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

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Abstract

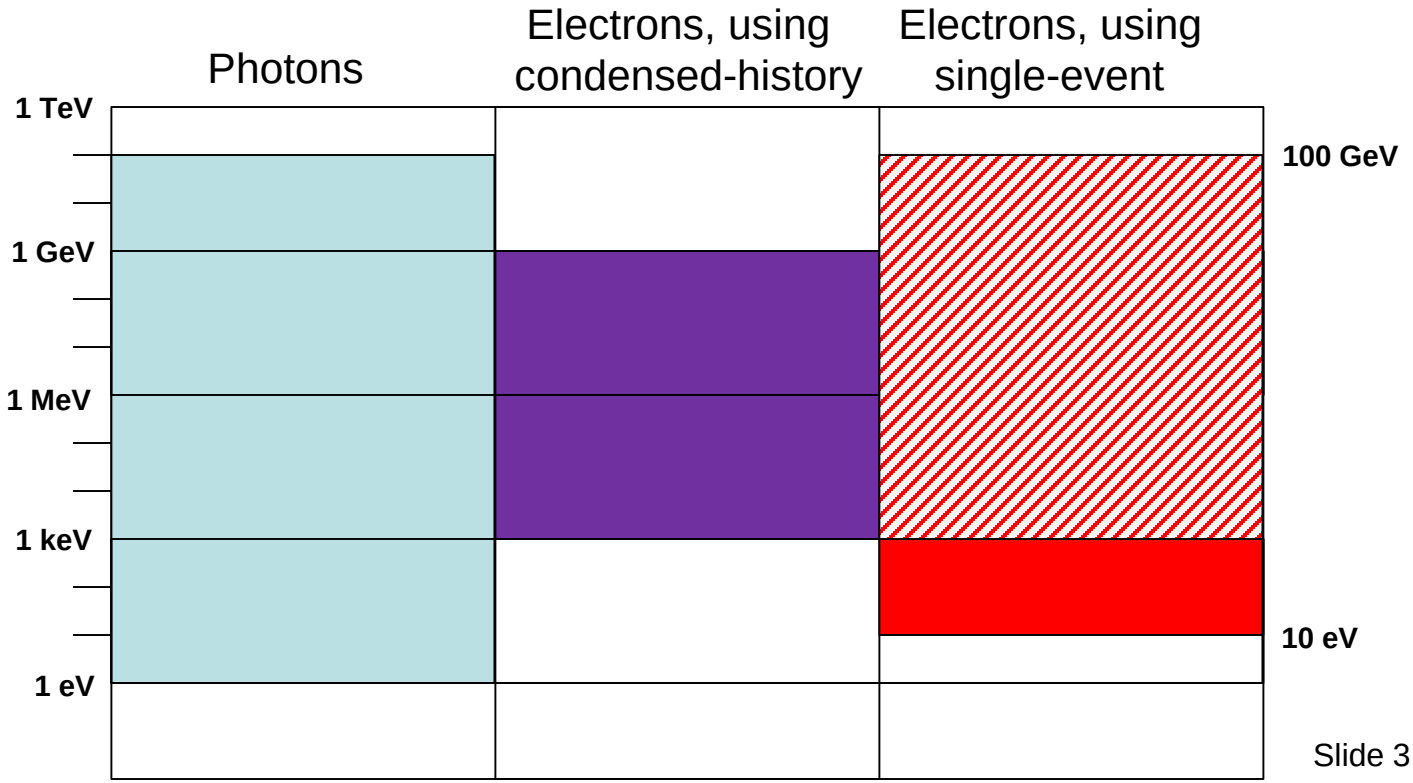
After the initial release of the first production version of MCNP6 and its subsequent beta release, the extended electron-photon-relaxation capabilities of the code have continued to be developed. With the availability of newer data, several enhancements and corrections to the methods have been installed 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 – 100GeV



