Treatment of non constant cross sections in analog and biasing Monte Carlo

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1 Introduction

The cross section of a process applying to charged particles is changing over a tracking step as the particles loose continuously energy. However the occurrence of a process is sampled in Geant4 from a cross section that is considered as constant over a step. This approximation can be corrected in the analog and biasing mode by using either the integral cross section method described in section 2) or by applying a weight correction factor (see section 3).

2 Integral CS mode used in analog Monte Carlo in Geant4

For correcting for the variation of the cross section over a step the integral cross section mode is used by default in Geant4 for electromagnetic processes applying to charged particles. In this mode the cross section $\sigma_i^t$, used to sample the occurrence of the process $i$ is set to an upper limit $\sigma_{\text{max}}^i$ of the real cross section over the step $[l_0, l]$. When the process $i$ occurs, an additional test is performed in the post step do it method to check if the process applies or not. In this test the following random check is performed:

$$\text{rand}(0, 1) \leq \frac{\sigma_i^t(l)}{\sigma_{\text{max}}^i}$$

with $\text{rand}(0, 1)$ defining a variable generated randomly over $[0, 1]$ with linear sampling. If the test is passed the process is applied while in the contrary the process is not applied and the tracking of the primary particle continues. This procedure is equivalent to correct at $l$ the effective cross section $\sigma_{\text{max}}^i$ by the factor $\frac{\sigma_i^t(l)}{\sigma_{\text{max}}^i}$. As $l$ is sampled randomly it ensures a correction of the cross section at all positions.

It is quite obvious that the probability of non interaction $P_{NI}(l_0, l)$ over the step $[l_0, l]$ is also corrected in the right way by applying the integral cross section...
method as the correction of the cross section is applied for all $l$. However this can be also proved analytically. When applying the integral cross section mode the probability $P_{NI}^i(l_0, l)$ of non-interaction for the process $i$ over the step $[l_0, l]$ is given by the sum of the probability that a particle arrives at $l$ with no rejection test for the process $i$ applied at all over $[l_0, l]$, plus all the cases where before arriving at $l$ the occurrence of the process $i$ has been rejected once, twice, ..., by $n$ times. The probability $P_{NI,0}^i(l_0, l)$ of non interaction for the process $i$, over $[l_0, l]$, without any rejection of the process, is the non interaction probability when the cross section is set to $\sigma_{i,\text{max}}$ all over the step. It writes

$$P_{NI,0}^i(l_0, l_1) = e^{-\sigma_{i,\text{max}}(l-l_0)}$$  \hspace{1cm} (2)$$

The probability $P_{NI,1}^i(l_0, l_1)$ of non interaction for the process $i$ over $[l_0, l]$, with one rejection of the process taking place, writes

$$P_{NI,1}^i(l_0, l_1) = e^{-\sigma_{i,\text{max}}(l-l_0)} \int_{l_0}^{l_1} \left[ \sigma_{i,\text{max}} - \sigma_i(l_1) \right] dl_1$$  \hspace{1cm} (3)$$

The probability $P_{NI,2}^i(l_0, l_1)$ of non interaction for the process $i$ over $[l_0, l]$, with two rejections of the process taking place, writes

$$P_{NI,2}^i(l_0, l_1) = e^{-\sigma_{i,\text{max}}(l-l_0)} \int_{l_0}^{l_1} \left[ \sigma_{i,\text{max}} - \sigma_i(l_1) \right] \int_{l_1}^{l_2} \left[ \sigma_{i,\text{max}} - \sigma_i(l_2) \right] dl_2 dl_1$$

$$= \int_{l_0}^{l_1} \left[ \sigma_{i,\text{max}} - \sigma_i(l_1) \right] P_{NI,1}^i(l_0, l_1) dl_1$$  \hspace{1cm} (4)$$

And by extension the probability of non interaction for the process $i$ over $[l_0, l]$, with $n$ rejections of the process taking place, writes

$$P_{NI,n}^i(l_0, l_1) = e^{-\sigma_{i,\text{max}}(l-l_0)} \int_{l_0}^{l_1} \left[ \sigma_{i,\text{max}} - \sigma_i(l_1) \right] \int_{l_1}^{l_2} \left[ \sigma_{i,\text{max}} - \sigma_i(l_2) \right] \int_{l_2}^{l_3} \left[ \sigma_{i,\text{max}} - \sigma_i(l_3) \right] \int_{l_3}^{l_{n-1}} \left[ \sigma_{i,\text{max}} - \sigma_i(l_{n-1}) \right] dl_{n-1} dl_{n-2} \ldots dl_1$$

$$= \int_{l_0}^{l_1} \left[ \sigma_{i,\text{max}} - \sigma_i(l_1) \right] P_{NI,n-1}^i(l_0, l_1) dl_1$$  \hspace{1cm} (5)$$

