A Monte Carlo Model for Gamma-Ray Klein-Nishina Scattering Probabilities to Finite Detectors

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This report introduces the Monte Carlo simulating processes for gamma-ray Klein-Nishina scattering probabilities to finite detectors and a few modifications for producing photon mode and gamma production data from the neutron collision. Those approaches have been used in MCNP code. The calculation results are given according to the primary continuous photons, the line photons and the Compton photons, respectively. The results are compared with that of MCNP code. It indicates that the approach is valid and efficient for deep-penetration problems.

KEYWORDS: Monte Carlo method, finite detectors, gamma-ray Klein-Nishina scattering, producing photon mode, primary continuous photons, line photons, Compton photons

I. INTRODUCTION

The Collision Estimator and Track Length Estimator are the common methods in the traditional Monte Carlo calculation of finite detector responses. The former tallies only when the particle collision happens inside the detector, and the later tallies only when the particle trace crosses the detector. The efficiency of the track length estimator is higher than that of the collision estimator (MCNP code uses the Track Length Estimator(4)). However the tallying rates of two estimators are respectively lower for deep-penetration problems of small size detected regions. The statistical estimator is one of the most effective variance reduction techniques in the Monte Carlo calculation of finite detector responses. It is different from the mentioned two estimators in tallying; it can tally in every scattering except the scattering happens inside the detector because the estimation has been already taken into account prior to this particle scattering. This technique can be used for the various neutron or γ-ray scatters. At present the statistical estimator about the γ-ray Klein-Nishina(K-N) scattering, which is thought the most complex in all neutron and γ-ray scatters, has been considered in our code. It involves the calculation of the probability of the photon to be detected after Compton scattering. Due to this probability being very complex, we try to use the Monte Carlo method to simulate the probability in accordance with the thought of Shyu(2) and put this method into MCNP code. In addition, the Gamma Production Data (GPD) from the neutron collision has been updated in the MCNP code. The secondary γ-ray production uses the Expected Value Technique (EVT)(5). Although the number of the γ-rays increases greatly, it avoids some statistical fluctuations for the γ-ray spectrums. In this paper the sample results are given and discussed for the present technique. The results of three different type problems are compared with that of MCNP code.

II. GENERAL SAMPLING SCHEMES

1. Expected Value Technique (EVT)

Suppose E1, E2, ..., En are n independent, mutually exclusive events with probabilities P1, P2, ..., Pn, respectively, \( \sum P_i = 1 \). Clearly, if a random number \( \xi \in [0, 1) \) is such that

\[ \sum_{i=1}^{k-1} P_i \leq \xi < \sum_{i=1}^{k} P_i, \]

then \( \xi \) determines the event \( E_k \). This random process is referred as direct sampling, inevitably results in some statistical fluctuations.

Assuming the cumulative weight at the present is \( W \), the EVT can be employed by starting n independent random walks from this point with the starting weight

\[ W_i = P_i W, \quad \text{for } i = 1, \ldots, n \]

respectively.

At present, the EVT is primarily used to produce photons from the neutron collision in our work. The secondary γ-rays are produced by their real probabilities

\[ p_{ij} = \frac{\Sigma_{t,i} N_j \sigma_{t,i}}{\Sigma_t}, \]

where \( \sum_{i,j} p_{ij} = 1 \), \( \Sigma_t = \sum_{i,t,i} \), and \( \Sigma_{t,i} = \sum_{j} N_j \sigma_{t,i}^j \)
\( \sigma_{i,j} \) is the microscopic gamma production cross section about the nucleus \( i \) and the reactive channel \( j \) corresponding to the nucleus \( i \), \( \Sigma_t \) and \( \Sigma_{t,i} \) are the neutron macroscopic total cross sections of collision material zone and the nucleus \( i \), respectively, and \( N_j \) is the atomic fraction of the reactive channel \( j \) for the nucleus \( i \).

### 2. Statistical Estimator

It is assumed that the detector is the right cylinder detector (It is also applicable to the sphere detector), where its radius and height are as \( R \) and \( H \), respectively, the major axis vector of the detector is as \( \vec{\Omega}_d = (u_t, v_t, w_t) \) in the Cartesian coordinates (see Fig. 1).