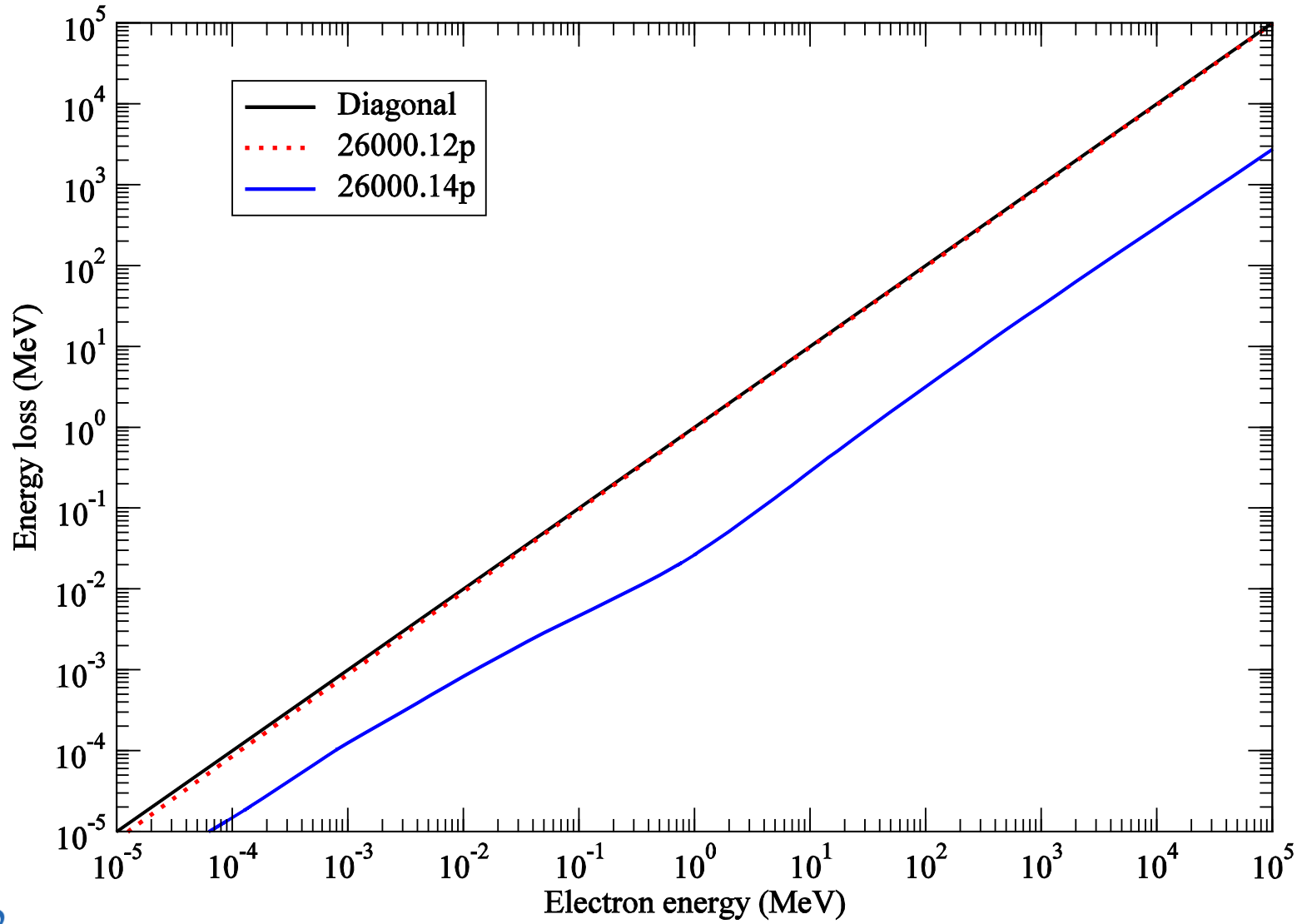
Existing data: EPRDATA12 / MCNP6.1

- 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

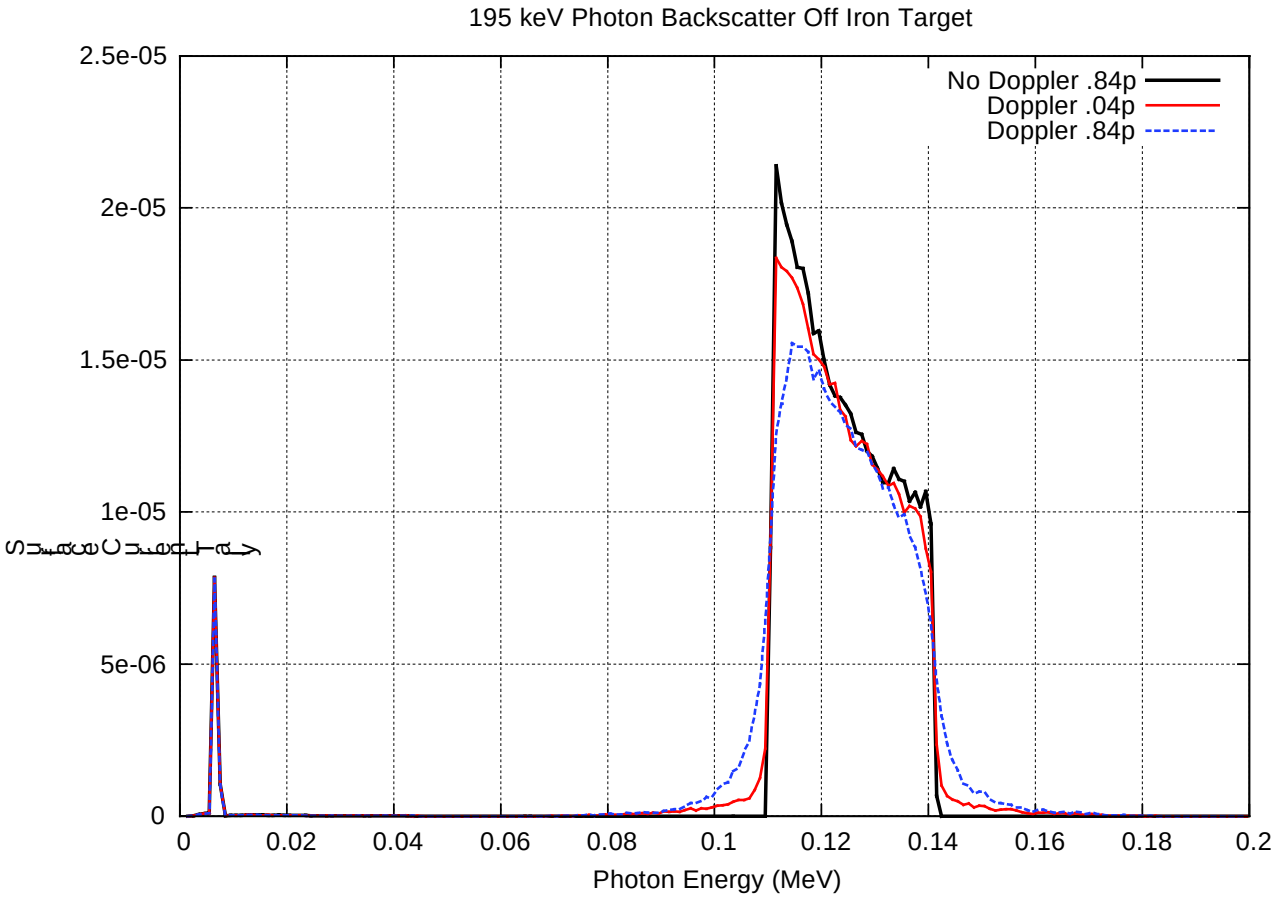
New data: EPRDATA14 / MCNP6 6.2

- 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



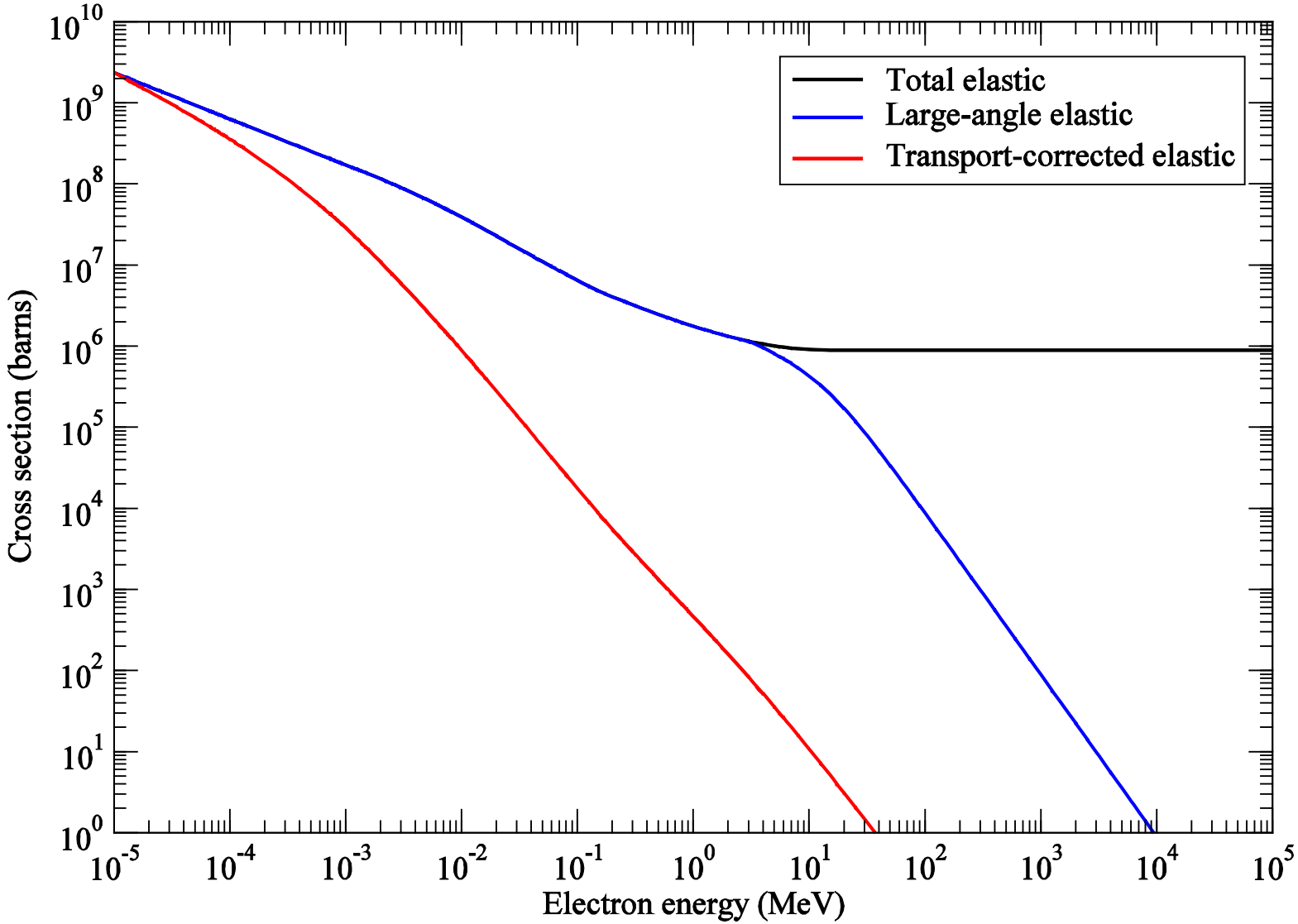
From Kiedrowski et al. LA-UR-12-00121



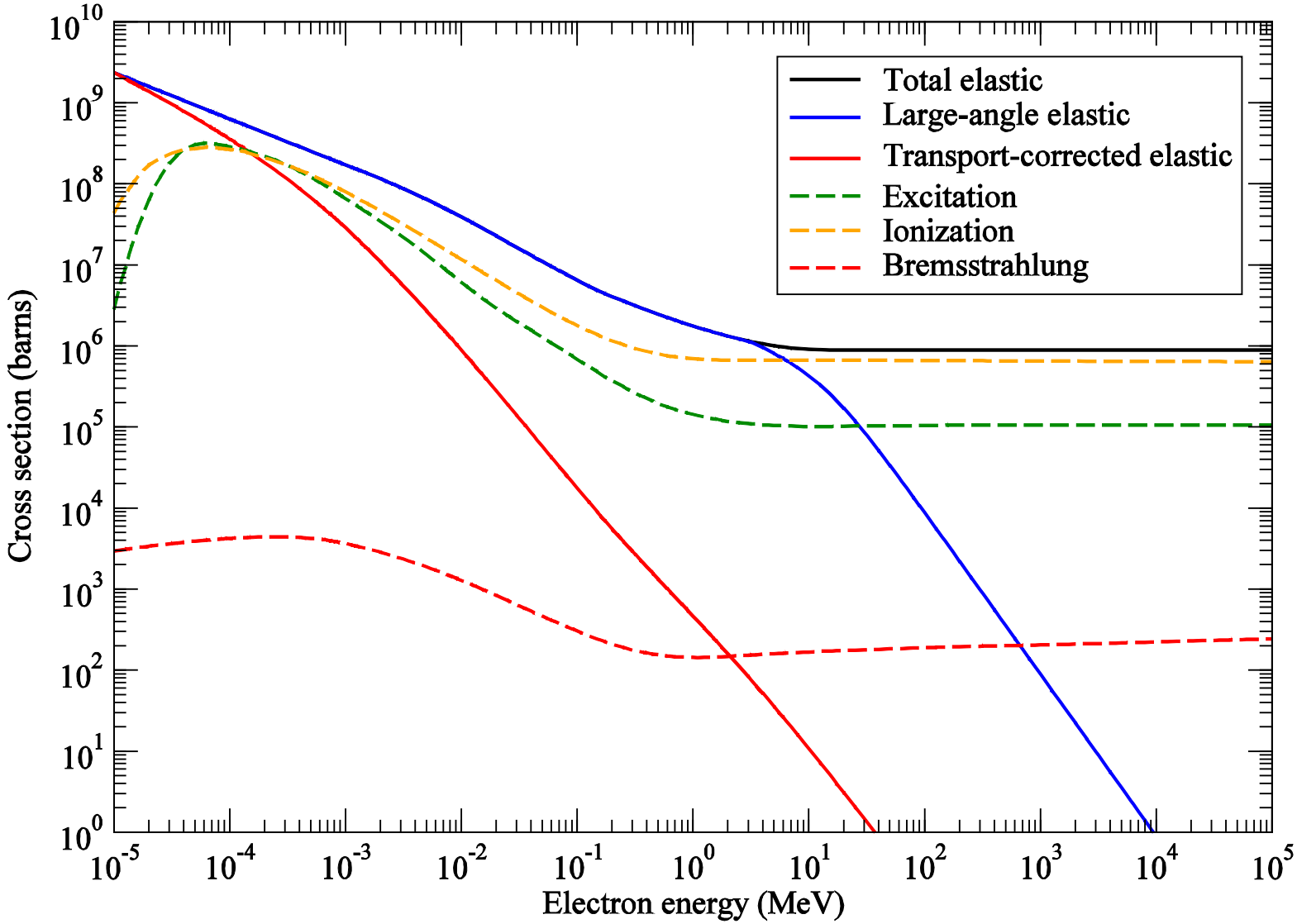
Three kinds of electron elastic cross section

- 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 σ_{Tran} selected, call isos
- Total elastic cross section $\sigma_{Tot}(E) = \sigma_{LA}(E) + \sigma_{peak}(E)$
  - If σ_{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



Electron Cross Sections in Iron



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:

534 or -101 K	535 or -102 L1	536 or -103 L2	537 or -104 L3
538 or -105 M1	539 or -106 M2	540 or -107 M3	541 or -108 M4
