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Title: An update to the computation of the Goudsmit-Saunderson distribution in MCNP ® version 6.2

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An update to the computation of the Goudsmit-Saunderson distribution in MCNP® version 6.2

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1 Background

In MCNP6.2 [1], electron angular deflection is determined by sampling the Goudsmit-Saunderson distribution [2, 3]. The Goudsmit-Saunderson distribution is obtained by solving an infinite medium transport equation for mono-energetic electrons undergoing only elastic collisions. The solution

$$A_{GS}(\mu, s) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} e^{-sG_\ell} P_\ell(\mu), \tag{1}$$

is a function of pathlength, s, momentum-transfer moments, G_ℓ, and the deflection cosine, $\mu = \cos\theta$, and gives the probability that a multiply-scattered electron is deflected through some angle, θ, after traveling a distance, s. The momentum transfer moments are given by

$$G_\ell = 2\pi N \int_{-1}^{1} d\mu \, [1 - P_\ell(\mu)] \, \sigma_{el}(E, \mu), \tag{2}$$

where $\sigma_{el}(E, \mu)$ is the single-scatter DCS for an electron with energy E and N is the number of atoms per unit volume. The benefit of using the Goudsmit-Saunderson distribution is that it is not derived in the small angle approximation, so it is exact for any angle, and it can be applied to any DCS. In theory, it is valid for any pathlength (there are numerical issues associated with generating the distribution for small pathlengths).

For many years, the prescription to determine the truncation point [4] in Eq. (1) has been given by

$$\ell_{max} = \max\left(10, \exp\left[1.794 - 0.397 \ln(\eta)\right]\right). \tag{3}$$

In MCNP6.2, the default behavior is actually more restrictive than the above equation and given by

$$\ell_{max} = \max\left(10, \min(240, \exp\left[1.794 - 0.397 \ln(\eta)\right])\right). \tag{4}$$

Under these conditions, no more than 240 terms are used in computing Eq. (1). While this is sufficient for a wide range of source energies and default pathlength

sizes, users can easily introduce input parameters such that 240 terms are no longer sufficient.

Therefore, an additional DBCN option (entry 90) was introduced in MCNP6.2 to allow for an arbitrary number of terms in the computation of the Goudsmit-Saunderson distribution. We show the impact of modifying the number of terms used to compute the Goudsmit-Saunderson distribution.

2 Impact of update

To demonstrate how the number of terms used to compute the Goudsmit-Saunderson distribution impacts results, we study a thin foil problem where the outgoing angular distribution is observed for 20-MeV electrons. The foil thickness is roughly 1.5 times the default substep size for a 20-MeV electron in gold (∼2.8e-3 cm). Therefore, for the default substep size, electrons are guaranteed to undergo at least one collision before encountering a boundary (at which point an approximation is applied). In theory, one can improve the accuracy of the MCNP6.2 electron transport method by reducing the substep size. However, one must assume that the underlying data is valid. We show that when a user reduces the substep size, the angular distribution observed is different than expected. The primary reason being that the underlying data was not computed using a sufficient number of terms. We aslo show that the distribution is recovered when the number of terms is increased from hundreds to thousands.

In fig. 1, angular distributions are presented for three cases: (1) ESTEP=13, L=240, (2) ESTEP=13, L=10000, and (3) ESTEP=208, L=10000. Here, the reference solution is assumed to be ESTEP=208, L=10000. Note that there is subtle disagreement between the reference solution and the two other solutions where ESTEP=13 and L=240 or L=10000.

In fig. 2, angular distributions are presented for three cases: (1) ESTEP=104, L=240, (2) ESTEP=104, L=10000, and (3) ESTEP=208, L=10000. Again, the reference solution is assumed to be ESTEP=208, L=10000. Now, note that the disagreement between the reference solution and ESTEP=104, L=240 grows while the disagreement between the reference solution and ESTEP=104, L=10000 is reduced.

In fig. 3, angular distributions are presented for two cases: (1) ESTEP=208, L=240 and (2) ESTEP=208, L=10000. Once again, the reference solution is assumed to be ESTEP=208, L=10000. Now, note that the disagreement between the reference solution and ESTEP=104, L=240 grows considerably.

3 Conclusions

Here, we showed that stabilizing the underlying angular deflection distributions used in transport improves simulation results, particularly, when default parameters are adjusted such that the substep size is reduced. Stabilization is achieved by adding more terms when computing the Goudsmit-Sanderson distribution. The default number of terms remains as 240 with the option of controlling the number of terms via DBCN(90). Once additional studies are completed that demonstrate the stabilization effect is real and not a result of numerical artifacts such as truncation error, the default number of terms will be adjusted