Suppose a photon happens Compton scattering at point \( \vec{r}_p \). The expected value of the unscattered detection probability of a photon is

\[
P(v, \rho) = \frac{1}{\Omega} \int_{\min}^{\max} \int_{\rho_{\min}(v)}^{\rho_{\max}(v)} pc(v, \rho) \exp \left\{ - \sum_{i=1}^{n} \Sigma_t(i)(E(v, \rho)) l_i(v, \rho) \right\} \, dv \, dp,
\]

where \( pc(v, \rho) \) is the probability density function (pdf) of a photon that happens Compton scattering at \( \vec{r}_p \) toward the detector through the angles \( (v, \rho) \) which represents the cosine of the polar angle \( \theta \) and an azimuthal angle \( \phi \) measured from the direction \( \Omega_d \); let

\[
\Omega_D = \int_{\rho_{\min}(v)}^{\rho_{\max}(v)} \int_{\rho_{\min}(v)}^{\rho_{\max}(v)} dv \, dp,
\]

where \( \Omega_D \) is the solid angle subtended by detector response to the scattering point \( \vec{r}_p \), \( \exp \left\{ - \sum_{i=1}^{n} \Sigma_t(i)(E(v, \rho)) l_i(v, \rho) \right\} \) is the probability that the photon is transmitted to the detector at the direction angle \( (v, \rho) \) without collision, with \( \Sigma(t)(E) \) and \( l(v, \rho) \) being the macroscopic total cross section of zone \( i \) and path length through the zone \( i \), respectively and \( n \) is the total number of zones from \( \vec{r}_p \) to the surface of detector.

Firstly, the integral of Eq.(4) requires the determination of the limiting polar and azimuthal angles subtented by detector, then it needs giving out the expression of \( pc(v, \rho) \). The integral limits of Eq.(4) can be determined by Ref.(1). The \( \gamma \)-ray K-N scattering law in angle system \((\mu, \phi)\) has been known as

\[
K(\alpha, \phi) = \frac{2}{\alpha} \frac{(\alpha - \alpha')^2 + \alpha^2 - 2\alpha^2 \alpha'^2}{\alpha'^3}
\]

where \( r_0=2.81794 \times 10^{-13} \) cm is the "classical electron radius";

\[\alpha'=E'/0.511008, \alpha=E/0.511008, \quad E'\text{ and } E \text{ are the incident photon energy and the emit photon energy, respectively.} \]

### Fig. 1 Illustration of the limiting polar and azimuthal angle subtended by a right cylinder detector as measured from \( \Omega_d \)

### Fig. 2 Illustration of the relationship between the two angle systems
Clearly, it is difficult to be integrated analytically for Eq. (4) over both v and p. So it is only solved by numerical methods. In the article of Mickael et al., \( p_C(v, \rho) \) is fitted to a fourth-order polynomial about \( \mu(v, \rho) \), then it is integrated over v and p, respectively. The process is very complex and only successful for \( \alpha \leq 2 \). Here the Monte Carlo method is used to simulate the integral in accordance with the suggestions of Shyu (2).

III. THE MONTE CARLO SIMULATION FOR GAMMA-RAY K-N SCATTERING

Because \( p_C(v, \rho) \) is a pdf about v and \( \rho \), let

\[
c_1 = \int_{v_{\min}}^{v_{\max}} \int_{\rho_{\min}(v)}^{\rho_{\max}(v)} p_C(v, \rho) dv \rho.
\]

Then

\[
p_{\tilde{C}}(v, \rho) = c_1^{-1} p_C(v, \rho),
\]

\( p_{\tilde{C}}(v, \rho) \) is a pdf in \( \Omega_D \). Let

\[
x(v, \rho) = \exp \left\{ -\sum_{i=1}^{n} \frac{\sigma_i E(v, \rho) l_i(v, \rho)}{\mu} \right\}.
\]

The integral of Eq. (4) can be expressed as

\[
P = c_1 \int_{v_{\min}}^{v_{\max}} \int_{\rho_{\min}(v)}^{\rho_{\max}(v)} \bar{p}_C(v, \rho) x(v, \rho) dv \rho
\]

\[
= c_1 E[x(v, \rho)],
\]

where \( E(x) \) expresses the mathematical expectation of \( x \).

