

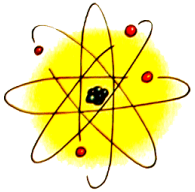

Joint ICTP-IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications
28 October – 8 November 2024
ICTP, Trieste, Italy

Lecture 5

Photon physics

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National Research Council Canada


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Gouvernement du Canada
Carleton University
Université de Montréal
nova scotia health

General aspects of photon interactions with matter

- Indirectly ionizing through the generation of secondary particles (electrons, positrons, neutrons).
- Involve either the nuclei or orbital electrons of the atoms in the medium.
- Interactions with nuclei might be direct photon–nucleus (photo-disintegration), or with the electrostatic field of the nucleus (pair production).
- Interaction with losely–bound orbital electrons ($E_{\mathrm{B}} \ll h\nu$): Thomson scattering, Compton scattering, tripplet production.
- Interaction with tightly–bound orbital electrons ($E_{\mathrm{B}} \lesssim h\nu$): photo-electric effect, Rayleigh scattering, bound Compton scattering.

Attenuation coefficients (a.k.a interaction cross sections)

- **Atomic attenuation coefficient** $\mu_i^{\mathrm{a}}(E)$: "effective area" of atoms or molecules as seen by photons with energy E with respect to interactions of type i (measured in length^2).

- **Linear attenuation coefficient** $\mu_i(E)$: average number of photon interactions of type i per unit length for photons with energy E (measured in length^{-1})

$$\mu_i(E) = \mu_i^{\mathrm{a}}(E) \cdot n$$

  where n is the atomic density (number of atoms per unit volume).

- These coefficients are often referred to as **microscopic** cross section $\sigma_i(E)$ and **macroscopic** cross section $\Sigma_i(E)$, respectively, following the nomenclature commonly in use in nuclear physics.

Interaction probability

- **Total atomic attenuation coefficient** $\mu^{\mathrm{a}}(E)$: given by the sum of the individual interactions:

$$\mu^{\mathrm{a}}(E) = \sum_i \mu_i^{\mathrm{a}}(E)$$

- **Total attenuation coefficient** $\mu(E)$: given by the sum

$$\mu(E) = \sum_i \mu_i(E)$$

- **Interaction probabilities** (branching ratios) $w_i(E)$: probability that the interaction is of type i when a photon of energy E interacts with the surrounding medium, e.g.,

$$w_i(E) = \frac{\mu_i^{\mathrm{a}}(E)}{\mu^{\mathrm{a}}(E)} = \frac{\mu_i(E)}{\mu(E)}$$

Energy and direction after an interaction

Differential microscopic cross sections can be used to obtain the energy and angular distribution after an interaction of type i. For example,

$$\frac{1}{\sigma_i(E)} \frac{\mathrm{d}\sigma_i(E, E')}{\mathrm{d}E'} \mathrm{d}E'$$

is the probability that a photon of energy E will scatter into energy interval $\mathrm{d}E'$ around E' after interaction type i.

Equivalently:

$$\frac{1}{\sigma_i(E)} \frac{\mathrm{d}\sigma_i(E, \Omega)}{\mathrm{d}\Omega} \mathrm{d}\Omega$$

is the probability that a photon of energy E will scatter into angular interval $\mathrm{d}\Omega$ around Ω after interaction type i.

Photon transport

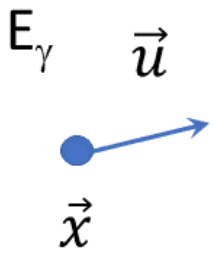
- Photons are neutral particles that travel through matter in straight lines
- Significantly simpler than transport of charged particles, which follow complicated trajectories as they continuously slow down in a medium due to atomic excitation or ionization
- Neutral particles are characterized by their mean-free-path λ while charged particles are characterized by their mass stopping power L/ρ and their range R_{CSDA}
- Since distance to interaction d follows the **exponential distribution**

$$f(d) = \mu\, e^{-\mu\, d}$$

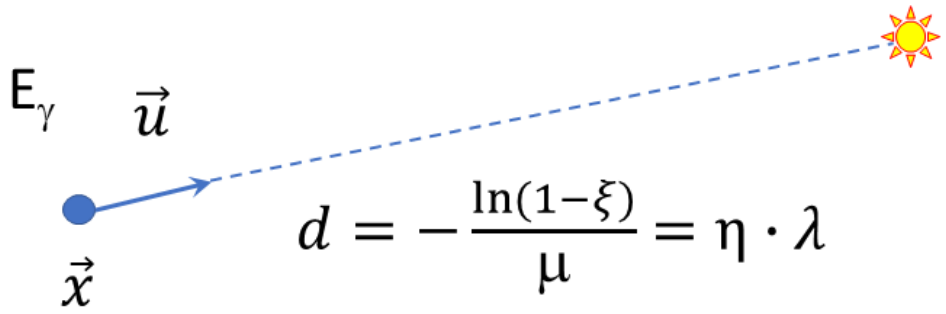
where μ is the **linear attenuation coefficient**, the mean-free-path λ is given by

$$\lambda = \frac{1}{\mu}$$

Photon transport mechanics

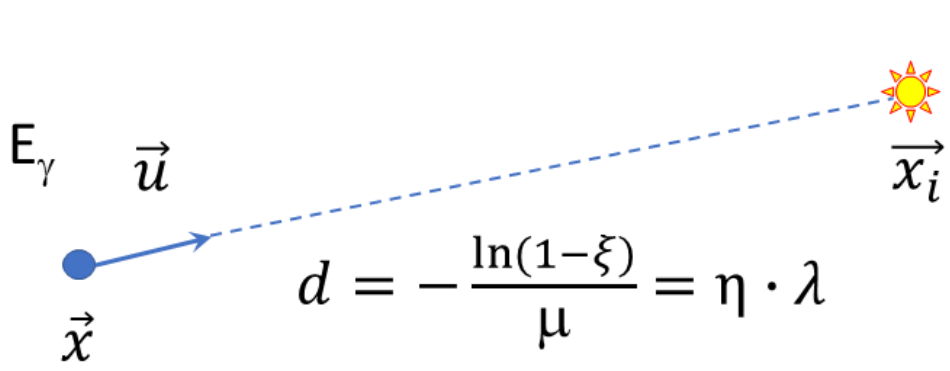


Photon transport mechanics



Where $\xi \sim U[0,1)$

Photon transport mechanics



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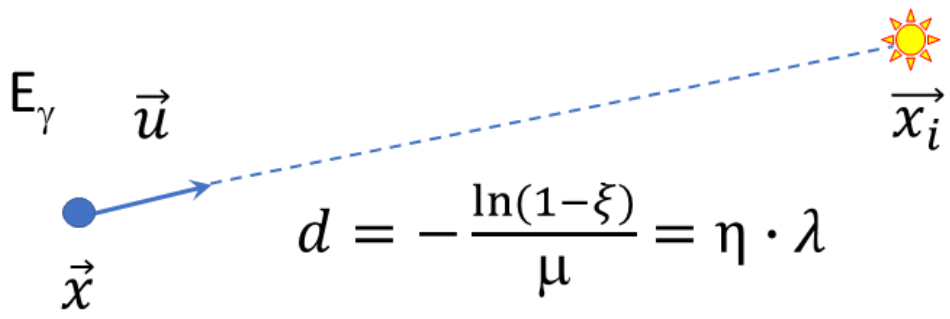
Photon transport mechanics



$$d = -\frac{\ln(1-\xi)}{\mu} = \eta \cdot \lambda$$

Where $\xi \sim U[0,1)$

$$\omega_i = \frac{\mu_i}{\mu}$$

Resulting particles

$E_1, \vec{u}_1$
$E_2, \vec{u}_2$
.
.
.
$E_n, \vec{u}_n$

Total photon cross sections in EGSnrc

- **By default** the total cross sections for pair and triplet production, photoabsorption and Rayleigh from the NIST photon cross sections database XCOM, and the total cross section for Compton is derived from a theoretical model.
- User has the option to use **alternative cross sections,** with tabulations by Storm & Israel or EPDL-97, both provided with EGSnrc. To select cross sections, add

  ```
  photon cross sections = xcom | si | epdl | [user_prefix]
  ```

