

LA-UR-25-23077

Approved for public release; distribution is unlimited.

Title: An update to delta-ray production in MCNP6

Author(s): Lively, Michael Aaron

Intended for: Report

Issued: 2025-04-17 (rev.1)



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

An update to δ -ray production in MCNP6

Michael A. Lively (XCP-3)

April 1, 2025

Abstract As originally introduced in MCNP6.2, the δ -ray production subroutine had a number of flaws related to treatment of particle or nuclear spin contributions to the production cross section. A recent update by the author to the MCNP6 code corrects these flaws. This report documents those changes for the benefit of MCNP6 users who use the delta ray production capability. Additionally, this report aims to provide a more comprehensive documentation of the delta ray production, building on the prior documentation by C. Anderson and coworkers. On this latter point, the goal is to save future MCNP developers from a visit to the library to dig out ancient texts from 1952, or at least to provide useful points of reference should such a visit be necessary.

1 Introduction

A charged particle traveling through matter transfers energy to bound atomic electrons through a series of inelastic collisions. When the transferred energy is greater than the ionization energy, a secondary electron is ejected from its atomic orbit. Secondary electrons with sufficient kinetic energy to travel a significant distance* from their points of origin are called knock-on electrons or δ -rays.

Since MCNP code version 4B [1], electron and positron transport has included knock-on electron generation. However, support for δ -ray production by heavy charged particles was only added in MCNP6.2 [2]. This implementation is based on the analytical expressions given by B. Rossi [3] and A. Kamal [4][†].

The original implementation suffered from a number of errors affecting the spin-dependent contribution to the δ -ray production cross section:

- Most concerning, while a term for the additional cross-section contribution from a hadron or nuclear spin number of 1/2 was provided, this contribution was only applied for incident protons, ignoring the wide range of other spin-1/2 hadrons and ions present in the MCNP code.
- The expression for the spin-dependent contribution was incorrect and not in agreement with [2]. An unqualified high-energy approximation was used instead.

* A “significant distance” is application-dependent, but as a rule of thumb implies an electron range on the order of the primary charged particle range. For example, a 1-MeV α particle has a range in iron of about 1.5 μm ; an electron with similar range has a kinetic energy of about 20 keV.

[†]While the authors of [2] also cite ICRU Report 37 [5], this citation is largely incidental, as the formulation given in [3] is not only entirely sufficient but in fact more comprehensive.

- Particles with nonzero spin greater than 1/2 are not treated, most critically including deuterons (spin-1) as well as most heavy ion species.

In light of recent changes to the MCNP source code to rectify these deficiencies, this report provides an updated documentation source superseding the prior work [2]. Furthermore, this report aims to provide a comprehensive overview of the δ -ray production physics implemented in the MCNP code which goes beyond the cursory overview of the prior work. This will enable MCNP developers and other source code users to readily understand the physical origins of each term in the present source code implementation.

2 Theory

2.1 The collision cross section

Note to readers: The analytical formulations given here are found in sections 2.2 and 2.3 of [3]. In particular, see Equations (2.2.4), (2.3.1), and (2.3.6) through (2.3.9) in that text.

Consider a charged particle of mass M and atomic number Z_i traveling through a material with speed v and kinetic energy E . The (macroscopic) cross section for an inelastic energy transfer T to an atomic electron is given by

$$d\Sigma_{\text{inel}}(\beta, T) = C_{\text{inel}} \frac{Z_i^2}{\beta^2} \frac{dT}{T^2} K_s(\beta, T) \quad (1)$$

where $\beta \equiv v/c$ is the ratio of the incident particle speed to the speed of light in a vacuum (c), $C_{\text{inel}} \equiv 2\pi r_e^2 m_e c^2 N \langle Z \rangle$ where r_e is the classical electron radius, m_e is the electron mass, N is the material atomic density, and $\langle Z \rangle$ is the average atomic number of the material (such that $N \langle Z \rangle$ gives the material electron density). The spin-dependent term, K_s , is given by

$$K_s(\beta, T) = \begin{cases} 1 - \beta^2 \frac{T}{T_{\text{max}}}, & s = 0 \\ 1 - \beta^2 \frac{T}{T_{\text{max}}} + \frac{1}{2} \left(\frac{T}{E_{\text{tot}}} \right)^2, & s = \frac{1}{2} \\ \left(1 - \beta^2 \frac{T}{T_{\text{max}}} \right) \left(1 + \frac{1}{3} \frac{T}{E_c} \right) + \frac{1}{3} \left(\frac{T}{E_{\text{tot}}} \right)^2 \left(1 + \frac{1}{2} \frac{T}{E_c} \right), & s = 1 \end{cases} \quad (2)$$

where T_{max} is the maximum kinematically allowed energy transfer, given by

$$T_{\text{max}} = \frac{2m_e c^2 (\gamma^2 - 1)}{1 + 2\gamma\mu + \mu^2} \quad (3)$$

where $\gamma \equiv 1/\sqrt{1 - \beta^2}$ and $\mu \equiv m_e/M$, $E_{\text{tot}} = E + Mc^2$, and the factor $E_c = Mc^2/\mu$ defines a critical energy value above which the spin-spin interaction dominates the Coulomb interaction. Note that while some hadrons and most heavy ion nuclei may have spin numbers greater than 1, to the best of the author's knowledge no expressions for the inelastic energy transfer cross section for these conditions is provided in the literature. A list of heavy charged particles available for transport in MCNP6, including their charge and spin numbers, is provided in Table 1. The behavior of T_{max} as a function of incident energy for various particle types is shown in Figure 1. Note the low-energy limit ($T_{\text{max}}/E \rightarrow 4\mu$) and the high-energy limit ($T_{\text{max}}/E \rightarrow 1$) which can be found from Equation (3).