By using the Monte Carlo method the Eq.(16) can be approximated to

\[
P \approx c_1 \frac{1}{N} \sum_{k=1}^{N} x(v_k, \rho_k), \quad N \propto \Omega_D,
\]

where \( N \) is the total sample numbers, \( v_k, \rho_k \) are the sample values from the pdf \( p_{\tilde{C}}(v, \rho) \), respectively.

Its relative standard error is

\[
\varepsilon \approx \left\{ \frac{\sum_{k=1}^{N} x^2(v_k, \rho_k)}{\left( \frac{\sum_{k=1}^{N} x(v_k, \rho_k)}{N} \right)^2} - 1 \right\}^{\frac{1}{2}}.
\]

Due to the \( \bar{p}_{\tilde{C}}(v, \rho) \) being also very complex, it is impossible to sample \( v_k, \rho_k \) from \( p_{\tilde{C}}(v, \rho) \) directly. The biasing sample must be used. It means that a pdf \( h(v, \rho) \) with the same domain of definition as \( p_{\tilde{C}}(v, \rho) \) and easy sampling about v, \( \rho \) needs to be instructed. Then the integral of Eq. (4) is changed into

\[
P = \int_{v_{\min}}^{v_{\max}} \int_{\rho_{\min}(v)}^{\rho_{\max}(v)} h(v, \rho) \frac{p_{\tilde{C}}(v, \rho)}{h(v, \rho)} x(v, \rho) dv \rho,
\]

\[
= E \left[ \frac{p_{\tilde{C}}(v, \rho)}{h(v, \rho)} x(v, \rho) \right],
\]

\[
\approx \frac{1}{N} \sum_{k=1}^{N} w_{adj}(v_k, \rho_k) x(v_k, \rho_k), \quad N \propto \Omega_D,
\]

where \( w_{adj}(v_k, \rho_k) = \frac{p_{\tilde{C}}(v_k, \rho_k)}{h(v_k, \rho_k)} \) is the adjusting weight factor and \( v_k, \rho_k \) are the sample values from \( h(v, \rho) \). The biasing pdf \( h(v, \rho) \) is usually taken as

\[
h(v, \rho) = 1/\Omega_D,
\]

obviously, \( h(v, \rho) \) is also a pdf in \( \Omega_D \). The sample values of \( v_k, \rho_k \) are easily given by

\[
v_k = v_{k_{\min}} + \xi_{1_{\min}} (v_{k_{\max}} - v_{k_{\min}}),
\]

\[
\rho_k = \rho_{k_{\min}}(v_k) + \xi_{2_{k_{\min}}} (\rho_{k_{\max}}(v_k) - \rho_{k_{\min}}(v_k)),
\]

\[
k = 1, \cdots, N,
\]

where \( \xi_{1_{\min}}, \xi_{2_{k_{\min}}} \) are the random numbers of the interval \([0,1]\).

Substituting Eq.(21) into Eq.(19), the integral value of Eq.(4) can be obtained approximately.

IV. SAMPLE RESULTS

A few approaches have been applied to MCNP code. The new code is named as STAT. Here we give out three different sample problems. The computer used was the VAX 7610.

In the first problem of the coupled neutron and \( \gamma \)-ray transport, it is a deuterium-tritium (D-T) neutron point source which it locates at \( x=23.4039 \) cm and with energy 14 MeV, the neutrons are biased to emit towards to a TNT sphere where its radius is 3.4039 cm and component is C\(_3\)H\(_6\)N\(_6\)O\(_6\) with a density of 1.816 g/cm\(^3\). The detector is a right cylinder which both its diameter and height are as 7.5 cm and its material consists of iodine-sodium (NaI) with a density of 3.67 g/cm\(^3\) (see Fig. 3), it tallies the currents from the \( \gamma \)-ray. Table 1 shows the comparison of STAT results with MCNP results.

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Figure 4 gives out the spectrums of two codes. The STAT results are given according to the continuous spectrum and the line spectrum, respectively. The MCNP results are summed for all contributions.