542 or -109 M5	543 or -110 N1	544 or -111 N2	545 or -112 N3
546 or -113 N4	547 or -114 N5	548 or -115 N6	549 or -116 N7
550 or -117 O1	551 or -118 O2	552 or -119 O3	553 or -120 O4
554 or -121 O5	555 or -122 O6	556 or -123 O7	557 or -124 O8
558 or -125 O9	559 or -126 P1	560 or -127 P2	561 or -128 P3
562 or -129 P4	563 or -130 P5	564 or -131 P6	565 or -132 P7
566 or -133 P8	567 or -134 P9	568 or -135 P10	569 or -136 P11
570 or -137 Q1	571 or -138 Q2	572 or -139 Q3	

Subshell electroionization cross sections:

-201 K	-202 L1	-203 L2	-204 L3
-205 M1	-206 M2	-207 M3	-208 M4
-209 M5	-210 N1	-211 N2	-212 N3
-213 N4	-214 N5	-215 N6	-216 N7
-217 O1	-218 O2	-219 O3	-220 O4
-221 O5	-222 O6	-223 O7	-224 O8
-225 O9	-226 P1	-227 P2	-228 P3
-229 P4	-230 P5	-231 P6	-232 P7
-233 P8	-234 P9	-235 P10	-236 P11
-237 Q1	-238 Q2	-239 Q3	

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 (radiative)
K from M2 (radiative)
K from M3 (radiative)
K from L1 with L1
K from L1 with L2
K from L1 with L3
K from L1 with M1
K from L1 with M2
K from L1 with M3
K from L2 with L2
K from L2 with L3
K from L2 with M1
K from L2 with M2
K from L2 with M3
K from L3 with L3
K from L3 with M1
K from L3 with M2
K from L3 with M3
K from M1 with M1
K from M1 with M2
K from M1 with M3
L1 from L2 (radiative)
L1 from L3 (radiative)
L1 from M2 (radiative)
L1 from M3 (radiative)
L1 from L2 with M1
L1 from L2 with M2
L1 from L2 with M3
L1 from L3 with M1
L1 from L3 with M2
L1 from L3 with M3
L1 from M1 with M1
L1 from M1 with M2
L1 from M1 with M3
L2 from L3 (radiative)
L2 from M1 (radiative)
L2 from M3 (radiative)
L2 from M1 with M1
L2 from M1 with M2
L2 from M1 with M3
L3 from M1 (radiative)
L3 from M2 (radiative)
L3 from M3 (radiative)
L3 from M1 with M1
L3 from M1 with M2
L3 from M1 with M3