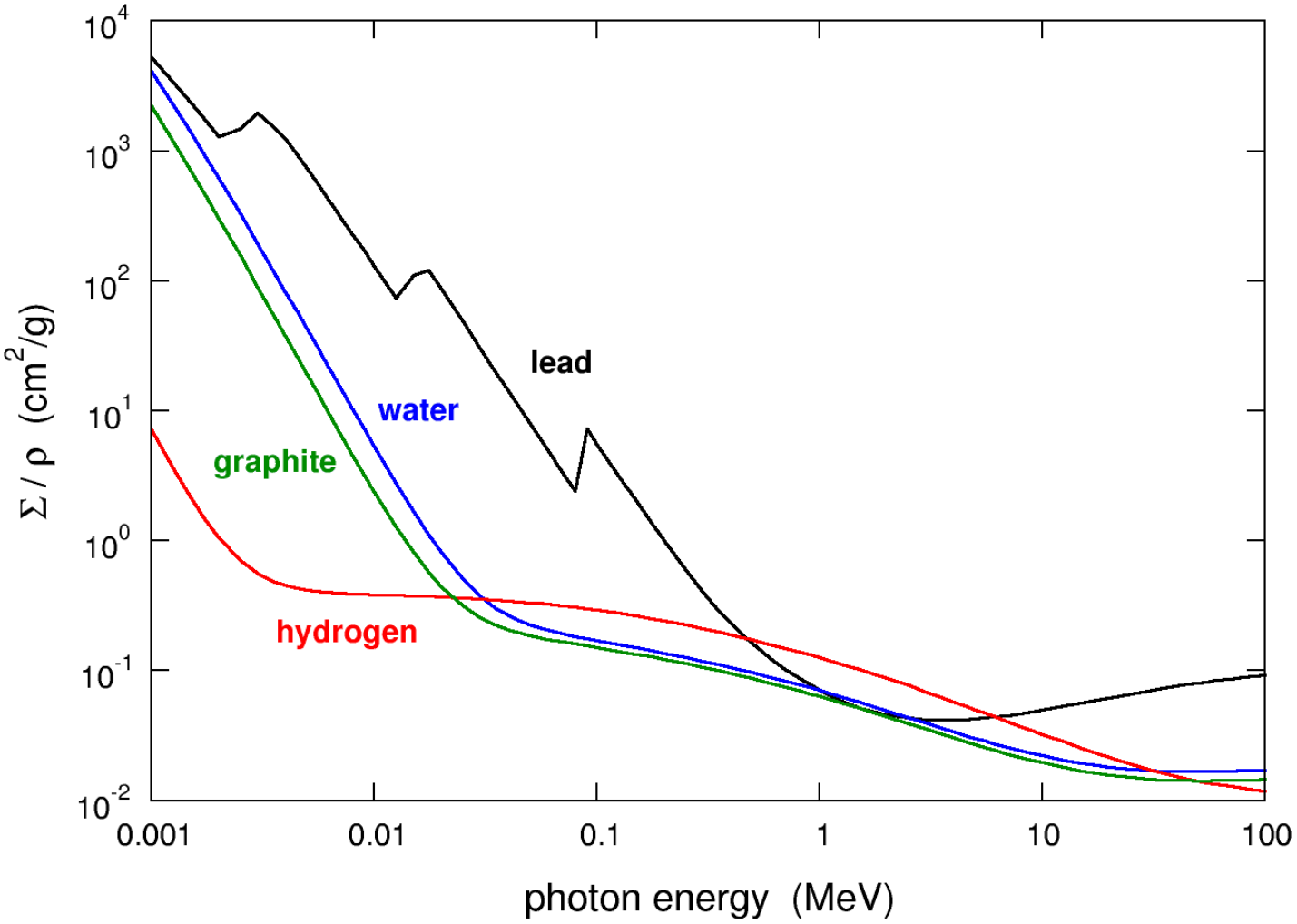
  to the transport parameter section of the input file. The input string read is taken as the prefix to the files `*_{pair,photo,rayleigh,triplet}.data`.
- Users may include **their own tabulations** using `user_prefix` which can be any string, for instance `joe`. These can be requested in the MC transport parameters input block

  ```
  photon cross sections = joe
  ```

- Cross section files are located in folder `$HEN_HOUSE/data/`

Total photon cross sections

(EGSnrc application `examin`)



Photon interactions

In the energy range, relevant to Medical Physics, photons interact with surrounding matter via four basic processes:

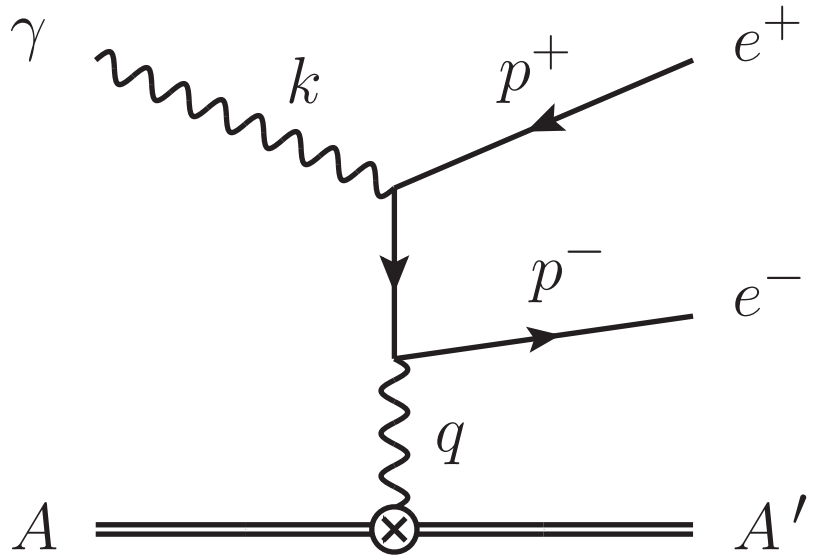
- **Materialization** into electron–positron pairs in the nuclear and electron field
- **Compton (incoherent)** scattering of atomic electrons
- **Photoelectric** absorption
- **Rayleigh (coherent)** scattering of atoms or molecules

On the high-energy end a fifth interaction possibility arises:

- **Photonuclear** absorption

Of concern in high-energy clinical linacs (above 10 MV).

Materialization into e^+e^- pairs: pair production



- Only possible when $k \geq 2\,m_0 = 1.022\ \mathrm{MeV}$
- Scales as Z^2
- Dominates at **high photon energies**

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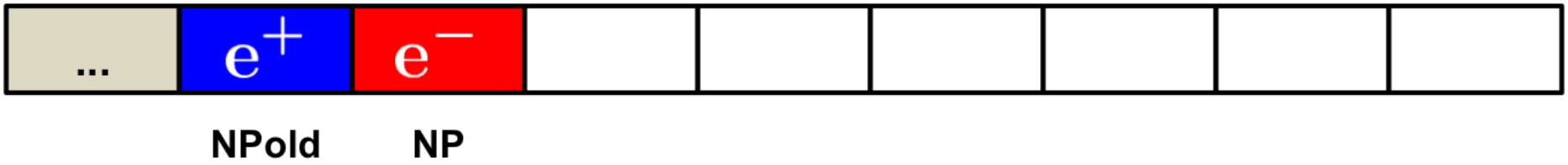


Pair production is always “On” in EGSnrc

The cross sections can be selected from:

```
Pair cross sections = BH | nrc
```

`BH (default):` **Bethe-Heitler (BH)** cross sections based on extreme relativistic first Born approximation, Coulomb corrected above 50 MeV.

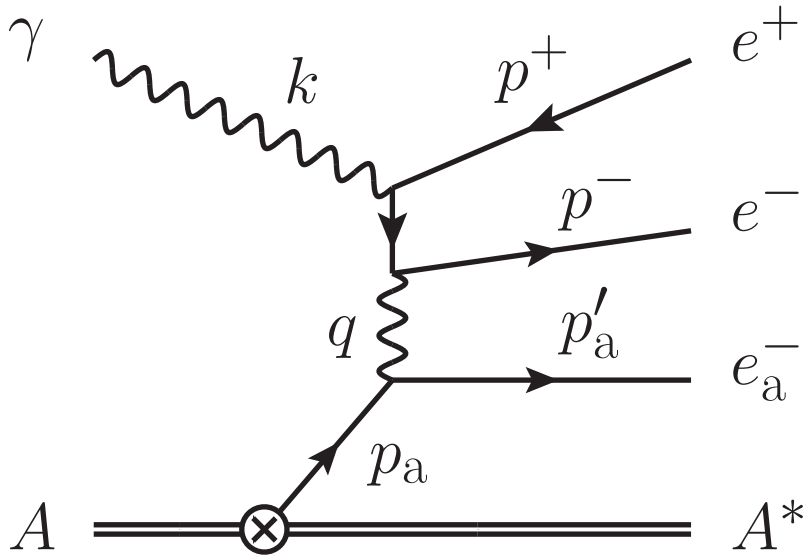
`nrc:` Option to use an exact formulation based on the exact PWA calculations by Øverbø, Mork and Olsen (OMO) for the unscreened nuclear potential modified by a multiplicative screening correction extended at NRC up to 85 MeV.

