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Title: Recent Developments in Low-Energy Electron/Photon Transport for MCNP6

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Recent Developments in Low-Energy Electron/Photon Transport for MCNP6

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Abstract

Recently a variety of programmatic needs have driven the development of improved methods for low-energy photon/electron transport in the Los Alamos Monte Carlo particle transport code MCNP6. Aspects of this development include a significant reworking of the MCNP coding to allow for consideration of much more detail in atomic relaxation process, new algorithms for reading and processing new Evaluated-Nuclear-Data-File photon, electron, and relaxation data capable of supporting such detailed models, and extension of the electron/photon transport energy range below the traditional 1-kilovolt limit in MCNP, with the goal of performing transport of electrons and photons down to energies in the few-electron-volt range. The work has also required review and development of standard MCNP-readable data formats to support new features and preparation for the development of special-purpose data libraries. In this presentation we will describe these new developments and illustrate their effects with a selection of example transport problems.

Plan of the Presentation

- Sources.
- Photon Enhancements.
- Atomic Relaxation.
- Electron Enhancements.
- Future Work.

Sources of Data

- mcplib:
  - coherent/incoherent, photoelectric, pair production, form factors
    - Storm and Israel, Los Alamos document LA-3753 (1967).
    - ENDF/B IV: Hubbell et al. *J. Phys. Chem. Ref. Data* **4**, 471 (1975).
  - fluorescence
    - Everett and Cashwell, Los Alamos document LA-5240-MS (1973).
- mcplib02:
  - coherent/incoherent, photoelectric, pair production
    - EPDL89: Cullen *et al*. LLNL document UCRL-50400, **6** (1989).
    - Implementation: Los Alamos document X-6:HGH-93-77 (1993).
- mcplib03:
  - Compton Doppler broadening data
    - Biggs *et al*. *Atomic Data and Nuclear Data Tables* **16** #3, 201 (1975).

Sources of Data

- mcplib04:
  - New data, same coverage and format
    - EPDL97: Cullen *et al*. LLNL document UCRL-50400 **6**,Rev. 5 (1997).
    - ENDF/B VI.8: Members of CSEWG, National Nuclear Data Center, Brookhaven document BNL-NCS-44945-01/04-Rev. (1990).
- mcplib12:
  - Extensions, additions, relaxation, and electrons
    - ENDF/B VI.8: Members of CSEWG, National Nuclear Data Center, Brookhaven document BNL-NCS-44945-01/04-Rev. (1990).
    - Los Alamos documentation: in progress.
    - Quick-Start Guide: LA-UR-12-21068 (2012).

Previous Photon Libraries

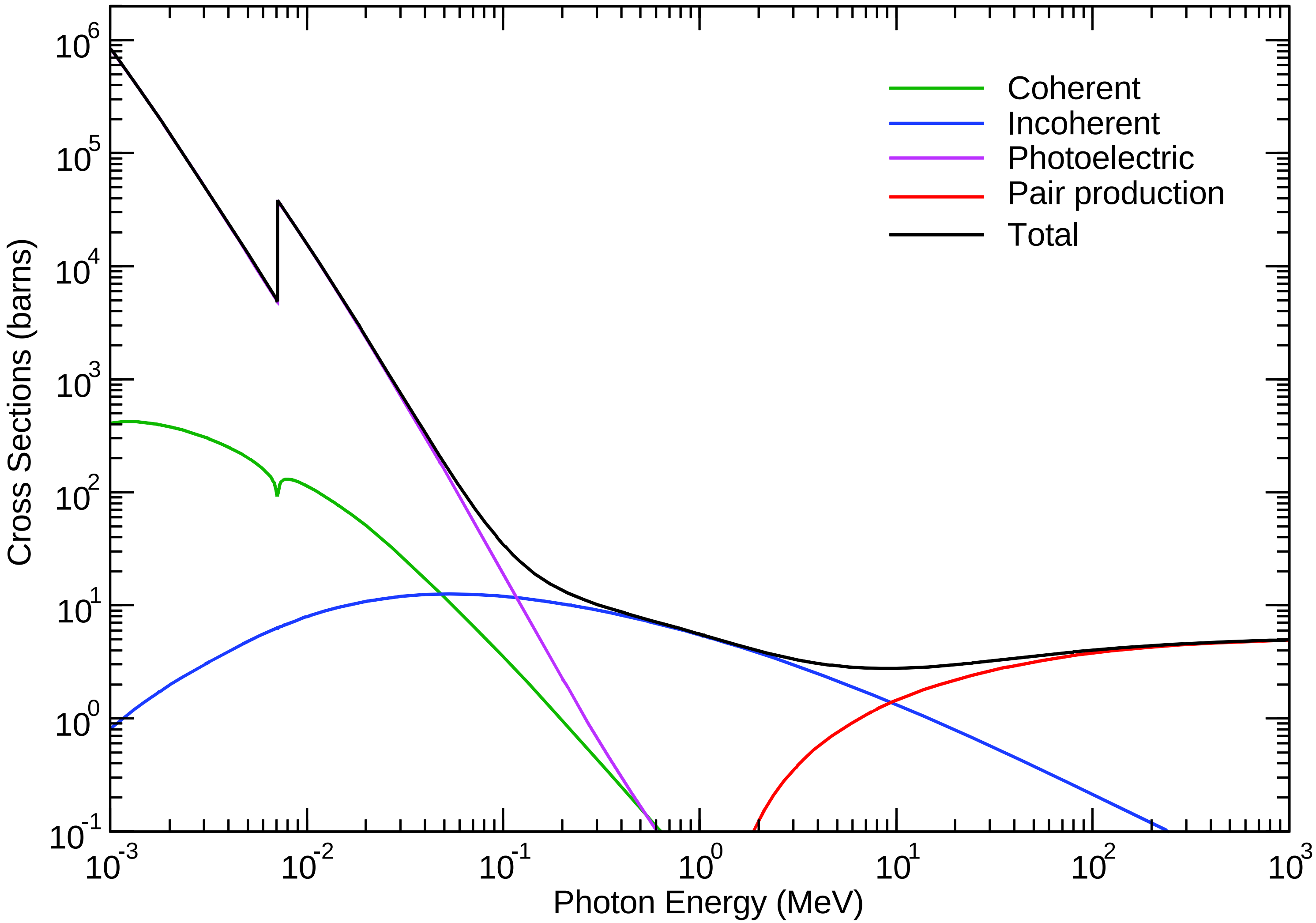
- mcplib: Z = 1 – 94 (e.g. 26000.01p)
  - coherent/incoherent, photoelectric, pair production, heating,
  - form factors, fluorescence
  - E = 1 keV – 100 MeV for 87 elements
  - E = 1 keV – 15 MeV for Po, At, Fr, Ra, Ac, Pa, Np
- mcplib02: Z = 1 – 94 (e.g. 26000.02p)
  - E = 1 keV – 100 GeV for 94 elements
- mcplib03: Z = 1 – 94 (e.g. 26000.03p)
  - Includes Compton Doppler broadening data.
  - E = 1 keV – 100 GeV for 94 elements
- mcplib04: Z = 1 – 100 (e.g. 26000.04p)
  - Changes existing data for consistency with ENDF/B VI.8 release.
  - E = 1 keV – 100 GeV for 100 elements