Resolving the approach to the elastic peak

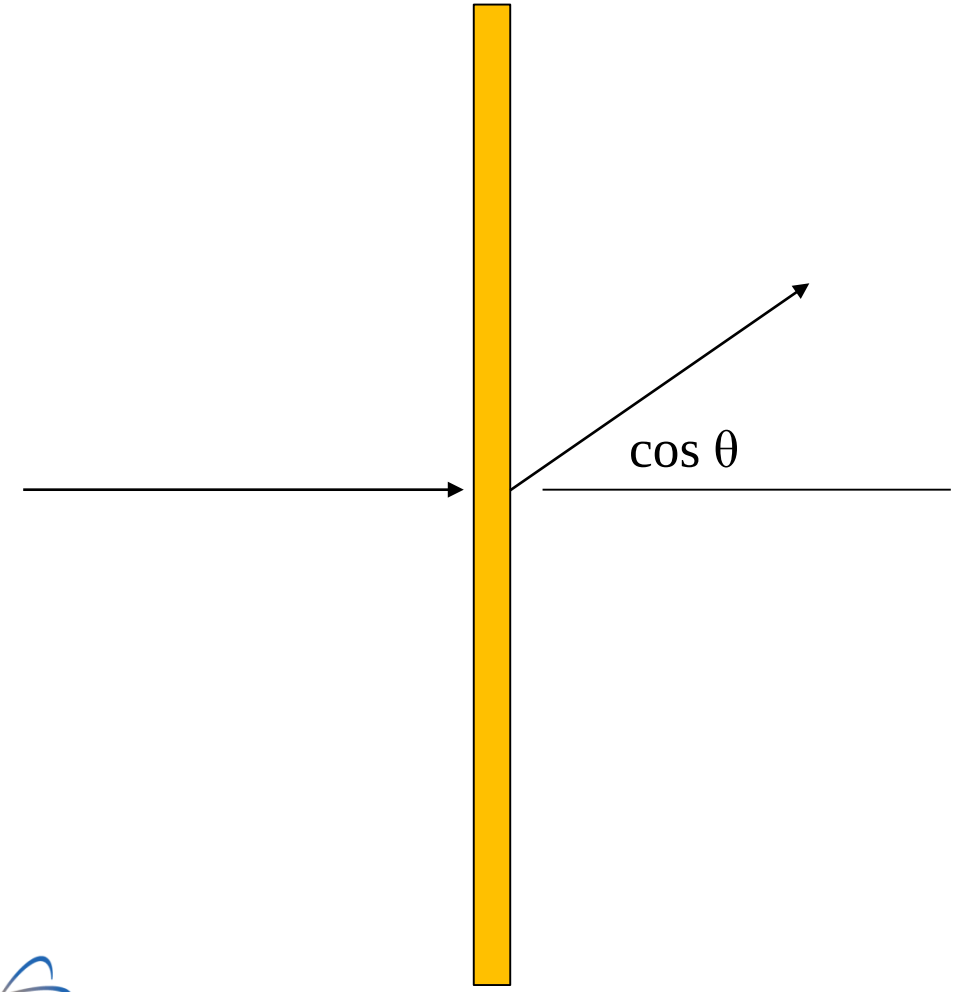
Example: 21.25 MeV in Lead

26000.12p		26000.14p	
-	-	9.9999650E-01	3.2630487E-01
9.9999700000E-01	2.2476624998E-01	9.9999710E-01	3.8934088E-01
-	-	9.9999760E-01	4.6400789E-01
-	-	9.9999800E-01	5.4795830E-01
9.9999800000E-01	3.3207649512E-01	9.9999830E-01	6.3374406E-01
-	-	9.9999860E-01	7.5199837E-01
-	-	9.9999880E-01	8.5821188E-01
9.9999900000E-01	5.8426678339E-01	9.9999900E-01	1.0000000E+00
1.0000000000E+00	1.0000000000E+00	-	-

