The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
Chattanooga, Tennessee, April 17–21, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

DIRECT AND ADJOINT SAMPLING OF COHERENT AND INCOHERENT PHOTON SCATTERING

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ABSTRACT

Exact techniques of coherent and incoherent photon scattering sampling in Monte Carlo method are developed. The similar methods are developed for adjoint photon scattering problem. Both approaches are based on direct use of information from evaluated nuclear data files in ENDF-6 format. The computation time for incoherent adjoint sampling is the same that Koblinger's approach needs for the Klein-Nishina distribution.

Key Words: Monte Carlo method, direct and adjoint coherent and incoherent photon scattering sampling

1 INTRODUCTION

At first, we consider the different approaches to the direct incoherent photon sampling and, in particular, the approaches to the Klein-Nishina distribution sampling. Secondly, we consider the approach to the sampling of adjoint incoherent scattering. At last we view the sampling of direct and adjoint coherent photon scattering.

2 INCOHERENT SCATTERING SAMPLING

Differential cross-section of incoherent scattering is represented in File 27 of ENDF-6 format files as

$$\frac{d\sigma_{InCoh}}{d\Omega} = S(q,z)\frac{d\sigma_{KN}}{d\Omega},$$

where $\frac{d\sigma_{KN}}{d\Omega}$ is the differential angle of Klein-Nishina (KN) distribution :

$$\frac{d\sigma_{KN}}{d\Omega} = \frac{\pi r_0^2}{2}\frac{\left(1+\cos^2\theta\right)}{\left[1+E(1-\cos\theta)\right]^2}\left\{1+\frac{E^2(1-\cos\theta)^2}{\left(1+\cos^2\theta\right)\left[1+E(1-\cos\theta)\right]}\right\}.$$

Below as a rule we will use the rejection method for the sampling of random values. Hence it is not important to normalize the probability density function to the unity. Omitting the normalization factor we will call further the functions $f_E(E,E'),\ f_\mu(E,\mu),\ f_q(E,q)$ as energy, angle and momentum density functions for the Klein-Nishina distribution. Above we have used the designations : *S(q,z)* – the incoherent scattering function,

$q = \sqrt{(E - E')(E - E' + 2)}$ – the momentum of recoil electron; *E, E'* – photon energies in unit m_0c^2.

Let us settle on the quality behavior of $f_E(E,E'),\ f_\mu(E,\mu),\ f_q(E,q)$ graphs and corresponding incoherent scattering densities that are obtained from multiplication $f(\cdot,\cdot)$ to the *S(q,z)*. All three densities KN (f_μ , f_E , f_q) have necessary behaviors to use the rejection method with linear majorant. But algorithms of rejection method for the different KN-densities have the different effectiveness in terms of useful work (see Table 1). The most effective algorithm is the one based on the energy-form of KN density.

We have another situation for incoherent scattering densities. It is necessary to construct complicated linear majorants to use the rejection method for angle- and energy-form of incoherent scattering distributions (see Figure 1). On the other hand the momentum-form of incoherent density function is monotone increasing function on the whole interval of *q* and its linear majorant is

$$\varphi(q) = qS(q_{\max}, z) \cdot \frac{f_q(E, q_{\max})}{q_{\max}}.$$

In this case

$$f_\mu(E,\mu) = \pi r_0^2 \left(\frac{E'}{E}\right)^2 \left(\frac{E'}{E} + \frac{E}{E'} + \mu^2 - 1\right),$$

$f_\mu(E,\mu)d\mu = f_E(E,E')dE'$ hence $f_E(E,E') = f_\mu(E,\mu)\left|\frac{d\mu}{dE'}\right|$;

$\left|\frac{d\mu}{dE'}\right| = \frac{1}{E'^2}$ and

$$f_E(E,E') = \pi r_0^2 \frac{1}{E^2}\left(\frac{E'}{E} + \frac{E}{E'} + \mu^2 - 1\right) = \pi r_0^2 \frac{1}{E^2}\left[\frac{E'}{E} + \frac{E}{E'} + 2\left(\frac{1}{E} - \frac{1}{E'}\right) + \left(\frac{1}{E} - \frac{1}{E'}\right)^2\right].$$