Table 1: Heavy charged particles available for transport in MCNP6. Particles which decay on production (e.g., Σ^\pm , Ξ^\pm , Ω^-) are not listed.

ipt	Name	Symbol	Mass (MeV/ c^2)	Charge (Z_i)	Spin (s)
4	negative muon (μ^-)		105.658389	-1	1/2
9	proton (p^+)	H	938.27231	+1	1/2
16	positive muon (μ^+)	!	105.658389	+1	1/2
19	anti proton (\bar{p})	G	938.27231	-1	1/2
20	positive pion (π^+)	/	139.56995	+1	0
22	positive kaon (K^+)	K	493.677	+1	0
31	deuteron (d)	D	1875.627	+1	1
32	triton (t)	T	2808.951	+1	1/2
33	helion (^3He)	S	2808.421	+2	1/2
34	alpha particle (α)	A	3727.418	+2	0
35	negative pion (π^-)	*	139.56995	-1	0
36	negative kaon (K^-)	?	493.677	-1	0
37	heavy ions	#	varies	varies	varies

2.2 The δ -ray production yield

The number of δ -rays produced by a charged particle which travels a given step length Δx can be estimated as

$$N_\delta(E) = \Sigma_{\text{inel}}(\beta)\Delta x \quad (4)$$

which is necessarily only an estimate as it neglects the energy loss along the particle track. $\Sigma_{\text{inel}}(\beta)$ is the total energy-dependent inelastic cross section for δ -ray production, given by

$$\Sigma_{\text{inel}}(\beta) = \int_{T_{\text{cut}}}^{T_{\text{max}}} d\Sigma_{\text{inel}}(\beta, T) \quad (5)$$

where T_{cut} is a minimum δ -ray energy set by the user. Using Equation (1) this becomes

$$\Sigma_{\text{inel}}(\beta) = C_{\text{inel}} \frac{Z_i^2}{\beta^2} \int_{T_{\text{cut}}}^{T_{\text{max}}} \frac{K_s(\beta, T)}{T^2} dT \quad (6)$$

The results of this integration for $s \in \{0, \frac{1}{2}, 1\}$ are as follows:

$$s = 0 : \quad N_\delta(E) = C_{\text{inel}}\Delta x \frac{Z_i^2}{\beta^2} \left[\left(\frac{1}{T_{\text{cut}}} - \frac{1}{T_{\text{max}}} \right) - \frac{\beta^2}{T_{\text{max}}} \ln \left(\frac{T_{\text{max}}}{T_{\text{cut}}} \right) \right] \quad (7a)$$

$$s = \frac{1}{2} : \quad N_\delta(E) = C_{\text{inel}}\Delta x \frac{Z_i^2}{\beta^2} \left[\left(\frac{1}{T_{\text{cut}}} - \frac{1}{T_{\text{max}}} \right) - \frac{\beta^2}{T_{\text{max}}} \ln \left(\frac{T_{\text{max}}}{T_{\text{cut}}} \right) + \frac{T_{\text{max}} - T_{\text{cut}}}{E_{\text{tot}}^2} \right] \quad (7b)$$

