Photon transport mode in Serpent 2

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Outline

- Photon physics in Serpent
- Doppler broadening in Compton scattering
- Thick-target bremsstrahlung approximation
- Comparison to MCNP6

Photon transport mode

- Detailed photon physics is included in version 2.1.24
- Photon transport for elements from $Z = 1$ to 98
- Energy range of photons from 1 keV to 100 MeV
- Data:
  - Most of the interaction data is from ENDF-B-VII.1 (form factors, incoherent scattering functions, photoelectric cross sections and atomic relaxation data)
  - Other sources for data not found in ENDF-B-VII.1 (Compton profiles, bremsstrahlung data and electron stopping powers)
  - Matlab script is used for preprocessing of some of the data and for converting the data to a simpler format
  - Total cross sections of photon interactions from an MCNP-library, e.g. mcplib12

Interaction physics

Rayleigh scattering (elastic scattering from the electron cloud of an atom)

- Direction is sampled using the form factor approximation

Compton scattering (inelastic scattering from an atomic electron)

- Direction is sampled using the incoherent scattering function approximation
- Doppler broadening of the photon energy is taken into account

Photoelectric effect

- Electron shell is selected with a probability given by its cross section, all subshells are included

Pair production

- The energies and directions of the electron and positron are sampled using appropriate theoretical distributions
- Positron annihilation at rest generates two 0.511 MeV photons

Secondary photons

Atomic relaxation

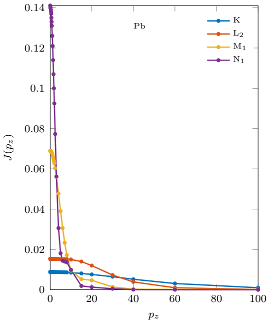
- Compton scattering and photoelectric effect cause vacancies in electron shells
- Relaxation cascade through radiative (fluorescence) and non-radiative (Auger, Coster–Kronig) transitions
- Transitions are sampled according to the probabilities given by ENDF/B-VII.1, all possible transitions are included

Thick-target bremsstrahlung approximation (TTB)

- Electrons are generated through Compton scattering, photoelectric effect, pair production and non-radiative transitions
- Bremsstrahlung photon production is important especially for high-Z atoms at energies above $\sim$1 MeV
- The number of bremsstrahlung photons and the photon energies are sampled from the distributions given by the continuous slowing down approximation (CSDA)
- Angular distribution is omitted; the direction of the bremsstrahlung photon is equal to the direction of the electron

Doppler broadening in Compton scattering

- The momentum of the electron broadens the energy spectrum, important below 1 MeV for heavy elements
- Energy broadening is included using Compton profiles $J(p_z)$
  - $J(p_z)$ is a PDF 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 and $\mathbf{q}$ is the momentum transfer vector of the photon
  - Scattered photon energy can be solved from p_z
- The minimum of p_z is $p_{z,\mathrm{min}} \approx -137$, the maximum depends on the incident photon energy, binding energy and scattering angle
- Compton profile data available only between $p_z = 0$ and $100 \Rightarrow$ extrapolation used in Serpent
- MCNP samples p_z only between -100 and 100
- Most of the sampled values of p_z will fall between -100 and 100



Comparison of Doppler models

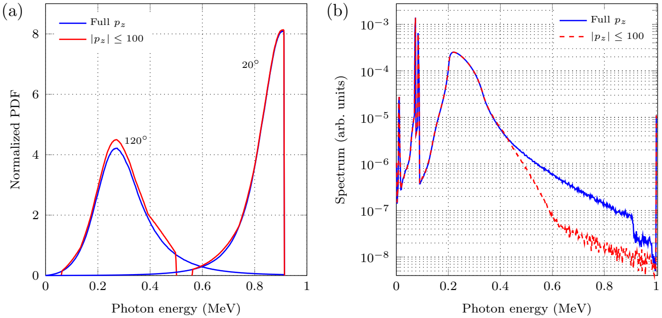


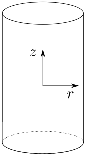
Figure : (a) Energy distribution of 1 MeV photons scattered from K-shell electrons of lead at 20° and 120°. (b) Energy spectrum of photons scattered between 90° and 180° from a lead target for a 1 MeV photon beam.