Photon Enhancements

- Extension of existing data: from ≥ 1 keV down to ≥ 1 eV
  - Coherent scattering
  - Incoherent scattering
  - Photoelectric absorption
- New kinds of photoatomic data
  - Subshell-wise photoelectric cross sections
    - Detailed sampling of initial vacancy now possible
  - Complete information for electron subshells
    - Binding energies, electron populations, transitions, etc.
    - Accurate kinematics for photoelectron
- Extended scattering form factors
  - Coherent and incoherent scattering
  - Complete range of energy and angle
  - Accurate interpolation (especially for coherent scattering)

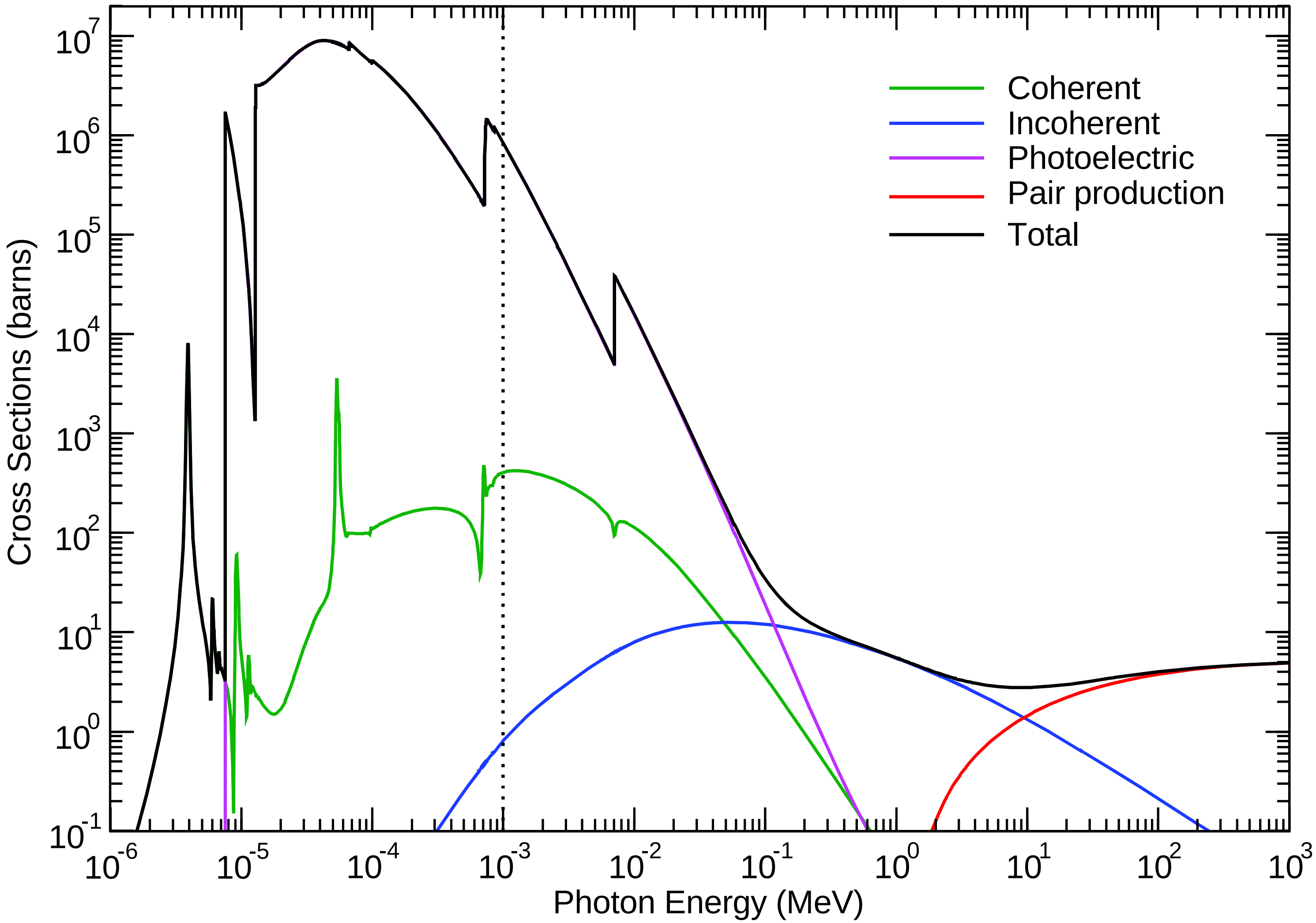
Photon Cross Sections in Iron

Data as in MCPLIB04



Photon Cross Sections in Iron

Data from ENDF/B VI.8

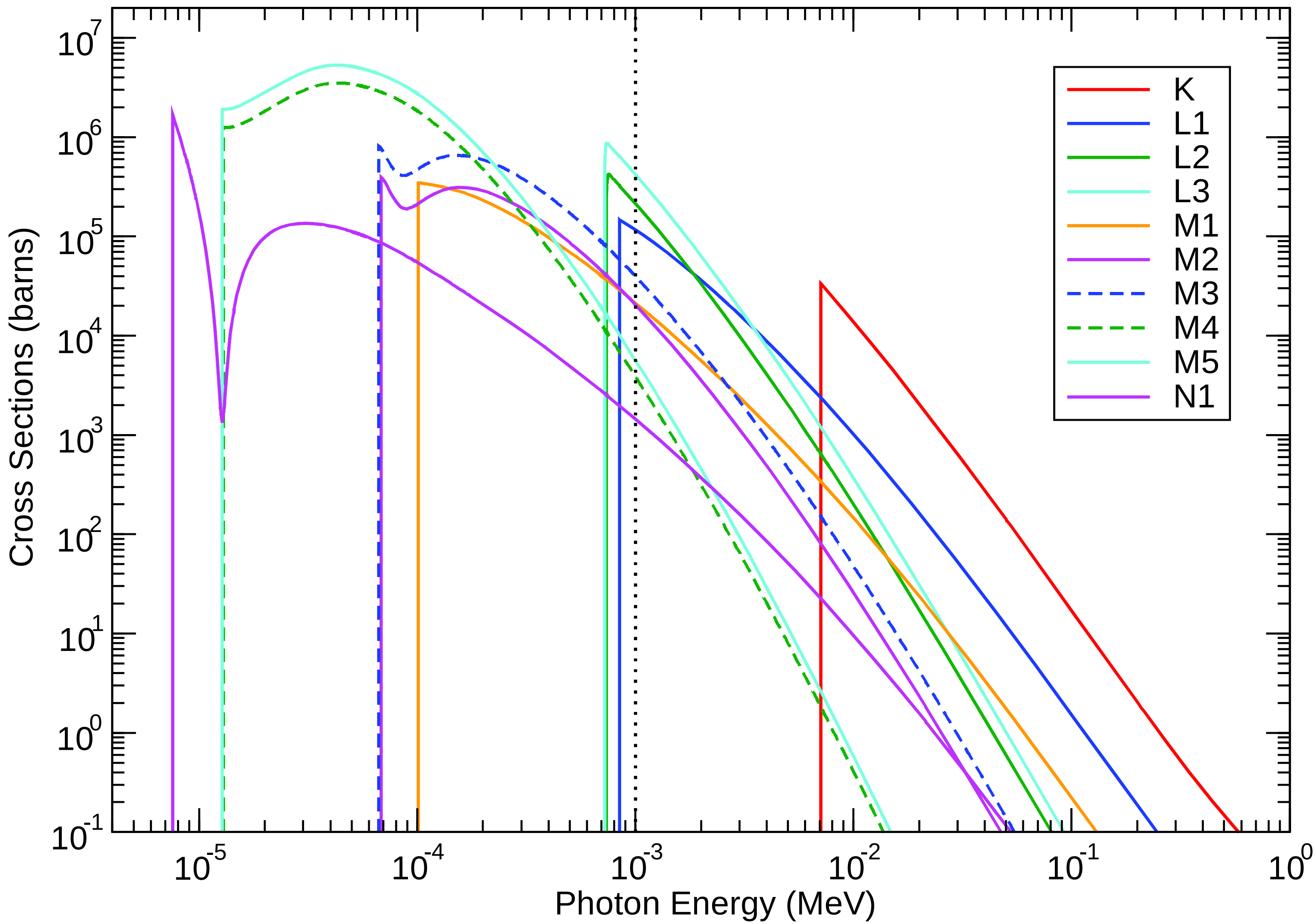


Plausible Uncertainties of Photoelectric XS (%)

Energy Range	Solid	Gas
10 – 100 eV	1000	20
100 – 500 eV	100 – 200	10 – 20