You can select the **angular sampling** method:

```
Pair angular sampling = KM | Simple | Off
```

- `KM`: The more sophisticated distribution from Koch and Motz is derived from an extreme relativistic approximation. It is better at high energies, above 50 MeV.
- `Simple`: The default selection (based on the leading term of the angular distribution) is most likely good enough for any application. The additional CPU cost compared to sampling a fixed angle is negligible.
- `Off`: Using the fixed angle approximation (inherited from EGS4) is never a good idea.

Materialization into e^+e^- pairs: triplet production



- Only for $k \geq 4\,m_0 = 2.044\ \mathrm{MeV}$
- Scales as Z
- **Always** much weaker than pair production (except for low Z)

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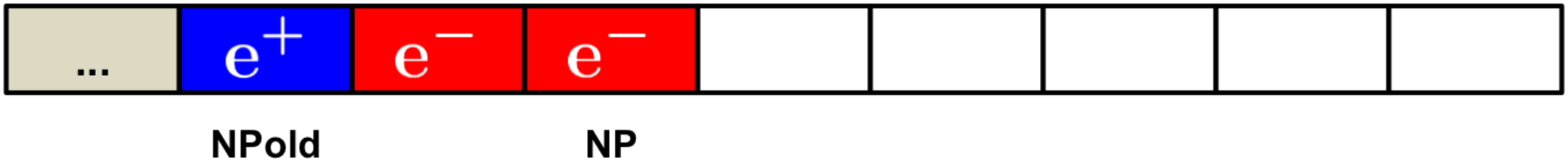


Triplet production is “Off” in EGSnrc by default

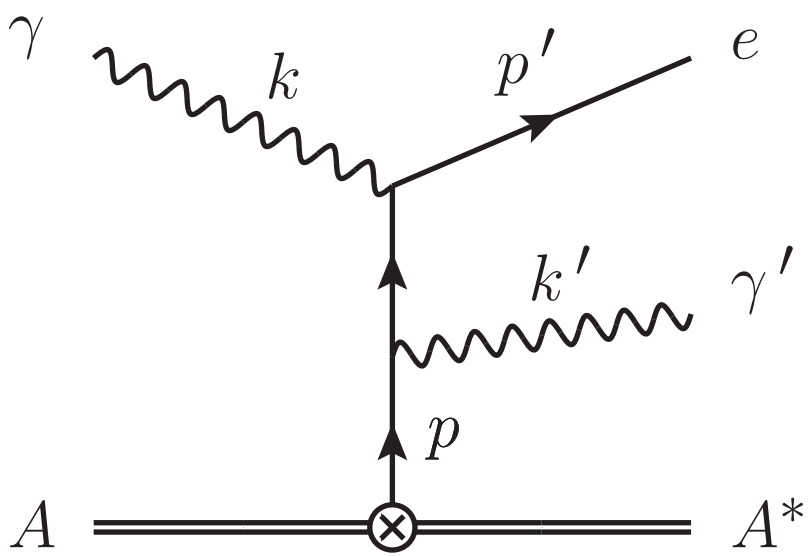
By default, the triplet production is taken into account within the pair cross-section, but the extra electron is not created.

To turn the explicit simulation of triplets On and Off:

```
Triplet production = On | Off
```

- Explicit triplet production creates correlations between individual particle histories due to the Markov chain sampling technique.
- Explicit triplet production effects can be observed in the build-up region of megavoltage photon beams.
- Explicit triplet production has a negligible impact in all cases studied so far.

Compton (incoherent) scattering



- Occurs for **all** photon energies
- Scales as Z
- Dominates at **intermediate photon energies**

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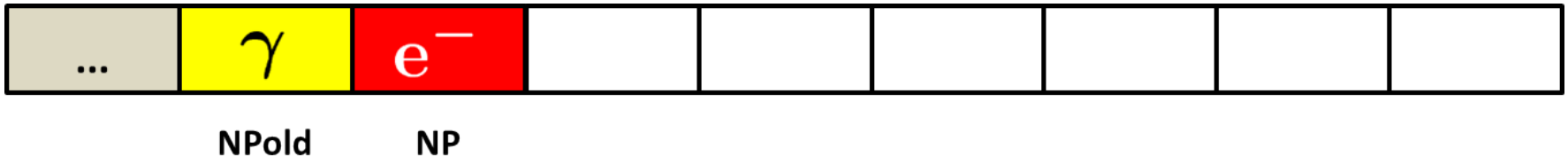


Bound Compton scattering in EGSnrc

Electron binding reduces the Compton cross-section (most strongly suppressed for forward angles). Binding effects are negligible for energies above a few hundred keV.

By default EGSnrc uses the **relativistic impulse approximation (RIA),** which takes into account binding and Doppler broadening. It is about 2 times slower than sampling interactions with free electrons. This can be significant for photon-only simulations.

Optionally, one can select a different incoherent scattering model:

```
Bound Compton scattering = off | simple | on | norej
```

- `off`: Klein-Nishina sampling (free electron).
- `simple`: simple bound model, no Doppler broadening (similar to XCOM).
- `on`: relativistic impulse approximation.
- `norej`: same as `on`, but more efficient (`default`).

To use alternative Compton cross sections, e.g., from the file `joe_compton.data` , add `Compton cross sections = joe` to the transport parameter section of the input file.

Further refinements to Compton scattering model

EGSnrc allows the user to include radiative corrections for Compton scattering in the one-loop approximation. These corrections are by default turned off.

- Radiative corrections up to O(α^3) based on the original Brown & Feynman equations (Phys. Rev. Vol. 85, No. 2, 231-244, 1952) can be taken into account which effectively reduce the cross section at large photon scattering angles.

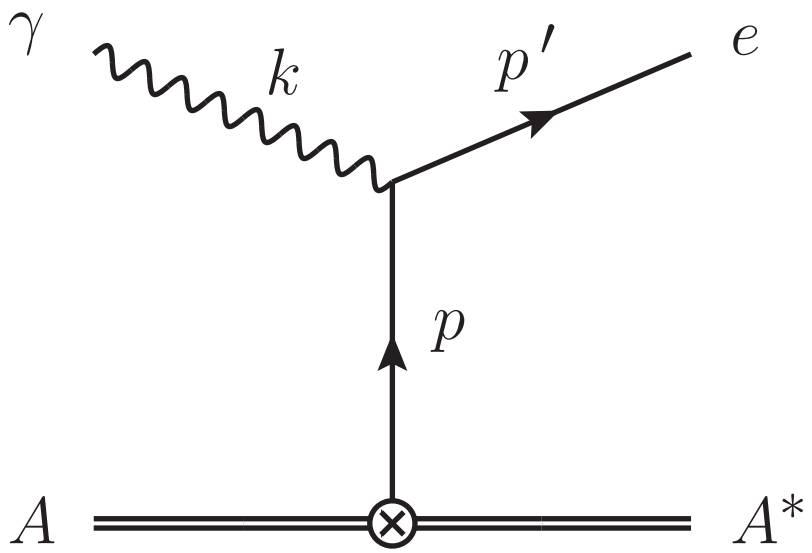
- Partially compensated by the inclusion of double Compton scattering process in which incident photon produces two photons when it interacts with the atomic electron.

