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# An Update to the Electron/Photon/Relaxation Data Library ACE Format Description for MCNP6

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**Abstract** Release versions of MCNP6 have included new electron-photon-relaxation data and single-event electron transport physics. The first released version of these data, called EPRDATA12, has been previously documented, but the succeeding release called EPRDATA14 required changes to the data file format which have not been documented. This report addendum documents the additional parameters and data in EPRDATA14 which are also relevant for upcoming future electron-photon-relaxation data file releases.

## 1 Introduction

The Electron-Photon-Relaxation ACE library file format was introduced with the release of MCNP6.1 to improve the photon-electron transport and enable the implementation of a new single-event method for electron transport [1]. The library file provided with this code release, EPRDATA12, has been documented previously [2]. However, the MCNP6.2 code version released with a new library file, EPRDATA14 [3], which contained several additions to the format that have not yet been documented outside of data processing codes. This report addendum is intended to provide the documentation of these format additions which are necessary to load the EPRDATA14 library and upcoming future releases.

## 2 Updates to Contents of an Electron-Photon-Relaxation Data Table

Changes are described in reference to Tables 1–4 of [2], to provide an easy point of reference to compare the EPRDATA12 and EPRDATA14 formats.

### 2.1 Changes to Table 1. Definition of Elements in the NXS array.

- NXS(6) = $\{1, 3\}$: New format flag. NXS(6) = 1 indicates the EPRDATA12 format. NXS(6) = 3 indicates the EPRDATA14 and later format with the changes described herein.
- NXS(13) = $N_{inc}$: Number of points in the tabulated photon incoherent form factor.
- NXS(14) = $N_{coh}$: Number of points in the tabulated photon coherent form factor.

### 2.2 Changes to Table 2. Definition of Elements in the JXS array.

- JXS(2): Location of photon incoherent form factors.
- JXS(3): Location of photon coherent form factors.

While these values retain the same definition in the newer format version, the calculations given for $N_{inc}$ and $N_{coh}$ (i.e., $N_{inc} = [JXS(3) - JXS(2)]/2$ and $N_{coh} = [JXS(4) - JXS(3)]/3$) are not guaranteed to hold and are superseded by the values of NXS(13) and NXS(14), respectively. While the reason for this change has never been explicitly documented, presumably this is done to allow for additional detail in the form factor data for future iterations of EPRDATA libraries.

- JXS(27): Location of additional electron elastic cross sections.

EPRDATA14 includes two new forms of the electron elastic cross sections: transport-corrected cross sections, and total cross sections including small-angle scattering [3].

### 2.3 Changes to Table 3. (Sub)Blocks within the Second Block of Data.

- The LPIPS block, beginning at JXS(8) and containing the probabilities of interaction for shells for the Doppler broadening model, now gives these probabilities as a cumulative distribution [3], following the convention established in the **mcplib63** and **mcplib84** libraries. Formerly, in the EPRDATA12 library this block was treated as differential data. This has no effect on running MCNP6 itself, which is capable of distinguishing between cumulative and differential forms, but is important for any code seeking to interpret EPRDATA14 and later EPR libraries.

- A new block, here named ELASX[1], begins at JXS(27) and contains transport-corrected and total (including small-angle scattering) cross sections for electron elastic scattering. These additional elastic cross sections fall on the same common energy grid as the cross sections contained in block ESZE located at JXS(19).

### 2.4 Changes to Table 4. Map of the Contents of the Second Block of Data.

The end of the second block of data consists of two segments of $N_e$ elastic cross section values falling on the same common energy grid as the other electron cross sections in block ESZE.

Table 1: Transport-corrected elastic cross section contents in the second data block.

| | | |
|---|---|---|
| $\sigma_{elas,tr}(1)$<br>$JXS(27)$ | Electron transport-corrected<br>elastic cross section | ... $\sigma_{elas,tr}(N_e)$<br>$JXS(27)+N_e-1$ |

Table 2: Total elastic cross section contents in the second data block.

| | | |
|---|---|---|
| $\sigma_{elas,tot}(1)$<br>$JXS(27)+N_e$ | Electron total elastic<br>cross section | ... $\sigma_{elas,tot}(N_e)$<br>$JXS(27)+2\cdot N_e-1$ |

Note that the electron elastic cross section data ($\sigma_{elas}$ contained at $JXS(19)+2\cdot N_e$ through $JXS(19)+3\cdot N_e-1$ are properly termed the large-angle elastic scattering cross section, distinct from the total elastic cross section which includes contributions from small-angle scattering. The difference is significant chiefly at high electron energies where the elastic scattering angular distribution is strongly forward-peaked. Finally, the transport-corrected cross section is defined as $\sigma_{elas,tr}=\sigma_{elas}(1-\bar{\mu})$ where $\bar{\mu}=\langle\cos\theta\rangle$ is the average scattering cosine.

## 3 Conclusion

The report addendum documents changes in the electron-photon-relaxation ACE library data file format for EPRDATA14 and later EPR library versions. As an addendum to the earlier documentation report [2], this information achieves the knowledge transfer necessary for the MCNP Development Team and Nuclear Data Team at LANL to continue working with this data format, and enables other users of the EPRDATA libraries to parse the data files for their own understanding and analysis.

[1]Note that the name of the block is arbitrary and has no bearing on interpretation of the EPRDATA file. Here, we choose "ELASX" to represent "elastic, extended".

# References


[1] H. Grady Hughes, III. Recent developments in low-energy electron/photon transport for MCNP6. *Progress in Nuclear Science and Technology*, 4:454–458, 2014.

[2] H. Grady Hughes III. An electron/photon/relaxation data library for MCNP6. Technical Report LA-UR-13-27377 (Rev. 1), Los Alamos National Laboratory, Los Alamos, NM, United States, September 2015.

[3] H. Grady Hughes III. Improvements in electron-photon-relaxation data for MCNP6. Technical Report LA-UR-16-20840, Los Alamos National Laboratory, February 2016.