0.5 – 1.0 keV	10 – 20	5
1.0 – 5.0 keV	5	5
5 – 100 keV	2	2
0.1 – 10 MeV	1 – 2	1 – 2
10 – 100 GeV	2 – 5	2 – 5

Subshell Photoelectric Cross Sections in Iron

Data from ENDF/B VI.8



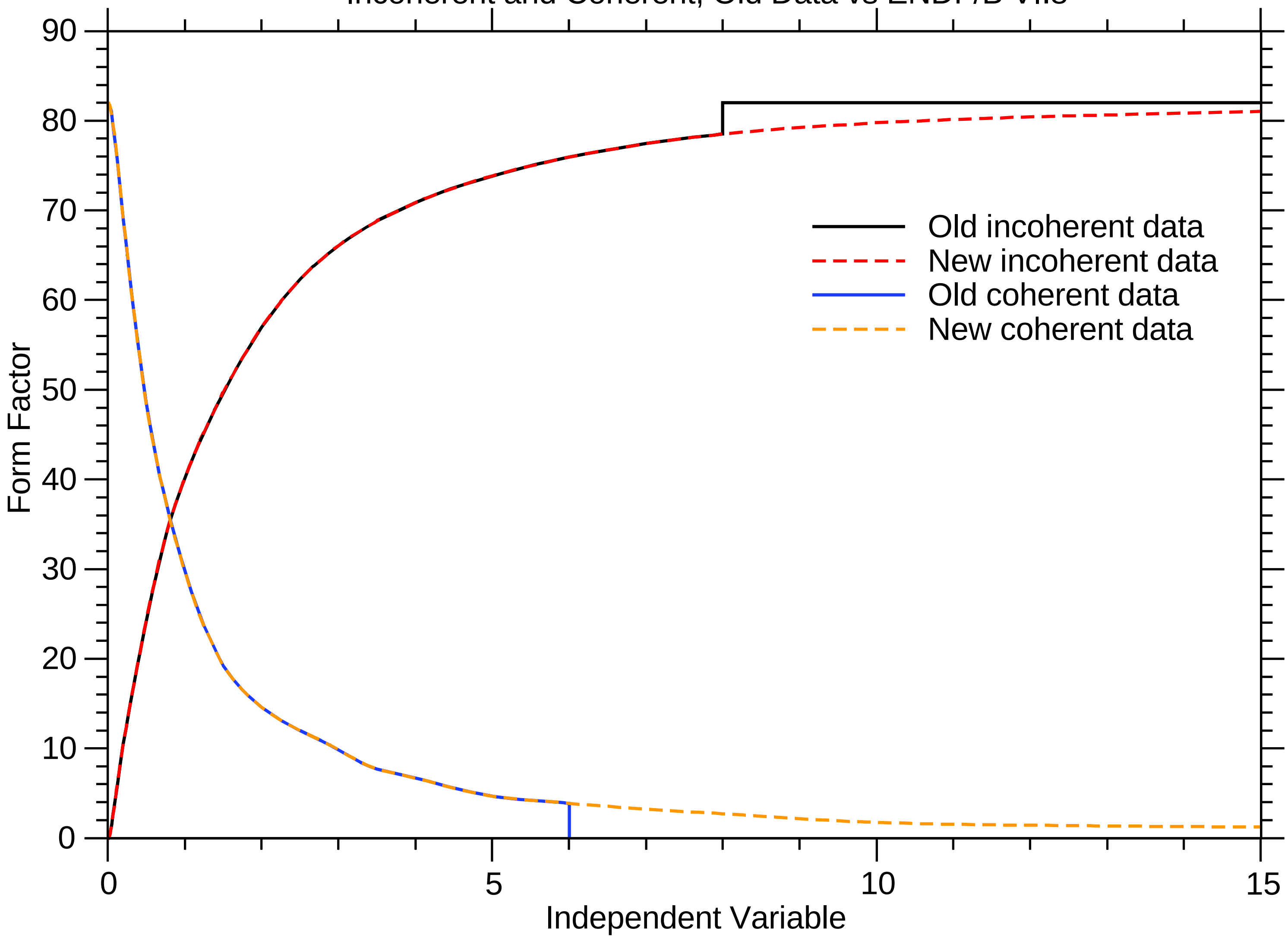
Photon Scattering Form Factors

- Incoherent: $\sigma(Z,\alpha,\mu) \sim I(Z,v)\,(\alpha'/\alpha)^2\,(\alpha'/\alpha + \alpha/\alpha' + \mu^2 - 1)$
- Coherent: $\sigma(Z,\alpha,\mu) \sim C^2(Z,v)\,(1 + \mu^2)$
- …where $\alpha = E/m_e c^2$; $\alpha' = E'/m_e c^2$

  $\mu = \cos(\theta)$; $v = \kappa\ \alpha\,(1 - \mu)^{1/2}$

  $\kappa = 10^{-8}\, m_e c/(2^{1/2}\, h) \approx 29.1445$
- Old incoherent data: tabulated for $v = 0 \ldots 8$
  - Full tabular angular coverage for $E \leq \sim 99$ keV
- Old coherent data: tabulated for $v = 0 \ldots 6$
  - Full angular coverage for $E \leq \sim 74$ keV
    - e.g. at 250 keV, no coherent scattering beyond ~ 35°
- First extension: Hendricks and Kahler

