Analytic Results

A computer code was written to directly calculate the analytic solution for all possible tracks. The analytic code consisted of recursive subroutine calls indexing over all possible particle collisions. The code calculated the collisional probability distribution, energy deposited, and the axial and radial escape energy distribution. The second region uses the axial leakage from the first region as an initial source spectrum. The analytic code was verified by comparing with hand calculations, summation of the history probabilities, and with a separate Monte Carlo calculation [5].

The single region problem generates 110 possible particle histories. There are 0 to 7 collisions possible with five discrete energies: 3.2, 1.6, 0.8, 0.4, and 0.2 MeV. Table 1 compares the analytic probabilities of collision. Each method should produce a distribution that sums to unity. Tables 2 and 3 show the axial and radial results and compares with the results from MCNP. Table 4 gives the pulse height distribution for a single region. Tables 5 and 6 gives the probability of collision and pulse height distribution for two detector regions.

5 Summary and Future Pulse Height Tally Verification Work

This paper had described an analytic pulse height verification problem and provided analytic derivations with numerical results. The analytic results have been verified in three ways. Several MCNP tallies have been verified using this analytic solution. The MCNP tally results cover the analytic results the expected fraction of the time. Sixty eight percent of the results are within one standard deviation; ninety five percent of the results are within two standard deviations.

This paper has also described the importance of analytic verification in code development. The simplified interaction mechanisms offers additional possible verification problems. Additional work includes the analytic calculation of the particle flux distribution and comparison with MCNP volume and surface flux tallies. The creation of unique pulses for every collision would clearly identify each particle track. The addition of a backscatter event would add more realism to the simplified physics. Finally, the verification of the unreleased MCNP 5 new pulse height with variance reduction option [6] has not been tested.

Table 1
Comparison of Probability of Collision: hand calculation, Fortran code, Monte Carlo simulation

# collisions	Hand Calculation	Analytic Calculation	Monte Carlo Calculation
0	0.5	0.5	0.500891
1	0.290616	0.29061548	0.2906586
2	0.113617	0.11361796	0.1146971
3	0.066150	0.066150332	0.0642505
4	0.023558	0.023557394	0.0239030
5	0.005213	0.0052131751	0.0054208
6	0.000770	0.00079103928	0.00090978
7	0.000055	0.000054629585	0.00008411
Total	**0.999979**	**1.000000009965**	**1.00081489**

Table 2
Probability of Axial Escape (Current) for Single Region Detector

Energy (MeV)	**MCNP's Result**	**Analytic Probability**
0	0.13460540	
0.2	0.040542254	*0.0652055 err 0.0016
0.4	0.036783283	0.0368315 err 0.0016
0.8	0.18409699	0.184052 err 0.0007
1.6	0.10397208	0.103843 err 0.0009
3.2	0.5	0.500142 err 0.0003
Total	**1.000000007**	**1.0000413**

Table 3
Probability of Radial Escape (Current) for Single Region Detector

Energy (MeV)	**MCNP's Result**	**Analytic Probability**
0	0.77284711	
0.2	0.064652901	*0.0917925 err 0.0013
0.4	0.037500002	0.0374989 err 0.0016
0.8	0.125000000	0.125038 err 0.0008
Total	**1.000000013**	**1.0000004**

Table 4
Pulse Height Distribution for Single Region Detector

Energy (MeV)	**Analytic Probability**	**Monte Carlo Result**	**MCNP's Result**
0	0.500000000	.500013	0.500142 err 0.0003
1.6	0.190615480	.190584	0.190518 err 0.0007
2.0	0.059593688	.0607156	0.0607738 err 0.0012
2.2	0.027446216	.0251430	0.0250999 err 0.0020
2.4	0.067084001	.068621	0.0685586 err 0.0012
2.6	0.010564592	.00999577	0.0100443 err 0.0031
2.8	0.023878481	.0241578	0.0241592 err 0.0020
3.0	0.0060571134	.00574761	0.00578880 err 0.0041
3.2	0.114760440	.115023	0.114915 err 0.0009
Total	**1.0000000114**	**1.00000078**	**0.9999996**

Table 5
Probability of Collision for Two Region Detector: Analytic Results

# collisions	**Analytic Calculation**
0	0.5000001400
1	0.3394592670
2	0.1014569285
3	0.0435443903
4	0.0124861873
5	0.0026305025
6	0.0003955194
7	0.0000273148
Total	**1.0000002498**

