New photon transport model in Serpent 2

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Motivation

- On average, 8 prompt fission photons over an energy range from 0.1 to 10.5 MeV are released per one thermal-neutron-induced fission of ^{235}U.
- Fission products also produce gamma photons
- High-energy photons have long path lengths

$\Rightarrow$ Gamma-heating : energy is deposited far away from the location of fission

- Important applications in dosimetry, shielding and medical physics

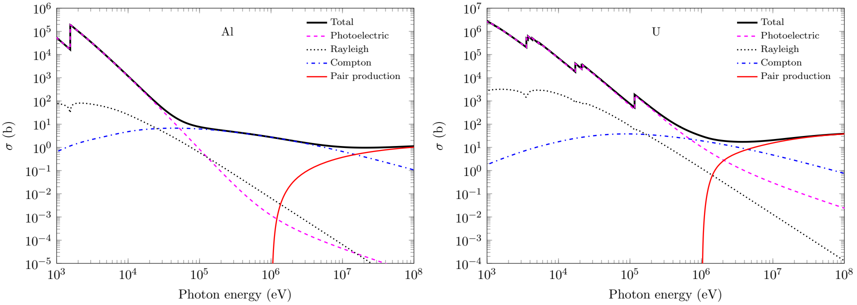
Outline

- General stuff
- Photon interactions:
  - Rayleigh scattering
  - Compton scattering
  - Photoelectric effect
  - Pair production
- Secondary processes:
  - Atomic relaxation
  - Thick-target bremsstrahlung
- Data
- Comparison to MCNP4C - first results

General stuff

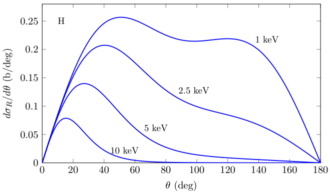
- Energy range of photons from 1 keV to 100 MeV
- Only unpolarised photons are considered
- Photonuclear interactions are disregarded for now
- Some parts are still under development

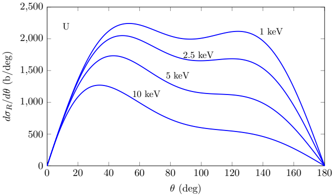
Interaction cross sections



Rayleigh scattering

- Elastic scattering from the electron cloud of an atom
- Form factor approximation resulting from the first-order Born approximation:
  - $\frac{d\sigma_{\mathrm{R}}}{d\Omega} = \frac{d\sigma_{\mathrm{Th}}}{d\Omega} |F(q,Z)|^2 = \frac{r_{\mathrm{e}}^2}{2}(1+\cos^2\theta)\,|F(q,Z)|^2$,
    where $q = |\mathbf{k} - \mathbf{k}'| = 4\pi\sin(\theta/2)/\lambda$ is the momentum transfer vector
  - $F(0,Z) = Z$, F decreases monotonically with increasing q
  - Valid only above K-edge, but is usually used as such
  - Straightforward to sample using rejection sampling