Photon Form Factors for Lead



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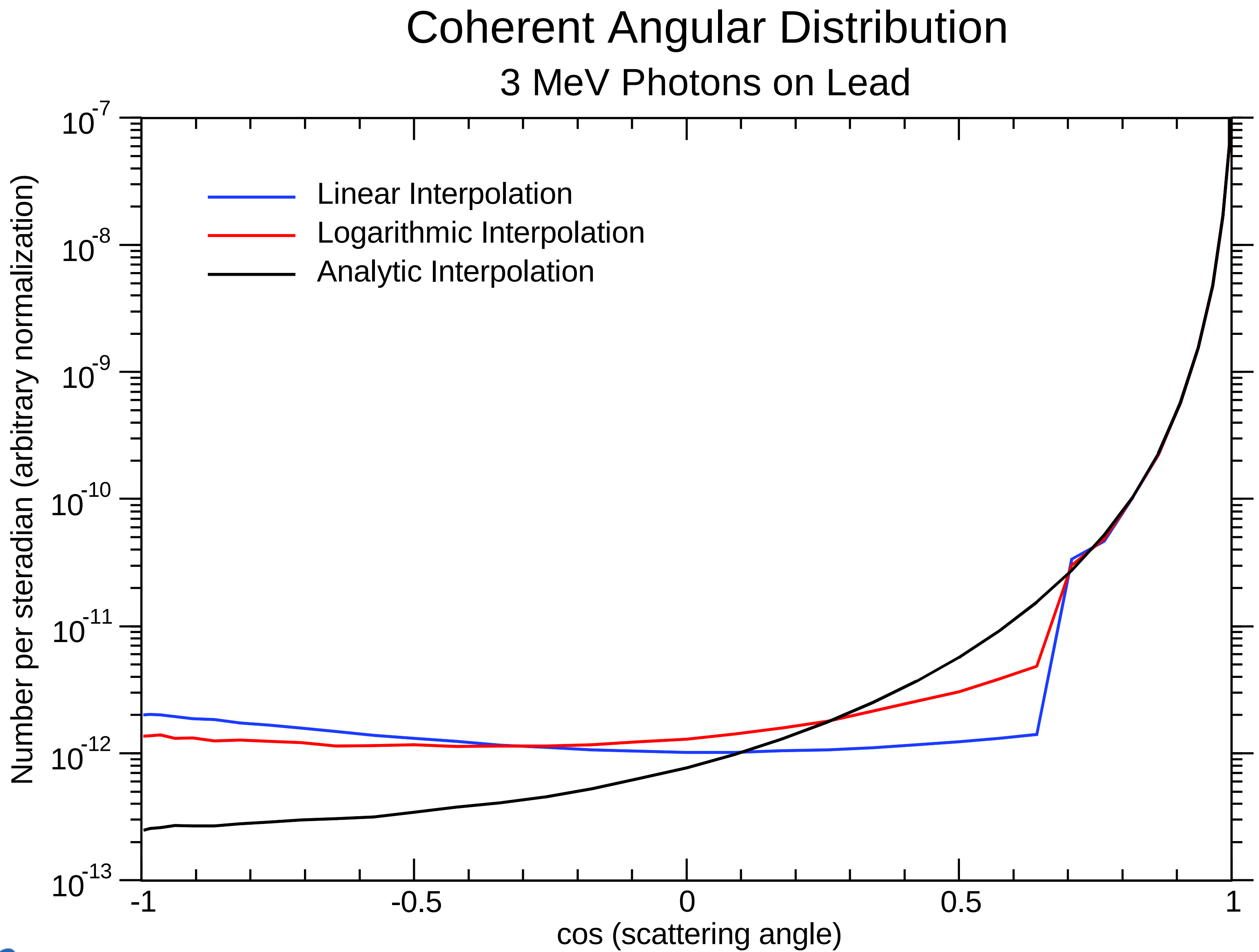
Interpolation Matters

- Incoherent scattering for transport: $I(Z,v)\ K(\alpha, \alpha', \mu)$
  - Sample from $K(\alpha, \alpha', \mu)$
  - Reject on normalized $I(Z,v)$ Log/log interpolation
- Incoherent scattering for detectors: $I(Z,v)\ K(\alpha, \alpha', \mu)$
  - Evaluate normalized $K(\alpha, \alpha', \mu)$
  - Evaluate normalized $I(Z,v)$ Log/log interpolation
- Coherent scattering for transport: $C^2(Z,v)\ T(\mu)$
  - Sample from $C^2(Z,v)$ Analytic interpolation
  - Reject on normalized $T(\mu)$
- Coherent scattering for detectors: $C^2(Z,v)\ T(\mu)$
  - Evaluate normalized $C^2(Z,v)$ Log/log interpolation
  - Evaluate normalized $T(\mu)$



Coherent Angular Distribution
3 MeV Photons on Lead
Linear Interpolation
Logarithmic Interpolation
Analytic Interpolation
Number per steradian (arbitrary normalization)
cos (scattering angle)
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
-1
-0.5
0
0.5
1