To include radiative corrections and double Compton scattering:

- `Radiative Compton corrections= On | Off`

- `Makefile` of the application must include file `$(EGS_SOURCEDIR)rad_compton1.mortran` in the SOURCES list, just before `$(EGS_SOURCEDIR)get_inputs.mortran`

Photoelectric absorption



- Occurs at all energies, but probability is exceedingly small at high energies
- Scales as Z^n, $n \sim 3 \cdots 5$
- Dominates at **low photon energies**

Photoelectron direction

By default sampled from the Sauter distribution [*]:

- Valid only for the K-shell
- Derived from an extreme relativistic approximation ($\beta \approx 1$)
- Good agreement with absorption measurements down to 92 keV

The photoelectric effect is only dominant at low energies, where the angular distribution of electrons rapidly becomes isotropic due elastic scattering. But the CPU cost is negligible, so angular sampling of the photoelectron is On by default.

turned On or Off using:

```
Photoelectron angular sampling = On | Off
```

When turned off, photoelectron inherits the photon's direction

[*] See EGSnrc manual for further details

Photoelectric absorption in EGSnrc

- Atomic relaxations turned OFF: photoelectron created with the photon's energy

```
Atomic relaxations = Off
```

STACK

Npold = NP

- Atomic relaxations considered: interaction with atomic shells

```
Atomic relaxations = On
```

STACK

NPold **Npold + 1** **NP**

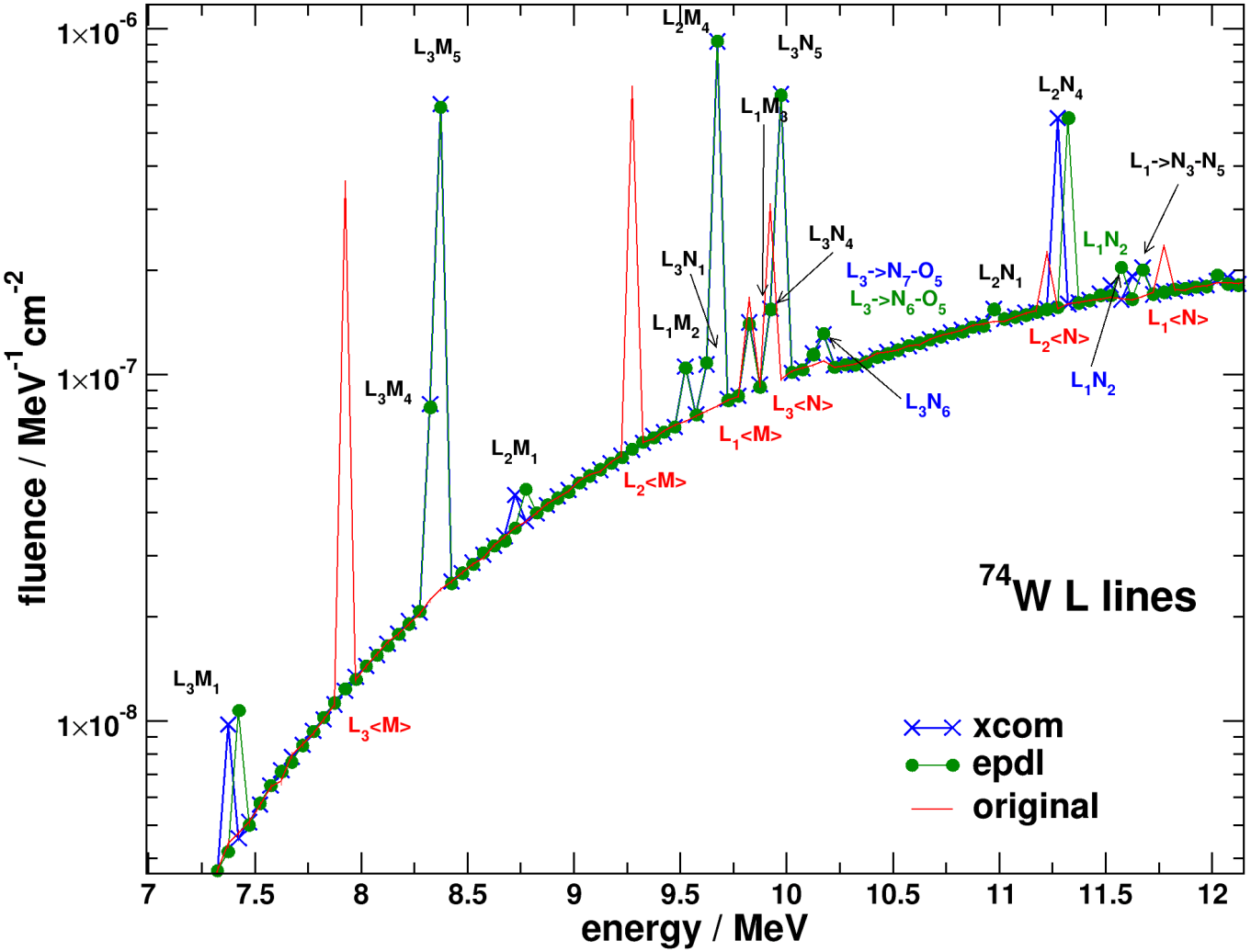
Atomic relaxations

The input options for atomic relaxations are:

```
Atomic relaxations = Off | [On | eadl] | simple
```

- Relaxation cascade of inner shell vacancies generates fluorescent photons, Auger or Coster-Kronig electrons. Of importance if their ranges are not small compared to the geometrical scale of the problem.
  - Currently in photo-absorption, bound Compton scattering, electron impact ionization
  - Future: triplet production, electron-electron bremsstrahlung
- If `simple`: All radiative and non-radiative transitions to/from K-, LI-, LII-, LIII-, and “average” M and N-shells with binding energies above 1 keV.
- If `On|eadl`: All radiative and non-radiative transitions to/from all available shells with binding energies above 1 keV.
- Cannot be `Off` when bound Compton or electron impact ionization requested!

Atomic relaxations



Photoelectric interaction with atomic shells

By default, the interacting shell is explicitly sampled using energy independent interaction probabilities ν_i with the K-, LI-, LII-, LIII-, and "average" M-shell with binding energies above 1 keV.

The input entries in the `Transport Parameters` input block influencing how the interaction occurs are:

```
Photon cross sections = xcom | epdl | si
Atomic relaxations    = simple | eadl
```

Atomic shells involved in the interaction depend on the atomic relaxation option selected:

Relaxation	simple	EADL
Initial vacancy	K,L1..L3,<M>	K,L1..L3
Final vacancy	K,L1..L3,<M>,<N>	K,L1..L3,M1..M5,N1..N7..

Photoelectric interaction with atomic shells

Option to use Sabbatucci and Salvat **renormalized** * shell-wise cross sections allowing to determine energy-dependent interaction probabilities for all available shells by setting:

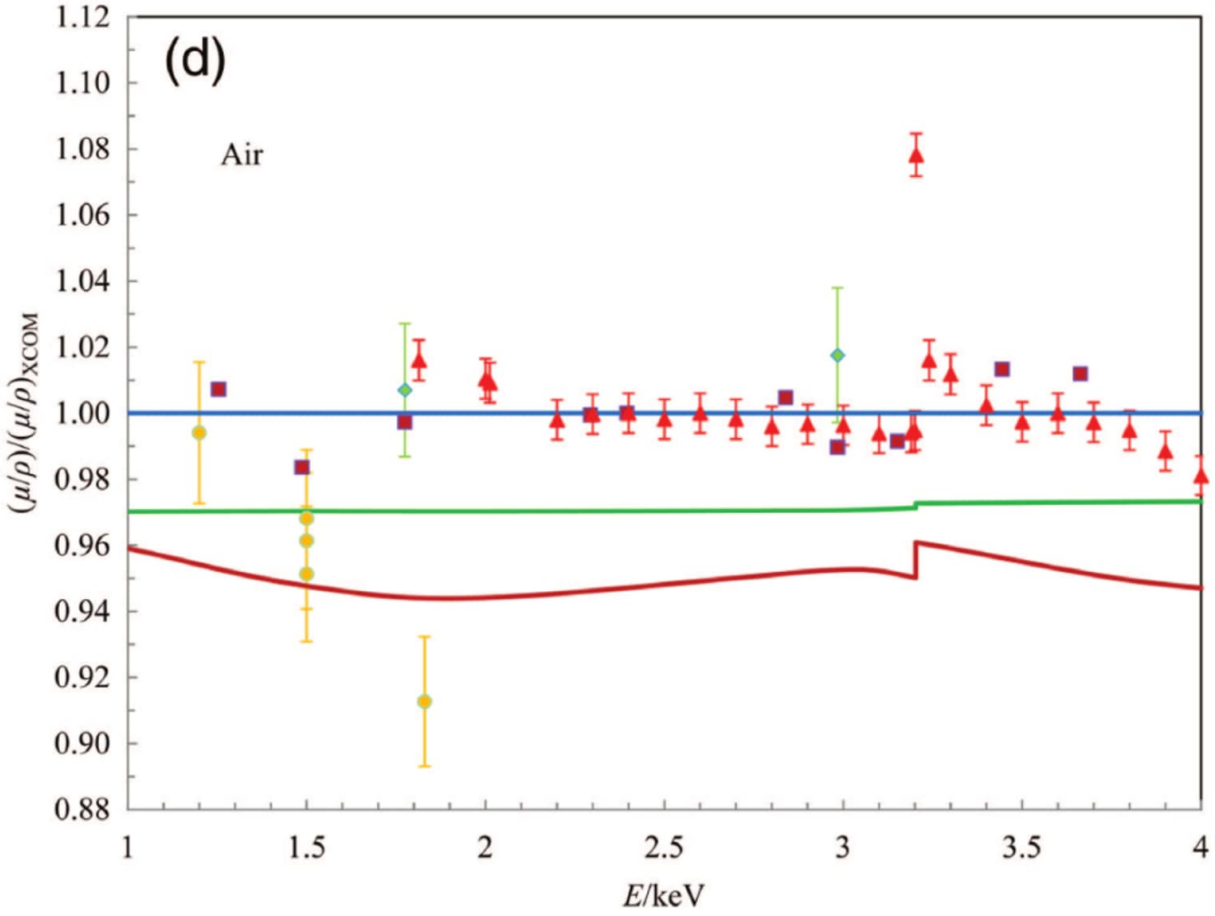
```
Photon cross sections = mcdf-xcom | mcdf-edpl
Atomic relaxations    = eadl
```