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



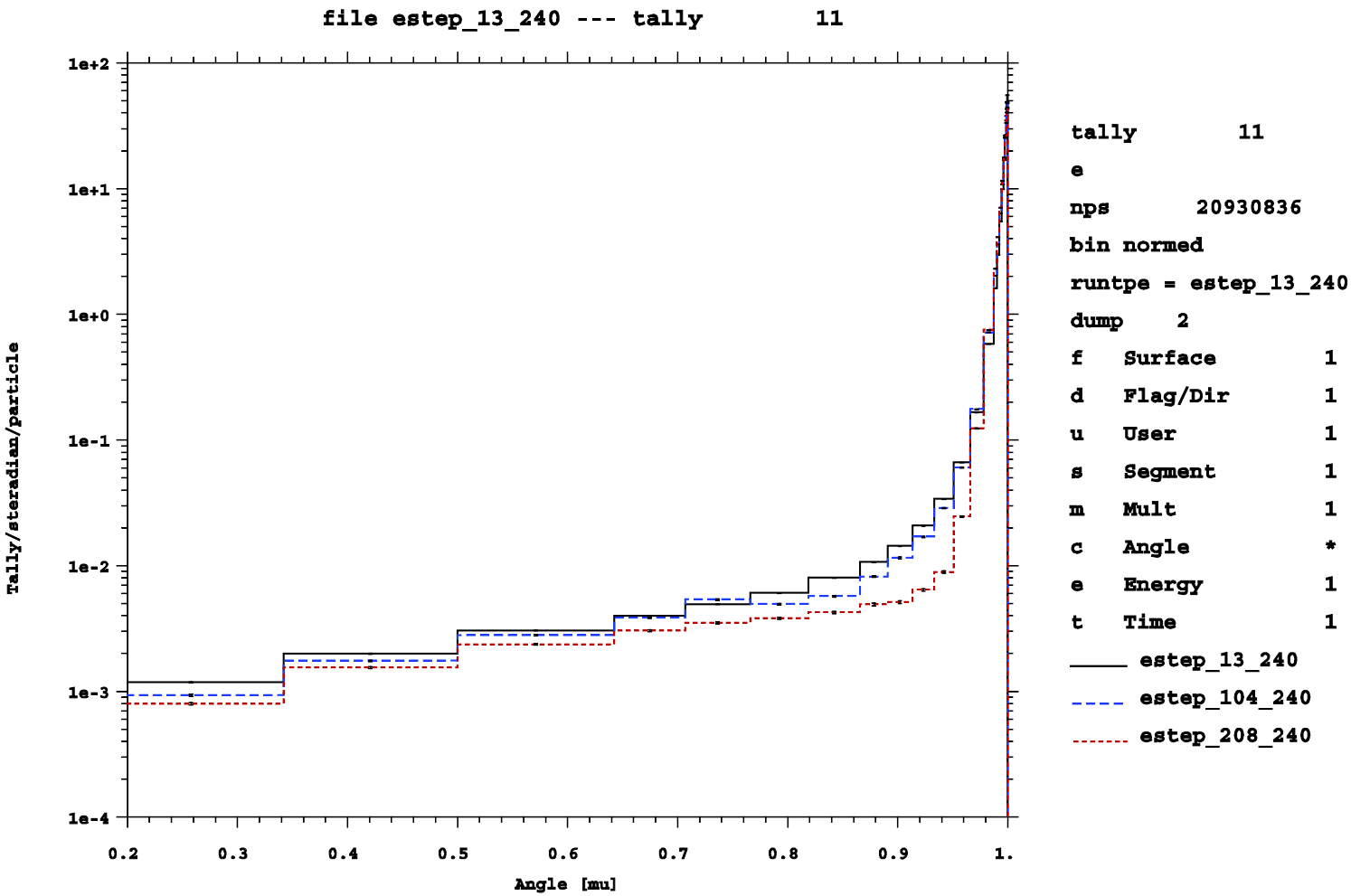
15 MeV electrons

0.002835 cm gold foil

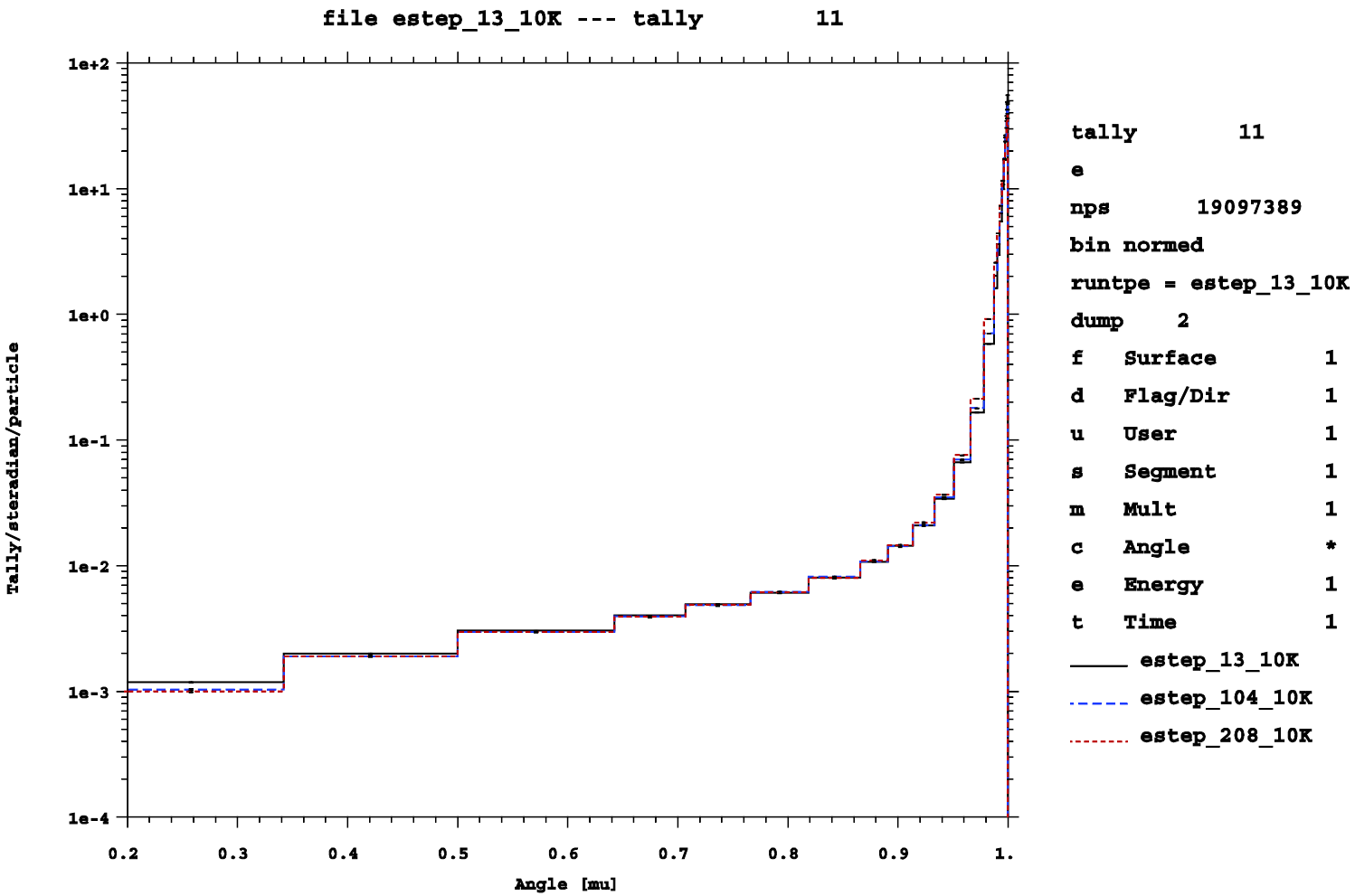
at 19.33 gm / cm^3

Calculate the angular distribution using MCNP6 with a variety of transport options.