Atomic Relaxation

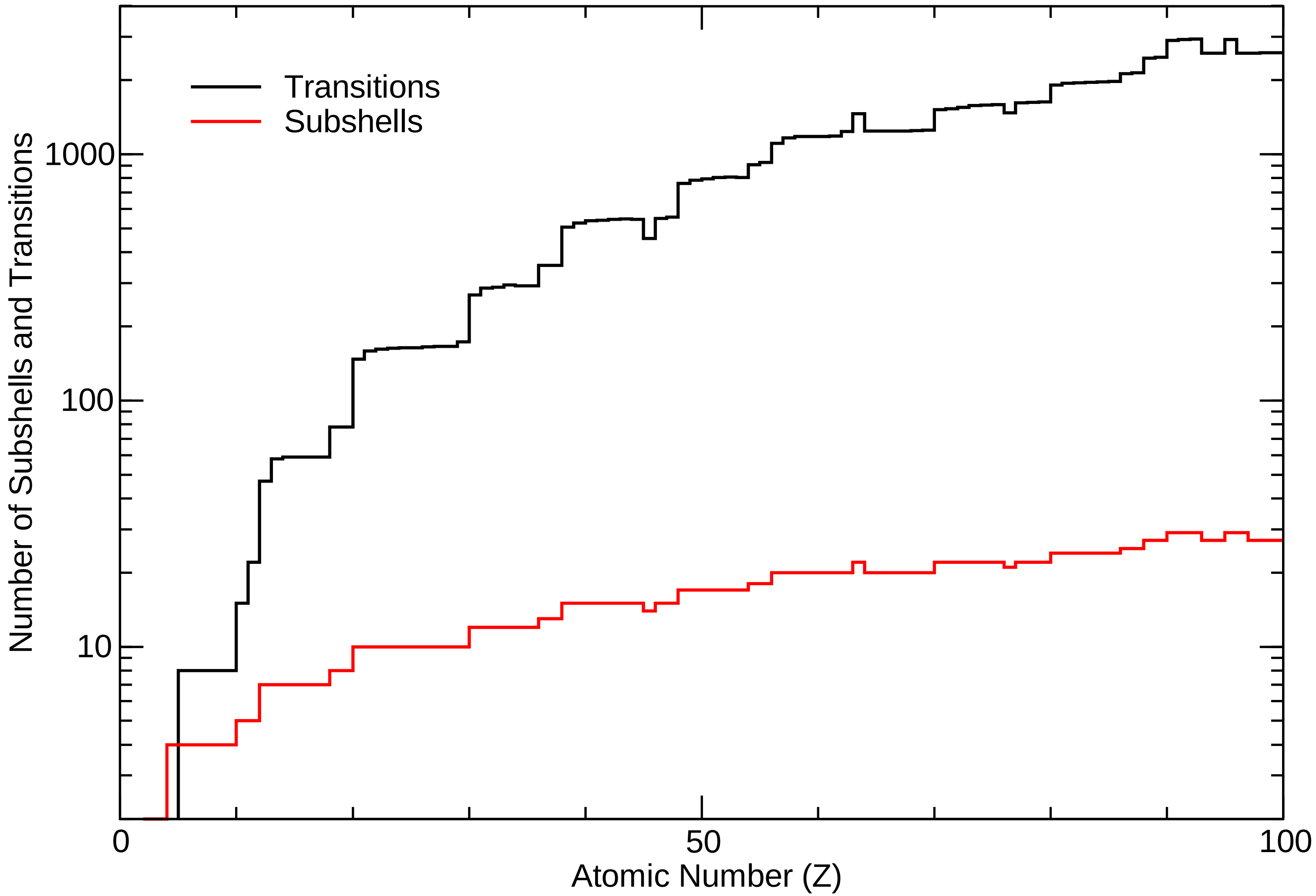
- Consistent data for electron subshells
  - Binding energies
  - Electron populations
  - Number of transitions
  - Photoelectric subshell cross sections down to 1 eV
- Consistent data for transitions
  - Transitions with photon fluorescence (radiative)
  - Auger and Coster-Kronig transitions (non-radiative)
- Full analog sampling of the relaxation cascade
- New process: Compton-induced atomic relaxation

Old MCNP Fluorescence Model

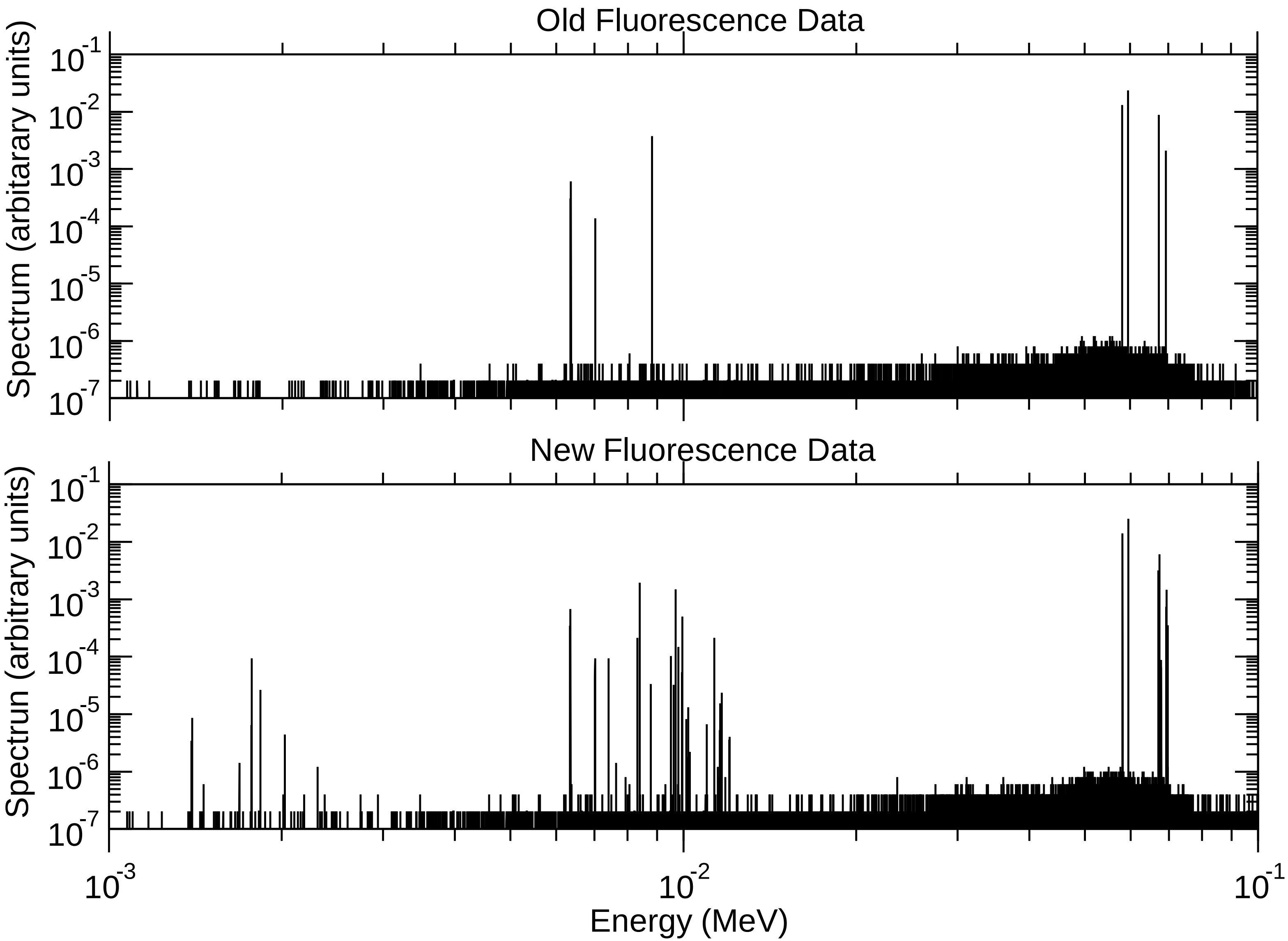
Z = 1 – 11:	no fluorescence	
Z = 12 – 19:	1 line	< K ← L2, K ← L3 >
Z = 20 – 30:	3 lines	K ← L2, K ← L3
		< K ← M2, K ← M3, K ← M4 >
Z = 31 – 36:	4 lines	K ← L2, K ← L3
		< K ← M2, K ← M3, K ← M4 >
		< L1, L2, L3 > ← < higher lines >
Z = 37 – 100:	5 lines	K ← L2, K ← L3
		< K ← M2, K ← M3, K ← M4 >
		< K ← N2, K ← N3 >
		< L1, L2, L3 > ← < higher lines >