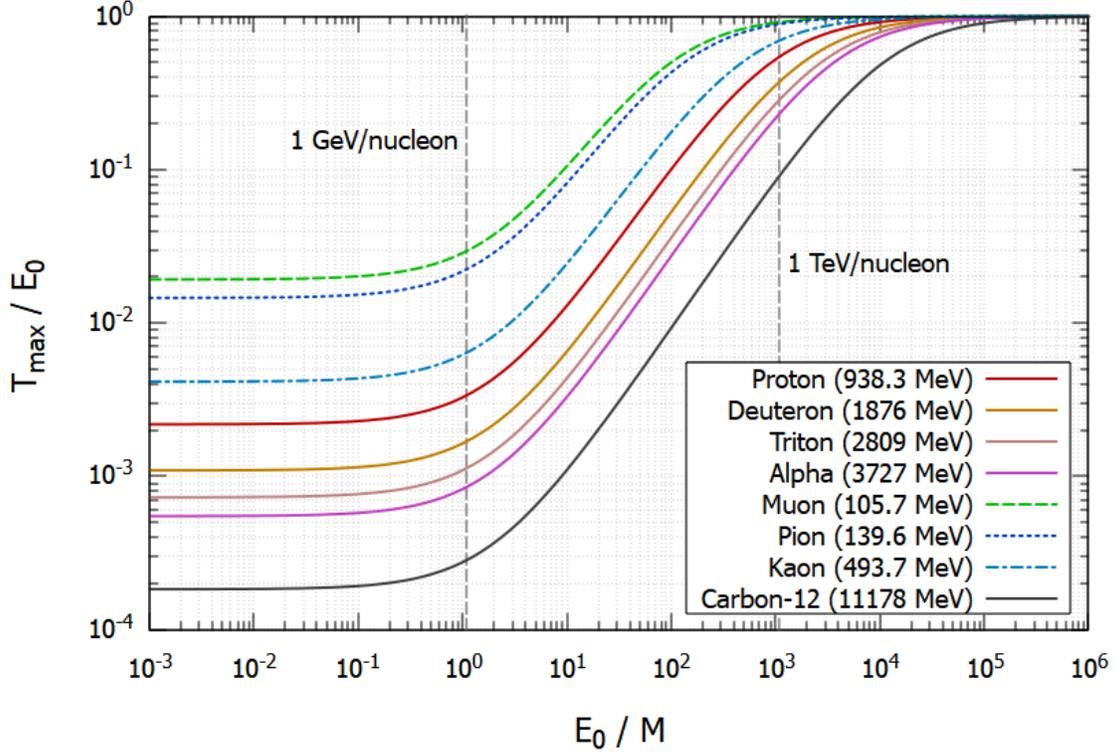


Figure 1: Maximum possible energy transfer to delta ray electrons as a function of incident energy for various incident charged particle types (from Equation (3)). The incident energy is given as a ratio over the particle mass, and the maximum energy transfer is given as a ratio over the (unnormalized) incident energy. Energy values after each particle name in the key indicate the particle mass times c^2 .

$$\begin{aligned}
 s = 1 : \quad N_\delta(E) = C_{\text{inel}} \Delta x \frac{Z_i^2}{\beta^2} & \left[\left(\frac{1}{T_{\text{cut}}} - \frac{1}{T_{\text{max}}} \right) - \left(\frac{\beta^2}{T_{\text{max}}} - \frac{1}{3E_c} \right) \ln \left(\frac{T_{\text{max}}}{T_{\text{cut}}} \right) \right. \\
 & \left. - \frac{T_{\text{max}} - T_{\text{cut}}}{3} \left(\frac{\beta^2}{T_{\text{max}} E_c} - \frac{1}{E_{\text{tot}}^2} \right) + \frac{T_{\text{max}}^2 - T_{\text{cut}}^2}{12 E_{\text{tot}}^2 E_c} \right] \quad (7c)
 \end{aligned}$$

In principle, the results could be extended indefinitely for increasing $s > 1$, but there do not appear to be any expressions for these cases in the extant literature.

2.3 δ -ray generation logic

MCNP generates N_δ δ -rays by looping over the logic below for each generated electron. The δ -ray energy is sampled from a $1/E$ integral distribution,

$$T = \left[\frac{1}{T_{\text{cut}}} - \mathcal{R} \left(\frac{1}{T_{\text{cut}}} - \frac{1}{T_{\text{max}}} \right) \right]^{-1} \quad (8)$$

where $\mathcal{R} \in [0, 1)$ is a single-use pseudorandom number generated by MCNP. The δ -ray energy is subject to rejection sampling with the rejection probability $P_{\text{rej}}(T) = K_s(\beta, T)$. The sampled value of T is accepted only if $\mathcal{R}P_{\text{max}} < P_{\text{rej}}(T)$, where P_{max} is the maximum value of $P_{\text{rej}}(\beta, T)$ over the domain $T_{\text{cut}} \leq T \leq T_{\text{max}}$. Note that this is a change from the prior implementation, which used $P_{\text{max}} = 1$. The former approach was not only inefficient, but potentially incorrect for extremely high energies.

The accepted electron gains speed $v' = \beta'c$ with $\beta' = \sqrt{T(T + 2m_e c^2)} / (T + m_e c^2)$. The δ -ray starting position is sampled as $\mathcal{R}\Delta x$ along the incident particle substep path length. The electron starting direction is set by the energy [4], with the angle respective to the incident particle track set by

$$\cos \theta = \left(\frac{T}{2m_e v'^2} \right)^{1/2} \quad (9)$$

and the azimuthal angle $\phi \in [0, \pi)$ about the incident particle track sampled uniformly. This completes the physical description of the δ -ray production process (although the associated subroutine performs additional bookkeeping steps not covered here). The generated electron is then banked for future transport.

Note that, as is common in MCNP and in Monte Carlo methods generally, the total sampled energy of the generated δ -rays will not equal, and may even exceed, the inelastic energy loss of the incident charged particle along the substep path length. In the event that the total δ -ray energy exceeds the inelastic energy loss, MCNP warns the user. Most often, this warning may arise because the value of T_{cut} is set too low and a large number of low-energy electrons are generated.