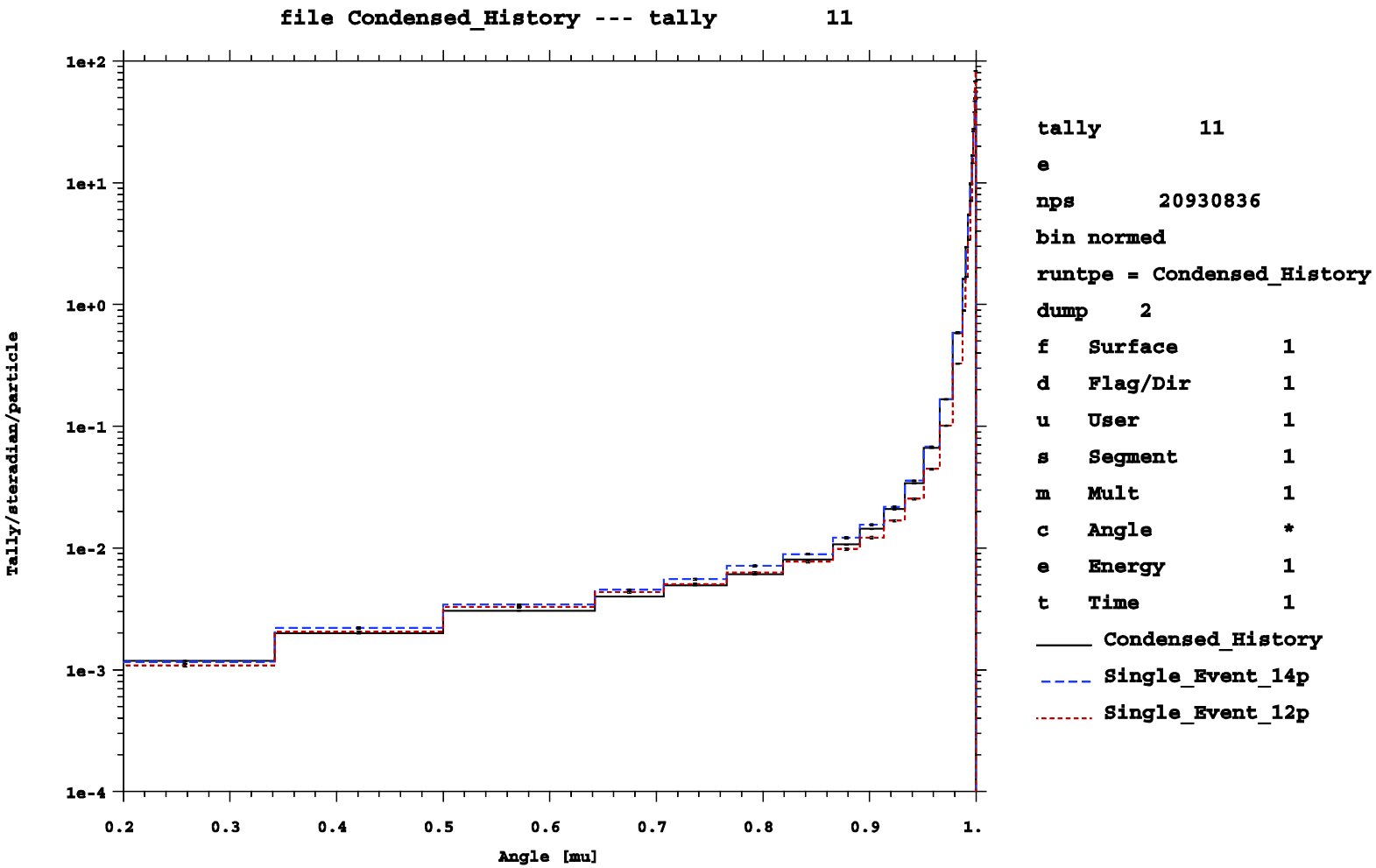
Compare estep=13, =104, =208. dbcn(90)=240



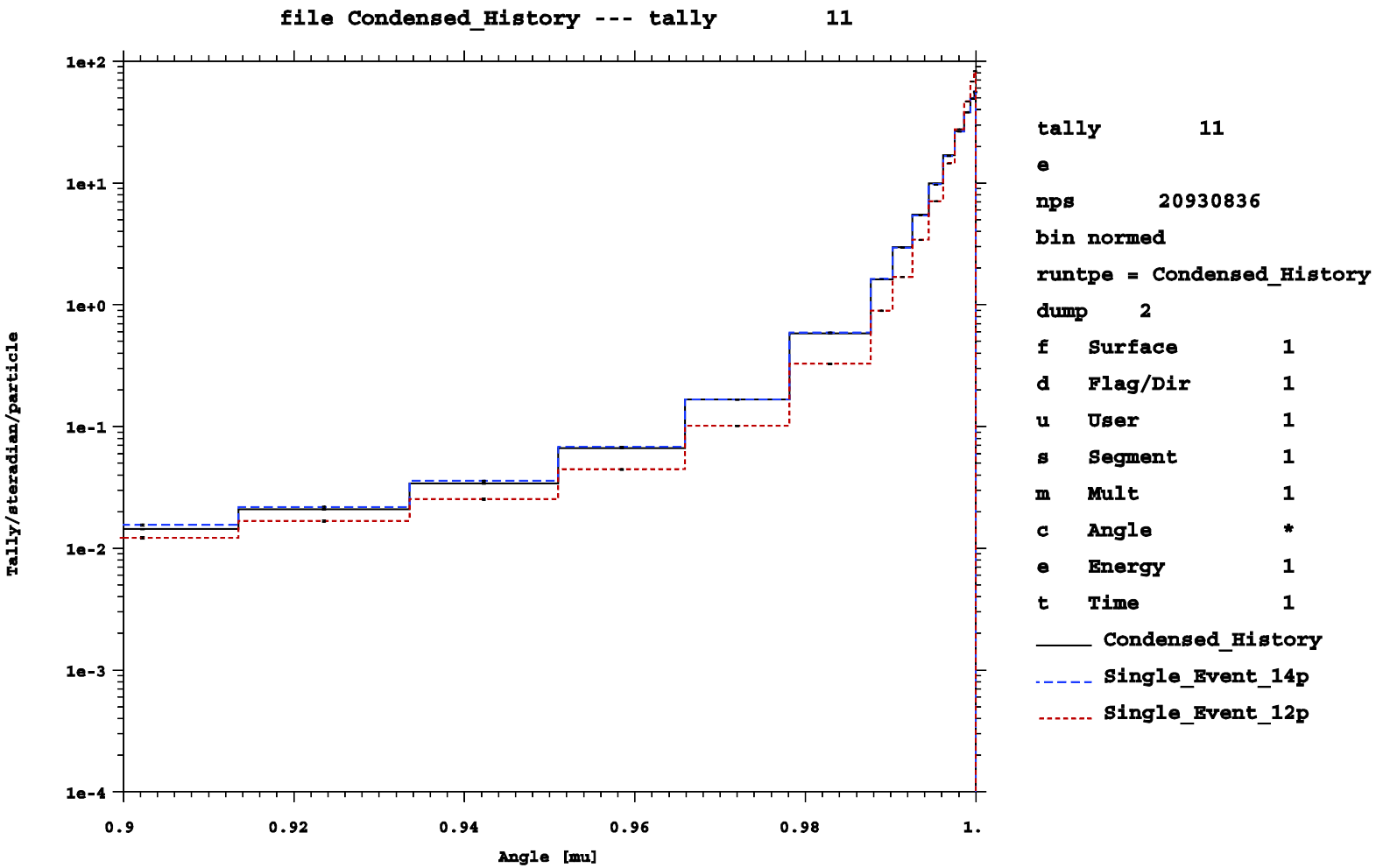
Compare estep=13, =104, =208. dbcn(90)=10000