Finally

$$f_q(E,q) = f_\mu(E,\mu)\left(\frac{1}{E'}\right)^2 \frac{q}{\sqrt{q^2+1}}.$$

According to the formalism of ENDF-6 format LOG-LOG (except for two first points) interpolation scheme should be used to calculate *S(q,z)*

$$S(q) = \alpha_i \cdot q^{\beta_i},\ \ \beta_i = \ln(S_{i+1}/S_i)\cdot \ln^{-1}(q_{i+1}/q_i),\ \ \alpha_i = S_i \cdot q_i^{-\beta_i}.$$

And differential incoherent cross-section is

$$\frac{d\sigma_{InCoh}(E,E',q)}{dq} = S(q,z)\cdot f_q(E,q) = \frac{\pi r_0^2}{E^2}\cdot \alpha_i \cdot q^{\beta_i}\left[\frac{E'}{E} + \frac{E}{E'} + 2\left(\frac{1}{E} - \frac{1}{E'}\right) + \left(\frac{1}{E} - \frac{1}{E'}\right)^2\right]\frac{q}{\sqrt{q^2+1}},$$

where

$$E' = E + 1 - \sqrt{q^2+1}.$$

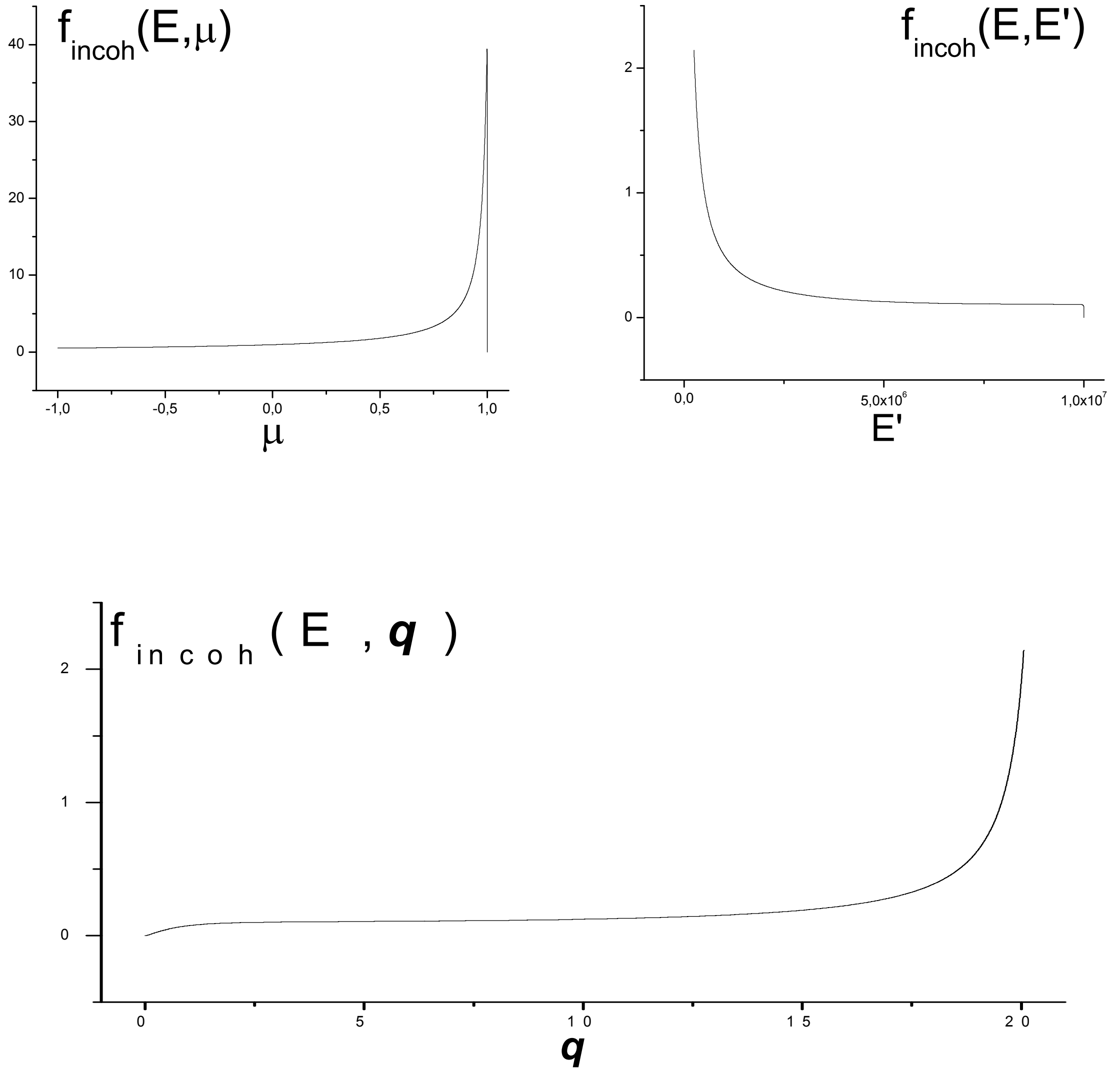

Figure 1. Angle- , Energy- and Momentum-form of incoherent scattering distributions

Table I. Sampling time (rel. unit) for incoherent photon scattering

Energy	Angle form				Energy form				Momentum form			
	KN	H	Fe	Pb	KN	H	Fe	Pb	KN	H	Fe	Pb
10 eV	25	$7.6\cdot10^5$	$1.8\cdot10^6$	$3.8\cdot10^6$	9	$3.7\cdot10^5$	$9.7\cdot10^5$	$3.6\cdot10^6$	10	24	24	24
100 eV	25	$1.8\cdot10^4$	$4.3\cdot10^4$	$9.3\cdot10^4$	9	$1.3\cdot10^4$	$3\cdot10^4$	$6.4\cdot10^4$	17	63	65	64
1 keV	25	224	600	1220	9	152	424	855	14	67	67	66
10 keV	24	46	77	113	9	29	53	79	14	53	62	62