2.4 Limitations

First, note that the effect of the spin-dependent contribution is in most cases difficult to observe if not invisible. Identifying parameter spaces where spin-dependent effects are visible is therefore crucial for effective verification and validation of this implementation. Principally, the spin-dependent contribution affects generation of the highest-energy δ -rays by very high-energy incident charged particles. For example, the yield of δ -rays with $T > 1$ GeV by 30-TeV protons may vary by $\sim 1\%$ when computed with $s = \frac{1}{2}$ versus that computed with $s = 0$. This difference, while slight, can be significant in certain applications, e.g., cosmic ray cascade problems.

The inelastic energy transfer cross section used for δ -ray production is hardwired into the MCNP code. This means that the current implementation omits a number of known corrections to the common Bethe collisional stopping power formulation, including [5]:

- The shell correction (C/Z), accounting for the fact that incident particle velocities are not necessarily large compared to atomic electron velocities, particularly for inner-shell electrons.
- The density effect ($\delta/2$), accounting for polarization of the material in the neighborhood of a swift charged particle.
- The Barkas (Z^3) correction, accounting for the difference in stopping powers between negatively and positively charged particles.

- The Bloch correction (Z^4), accounting for perturbation of the atomic electron wave-functions by the incident particle.

In practice, the impact of most of these corrections should be fairly minor, as the shell, Barkas, and Bloch corrections all become less significant as the incident particle energy increases whereas δ -ray production is most significant at high incident energies. However, the density-effect parameter δ increases with kinetic energy and becomes significant when $E \gtrsim Mc^2$, thus its omission is concerning in the high-energy regime where δ -ray production is most important.

The treatment of heavy ions ($Z > 2$) retains some caveats. Most importantly, there does not seem to be a theoretical treatment of nuclear spin contributions to the inelastic energy transfer cross section for $s > 1$, while it is common for larger nuclei to have nuclear spin numbers greater than 1. The current solution is crude: for each of the proton (Z) and neutron (N) numbers, an even nucleon number contributes 0 to the spin number while an odd nucleon number contributes an additive 1/2 to the spin. For example: Fe-56 ($Z = 26$, $N = 30$) has a nuclear spin of zero, Fe-57 ($Z = 26$, $N = 31$) and Co-57 ($Z = 27$, $N = 30$) are assigned nuclear spin values of 1/2 (actual values: 1/2 and 7/2, respectively), and Co-58 ($Z = 27$, $N = 31$) is assigned a nuclear spin of 1 (actual value: 2).

An additional caveat for heavy ions is that the nuclear mass is not known by the MCNP code. MCNP uses the rough approximation that $M \approx A \times u$, where A is the mass number and u is the atomic mass unit. This approximation is usually not a significant source of error.

3 Verification and validation

3.1 Range of applicability for spin-dependent contributions

To summarize the changes in the calculation of spin-dependent contributions, to be interrogated as a verification exercise:

- Most heavy charged particles are subject to the spin-dependent contribution term, whereas previously only the spin-1/2 contribution was applied to protons only.
- The new spin-1 contribution term applies to deuterons and certain heavy ions.
- The E_{tot} factor in the spin-1/2 contribution is correctly the sum of the incident particle kinetic and rest mass energies, instead of kinetic energy only as previously.

Examination of these points suggests a minimal verification approach:

- At least one spin-0 particle type should be tested to verify that there is no impact where the physics are unchanged (although test results will still vary from the previous implementation due to the improvements made for rejection sampling).
- Protons (spin-1/2) should be tested to verify that the E_{tot} correction is visible.
- An additional spin-1/2 particle should be tested, which was formerly treated as spin-0, to verify that the change in per-particle-type spin treatment is visible.

Table 2: Listing of charged particles selected for verification of the spin-dependent contribution to the delta ray production cross section, including proton/charge (Z_i), neutron(N_i), and spin (s_i) numbers along with incident energy (E) and maximum energy transfer (T_{\max}) values.

Name	Z_i	N_i	s_i	E (TeV)	T_{\max} (TeV)
proton (p^+)	+1	0	1/2	10	9.20786
deuteron (d)	+1	1	1	40	36.8324
alpha (α)	+2	2	0	160	147.474
negative muon (μ^-)	-1	0	1/2	0.1	0.0902568
B-10 ion ($^{10}_5\text{B}$)	+5	5	1	800	723.256
B-11 ion ($^{11}_5\text{B}$)	+5	6	1/2	1000	906.852
C-12 ion ($^{12}_6\text{C}$)	+6	6	0	1200	1089.06
C-13 ion ($^{13}_6\text{C}$)	+6	7	1/2	1350	1220.32

- Deuterons (spin-1) should be tested to verify that the spin-1 contribution is visible.
- Heavy ions with each permutation of even and odd N , Z should be tested to verify that the heavy ion spin contribution approximation is visible.

Based on these criteria, a suitable minimal verification set might include: protons, deuterons, alphas, muons, boron-10, boron-11, carbon-12, and carbon-13. What then remains is to determine the energy domain in which each verified change is expected to be visible, keeping in mind the discussion at the beginning of Section 2.4. Noting that the spin-dependent contribution is important only for high values of the energy transfer T , the visibility of these contributions can be maximized by selecting the incident particle energy E such that $T_{\max} \geq 0.9E$. The selected particle types for a minimal verification set along with these incident energies are listed in Table 2. Note that the selected incident energies are quite high by the standards of MCNP; while the spin-dependent contribution remain relevant for lower incident energies, these values are selected to make the contribution distinct from statistical noise with a minimal calculation time.