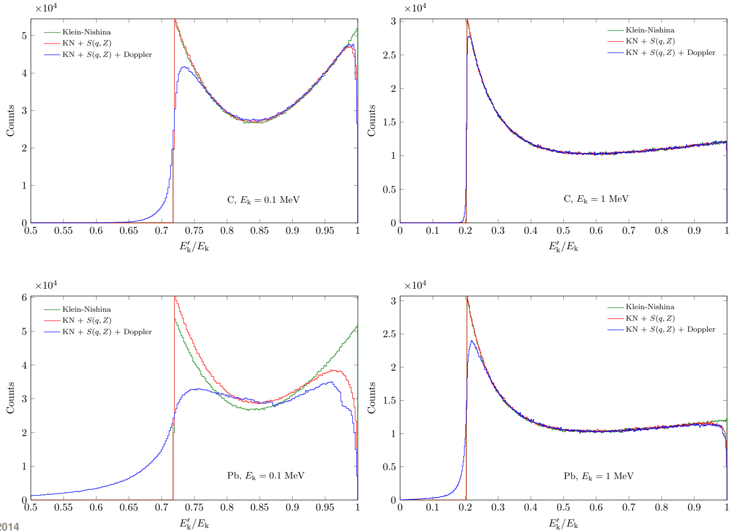
Compton scattering

- Scattering from a free electron is given by the Klein-Nishina formula
  - $\frac{d\sigma_{\mathrm{Co}}^{KN}}{d\Omega} = \frac{r_{\mathrm{e}}^2}{2}\left(\frac{E_{\mathrm{k}}'}{E_{\mathrm{k}}}\right)^2\left(\frac{E_{\mathrm{k}}'}{E_{\mathrm{k}}} + \frac{E_{\mathrm{k}}}{E_{\mathrm{k}}'} - \sin^2\theta\right)$
  - Reasonably accurate only above a few MeV
- Incoherent scattering function $S(q, Z)$ takes into account the effects of the binding energies of electrons
  - $\frac{d\sigma_{\mathrm{Co}}}{d\Omega} = \frac{d\sigma_{\mathrm{Co}}^{KN}}{d\Omega} S(q, Z)$
  - $S(q \to 0, Z) \to 0$, $S(q \to \infty, Z) \to Z$
- The momentum of the electron broadens the energy spectrum of the scattered photon
  - This Doppler energy broadening can be included with Compton profiles $J(p_z)$
  - $J(p_z)$ is a probability distribution for the projection $p_z = -\frac{\mathbf{p}_{\mathrm{e}} \cdot \mathbf{q}}{q}$, where $\mathbf{p}_{\mathrm{e}}$ is the pre-collision momentum of the electron
  - Scattered photon energy can be solved using the conservation of energy and momentum

Compton scattering - method

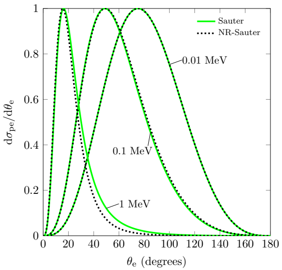
- Scattering angle:
  - Angle is sampled from the Klein-Nishina formula
  - Rejection sampling using the scattering function
- Doppler broadened photon energy:
  - The electron subshell is sampled according to the Compton profiles and number of electrons per shell
  - p_z is sampled from the Compton profile corresponding to the sampled subshell
  - Photon energy is calculated using p_z and the sampled angle
- Electron is emitted in the direction of $\mathbf{q}$ with an energy of $T_\mathrm{e} = E_\mathrm{k} - E'_\mathrm{k} - U_i$
- Vacancy is treated with the atomic relaxation model
- Compton electron is treated with the thick-target bremsstrahlung approximation

Compton scattering - histograms of scattered photon energy, 5 million photons per each case



Photoelectric effect

- Subshell is sampled according to the subshell cross sections
- Only those subshells with ionization energies larger than the cut-off energy are considered
- If the ionization energy of the shell is above the cut-off, $T_\mathrm{e} = E_\mathrm{k} - U_i$, else $T_\mathrm{e} = E_\mathrm{k}$
- Sauter distribution is commonly used for the polar angle θ_e:
  - $\frac{d\sigma_{\mathrm{pe}}^{\mathrm{Sauter}}}{d\Omega_\mathrm{e}} \propto \frac{\sin^2\theta_\mathrm{e}}{(1-\beta\cos\theta_\mathrm{e})^4}\left[1+\frac{1}{2}\gamma(\gamma-1)(\gamma-2)(1-\beta\cos\theta_\mathrm{e})\right]$
  - Low sampling efficiency ($\sim 0.3 - 0.4$)
- We use the non-relativistic approximation of Sauter distribution:
  - $\frac{d\sigma_{\mathrm{pe}}^{\mathrm{NR\ Sauter}}}{d\Omega_\mathrm{e}} \propto \frac{\sin^2\theta_\mathrm{e}}{(1-\beta\cos\theta_\mathrm{e})^4}$
  - Efficiency 2/3
- Secondary processes: thick-target bremsstrahlung and atomic relaxation