100 keV	25	45	51	55	10	27	34	35	14	48	61	61
1 MeV	36	67	82	83	20	30	40	40	16	54	76	76
10 MeV	106	225	268	273	25	85	106	109	42	155	203	208
20 MeV	168	368	449	452	40	137	173	176	68	253	330	335
50 MeV	336	750	900	901	93	281	352	359	137	510	670	681
100 MeV	591	1300	1561	1599	209	500	620	639	241	910	1180	1209

We can write integrals $\int_{q_i}^{q_{i+1}} \frac{d\sigma_{InCoh}(E,E',q)}{dq}\cdot dq$ in explicit form through special functions after substitution $y=\sqrt{q^2+1}$ that allows using exact algorithms for sampling q. But

$$\sigma_{InCoh}^{(23\,file)}(E) \neq \sigma_{InCoh}^{(27\,file)}(E),$$

and there can be reached difference up to 5%. Hence we have to calculate $\sigma_{InCoh}^{(27\,file)}(E)$ at every E and after this we can sample the interval $[q_i,\ q_{i+1}]$. This approach is unacceptable because of length of calculation time.

2.1 Direct Incoherent Photon Scattering Algorithm

At the first we sample the collision nuclide and (if reaction of incoherent scattering took place) we calculate q_{max} and $f_q(k,q_{max})$ according to the photon energy (note that f is calculated without normalization) :

$$f_m = \frac{q_{\max}^{\beta_i+1}}{\sqrt{q_{\max}^2+1}}\left(1+2E+\frac{1}{1+2E}\right),$$

index i is found from condition $q_{\max}\in[q_i,q_{i+1}]$. If $0 = q_1 < q_{max} \le q_2$ hence $\beta_1 = 1$.