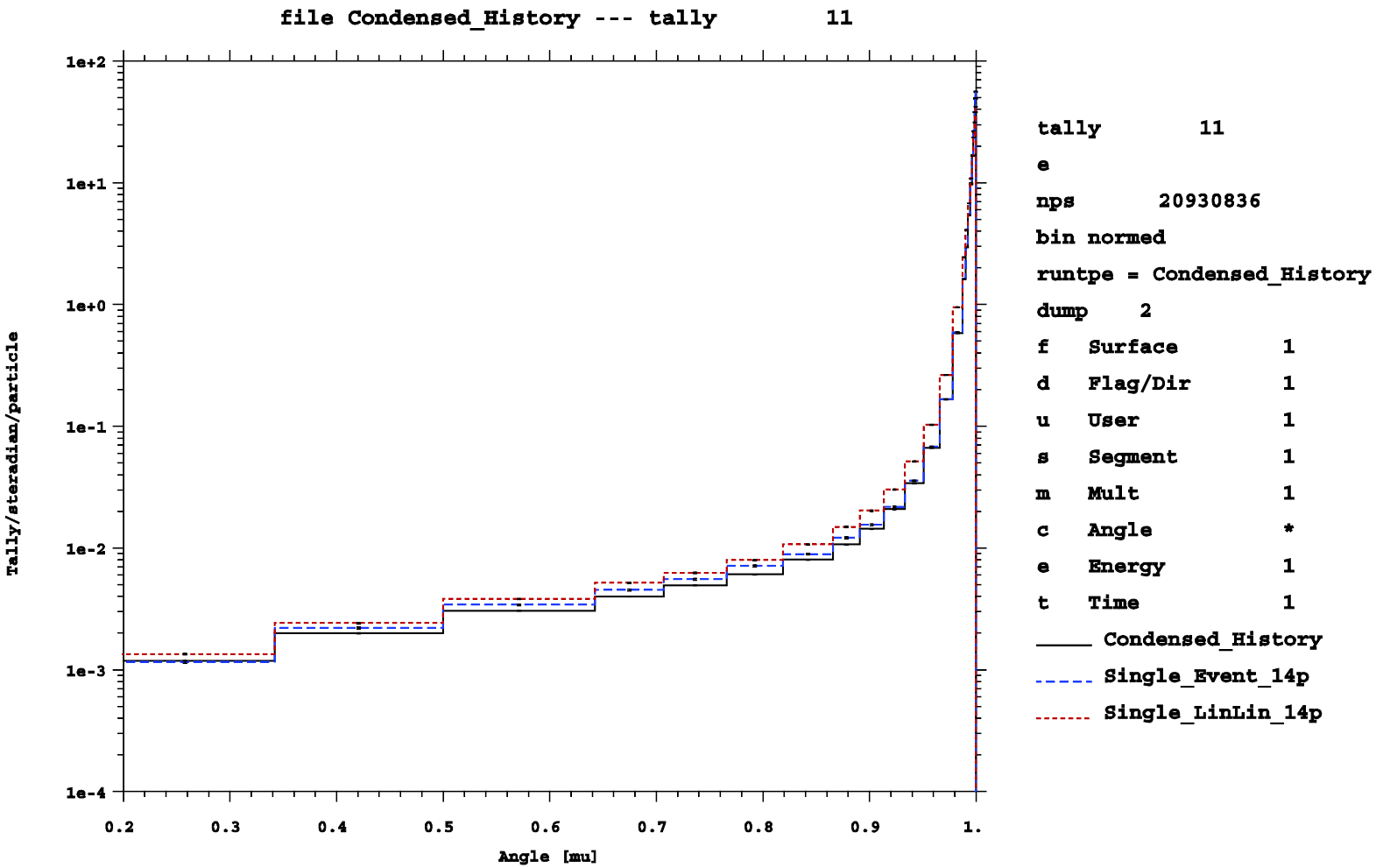
Compare C. H., single (12p), and single (14p).



Approaching the elastic peak



Compare CH, Single loglog vs Single linlin



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.”