3.2 Verification of the spin-dependent contribution

An example of a useful verification input deck for MCNP is given in Listing 1 (input decks used in this work are included as electronic attachments to this document). Calculation results obtained using input decks of this type are shown in Figure 2 through Figure 9. Each figure shows the probability distribution function for δ -ray emission (obtained by normalizing each tally value by its corresponding bin width) as well as the (arbitrarily scaled) differential energy transfer cross sections for $s \in \{0, 1/2, 1\}$. In each case, the trend in the δ -ray PDF at high energies matches the expected spin-dependent cross section. The new implementation is thus verified. A modification/combination of these input decks is incorporated into the MCNP regression testing suite. These new tests are named `inp408`, `inp409`, and `inp410` and are found under the `Testing/features/light_ions` directory of the MCNP6 repository.

Listing 1: Sample MCNP input deck for verification

```
1 Pencil beam problem for delta ray production by 800 TeV B-10 ions.
2 c Cell cards
3 10      1      -19.25  -100 210 -220      imp:e,#=1
4 99      0              #10              imp:e,#=0
5
6 c Surface cards
7 100     cz      1E-8
8 210     pz      0.0
9 220     pz      100.0
10
11 c Data cards
12 m1     74180    0.0012  74182    0.2650  74183    0.1431
13 74184   0.3064  74186    0.2843  elib=03e
14 mode   e #
15 phys:e 8E8
16 phys:# 8E8     15j    -1          $ Use CUT:E(2) to set the 'real' cutoff
17                1E10    $ Increase drnok for better statistics
18 cut:e   j      1E6
19 cut:#   j      1E6
20 lca     7j     -2
21 sdef    par=5010      pos=0 0 0   vec=0 0 1   dir=1   erg=8E8
22 f1:e    (100 210 220)
23 fc1     Energy distribution of delta rays produced by B-10 ions
24 e1      1E6     19ilog  1E8     8ilog   8E8
25 ft1     tag     4
26 fu1     0.00006 nt      $ Count only delta rays, ignore
27                $ electrons from nuclear reactions
28 nps     10
29 print
30 prdmp   2j     -1    j    1
```

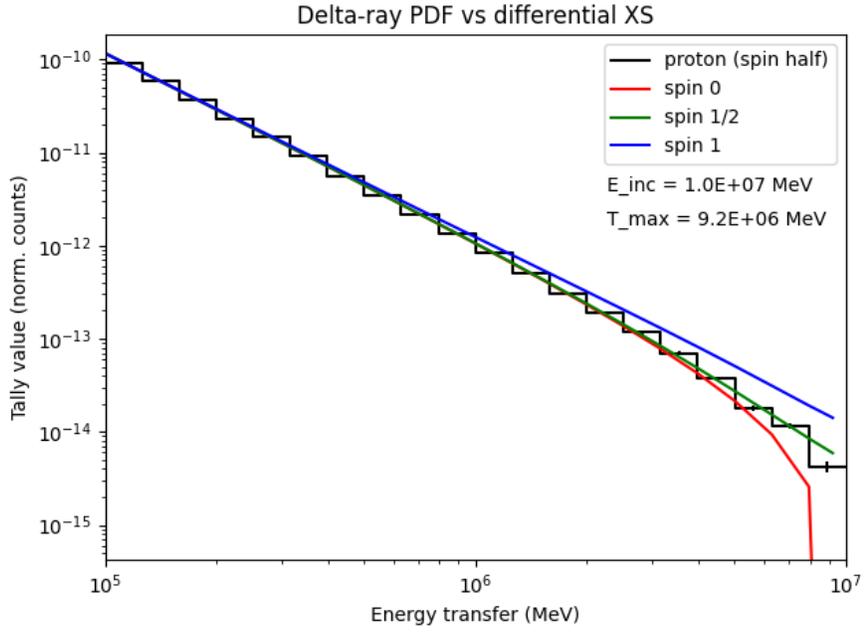


Figure 2: δ -ray production in MCNP by 10-TeV protons.