Electron–positron pair production

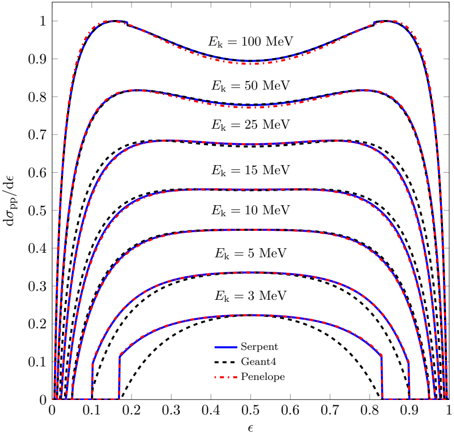
- Differential cross section for the electron reduced energy $\epsilon = (T_\mathrm{e} + m_\mathrm{e}c^2)/E_\mathrm{k}$ by Davies, Bethe and Maximon combined with the correction factor F_0 used by Penelope:

$$\frac{d\sigma_\mathrm{pp}}{d\epsilon} = \alpha Z^2 r_\mathrm{e}^2 \left[\left(2\epsilon^2 - 2\epsilon + 1\right) \left(\Phi_1(Z, \epsilon, \epsilon_\mathrm{min}) - \frac{4}{3}\ln Z - 4 f_\mathrm{C}(Z) + F_0(\epsilon_\mathrm{min}, Z) \right) + \frac{2}{3}\epsilon(1-\epsilon) \left(\Phi_2(Z, \epsilon, \epsilon_\mathrm{min}) - \frac{4}{3}\ln Z - 4 f_\mathrm{C}(Z) + F_0(\epsilon_\mathrm{min}, Z) \right) \right]$$

- Approximations for screening functions Φ_1 and Φ_2 by Butcher and Messel (also used by G4BetheHeitlerModel)
- Coulomb correction f_C used for all energies
- Sampling method:
  - Between 2 and 100 MeV, rejection sampling is employed: The maximum of $\frac{d\sigma_\mathrm{pp}}{d\epsilon}$ can be fitted by a rational function $\Lambda(E_\mathrm{k}, Z) = \frac{p_1(Z)E_\mathrm{k}^2 + p_2(Z)E_\mathrm{k} + p_3(Z)}{E_\mathrm{k}^2 + q_1(Z)E_\mathrm{k} + q_2(Z)}$
  - Below 2 MeV, uniform distribution is used
- Angular distribution: the leading term of the Sauter–Gluckstern–Hull distribution (used in ETRAN-based codes and Penelope)
- Annihilation: Two photons are generated isotropically in the opposite directions, both having an energy of $E_\mathrm{k} = m_\mathrm{e}c^2$

Electron–positron pair production - distribution comparison

- Comparison to G4BetheHeitlerModel and Penelope model for uranium, distributions are scaled to equal maximum

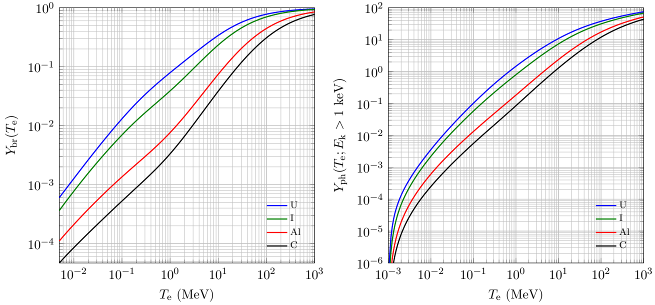


Atomic relaxation

- Vacancies are caused by photoelectric effect and Compton scattering
- Relaxation through radiative (fluorescence) and non-radiative (Auger, Coster-Kronig) transitions
- ENDF data provides probabilities and energies of transitions for all the subshells of each element
- Simulation procedure:
  - Transition is sampled if the binding energy of the vacancy subshell is larger than the cut-off energy
  - If the transition energy is larger than the cut-off, a photon or an electron is created
  - Repeated until vacancies are filled

Thick-target bremsstrahlung for electrons

- Thick-target bremsstrahlung approximation: no transport of electrons, only photons are generated
- Bremsstrahlung is important at high energies, especially for high-Z materials
- Electrons are generated by Compton scattering, photoelectric effect, pair production and non-radiative transitions
- Distributions for photon energies and angles can be generated using multiple electron scattering theory
- Another option is to use continuous slowing-down approximation (CSDA)