Differences in the TTB approximation between Serpent and MCNP6

- The average energy distribution is calculated using single-event bremsstrahlung distributions and electron stopping powers
- Stopping powers depend on the material density
  - Important at high energies and in compounds
  - Treated in MCNP6, not implemented in Serpent
- Radiative yield is smaller for positrons than for electrons because positrons lose more energy in collisions
  - In MCNP, electron and positron bremsstrahlung distributions are equal
  - In Serpent, a separate treatment for positrons can be chosen
- In Serpent, one bad approximation causes underestimation of the high-end of the bremsstrahlung spectrum
- Bremsstrahlung in compounds doesn't work well in 2.1.24, the method will be updated for 2.1.25

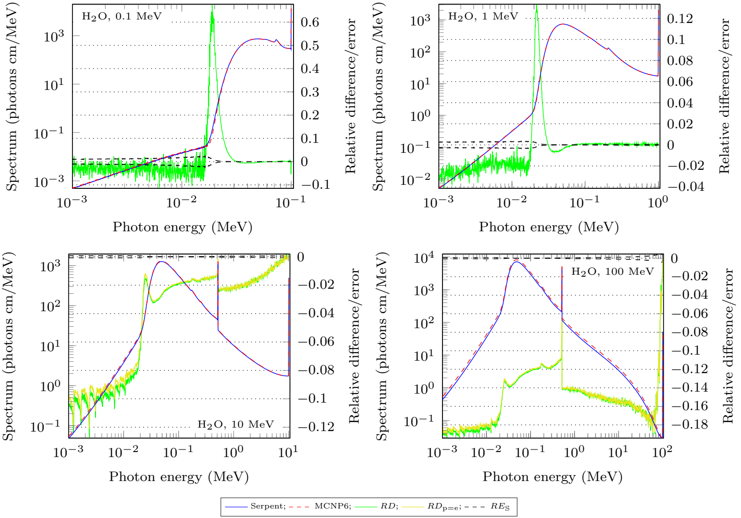
Test cases

- Energy distribution:
  - Isotropic, mono-energetic point source at the centre of a large sphere
  - Tested energies and materials: 100 keV, 1 MeV, 10 MeV and 100 MeV for water, uranium and uranium dioxide
  - Both positron bremsstrahlung models were tested at 10 and 100 MeV
- Energy-angular distribution:
  - Mono-directional point source at the centre of a cylinder
  - Spectrum and total flux tallied as a function of z and r
  - Test energies and materials: water at 100 keV, 1 MeV and 10 MeV, lead at 100 keV and 1 MeV

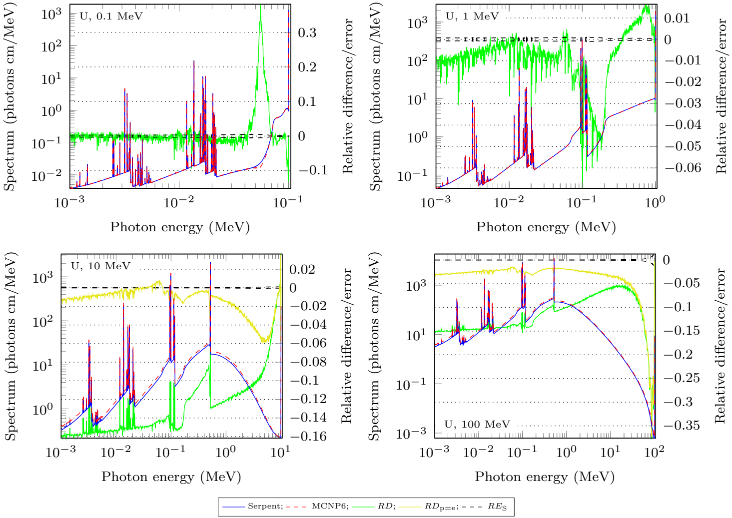


- Pre-compiled MCNP6.1 executable used in all cases with mcplib12-data
- Development version of Serpent used (2.1.25)
- Here, relative difference RD = (Serpent result - MCNP6 result)/MCNP6 result