Electron Subshells and Relaxation Transitions

From ENDF/B VI.8 Data



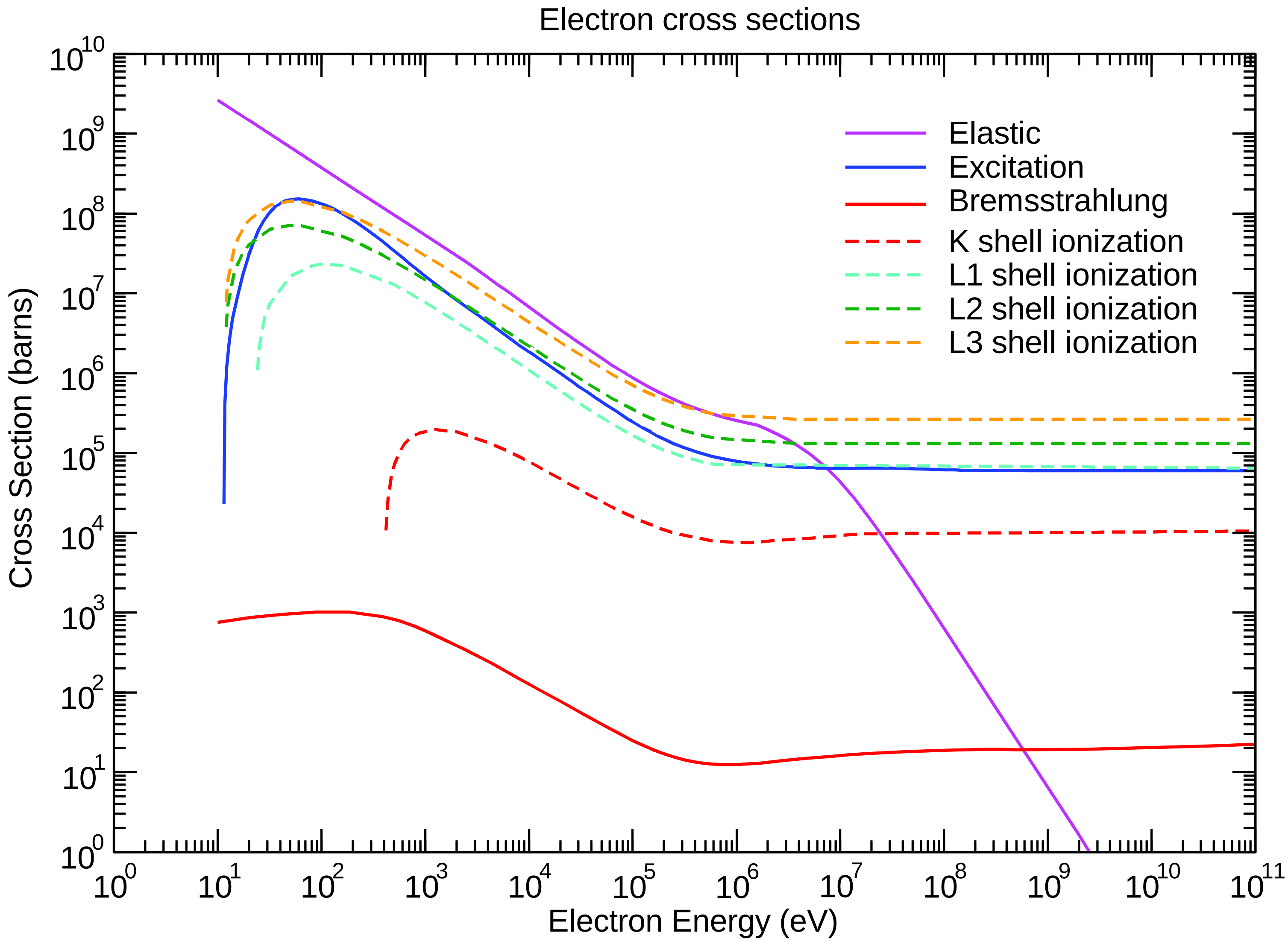
Iron / Tungsten Target, 100 keV photons



Electron Enhancements

- Microscopic electron cross sections down to 10 eV
- Electron elastic scattering
  - Electron angular distribution as function of electron energy
- Atomic excitation
  - Electron mean energy loss as function of electron energy
- Subshell-wise electroionization
  - Knock-on energy distribution as function of electron energy
  - Knock-on direction and primary energy loss from conservation
- Bremsstrahlung
  - Photon energy distribution as function of electron energy
  - Electron mean energy loss as function of electron energy
  - No photon angular distribution given

Atomic Nitrogen



Single-Event Electron Transport

- Get total cross section and distance to collision

  $\Sigma(i) = N(i) \cdot (\sigma_{elas}(i) + \sigma_{brem}(i) + \sigma_{exc}(i) + \sigma_{ion}(i))$

  $D = -\ln (\text{random}()) / (\Sigma(1) + \ldots + \Sigma(m))$

- Select target

  $R = \text{random}() \cdot (\Sigma(1) + \ldots + \Sigma(m))$

  $m = 1 \parallel R < \Sigma(1) \quad \longrightarrow \quad t = 1$

  otherwise find $\Sigma(1) + \ldots + \Sigma(t\text{-}1) \le R < \Sigma(1) + \ldots + \Sigma(t)$

- Select process

  $R = \text{random}() \cdot (\sigma_{elas}(t) + \sigma_{brem}(t) + \sigma_{exc}(t) + \sigma_{ion}(t))$

if $R < \sigma_{elas}$	process elastic collision
else if $R < \sigma_{elas} + \sigma_{brem}$	process bremsstrahlung
else if $R < \sigma_{elas} + \sigma_{brem} + \sigma_{exc}$	process excitation
else	process electro-ionization

Process Collisions

- Excitation
  - No angular deflection
  - No secondary particles
  - Apply energy loss as unique function of energy: $F_{exc}(E)$
  - (No sampling for this process)
- Electro-ionization
  - Sample for individual subshell
  - Sample knock-on energy from tabulation: $F_{knock}(E,\mu)$
  - Reduce incident energy by $E_{knock} + E_{binding}$
  - Get incident and knock-on directions from conservation
  - “Recursively” fill vacancy using new relaxation data

Process Collisions

- Elastic collision
  - No energy loss
  - No secondary particles
  - Sample deflection from tabulation: $F_{elas}(E,\mu)$
- Bremsstrahlung
  - No change in electron direction
  - Sample photon energy from tabulation: $F_{brems}(E)$
  - Reduce incident energy by E_{brems}
  - Sample photon direction in three energy ranges:
    - $E > 1$ GeV: $p(\mu) = \frac{1}{2}\,(1 - \beta^2) / (1 - \beta\mu)^2$
    - 1 keV $\leq E \leq$ 1 GeV: tabular distribution from condensed history
    - $E < 1$ keV: Currently $p(\mu)$
      Planned: dipole distribution