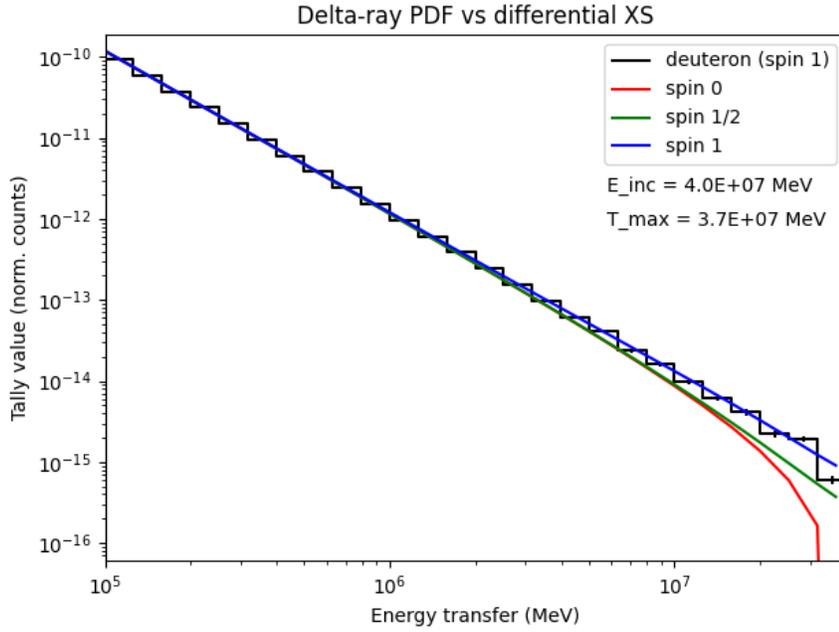


Figure 3: δ -ray production in MCNP by 40-TeV deuterons.

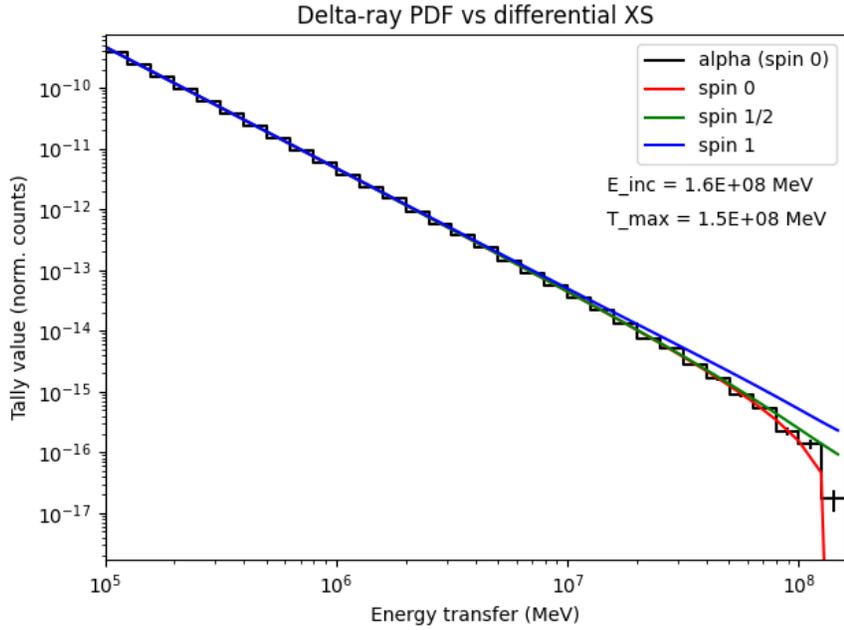


Figure 4: δ -ray production in MCNP by 160-TeV alpha particles.

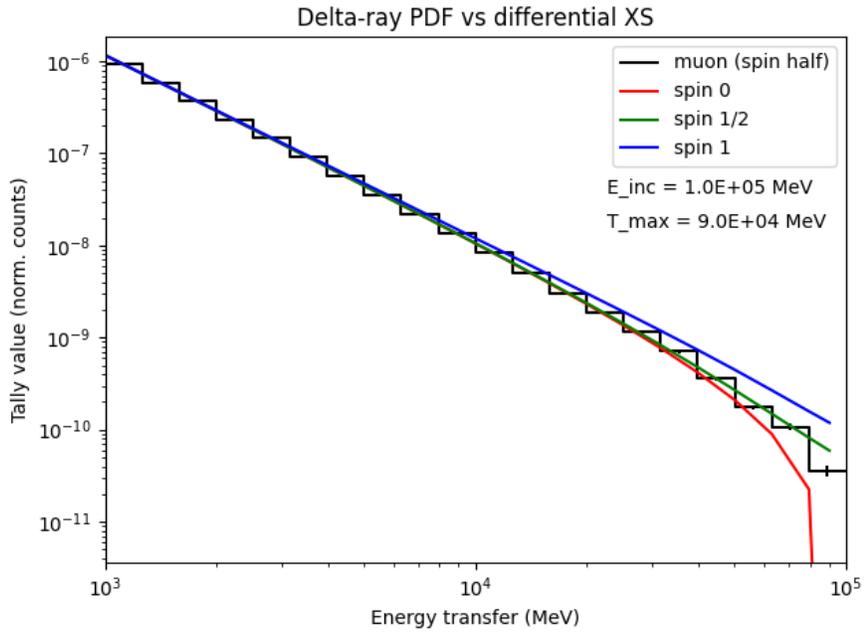


Figure 5: δ -ray production in MCNP by 100-GeV negative muons.