Atomic shells involved in the interaction:

Photoeffect	MCDF
Initial vacancy	K,L1..L3,M1..M5,N1..N7
Final vacancy	K,L1..L3,M1..M5,N1..N7..

* In principle, one can improve independent-electron cross sections using an energy-independent factor, obtained from atomic-structure calculations such as multi-configuration Dirac-Fock (MCDF) self-consistent model.

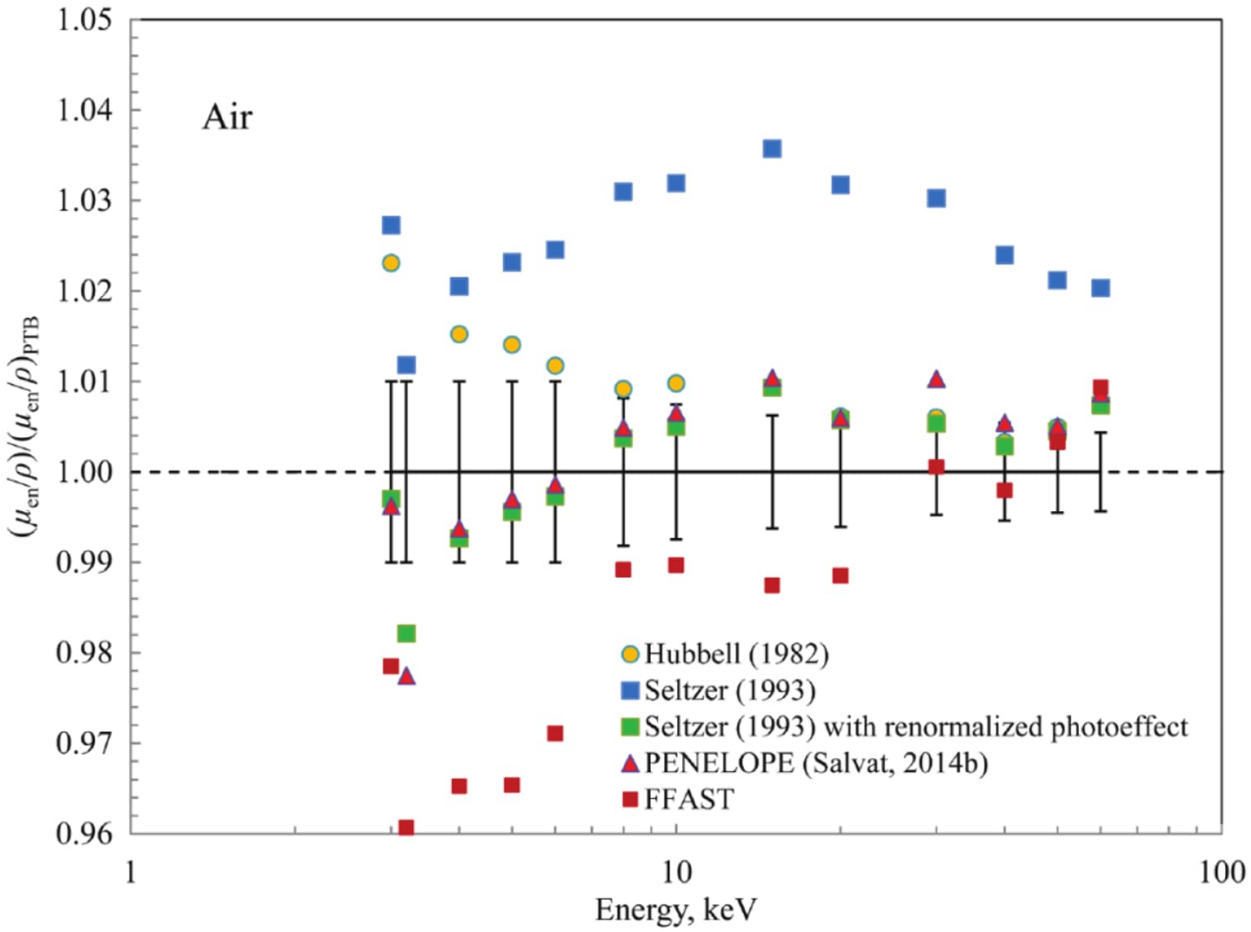
ICRU Report 90 (2016)



Kato et al 2010 (triangles)

- μ/ρ measurement at 0.3 %
- Synchrotron beams 1 keV - 3.9 keV
- Evidence for not normalizing
- Also observed by Hubbell and Salomon in 1969 below 1 keV

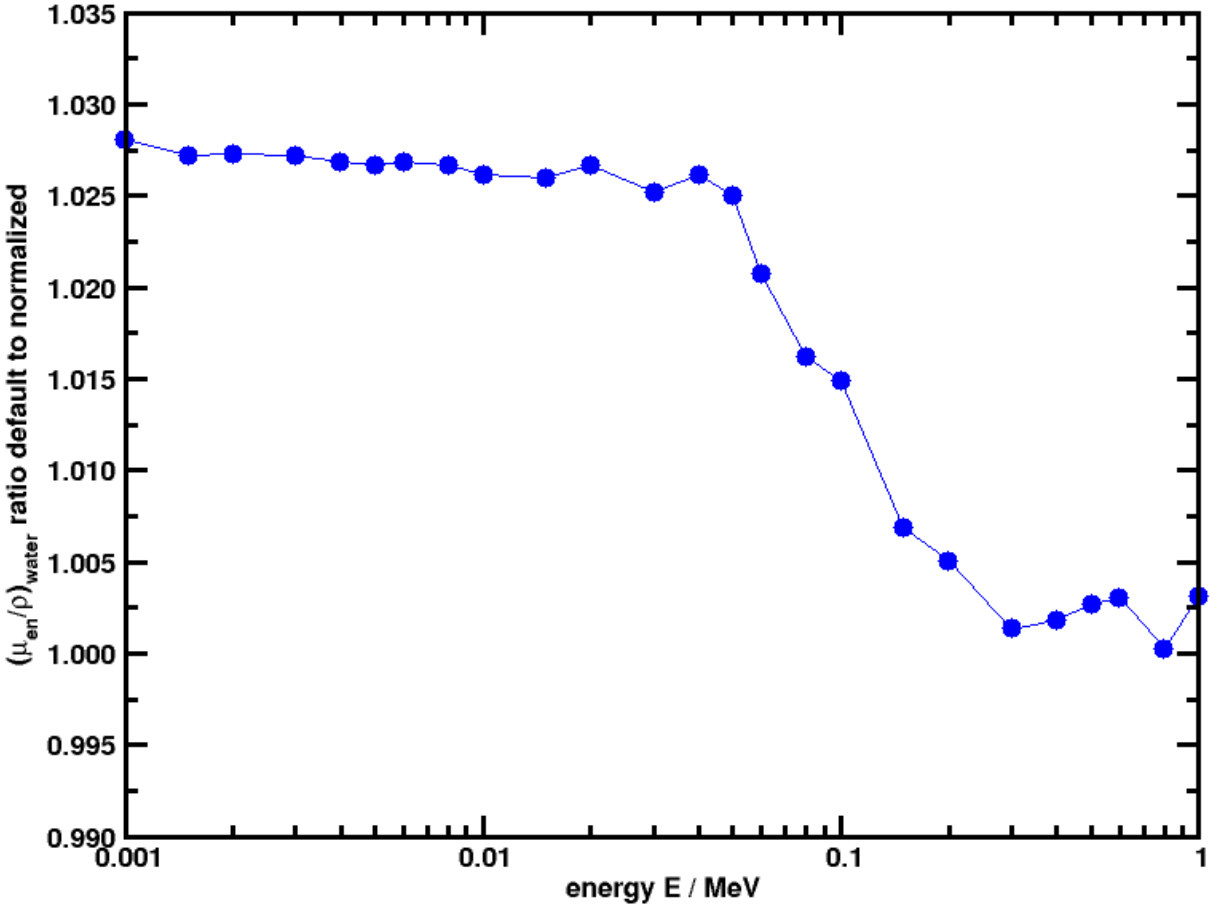
ICRU Report 90 (2016)