Thick-target bremsstrahlung - model

- Still under development
- Current incomplete (and incorrect) model:
  - Photon number yield calculated according to CSDA
  - The electron energies, at which bremsstrahlung occurs, are sampled from the photon number yield distribution
  - The photon energies are sampled from the single-bremsstrahlung distributions
  - Angular distribution and positrons are ignored for now

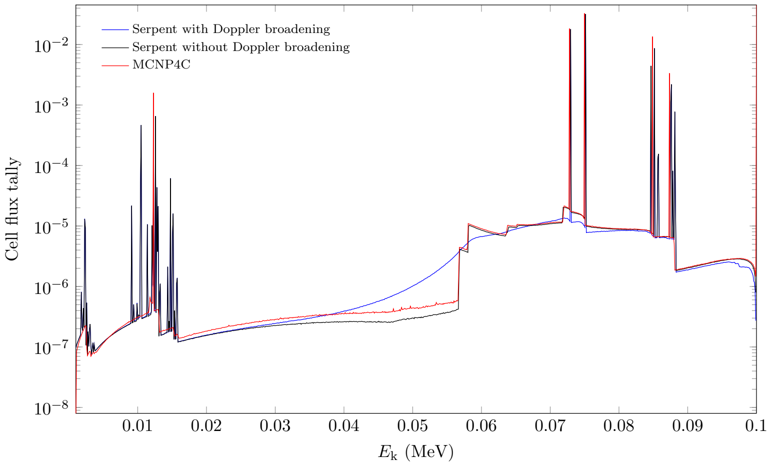
Data

- Form factors, incoherent scattering functions, photoelectric subshell cross sections and atomic relaxation data from ENDF-B-VII.1
  - A matlab script for some processing of the data and converting to a nicer format
  - Don't be afraid, this is just a temporary solution
- Compton profiles calculated by Biggs
- Why am I not NJOYing the data?
  - NJOY has (or at least had) old processing methods for form factors and incoherent scattering functions
  - NJOY 2012 manual states: "The fluorescence part is not coded yet. This section will be completed when the new fluorescence methods have been developed and installed in MCNP."
- Total cross sections of photon interactions from MCNP-libraries, e.g., mcplib84

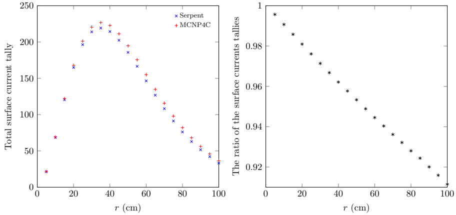
First results - comparison to MCNP4C

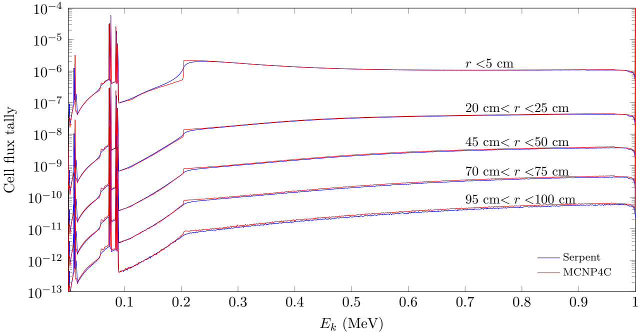
- The photon transport model in MCNP4C is in many ways different than the model presented here
- There could still be some bugs...
  $\Rightarrow$ Don't take the comparison too seriously
- Two test cases with an isotropic point source at the centre of a lead sphere with a density 1 g/cm^3
  - E_k = 100 keV, radius = 10 cm, cell flux tallied inside a sphere of radius 1 cm
  - E_k = 1 MeV, radius = 100 cm, total surface current tallied at 20 nested spherical surfaces, cell flux tallied between the surfaces
  - 1 billion photons
- The standard libraries were used in the MCNP4C calculations. In Serpent calculations, the data discussed in the previous slide (+ mcplib84)

100 keV point source



1 MeV point source





Summary

- A new photon transport model has been developed in Serpent, which covers the most important photon interactions and secondary processes
- Bremsstrahlung model is still under development
- Final comparison will be made with MCNP6
- Future work, e.g.:
  - Photonuclear interactions
  - Coupled neutron-photon transport
  - Variance reduction techniques