Than we sample random value q using linear probability density function (LPDF) that passes through the points $(0,\ 0)$ and $(q_{max}\ ,\ f_m)$. In this case optimal algorithm for the sampling from LPDF is a very elegant [2]. Let random values γ_1, γ_2 be uniform in (0,1). Let us assume $q=\gamma_1\cdot q_{\max}$ and $\eta=\gamma_2\cdot f_m$. If $\gamma_1 > \gamma_2$ then $q = (1-\gamma_1)q_{max}$, $\eta=(1-\gamma_2)\cdot f_m$ in another case. Value q

is the value of incoherent scattered photon momentum in case of $S(q,z)\cdot f_q(E,q)>\eta$, otherwise the value of q is rejected and we repeat the sampling of q from LPDF. Finally

$$E' = E + 1 - \sqrt{q^2+1} \quad \text{and} \quad \mu = 1 + \frac{1}{E} - \frac{1}{E'}.$$

Some results for nuclides H, Fe and Pb are presented in Table I.

2.2 Adjoint Incoherent Photon Scattering Algorithm

Energy form of probability density function of scattering pseudo-photon is proportional to the function

$$f_E(E,E') = \frac{1}{E^2}\left[\frac{E'}{E} + \frac{E}{E'} + \left(1 + \frac{1}{E} - \frac{1}{E'}\right)^2 - 1\right], \tag{1}$$

where E' is the energy of initial pseudo-photon (it is parameter here), E - energy of scattered pseudo-photon (it is variable here). Cosine of scattering angle is

$$\mu = \cos(\theta) = 1 + \frac{1}{E} - \frac{1}{E'}. \tag{2}$$

We have some difficulties in modeling E from (1) because integral of density function can be equal to infinity. Actually, as $-1 \le \mu$ than $E \le \dfrac{E'}{1-2E'}$. On the other hand $E \ge 0$ and hence

$E' \le E \le \dfrac{E'}{1-2E'}$ when $E' < \dfrac{1}{2}$.

Using (2) and condition $\mu \le +1$ we obtain that $E' \le E$. Hence, in the case $E' \ge \dfrac{1}{2}$ the integral $\int_{E'}^{\infty} f_E(E,E')dE$ is equal to infinity due to the second term in (1). To avoid this difficulty there was proposed to use modified formula $f_E^*(E,E') = \dfrac{E'}{E} f_E(E,E')$ that has finite integral by E in [1]. In that way statistical weight of pseudo-photon must be corrected according to the term $\dfrac{E}{E'}$. But now weight factor can be infinite at $E' \ge \dfrac{1}{2}$. This fact is not important in practice because as it is usual for practical tasks we have the maximum of energy source E_{max} and maximum value of weight term that is equal to $\dfrac{E_{max}}{E'}$.

In case of $E'<\frac{1}{2}$ the sampling of energy of scattering pseudo-photon is realized by inverse function methods.

From effectiveness point of view this approach is not the best as the a lot of calculation time is needed. So we proposed the new algorithm for sampling the adjoint incoherent scattering density of pseudo-photon.

Let us get from the formula (1) the angle-form density of pseudo-photon scattering :

$$f_{\mu}(\mu,E')=f_{E}(E,E')\left|\frac{dE}{d\mu}\right| ,$$

where $\left|\frac{dE}{d\mu}\right|=\left[\frac{E'}{1-E'(1-\mu)}\right]^2=E^2$.

Hence

$$f_{\mu}(\mu,E')=\left[\mu^2+\frac{1}{1-E'(1-\mu)}-E'(1-\mu)\right] . \qquad (3)$$

Integration limits of (3) are following :

$\mu\in[-1,1]$ when $E'<\frac{1}{2}$ and $E\in[E',\infty]\Rightarrow\mu\in\left[1-\frac{1}{E'};\ 1\right]$ in another case due to (2).

As we can see the expression (3) is finite at all values of μ when $E'<\frac{1}{2}$. But we have peculiarity when $E'\geq\frac{1}{2}$ at the point $\mu=1-\frac{1}{E'}$ due to denominator of (5). As the case of (1) in this point function (3) is infinite.