If we set $g(l) = \sigma_{i,\text{max}}^i - \sigma_i(l)$ in equation 5 we need finally to evaluate the following type of integral

$$G_n(l_0, l) = \int_{l_0}^{l_1} g(l_1) \int_{l_1}^{l_2} g(l_2) \int_{l_2}^{l_3} g(l_3) \ldots \int_{l_{n-1}}^{l_n} g(l_n) dl_n \ldots dl_2 dl_1$$  \hspace{1cm} (6)$$
By defining $G(l) = \int g(l)dl$ as the integral function of $g(l)$ we have

$$G_2(l_0, l) = \int_{l_0}^{l} g(l_1) \int_{l_1}^{l} g(l_2)dl_2dl_1$$
$$= \int_{l_0}^{l} g(l_1)[G(l) - G(l_1)]dl_1$$
$$= \int_{0}^{[G(l) - G(l_0)]} [G(l) - G(l_1)]d(G(l) - G(l_1))$$
$$= \frac{[G(l) - G(l_0)]^2}{2}$$
$$= \frac{[\int_{l_0}^{l} g(l_1)dl_1]^2}{2}$$

(7)

And by extension we get

$$G_3(l_0, l) = \int_{l_0}^{l} g(l_1) \int_{l_1}^{l} g(l_2) \int_{l_2}^{l} g(l_3)dl_3dl_2dl_1$$
$$= \frac{[G(l) - G(l_0)]^3}{3!}$$
$$= \frac{[\int_{l_0}^{l} g(l_1)dl_1]^3}{3!}$$

(8)

$$G_n(l_0, l) = \int_{l_0}^{l} g(l_1) \int_{l_1}^{l} g(l_2) \int_{l_2}^{l} g(l_3) \int_{l_3}^{l} g(l_4)\ldots\int_{l_{n-1}}^{l} g(l_n)dl_n..dl_{j..}dl_1$$
$$= \frac{[G(l) - G(l_0)]^n}{n!}$$
$$= \frac{[\int_{l_0}^{l} g(l_1)dl_1]^n}{n!}$$

(9)

Finally considering equations 9, 4, and 5 we obtain

$$P_{NI,2}^i(l_0, l) = e^{-\sigma_{\text{max}}^i(l-l_0)} \frac{[\int_{l_0}^{l} [\sigma_{\text{max}}^i - \sigma^i(l_1)]dl_1]^2}{2}$$

(10)

$$P_{NI,3}^i(l_0, l) = e^{-\sigma_{\text{max}}^i(l-l_0)} \frac{[\int_{l_0}^{l} [\sigma_{\text{max}}^i - \sigma^i(l_1)]dl_1]^3}{3!}$$

(11)

$$P_{NI,n}^i(l_0, l) = e^{-\sigma_{\text{max}}^i(l-l_0)} \frac{[\int_{l_0}^{l} [\sigma_{\text{max}}^i - \sigma^i(l_1)]dl_1]^n}{n!}$$

(12)

The total probability $P_{NI}(l_0, l)$ that the particles arrives at $l$ without occurrence
of the process $i$ becomes

$$P_{NI}^i(l_0, l) = \sum_{n=0}^{\infty} P_{NI,n}^i(l_0, l)$$

$$= e^{-\sigma_{\text{max}}^i(l-l_0)} \sum_{n=0}^{\infty} \left[ \int_{l_0}^{l} \sigma_{\text{max}}^i - \sigma_{\text{max}}^i(t_1) \right]^{n} \frac{n!}{n!}$$

$$= e^{-\sigma_{\text{max}}^i(l-l_0)} \int_{l_0}^{l} \sigma_{\text{max}}^i - \sigma_{\text{max}}^i(t_1) \right] dt_1$$

and we get finally the expected survival probability

$$P_{NI}^i(l_0, l) = e^{-\int_{l_0}^{l} \sigma_{\text{max}}^i(t_1) dt_1}.$$

The integral method described above can be used also for the forced interaction and the cross section biasing modes. It will work providing that when the rejection test is performed in the post step do it of the process the weight of particles have been already corrected for the other biasing effects. For the case of the forced interaction over a distance $L$ it is important to note that if a process occurrence is rejected by the cross section test at a position $l$ over $[0, L]$, the next occurrence of the process should be forced on the interval $[l, L]$.

3 Weight correction factor for cross section varying over a step

The integral cross section mode can not be applied for the flight free mode as no process occurs over $L$ and the rejection test are therefore not applied over the interval $[0, L]$ for compensating for the cross section variation. In this case the extra weight correction factor $w_1 = e^{\int_{l_0}^{l_1} \sigma_{\text{max}}^i - \sigma_{\text{max}}^i(t) dt}$ should be be applied, after the usual free flight weight correction factor $w_0 = e^{-\sigma_{\text{max}}^i}$.