Table 6
Pulse Height Distribution for Two Region Detector

Energy (MeV)	**Analytic Probability**	**MCNP's Result**
0.0	*0.561166189	0.561293 err 0.0004
0.2	0.0240955759	0.0238154 err 0.0020
0.4	*0.061957400	0.0629887 err 0.0012
0.6	0.0215683040	0.0196861 err 0.0022
0.8	0.0490454497	0.0500114 err 0.0014
1.0	0.0028098961	0.00279270 err 0.0060
1.2	0.0129718688	0.0129966 err 0.0028
1.4	0.0022677653	0.00217200 err 0.0068
1.6	0.1094255676	0.109602 err 0.0009
2.0	0.0297968460	0.0303551 err 0.0018
2.2	0.0137231110	0.0125378 err 0.0028
2.4	0.0335420060	0.0343277 err 0.0017
2.6	0.0052822959	0.00499650 err 0.0045
2.8	0.0119392397	0.0120529 err 0.0029
3.0	0.0030285574	0.00287250 err 0.0059
3.2	0.0573802425	0.0574987 err 0.0013
Total	**1.0000003151**	**0.9999991**

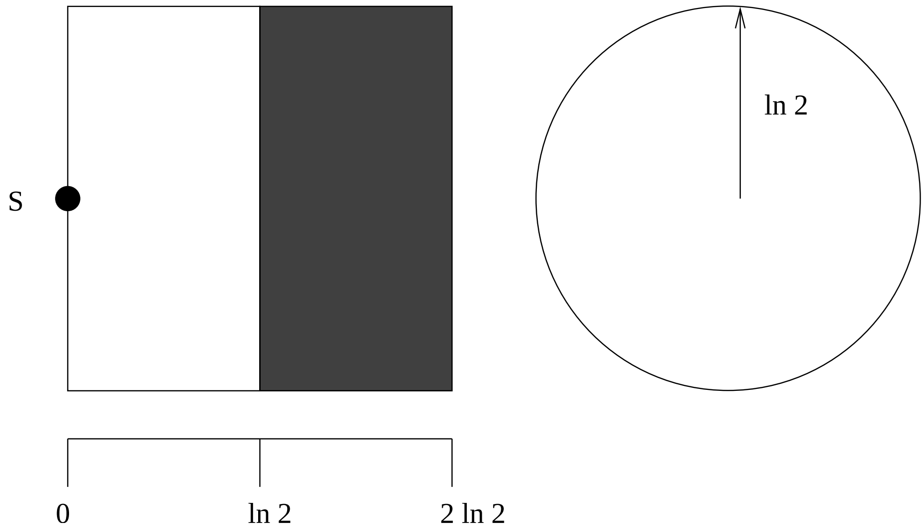

Fig. 1. Problem geometry

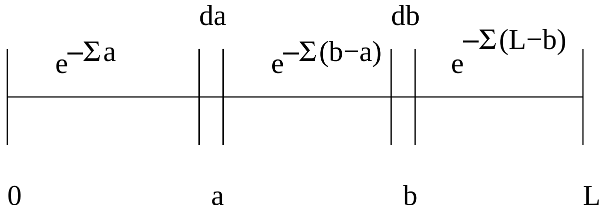

Fig. 2. Analytic solution

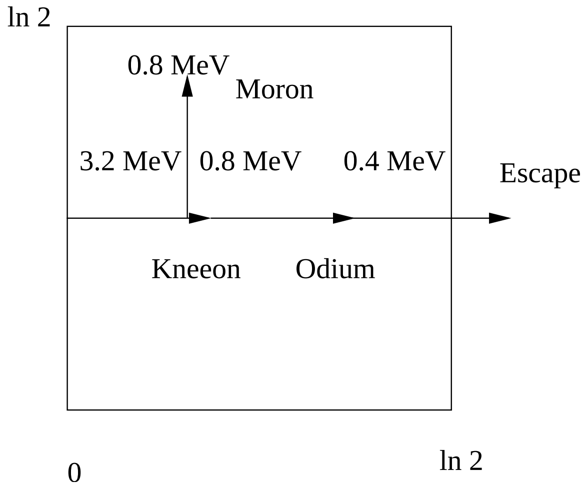

Fig. 3. Example History

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