Let us get to the density $f_x(x,E')$ using substitute $x=1-E'(1-\mu)$. At that time

$$f_x(x,E')=\frac{1}{E'}\left[\left(\frac{x-1}{E'}+1\right)^2+\frac{1}{x}+x-1\right] . \qquad (4)$$

In case $E'\geq\frac{1}{2}$, $x\in[0,1]$ from (4) we can see that $f_x(x,E')$ has peculiarity in point x=0. This fact fits with $\mu=1-\frac{1}{E'}$ and $E'\leq E<\infty$ for function (1). We have possibility to finite integral of density $f_x(x,E')$ for all values of $E'\geq\frac{1}{2}$ using statistical weight $W=\frac{1}{x}$.

Hence $\tilde{f}_X(x,E') = x \cdot f_X(x,E')$ is

$$\tilde{f}_X(x,E') = \frac{1}{E'}\left[x\left(\frac{x-1}{E'}+1\right)^2 + 1 + x^2 - x\right] \tag{5}$$

and $\tilde{f}_X(0,E') = \frac{1}{E'}$, $\tilde{f}_X(1,E') = \frac{2}{E'}$ that gives possibility to use rejection method with linear majorant for sampling X.

In case $E' < \frac{1}{2}$ we use energy form of density (1) and method of reverse function. When $E' \geq \frac{1}{2}$ in the expression (5) it is convenient to use method from [2]. The character of behavior of $\tilde{f}_X(x,E')$ is very close to linear function at $x \in [0,1]$ when E' increases. Rejection method with linear majorant is more effective than method of reverse function in this situation.

Thus the new modeling algorithm for pseudo-photon KN and incoherent scattering is following.

1. Let for $x \in [0,1]$ linear function $\varphi(x)$ be defined. Denote

$$\varphi(0) = \tilde{f}_X(0,E') = \frac{1}{E'}, \qquad \varphi(1) = \tilde{f}_X(1,E') = \frac{2}{E'}.$$

We sample η' and ξ':

$\xi' \sim U(0,1) \Rightarrow \xi' = \gamma_1$, $\eta' \sim U(0, \varphi(0)+\varphi(1)) \Rightarrow \eta' = \gamma_2 \cdot \frac{3}{E'}$ and calculate

$$\xi = \begin{cases} \xi' & \text{when } \eta' < \varphi(\xi') \\ 1-\xi' & \text{when } \eta' > \varphi(\xi') \end{cases}, \qquad \eta = \begin{cases} \eta' & \text{when } \eta' < \varphi(\xi') \\ \frac{3}{E'} - \eta' & \text{when } \eta' > \varphi(\xi') \end{cases}$$

2. In the case $\tilde{f}_X(\xi,E') \geq \eta$ we have $x = \xi$ with KN density (7). In another case - resample η' and ξ'.

3. In the case $\tilde{f}_X(x,E') \cdot S(q,z) \geq \eta$ we have $x = \xi$ with incoherent density f_{InCoh}. In another case - resample η' and ξ'.

4. Calculate new parameters of scattered pseudo-photon:

$$\mu = \frac{x-1}{E'} + 1, \; E = \frac{E'}{x} \text{ and } W = \frac{1}{x}.$$

3 COHERENT SCATTERING SAMPLING

There is no energy change during coherent photon scattering. Hence we can use the same algorithm both for the direct and adjoint photon transport equation.

The main idea of proposed approach is based on possibility of analytical integration of differential cross-section of coherent scattering that is represented in File 27 of ENDF-6 format files as

$$\frac{d\sigma_{Coh}(E,\mu)}{d\mu} = f(E,\mu) = \pi r_0^2 \left[\{F(q)+\mathrm{Re}(E)\}^2 + \{\mathrm{Im}(E)\}^2\right](1+\mu^2),$$

where $q = E[2(1-\mu)]^{1/2}$ is the recoil momentum of the atom; F(q) is a form factor; Re(E) – the real anomalous scattering factor; Im(E) – the imaginary anomalous scattering factor.