3.1 Monte Carlo integration of $w_1$

The weight correction factor $w_1$ can be computed randomly by simulating the flying of particle over $L$ with random rejections of the processes $i$ at succesives positions. The exact method to compute $w_1$ is described below. The weight correction factor start as $w_1 = 1$. A position $l_1$ is generated randomly over $[0, L]$ with a linear sampling. By this way the statistical weight of the selection of $l_1$ is equivalent to $dl/L$. The following random test is performed at $l_1$:

$$\text{rand}(0, 1) > \frac{\sigma_{\text{max}}^i(t_1)}{\sigma_{\text{max}}^i}$$

with $\text{rand}(0, 1)$ defining a variable generated randomly over $[0, 1]$ with a linear sampling. If the test is not passed the procedure is stopped and $w_1$ is kept equal
to 1. It corresponds to the case where the free flight to $L$ happens without any rejection of the process $i$. On the contrary if the test is passed the term $t_1 = \sigma_{\text{max}}^i L$ is added to $w_1$. This term contributes to $w_1$ as the cases where one rejection of the occurrence of the process $i$ take place during the free flight over $L$. As the probability that the test is passed is $1 - \frac{\sigma^i(l_1)}{\sigma_{\text{max}}^i}$ and as the statistical weight for the selection of $l_1$ is $\frac{dl}{L}$, the term $t_1$ is statistically equivalent to

$$\frac{\sigma_{\text{max}}^i L(1 - \frac{\sigma^i(l_1)}{\sigma_{\text{max}}^i})}{L} = [\sigma_{\text{max}}^i - \sigma^i(l_1)]dl$$  \hspace{1cm} (18)

Therefore the mean value of the term $t_1$ is

$$\bar{t}_1 = \int_{l_0}^L [\sigma_{\text{max}}^i - \sigma^i(l_1)]dl_1$$  \hspace{1cm} (19)

The procedure applied to the position $l_1$ is repeated over successive positions $l_2$, $l_3$, ..., $l_j$, ... that are generated randomly over $[l_1, L]$, $[l_2, L]$, ..., $[l_{j-1}, L]$ respectively. Successive positions $l_i$ are generated while the rejection test

$$\text{rand}(0, 1) > \frac{\sigma^i(l_j)}{\sigma_{\text{max}}^i}$$  \hspace{1cm} (20)

is passed. For each new position $l_j$ the term

$$t_j = (\sigma_{\text{max}}^i)^j L(L - l_1)(L - l_2)...(L - l_{j-1})$$  \hspace{1cm} (21)

is added to $w_1$, except for the last position where the test failed. Following the same logic than what was explained above for the term $t_1$ we can show that the mean value of $t_j$ is given by

$$\bar{t}_j = \int_0^L [\sigma_{\text{max}}^i - \sigma^i(l_1)]..\int_{l_{j-1}}^L [\sigma_{\text{max}}^i - \sigma^i(l_j)]dl_j..dl_1$$  \hspace{1cm} (22)

Finally we see from equations 22 and 5 that the mean value of $w_1$ writes

$$\bar{w}_1 = 1 + \sum_{j=0}^{\infty} \bar{t}_j = 1 + \sum_{j=1}^{\infty} \int_0^L [\sigma_{\text{max}}^i - \sigma^i(l_1)]..\int_{l_{j-1}}^L [\sigma_{\text{max}}^i - \sigma^i(l_j)]dl_j..dl_1$$

$$= \sum_{j=0}^{\infty} \frac{[\int_0^L [\sigma_{\text{max}}^i - \sigma^i(l)]dl]^j}{n!} = e^{\int_0^L [\sigma_{\text{max}}^i - \sigma^i(l)]dl}$$  \hspace{1cm} (23)

and we get the expected weight correction factor.
3.2 Integration of $w_1$ over the energy $E$

The Monte Carlo integration of $w_1$ that we have described in subsection 3.1, is done over the length $l$. In this integration the variation of the cross section is considered as a function of $l$ while in the real case it is a function of kinetic energy $E$ that is varying over $l$. As the variation of $E$ over $l$ is a random process (multiple scattering,...) it is better to perform the integration of $w_1$ over $E$ rather than over $l$. This implies that instead of generating randomly successive positions, successive energies $E_1$, $E_2$, ..., $E_j$ are generated randomly over $[E_i, E_f]$, $[E_1, E_f]$, $[E_j - 1, E_f]$ respectively, with $E_i$ and $E_f$ respectively the energy of the particle at the beginning and at the end of the step $[0, L]$. The statistical weight of the selection of $E_j$ is equivalent to $dE/(E_j - E_f)$ and the terms $t_j$ are set to

$$t_j = (\sigma_{\text{max}}^i)^j E - E_0 \frac{E - E_1}{dE_1/dl} \frac{E - E_2}{dE_2/dl} ... \frac{E - E_{j-1}}{dE_{j-1}/dl} \frac{E - E_f}{dE_f/dl}$$

(24)

in order to go back to the correct integration over $dl$. In this last equation the $dE_j/dl$ are obtained from precomputed $dE/dX$ table of Geant4 EMprocesses.