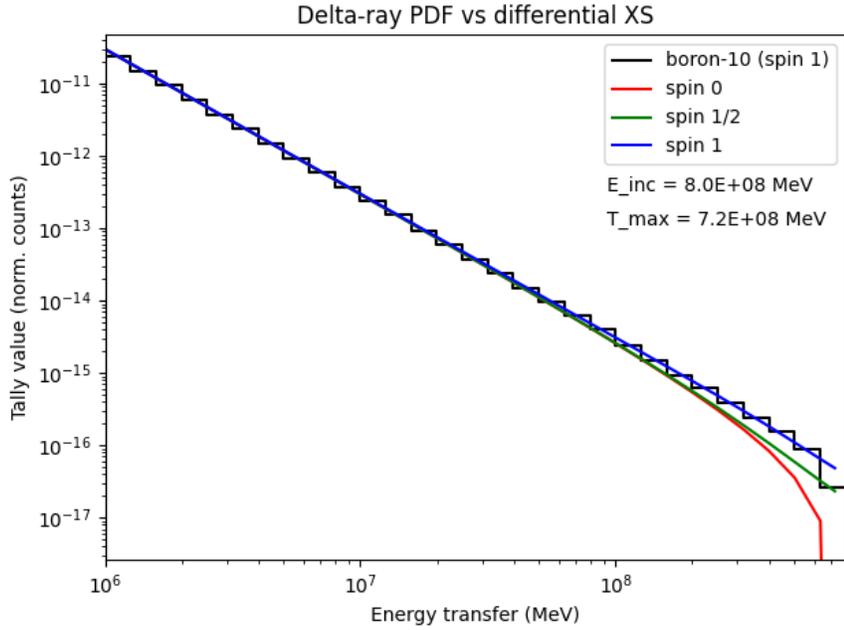


Figure 6: δ -ray production in MCNP by 800-TeV boron-10 ions.

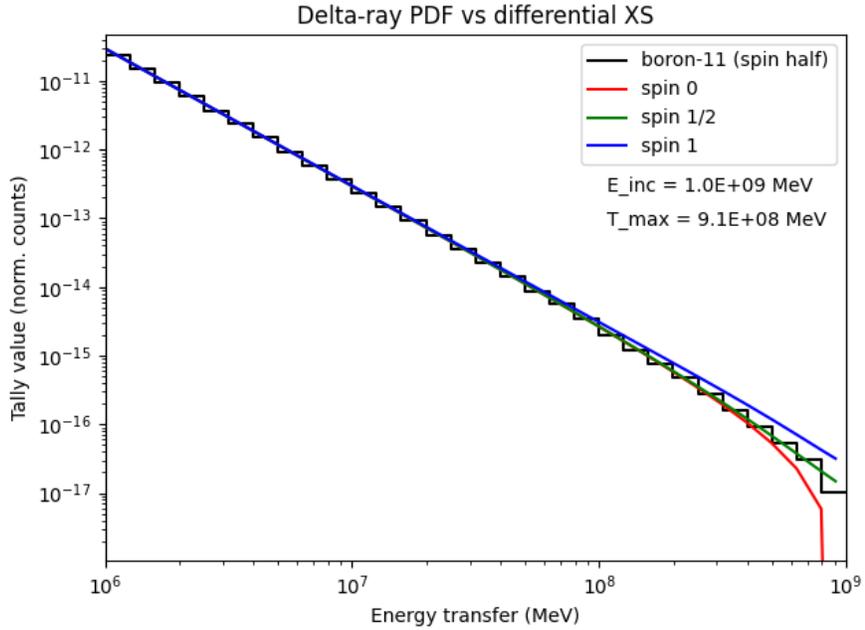


Figure 7: δ -ray production in MCNP by 1000-TeV boron-11 ions.

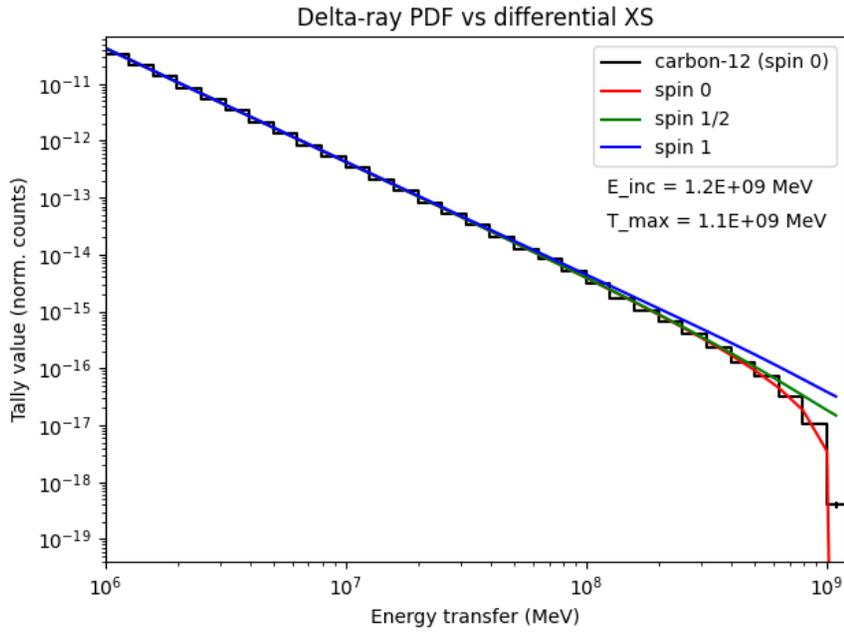


Figure 8: δ -ray production in MCNP by 1200-TeV carbon-12 ions.