The coherent scattering function is such, that for $\mu \approx 1$ it sufficiently grows at small angle interval, hence it is more efficient to use analytical integration by q. Let us get from the density *f(E, μ)* to the density *f(E, q)* using Jacobean $\left|\frac{d\mu}{dq}\right| = \frac{q}{E^2}$. In this way momentum density is

$$\frac{\pi r_0^2}{E^2}\cdot q\cdot\left(2+\frac{q^4}{4E^4}-\frac{q^2}{E^2}\right)\left[F^2(q)+2\mathrm{Re}(E)\cdot F(q)+\{\mathrm{Re}^2(E)+\mathrm{Im}^2(E)\}\right].$$

At the same time total coherent cross-section is $\sigma_{Coh}^{(27file)}(E) = \int_0^{q_{max}} f(E,q)dq$ and it is important that the difference between $\sigma_{Coh}^{(23file)}(E)$ and $\int \frac{d\sigma_{Coh}^{(27file)}(E)}{dq}dq$ is less than 0.01 – 0.05%. Hence we can use sampling of the number of interval $[q_i, q_{i+1}]$ without calculation of integral in $[0, q_{max}]$.

On the other hand we can write $\sigma_{Coh}^{(27file)}(E) = \sum_{q=0}^{q_{max}} P_i(E,q)$, where P_i is the probability with $q \in [q_i, q_{i+1}]$ and

$$\int_{q_i}^{q_{i+1}} f(E,q)dq = \int_{q_i}^{q_{i+1}} q\left(2+\frac{q^4}{4E^4}-\frac{q^2}{E^2}\right)\left[\alpha_i^2 q^{2\beta_i} + 2\alpha_i\cdot\mathrm{Re}\cdot q^{\beta_i} + (\mathrm{Re}^2+\mathrm{Im}^2)\right]\cdot dq =$$

$$q^2(\mathrm{Re}^2+\mathrm{Im}^2) - \frac{q^4}{4E^2}(\mathrm{Re}^2+\mathrm{Im}^2) + \frac{q^6}{24E^4}(\mathrm{Re}^2+\mathrm{Im}^2) + \frac{4\alpha_i\cdot\mathrm{Re}\cdot q^{\beta_i+2}}{(\beta_i+2)} -$$

$$- \frac{2\alpha_i \cdot \mathrm{Re} \cdot q^{\beta_i+4}}{E^2(\beta_i+4)} + \frac{\alpha_i \cdot \mathrm{Re} \cdot q^{\beta_i+6}}{2E^2(\beta_i+6)} + \frac{2\alpha_i^2 \cdot q^{2\beta_i+2}}{(2\beta_i+2)} - \frac{\alpha_i^2 \cdot q^{2\beta_i+4}}{E^2(2\beta_i+4)} + \frac{\alpha_i^2 \cdot q^{2\beta_i+6}}{4E^4(2\beta_i+6)},$$

where $\beta_i = \ln\left(\frac{F_{i+1}}{F_i}\right) \Big/ \ln\left(\frac{q_{i+1}}{q_i}\right)$, $\alpha_i = F_i \left(\frac{1}{q_i}\right)^{\beta_i}$.

This formula is right for all $q_2 < q_i < q_{max}$ i.e. for LOG-LOG interpolation law for $F(q)$. For the first interval ($0 = q_1 \le q \le q_2$) expression for P_1 has another form (omitted here). These formulae are intricate ones but they are appropriate for the calculations. Finally we calculate value of $\mu = 1 - q^2/2E^2$ after sampling value of q.

4 CONCLUSIONS

Five exact effective sampling methods are developed for the:

- Klein-Nishina distribution for Monte Carlo simulation of the direct and adjoint photon transport equation;

- incoherent photon scattering for Monte Carlo simulation of the direct and adjoint photon transport equation;

- coherent photon scattering for Monte Carlo simulation of the photon transport equation.

All algorithms are included to the Monte Carlo code BRAND [3,4].

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