PTB 2006, 2012

- μ_{en}/ρ measurements ($\approx 1.0\,\%$)
- Synchrotron beams 3 keV - 60 keV
- Evidence for normalizing

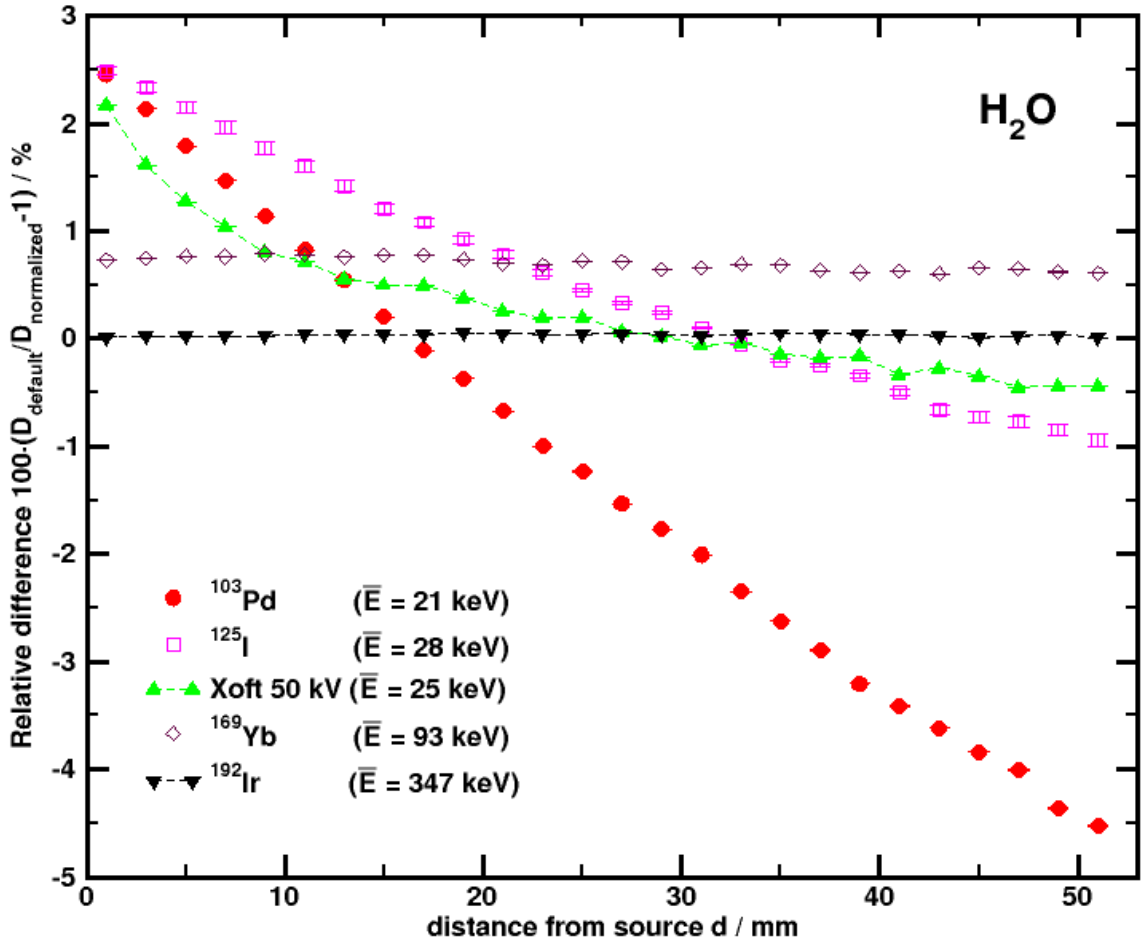
Does it matter?



- Absolute dose/kerma at low-energies: yes *
- LDR brachytherapy: yes
- Yb-169 brachytherapy sources? Maybe!
- HDR brachytherapy: no

* Valdes-Cortez *et al.* 2021 recommend 1.5 % type B uncertainties (k=2) in μ_{en}/ρ for air and water, and 2.0 % for graphite (*Phys. Med. Biol.* **66** 105014).

Does it matter?



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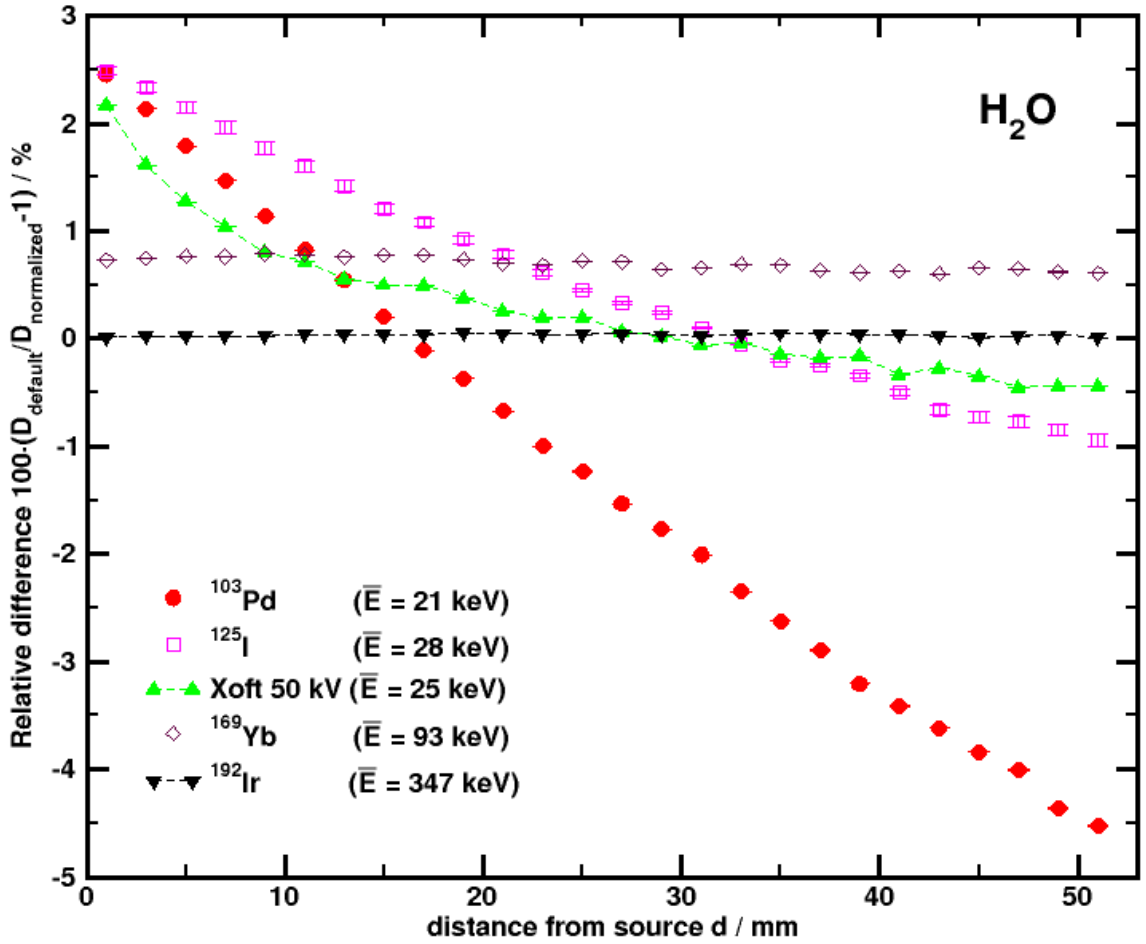
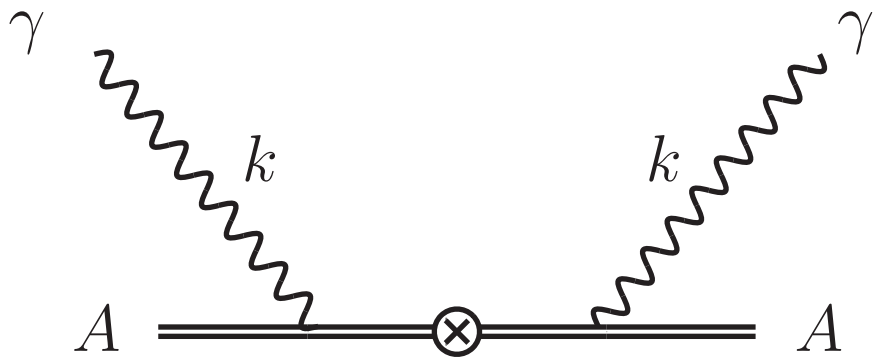