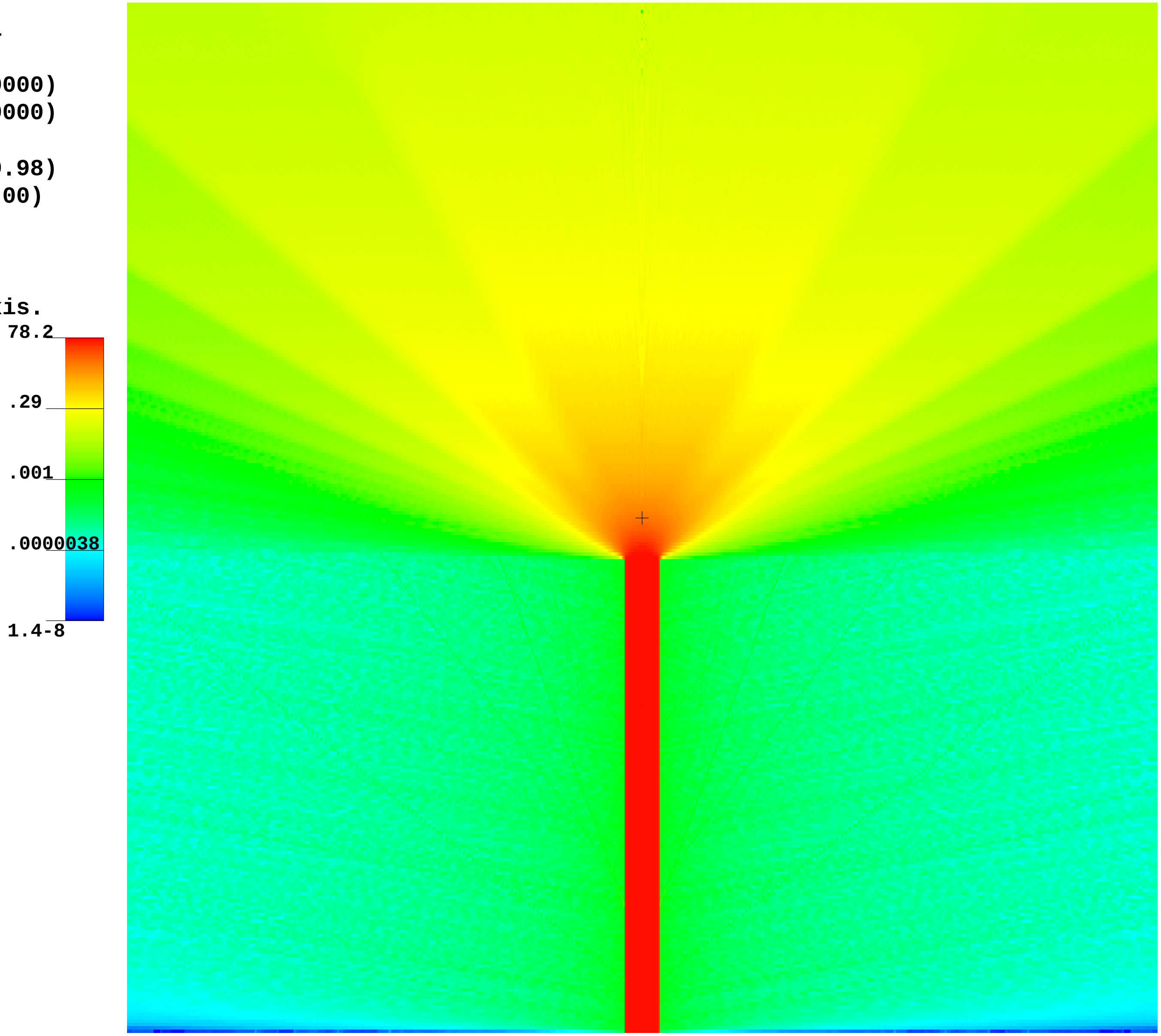
Brief User Guide

- Use the new data tables:
  - `M1    1000.12p  2   8000.12p  1`
  - `M1    1000  2   8000  1   plib  12p   elib  03e`
- Use the right problem modes:
  - `MODE   P  E`
  - `DBCN   17J  2  $  now the default`
- The default energy cutoff is still 1 keV:
  - `CUT:P  J  1.0e-06  $  1 eV`
  - `CUT:E  J  1.5e-05  $ 15 eV avoid the Sargasso Sea`
- Single-event starting point is adjustable:
  - `PHYS:E  10. 13J  2.0e-03  $  start at 2 keV`

07/23/12 16:23:48
60-MeV electrons in air.

probid = 07/23/12 15:15:41
basis: YZ
(0.000000, 1.000000, 0.000000)
(0.000000, 0.000000, 1.000000)
origin:
(0.00,   0.00,   499.98)
extent = (15.00,   500.00)

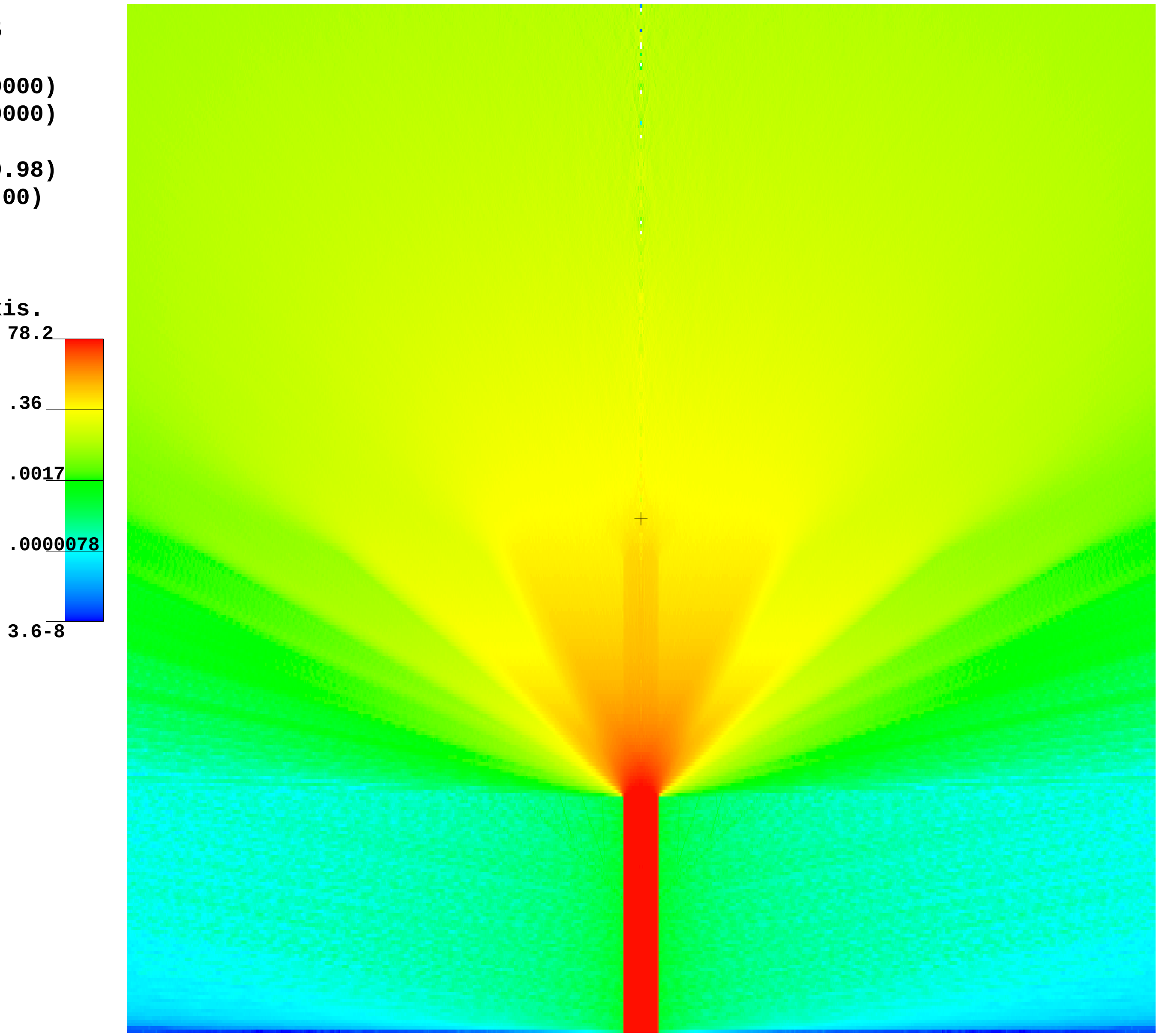
Mesh Tally   4
Electron flux on central axis.
nps   400000
runtpe = prod_default_r
dump   11



