New Electron-Photon-Relaxation Data for MCNP6: Verification and Validation

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Abstract

After the initial release of the first production version of MCNP6 and its subsequent beta release, the extended electron-photon-relaxation capabilities of the code have continued to be developed. With the availability of newer data, several enhancements and corrections to the methods have been installed into the code. In this paper we discuss these improvements, including the development of three distinct approaches to sampling electron elastic scattering, the correction of an earlier data resolution problem, and a few formal corrections to the earlier ACE data file. We also describe some of our plans for verification and validation testing of the new capabilities.
Existing data: EPRDATA12 / MCNP6.1

- Extended energy ranges
- XS: incoherent, coherent, photoelectric, pair production
- Extended scattering form factors
- Old-style fluorescence and Auger
- Heating numbers
- Compton Doppler broadening
- Shell-wise photoelectric cross sections
- Detailed atomic relaxation (for photons and SE electrons)
Energy Ranges for Transport

- **Photons**: 1 eV – 100 GeV
- **Condensed-history electrons**: 1 keV – 1 GeV
- **Single-event electrons**: 10 eV – 1 keV or above, potentially: 10 eV – 100 GeV
Existing data: EPRDATA12 / MCNP6.1

- XS: elastic, bremsstrahlung, excitation, electroionization
- Shell-wise electroionization cross sections
- Excitation average energy-loss table
- Large-angle elastic angular distributions
- Knock-on electron energy distributions
- Bremsstrahlung photon energy distributions
- Bremsstrahlung average energy-loss table
New data: EPRDATA14 / MCNP6 6.2

- **Sources:** EPICS2014 — ENDF and EEDL
- **Two variations on electron elastic scattering**
  - Transport-corrected cross section
  - Total cross section (large-angle + in-peak)
- **Tabulated elastic angular distributions better resolved**
- **Average bremsstrahlung energy-loss corrected**
  - Now consistent with excitation energy-loss table
  - Applies to large-angle elastic scattering
  - Not yet used by MCNP6
- **Compton Doppler broadening data bug pre-corrected**
  - Relevant to MCNP6
  - Primarily a matter of aesthetics
Bremsstrahlung "Energy Loss" in Iron

Energy loss (MeV) vs. Electron energy (MeV)

- **Diagonal**
- **26000.12p**
- **26000.14p**
195 keV Photon Backscatter Off Iron Target

No Doppler .84p
Doppler .04p
Doppler .84p
Three kinds of electron elastic cross section

- Large-angle elastic cross section \( \sigma_{LA}(E) \)
  - Restricted to scattering with \( \Delta \mu > 10^{-6} \)
  - Rapid fall-off at high energy
  - Already available in EPRDATA12

- Transport-corrected elastic cross section \( \sigma_{Tran}(E) \)
  - Preserves mean deflection angle
  - Smaller than \( \sigma_{LA}(E) \) or \( \sigma_{Tot}(E) \), i.e. faster execution
  - Simpler sampling: if \( \sigma_{Tran} \) selected, call isos

- Total elastic cross section \( \sigma_{Tot}(E) = \sigma_{LA}(E) + \sigma_{peak}(E) \)
  - If \( \sigma_{LA} \) selected, sample from tabulated angular distribution,
  - else sample from \( \frac{d\sigma}{d\mu} = \frac{A}{(\eta+1-\mu)^2} \)
Electron Cross Sections in Iron

- Total elastic
- Large-angle elastic
- Transport-corrected elastic

Cross section (barns) vs. Electron energy (MeV)

Slide 9
Electron Cross Sections in Iron

- Total elastic
- Large-angle elastic
- Transport-corrected elastic
- Excitation
- Ionization
- Bremsstrahlung

Cross section (barns) vs. Electron energy (MeV)
User interface for elastic cross sections

PHYS:E 12 entries mode_electron_elastic other entries

mode_electron_elastic = -1 : no elastic scattering
= 0 : large-angle elastic (default)
= 1 : transport elastic
= 2 : total elastic

Comments, warnings, fatal errors as appropriate.
The plotter knows — MT values:

504 or -1 Photon Incoherent Cross Section
502 or -2 Photon Coherent Cross Section
522 or -3 Photoelectric Total Cross Section
516 or -4 Photon Pair Production Cross Section
501 or -5 Photon Total Cross Section
-6 Average Photon Heating Numbers
-7 Electron Large Angle Elastic Cross Section
-8 Electron Bremsstrahlung Cross Section
-9 Electron Excitation Cross Section
-10 Electro-Ionization Cross Section
-11 Electron Total Cross Section (with Large Angle Elastic)
-12 Electron Bremsstrahlung Mean Energy Loss
-13 Electron Excitation Mean Energy Loss
-14 Electron Elastic Transport Cross Section
-15 Electron Total Elastic Cross Section
-16 Electron Total Cross Section (with Transport Elastic)
-17 Electron Total Cross Section (with Total Elastic)
Subshell photoelectric cross sections:

<table>
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<tr>
<th>Subshell</th>
<th>Symbol</th>
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<tr>
<td>L1</td>
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<tr>
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<tr>
<td>L3</td>
<td>537 or -104</td>
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<tr>
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<td>N4</td>
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<td>546 or -113</td>
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<tr>
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<td>549 or -116</td>
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<tr>
<td>O2</td>
<td>550 or -117</td>
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<tr>
<td>O3</td>
<td>551 or -118</td>
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<td>O4</td>
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<td>P11</td>
<td>567 or -134</td>
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<tr>
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<td>568 or -135</td>
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<tr>
<td>Q2</td>
<td>569 or -136</td>
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<tr>
<td>Q3</td>
<td>570 or -137</td>
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Subshell electroionization cross sections:

<p>| | | | | |</p>
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<td>-201</td>
<td>K</td>
<td>-202</td>
<td>L1</td>
<td>-203</td>
</tr>
<tr>
<td>-205</td>
<td>M1</td>
<td>-206</td>
<td>M2</td>
<td>-207</td>
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<tr>
<td>-209</td>
<td>M5</td>
<td>-210</td>
<td>N1</td>
<td>-211</td>
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<td>-213</td>
<td>N4</td>
<td>-214</td>
<td>N5</td>
<td>-215</td>
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<tr>
<td>-217</td>
<td>O1</td>
<td>-218</td>
<td>O2</td>
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</tr>
<tr>
<td>-237</td>
<td>Q1</td>
<td>-238</td>
<td>Q2</td>
<td>-239</td>
</tr>
</tbody>
</table>
Old MCNP Fluorescence Model

Z = 1 – 11: no fluorescence

Z = 12 – 19: 1 line  
< K ← L2, K ← L3 >

Z = 20 – 30: 3 lines  
K ← L2, K ← L3
< K ← M2, K ← M3, K ← M4 >

Z = 31 – 36: 4 lines  
K ← L2, K ← L3
< K ← M2, K ← M3, K ← M4 >
< L1, L2, L3 > ← < higher lines >

Z = 37 – 100: 5 lines  
K ← L2, K ← L3
< K ← M2, K ← M3, K ← M4 >
< K ← N2, K ← N3 >
< L1, L2, L3 > ← < higher lines >
Relaxation for $Z = 13$ in EPRDATA libraries

K from L2 (radiative) K from L3 with M1 L1 from M1 with M1
K from L3 (radiative) K from L3 with M2 L1 from M1 with M2
K from M2 (radiative) K from L3 with M3 L1 from M1 with M3
K from M3 (radiative) K from M1 with M1 L2 from L3 (radiative)
K from L1 with L1 K from M1 with M2 L2 from M1 (radiative)
K from L1 with L2 K from M1 with M3 L2 from M3 (radiative)
K from L1 with L3 L1 from L2 (radiative) L2 from M1 with M1
K from L1 with M1 L1 from L3 (radiative) L2 from M1 with M2
K from L1 with M2 L1 from M2 (radiative) L2 from M1 with M3
K from L1 with M3 L1 from M3 (radiative) L3 from M1 (radiative)
K from L2 with L2 L1 from L2 with M1 L3 from M2 (radiative)
K from L2 with L3 L1 from L2 with M2 L3 from M3 (radiative)
K from L2 with M1 L1 from L2 with M3 L3 from M1 with M1
K from L2 with M2 L1 from L3 with M1 L3 from M1 with M2
K from L2 with M3 L1 from L3 with M2 L3 from M1 with M3
K from L3 with L3 L1 from L3 with M3
Resolving the approach to the elastic peak

Example: 21.25 MeV in Lead

<table>
<thead>
<tr>
<th>26000.12p</th>
<th>26000.14p</th>
</tr>
</thead>
<tbody>
<tr>
<td>-</td>
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</tr>
<tr>
<td>9.99997000000E-01</td>
<td>2.2476624998E-01</td>
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<td>-</td>
<td>-</td>
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<tr>
<td>-</td>
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<tr>
<td>9.99999000000E-01</td>
<td>5.8426678339E-01</td>
</tr>
<tr>
<td>1.00000000000E+00</td>
<td>1.00000000000E+00</td>
</tr>
</tbody>
</table>
V&V Candidate List

- Lockwood et al. Energy deposition in extended media
- Aubry et al. Dose calculations
- Ross et al. Thin-foil multiple scattering
- Tabata et al. Charge deposition
- Gierga and Adams
  - Faddegon et al. Bremsstrahlung
  - O’Dell et al. Bremsstrahlung
  - Starfelt and Koch Bremsstrahlung
  - Ebert et al. Transmission and backscatter
  - MCNP transport parameter studies
A simple scattering test

15 MeV electrons

0.002835 cm gold foil
at 19.33 gm / cm\(^3\)

Calculate the angular distribution using MCNP6 with a variety of transport options.
Compare estep=13, =104, =208.  dbcn(90)=240

tally 11

xps 20930836
bin normed
runps = estep_13_240
dump 2
f Surface 1
d Flag/Dir 1
u User 1
s Segment 1
m Mult 1
c Angle *
e Energy 1
t Time 1

--- estep_13_240
--- estep_104_240
--- estep_208_240
 Compare estep=13, =104, =208. dbcn(90)=10000

file estep_13_10X --- tally 11

tally 11
*
exit 19097389
bin normed
runpts = estep_13_10X
dump 2
f Surface 1
d Flag/Dir 1
u User 1
s Segment 1
m Mult 1
c Angle 1
e Energy 1
t Time 1

--- estep_13_10X
--- estep_104_10X
--- estep_208_10X

Angle [mu]

Tally/standard/particle
Compare C. H., single (12p), and single (14p).
Approaching the elastic peak
Compare CH, Single loglog vs Single linlin

```
tally 11
s
nps 20930836
bin normed
runtpe = Condensed_History
dump 2
f Surface 1
d Flag/Dir 1
u User 1
s Segment 1
m Mult 1
c Angle 1
e Energy 1
t Time 1

Condensed_History
Single_Event_14p
Single_linlin_14p
```
Summary Points

• eprdata14 is enhanced over eprdata12.
  – Alternative approaches to electron elastic scattering.
  – Correction of an important numerical issue.

• MCNP6.2 will take advantage of eprdata changes.
  – New abilities in elastic scattering.
  – Improved resolution near the elastic peak.
  – Better attention to numerical aspects (e.g. interpolation).

• Preliminary testing is promising.

• Verification and validation testing is beginning.

• MCNP6.2 will be available “very soon.”