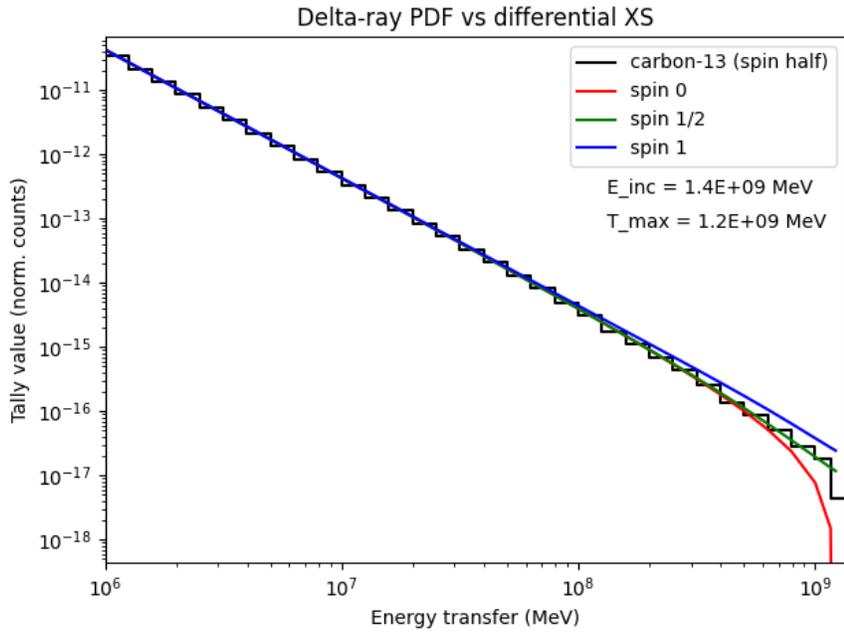


Figure 9: δ -ray production in MCNP by 1350-TeV carbon-13 ions.

On the topic of verification, note that the amended δ -ray production code passes the pre-existing set of 8 regression tests, aside from statistical divergences due to the improved rejection sampling algorithm and corrections to proton-induced δ -ray production due to the corrected use of E_{tot} . These pre-existing tests will remain in the MCNP regression testing suite, supplemented by verification of the new high-energy, spin-dependent functionality.

To support these tests, a new 18th parameter was added to the `PHYS` card for heavy charged particles, `drnok`, which allows scaling of the δ -ray yield by a specified factor. In these tests, the value was used to increase the yield of high-energy electrons to construct plots similar to those following, but the `drnok` option could just as easily be used to reduce the number of low-energy δ -rays generated. A further modification to implement energy biasing of the δ -rays is left for future development.

3.3 Validation

The validation work for “low” energies (< 1 GeV) is contained in [2] and is unaffected by the current work. Validation of the current work will require locating experimental data or other comparable modeling in the \geq TeV energy range, which the author so far has not located. Therefore, at present the validation effort remains a topic of future work.

4 Conclusion

The δ -ray production routine in the MCNP code has been updated to correctly hand spin-dependent contributions at very high incident energies. This work extends the previous formulation for spin-1/2 particles from protons to all spin-1/2 particles and nuclei, and adds a treatment for spin-1 particles (i.e., deuterons) and nuclei. The code changes also include minor bug fixes, feature improvements, and modernization/cleanup efforts. Verification tests confirm the correct implementation of the new spin-dependent terms, which reproduces the expected energy transfer probability distribution. Validation of these physics is a subject for future investigation pending the availability of experimental or theoretical data on which such a validation can be based.

A remaining future work item is the addition of energy biasing to the production of δ -rays (and ideally knock-on electrons as well). This is a desirable addition, since the energy distribution of δ -ray/knock-on electrons is heavily skewed towards the lower energies, while the higher energies are usually of greatest interest for transport calculations.

References

- [1] Judith F. Briesmeister et al. MCNPTM—A General Monte Carlo N-Particle Transport Code. Technical Report LA-12625-M, Los Alamos National Laboratory, Los Alamos, NM, USA, March 1997. Code Version 4B.
- [2] Casey Alan Anderson, Gregg Walter McKinney, James Robert Tutt, and Michael R. James. Delta-ray Production in MCNP 6.2.0. Technical Report LA-UR-16-28498, Los Alamos National Laboratory, Los Alamos, NM, USA, 2017. URL <http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-16-28498>.
- [3] Bruno Benedetto Rossi. *High-Energy Particles*. Prentice-Hall, Inc., Englewood Cliffs, NJ, USA, 1952.
- [4] Anwar Kamal. *Nuclear Physics*. Springer Berlin, Heidelberg, Germany, 2014. doi: 10.1007/978-3-642-38655-8.
- [5] M. J. Berger, M. Inokuti, H. H. Anderson, H. Bichsel, J. A. Dennis, D. Powers, S. M. Seltzer, and J. E. Turner. Stopping Powers for Electrons and Positrons. Technical Report ICRU-37, International Commission on Radiation Units and Measurements (ICRU), Bethesda, MD, USA, December 1984. URL <https://journals.sagepub.com/toc/crub/os-19/2>.