$$K(d) = \frac{\Phi_0 \cdot \frac{\mu_{\mathrm{en}}}{\rho} \cdot E}{e^{\mu \cdot d}}$$

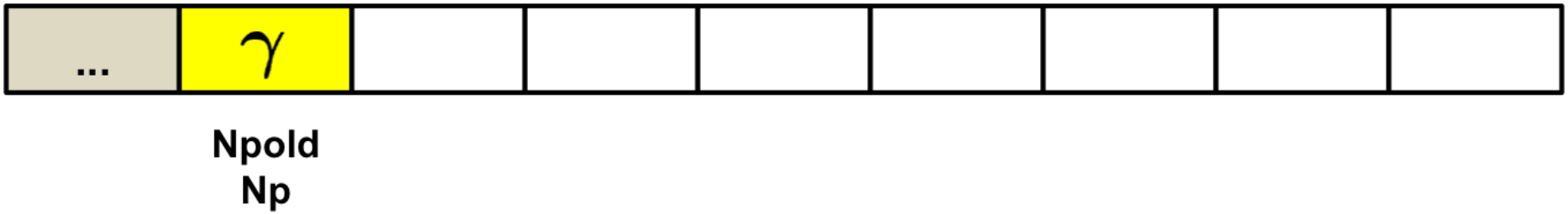
*Valdes-Cortez *et al.* 2021 recommend 1.5 % type B uncertainties (k=2) in μ_{en}/ρ for air and water, and 2.0 % for graphite (*Phys. Med. Biol.* **66** 105014).

Rayleigh (coherent) scattering



- Occurs for **all** photon energies, but probability is extremely small at high energies
- Scales as Z^2 (small angles) to Z^3 (large angles)
- **Never** dominates

STACK



Rayleigh scattering is “On” in EGSnrc by default

This effect can be turned on and off:

```
Rayleigh scattering = Off | On | custom
```

EGSnrc uses **atomic form factors** from the tabulations by Hubbell and Øverbø, which are derived from atomic form factors using the independent atom approximation.

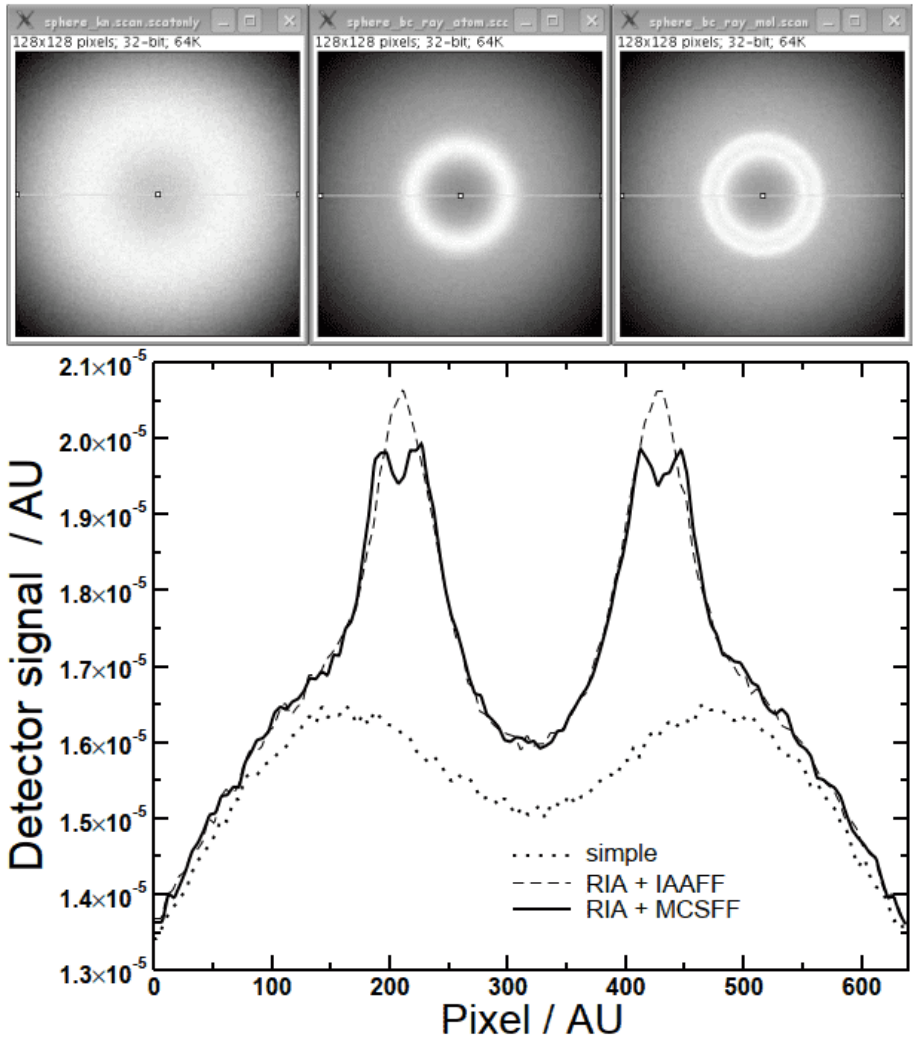
The `custom` option allows users to employ **their own form factor tabulations.** For example, to use the form factor data found in `file1` for the medium `medium1`, etc.:

```
Rayleigh scattering = custom
ff media names = medium1 medium2 ...
ff file names  = file1 file2 ...
```

Measured molecular form factors for 15 substances (including water) from Peplow and Verghese are distributed with EGSnrc.

Only use Rayleigh scattering when using bound Compton scattering: there is no such thing as a photon elastically scattering off a free electron!

Molecular form factors in imaging



Photonuclear absorption

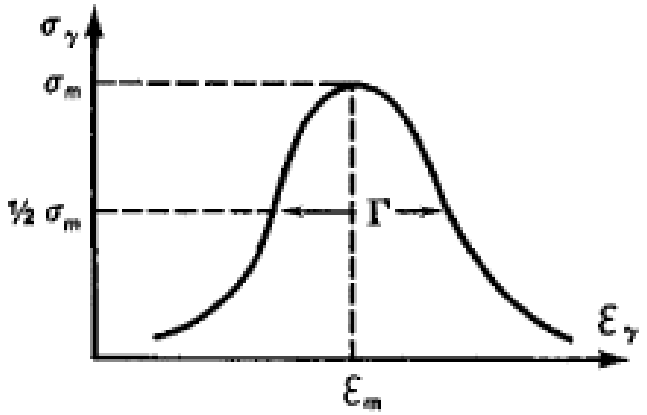
It is possible to account for photon attenuation due to photonuclear interactions (E. Ali):

- IAEA photonuclear cross sections by E. Ali (`iaea_photonuc.data`). Although user-provided cross sections can be used.
- The gamma mean free path (GMFP) in the medium is shortened accordingly.
- Photon is discarded without energy deposition and without generating secondary particles.