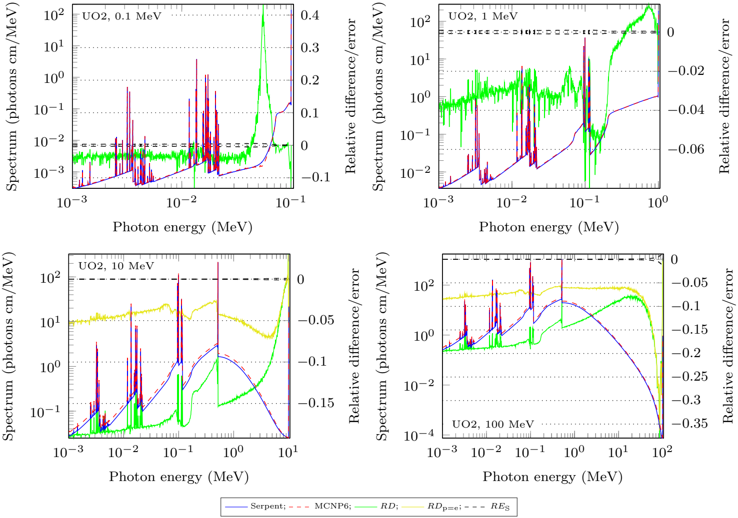
Photon spectrum in water



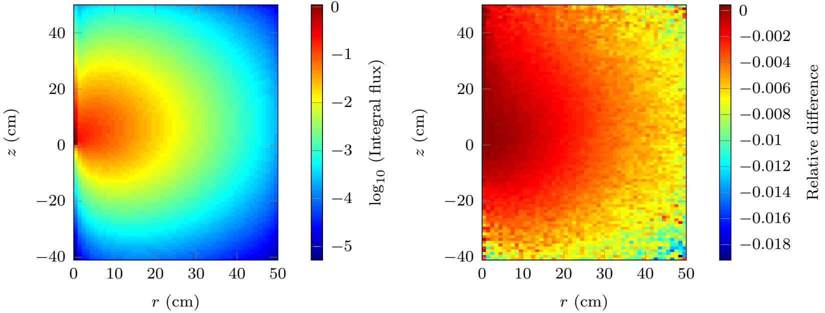
Photon spectrum in uranium



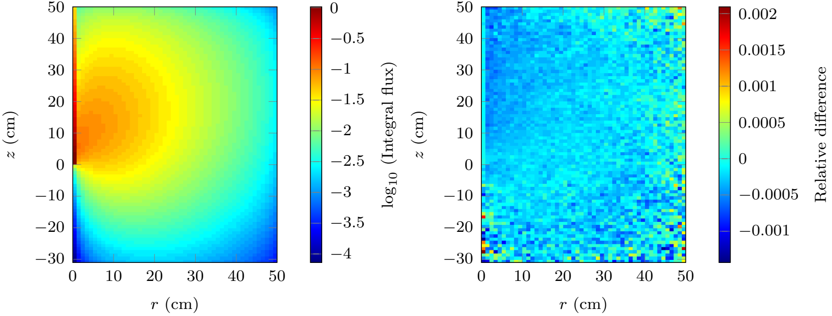
Photon spectrum in uranium dioxide



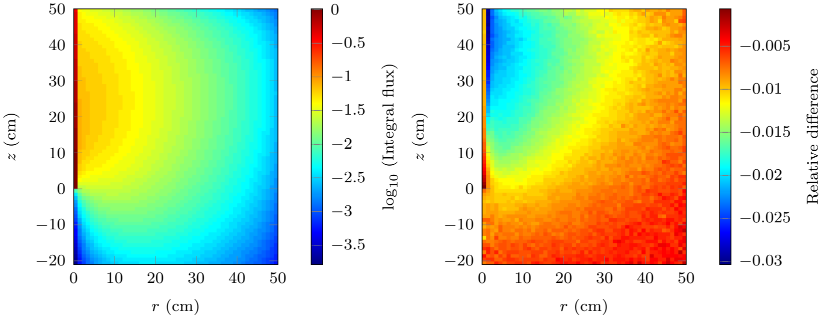
Total flux in water cylinder, 100 keV



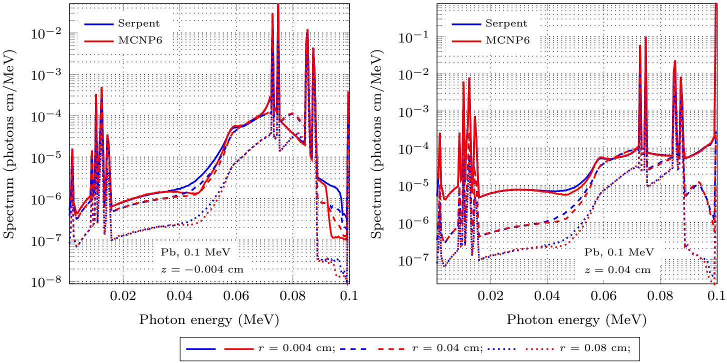
Total flux in water cylinder, 1 MeV



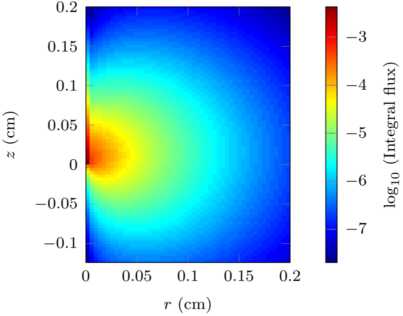
Total flux in water cylinder, 10 MeV

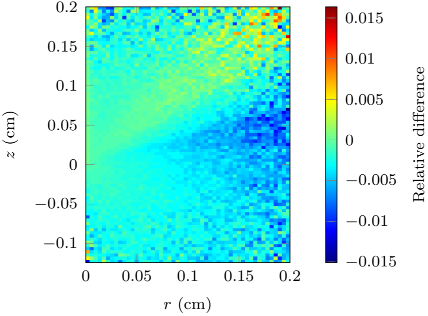


Spectrum in lead cylinder, 100 keV

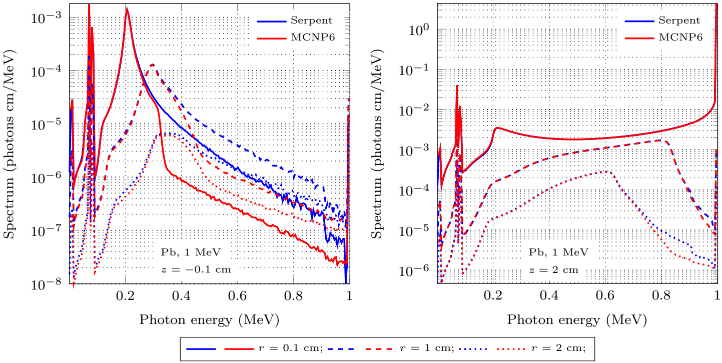


Total flux in lead cylinder, 100 keV

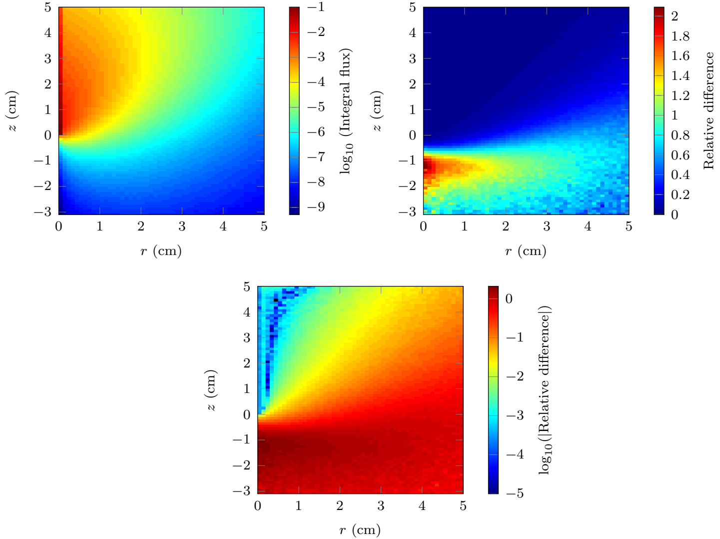




Spectrum in lead cylinder, 1 MeV

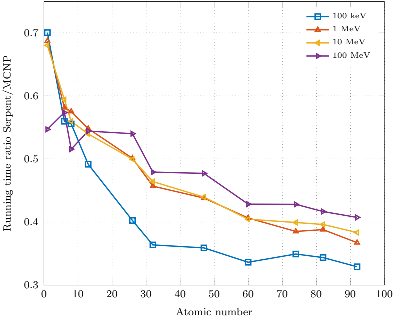


Total flux in lead cylinder, 1 MeV



Running time comparison in the spectrum (sphere) test case

- Single-core simulations without any tallies, number of photons 10^7–10^8
- The pre-compiled version of MCNP6 probably hasn't been compiled with full optimization
- Some of the photon physics routines in Serpent have not been fully optimized yet



Summary

- Reasonably good agreement with MCNP6
- Doppler broadening and TTB approximation are the main causes of the observed differences
- Stopping powers cause the largest differences, especially in compounds
- Future work:
  - TTB development
  - Comparisons with other photon transport codes needed for studying Compton scattering and positron bremsstrahlung