07/23/12 16:37:22
60-MeV electrons in air.

probid = 07/23/12 15:15:25
basis: YZ
(0.000000, 1.000000, 0.000000)
(0.000000, 0.000000, 1.000000)
origin:
(0.00, 0.00, 499.98)
extent = (15.00, 500.00)

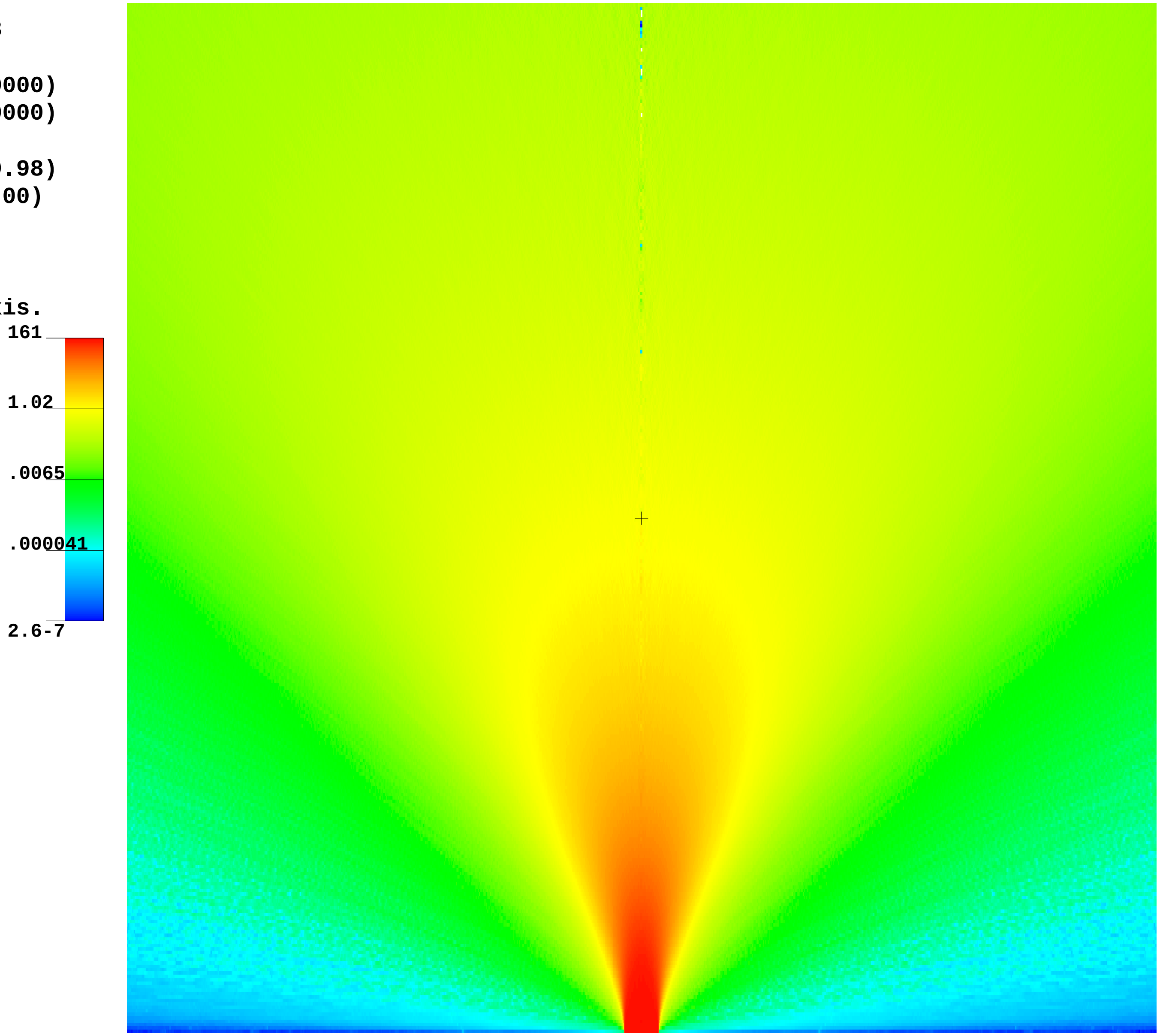
Mesh Tally 4
Electron flux on central axis.
nps 400000
runtpe = prod_double_r
dump 19



07/24/12 06:45:35
60-MeV electrons in air.

probid = 07/23/12 15:14:48
basis: YZ
(0.000000, 1.000000, 0.000000)
(0.000000, 0.000000, 1.000000)
origin:
(0.00, 0.00, 499.98)
extent = (15.00, 500.00)

Mesh Tally 4
Electron flux on central axis.
nps 400000
runtpe = prod_single_r
dump 207



Future Work — Finishing Touches

- Photon heating numbers
- Bremsstrahlung angular distribution at low energies
- Resolve electron elastic scattering peak
- New relaxation data with condensed-history electrons
- Molecular cross sections and relaxation
- Full integration of other MCNP features
- Formalities of ACE format libraries
- Electromagnetic fields (with single-event electrons)
- Single-event electrons at high energies

Future Work — Speculation

- Photon polarization
- Anomalous scattering factors
- Reflection/refraction
- Cerenkov and synchrotron radiation
- Impact electrons from heavy charged particles
- Variance reduction (computer speed)
- Finite temperatures, condensed matter, etc.
- Collective effects
- Transport in plasmas

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  - Cecile Toccoli
- Supporting agencies
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  - Los Alamos National Security, LLC / Department of Energy

This work is dedicated to the memory of Professor Joon Lee

from Kabacchi's photostream