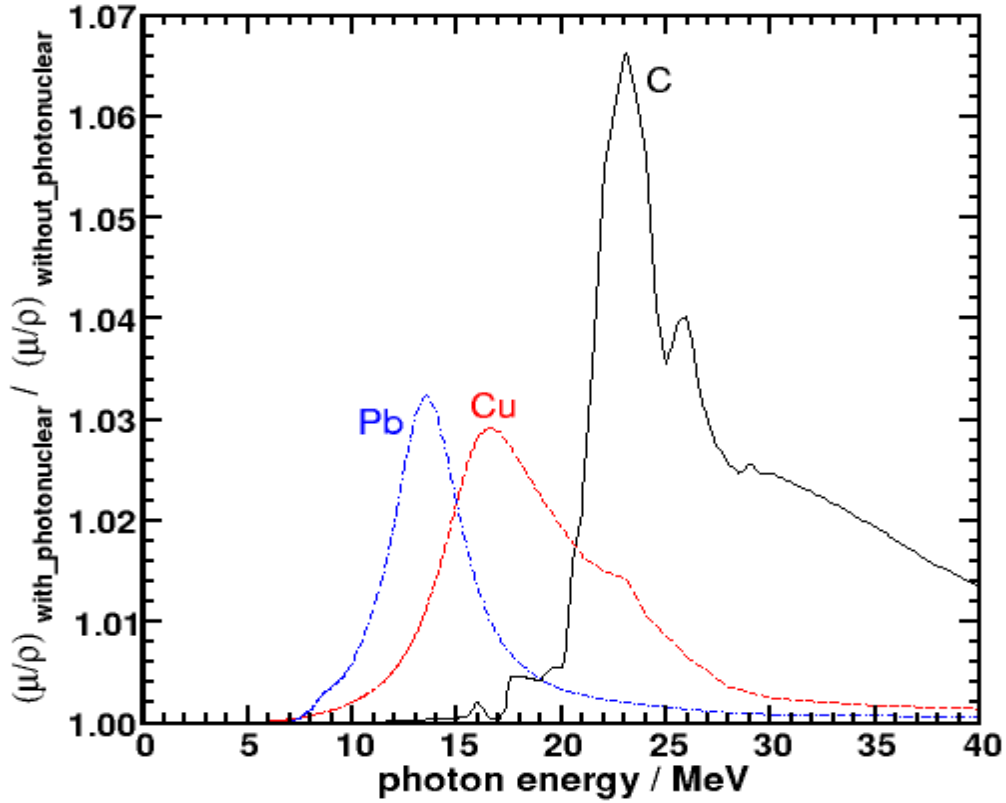
The user's inputs for the photonuclear option are handled in a way similar to the inputs for typical EGSnrc transport parameters:

```
Photonuclear attenuation = OFF (default) | ON | [ON|OFF] in regions
start region = ir1, ir3, . . .
stop region  = ir2, ir4, . . .
Photonuclear cross sections= photonuc_xsections
```

Photonuclear absorption



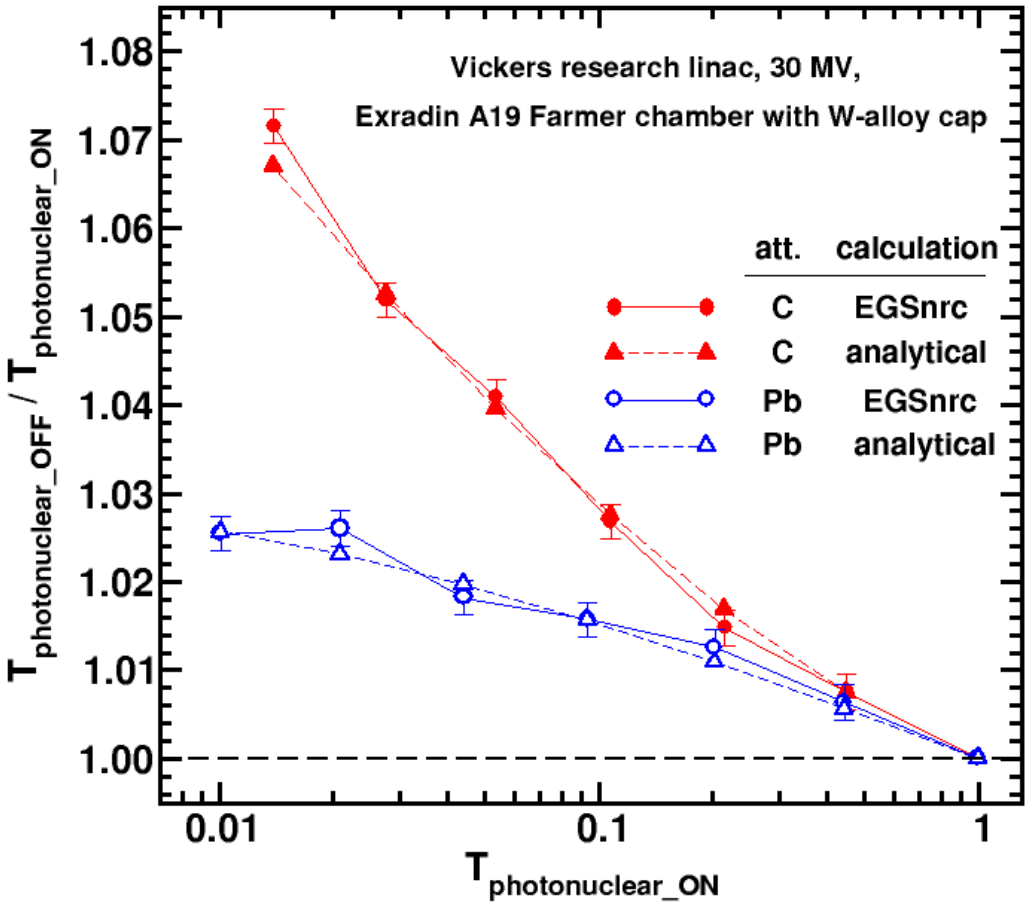
The photonuclear cross sections have a broad maximum known as the giant resonance usually spaning about 4 MeV to 8 MeV.



This interaction is of significance for photon energies of the order of tens of MeV.

Photonuclear absorption

Added to EGSnrc circa 2012 motivated by megavoltage transmission experiments conducted at NRC with our research linac (Vickers) in the MV energy range.



Highly sensitive experiment: extended dimensions ($\sim$3 m), extreme attenuation, and extreme collimation strongly amplify what would otherwise be small physics effects.

Default photon transport parameters

```
:start MC transport parameters:

Photon cross sections              =  xcom # mcdf-xcom?
Compton cross sections             =  default
Global Pcut                        =  AP # in MeV
Pair cross sections                =  BH
Pair angular sampling              =  Simple
Triplet production                 =  Off
Bound Compton scattering           =  norej
Radiative Compton corrections      =  Off
Rayleigh scattering                =  On
Atomic relaxations                 =  eadl
Photoelectron angular sampling     =  On
Photonuclear attenuation           =  Off
Photonuclear cross sections        =  default

:stop MC transport parameters:
```

Optimum parameters for clinical MV photon beams

```
:start MC transport parameters:

Photon cross sections              =  xcom
Compton cross sections             =  default
Global Pcut                        =  0.010 # in MeV
Pair cross sections                =  BH
Pair angular sampling              =  Simple
Triplet production                 =  Off
Bound Compton scattering           =  Off
Radiative Compton corrections      =  Off
Rayleigh scattering                =  Off
Atomic relaxations                 =  Off
Photoelectron angular sampling     =  Off
Photonuclear attenuation           =  Off
Photonuclear cross sections        =  default

:stop MC transport parameters:
```

Saves about 25 % CPU time for a 6 MV and a 16 MV beam.

Take-home messages

- EGSnrc uses `state-of-the-art` photon physics models
- Options to use different models allows comparison with other MC codes and historical results
- Options to use simpler models increasing calculation speed,

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Lecture 5

Photon physics

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