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Quick-Start Guide to Low-Energy Photon/Electron Transport in MCNP6

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ABSTRACT

A new feature of the particle transport code MCNP6 is the ability to transport photons and electrons below the traditional lower energy limit of 1 keV. Full discussions of this new capability, its supporting data, and its methods, especially the new single-event electron transport, a data-based method that replaces condensed-history in selected energy ranges, will appear in various publications in the near future. In this document, we present a few practical points that users of the new feature will need to know.

I. DATA MATTERS.

There are three separate aspects of the new electron/photon capability: extension of photon transport to lower energies, enhancement of the treatment of atomic relaxation processes, and introduction of a single-event electron transport method allowing electron transport at lower energies. All three of these features require new data, based on release 8 of ENDF/B VI. These data are provided in the new library eprdata12 (meaning Electron-Photon-Relaxation DATA), which contains ACE-format data tables (with the identifier .12p) for the first 100 elements. These tables are in a newly-developed format that includes not only photon transport data as in previous libraries such as mcplib04, but also complete relaxation data and electron interaction data as well. This new format is designed to work with MCNP6, but is not suitable for use with MCNP5 or MCNPX. Since these new tables may not be the default in any particular installed system, they should be requested on the material cards, either explicitly as here:

```
m1  1000.12p  2    8000.12p  1
```

or implicitly by using the plib specifier:

```
m1  1000.03e  2    8000.03e  1   plib 12p
```

The xsdir lines for eprdata12 are located in the new default xsdir_mcnp6.1 file in the MCNP6 data directory (…/MCNP_DATA/) in the MCNP6 distribution. Note that the new data are only for zero-temperature atomic targets, so temperature, condensed state, and molecular effects are not yet treated for photons or electrons in MCNP6.

II. PROBLEM MODE

Since the data tables required for the new methods are identified as .12p in ZAID specification, they are treated as photon data (albeit in a new format). Therefore transporting electrons to lower energies (or using the single-event method at any energy) requires the problem to have access to photon data, and the problem mode should be at least

```
mode p e
```

even if the user is not interested in the photon transport. The reverse is not required: if the user is only interested in photons, "mode p" is sufficient.

III. STRAGGLING MODE

The single-event electron transport method has been installed in the part of the code that works with the most detailed straggling logic for the electron energy loss. Therefore one must select dbcn(18)==2 to use the single-event method. This can be explicit, as in

```
dbcn  17j  2.
```

But this choice is now the default in MCNP6, so it is only necessary to avoid setting dbcn(18) to 0 or 1.

IV. ENERGY CUTOFFS

It is now possible to transport photons and electrons below 1 keV, but the default energy cutoff for both particle types is still 1 keV. Therefore to go to lower energies, the user must explicitly request lower cutoffs. For example to transport photons down to 10 eV and electrons down to 20 eV one would use cards like these:

```
cut:p  j  1.0e-05  $  10 eV expressed in MeV.
cut:e  j  2.0e-05  $  20 eV.
```

Without these cards, the code would set the cutoffs to the default 1.0e-03 MeV.

V. WHERE TO START SINGLE-EVENT TRANSPORT

By default MCNP6 continues to transport electrons by the condensed-history algorithms down to 1 keV, and switches to the new single-event method below that energy. User control of this energy boundary has been provided as the optional 15-th entry on the phys:e card. For example, to use condensed-history down to 10 keV and single-event transport below that energy, one could use a card like

```
phys:e   100.  13j  0.01  $  switch to single-event at 10 keV.
```

This raises the interesting possibility of attempting to run even medium-energy or high-energy problems entirely with single-event transport. This has not yet been explored.

On the other hand, the switch to single-event transport should never be lower than 1 keV, since condensed-history methods rapidly collapse below their traditional lower limit. There is not yet a fatal error for this attempt, but there will be in future versions of the code.

VI. GOING TOO LOW WITH ELECTRONS

The new lower limits for energy cutoffs are 1 eV for photons and 10 eV for electrons. For very low-energy electrons however, a physics-based practical difficulty can arise: one tends to run out of energy-loss-inducing processes. Bremsstrahlung is still present, but is completely dominated by electron elastic scattering, which has no energy loss. Electroionization, which is an important energy-loss channel, vanishes below the binding energy of the least-bound shell given in the data. Whether that event occurs above or below 10 eV is element-dependent. Excitation, another energy-loss process, can also vanish at some energy above 10 eV, depending on the element. The result of all this is that there can be a small energy range just above 10 eV in which the electron can no longer lose energy and only experiences a large number of elastic scatterings. Coupled with the very short step sizes that characterize the electron transport at low energies, the effect is that the transport suddenly grinds nearly to a halt because an electron has become trapped, taking a huge number of small steps with little or no opportunity to lose energy. Such an electron is very close to the energy cutoff, but cannot get there because it is spending all its time in elastic scatter. Some insight into these cross-section-related matters can be gained by examining Fig. 1 on the last page of this document. Preliminary practical experience indicates that setting the electron cutoff no lower than about 12 eV may be sufficient to avoid this occasional effect. Again note that the new data are only for cold atomic targets, and that potential future treatments of molecular and other low-energy physics will significantly alter this discussion.

VII. SUMMARY

To summarize this short user guide as succinctly as possible:

1. Ask for the right data tables on the material cards.
2. Use "mode p e" to make data available to electrons.
3. Make sure that dbcn(18)==2 for single-event transport.
4. Ask explicitly for energy cutoffs below 1 keV.
5. The 15-th entry on the phys:e card can control the start of single-event transport.
6. Be careful about going all the way down to 10 eV for electrons.

Figure 1. ENDF/B VI.8 electron cross sections for atomic nitrogen, showing elastic, excitation, bremsstrahlung, and ionization by individual shells.