In the second problem of the coupled neutron and γ-ray transport, it is a fictitious well-logging mode where the borehole is omitted and the formation consists of limestone (CaCO₃)(65%) and water (H₂O)(35%) with a mixture density of 2.0725 g/cm³. The detector is a right cylinder which both its diameter and height are as 7.62 cm and its material consists of NaI with a density of 3.67 g/cm³. A pulse isotropic neutron source with the energy 14 MeV locates at z=10 cm. The detector tallies the currents from the secondary γ-rays. Table 2 gives out the results.

In the third problem of γ-ray transport, the γ-rays are assumed to have an energy of 5 MeV and scatter isotropically. A sphere with a 100 cm radius is the homogeneous medium of hydrogen(H) with a density 0.5 g/cm³. The detector is a right cylinder which both its diameter and height are as 7.5 cm and its material is also hydrogen. The source locates at the sphere center (See Fig. 6). The results are given in Table 3.

### Table 1 Results of problem 1

<table>
<thead>
<tr>
<th>Primary continuous photons $J_{PC}$</th>
<th>Primary line photons $J_{PL}$</th>
<th>Compton photons $J_C$</th>
<th>Total $J_{TOT}$</th>
<th>Sample No.</th>
<th>Relative error(%)</th>
<th>CPU time (min)</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.80292 - 10</td>
<td>3.32892 - 6</td>
<td>2.18023 - 7</td>
<td>3.5471 - 6</td>
<td>710</td>
<td>1.27</td>
<td>88</td>
<td>STAT</td>
</tr>
<tr>
<td>3.5295 - 6</td>
<td>180000</td>
<td></td>
<td>0.89</td>
<td>88</td>
<td></td>
<td></td>
<td>MCNP</td>
</tr>
</tbody>
</table>

### Figure 3 Illustration of problem 1

### Table 2 Results of problem 2

<table>
<thead>
<tr>
<th>Primary continuous photons $J_{PC}$</th>
<th>Primary line photons $J_{PL}$</th>
<th>Compton photons $J_C$</th>
<th>Total $J_{TOT}$</th>
<th>Sample No.</th>
<th>Relative error(%)</th>
<th>CPU time (min)</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0814 - 10</td>
<td>5.4598 - 6</td>
<td>1.2902 - 5</td>
<td>1.83615 - 5</td>
<td>4070</td>
<td>7.61</td>
<td>500</td>
<td>STAT</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.72778 - 5</td>
<td>1361399</td>
<td>13.1</td>
<td>500</td>
<td>MCNP</td>
</tr>
</tbody>
</table>

### Table 3 Results of problem 3

<table>
<thead>
<tr>
<th>Primary photons $J_P$</th>
<th>Compton photons $J_C$</th>
<th>Total $J_{TOT}$</th>
<th>Sample No.</th>
<th>CPU time (min)</th>
<th>Relative error(%)</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5867 - 3</td>
<td>1.2908 - 3</td>
<td>3.8775 - 3</td>
<td>450</td>
<td>55</td>
<td>12.3</td>
<td>STAT</td>
</tr>
<tr>
<td>3.7237 - 3</td>
<td>6648305</td>
<td></td>
<td>55</td>
<td>0.64</td>
<td></td>
<td>MCNP</td>
</tr>
</tbody>
</table>
V. DISCUSSIONS AND CONCLUSIONS

The results indicate that the results of two codes are almost same in the range of errors. The statistical estimator is proved to be valid for deep-penetration problems of low detective tallying rate from sample problem 2. Its tallying rate is higher than that of the track length estimator of the MCNP code. Due to the results being given according to the primary continuous photons, the primary line photons and the Compton photons, respectively, the γ-ray energy spectrums are more accurate in some degree from sample problem 1. This approach is often applied to analyse the components of some materials, such as the exploration of the hidden exploders. Although the statistical estimator has been proved to be effective in reducing the variance compared to other estimators (e.g., track length estimator), it suffers from the long computing times needed to determine the mentioned probability in every Compton scattering. This disadvantage can be seen from the sample problem 3. So it is not appropriate to non deep-penetration problems.

The other three scattering, which are the isotropic scattering in the Lab system, the isotropic neutron scattering in the center-of-mass (c.m.) system, and the thermal neutron scattering according to the free gas model, are also considered to use the statistical estimator in our present work.

REFERENCES