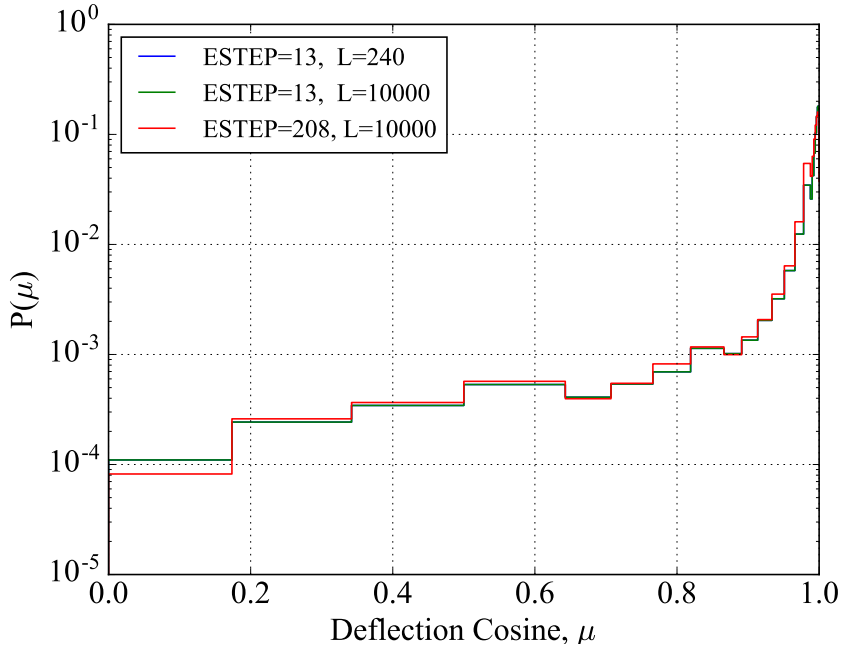

Figure 1: Comparison of outgoing electron angular distributions computed with ESTEP=13 and ESTEP=208, and L=240 or L=10000.

accordingly.

References

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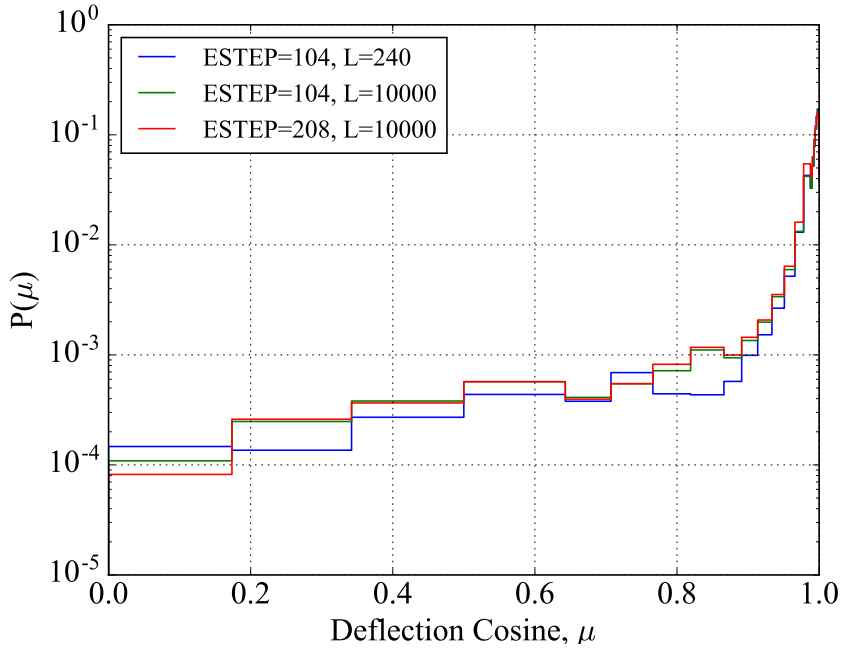

Figure 2: Comparison of outgoing electron angular distributions computed with ESTEP=104 and ESTEP=208, and L=240 or L=10000.

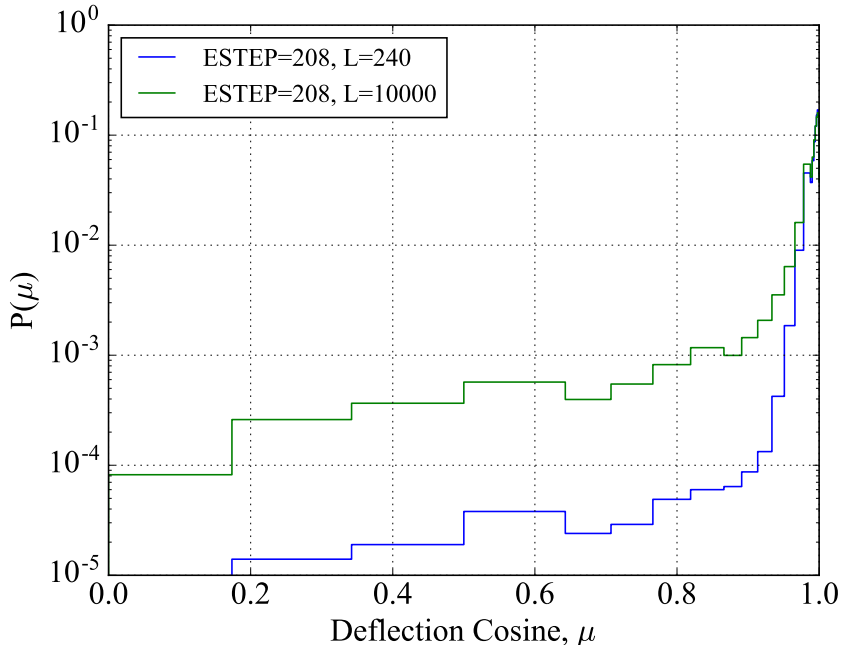

Figure 3: Comparison of outgoing electron angular distributions computed with ESTEP=13 and ESTEP=208, and L=240 or L=10000.