Recent development in Serpent photon transport mode

Toni Kaltiaisenaho

VTT Technical Research Centre of Finland

Serpent User Group Meeting, Gainesville, FL
November 6–9, 2017

Outline

- Photon physics in Serpent
- Improved thick-target bremsstrahlung approximation
- Beta bremsstrahlung
- Flux-to-Effective dose conversion factors
- Detector modeling with Serpent

Photon transport mode

- Photon transport for elements from Z = 1 to 99
- 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 and bremsstrahlung data)
    - Total cross sections of photon interactions are read from an MCNP-library, e.g. mcplib12

Photon 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

Improved TTB approximation (2.1.29)

- Electrons and positrons lose energy through ionization and excitation (collisions), and bremsstrahlung (radiative losses)
- Stopping power:

$$-\frac{dT}{ds} = n \int W \frac{d\sigma}{dW} dW \equiv S(T),$$

  where T is the electron energy and $d\sigma/dW$ is the differential cross section for the energy loss W.
- Total stopping power:

$$S_{\text{tot}}(T) = S_{\text{col}}(T) + S_{\text{rad}}(T)$$

- Radiative and total stopping powers are needed for calculating bremsstrahlung number yield and energy distribution
- In 2.1.28 and previous versions, elemental stopping powers given in NIST ESTAR database [1] were used, and additivity rule was applied for compounds and mixtures:

$$\frac{1}{\rho} S_{\text{rad/col}}(T) = \sum_j w_j \left[\frac{1}{\rho} S_{\text{rad/col}}(T) \right]_j ,$$

  where w_j is the mass fraction related to the jth constituent element.

Improved TTB approximation (2.1.29)

- Collision stopping power equation:

$$\frac{1}{\rho}S_{\mathrm{col}}\left(T\right)=\frac{2\pi r_{\mathrm{e}}^{2}m_{\mathrm{e}}c^{2}}{\beta^{2}}N_{\mathrm{A}}\frac{Z}{A_{\mathrm{M}}}\left[\ln\left(T/I\right)^{2}+\ln\left(1+\tau/2\right)+F\left(\tau\right)-\delta_{F}(T)\right],$$

  where $\tau = T/m_{\mathrm{e}}$, I is the mean excitation energy, and $\delta_F(T)$ is the density effect correction
- In 2.1.29, elemental mean excitation energies are from ESTAR. For compounds, additivity rule with slight modifications in some of the elemental I values is used.
- $\delta_F(T)$ depends on I, electron density, binding energies, ground state configuration, and conductivity of the material in a non-trivial way
- Sternheimer's model [2] is used for solving $\delta_F(T)$ for each material
- Collision stopping power is calculated with the equation above

$\Rightarrow$ Improved TTB energy distribution in compounds

- In 2.1.29, radiative stopping powers are integrated from bremsstrahlung cross section data

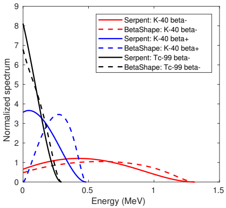
Beta bremsstrahlung

- Neutron-rich nuclides in spent fuel decay predominantly through beta decay
- Bremsstrahlung emitted by beta particles is of interest in shielding and decay heat calculations
- Evaluated beta spectrum data sparsely available
  - In the ENDF-B-VII.1 decay library, beta spectrum is given only for 280 of the about 1600 beta decaying nuclides (missing important nuclides, such as ^{90}Sr and ^{90}Y)
- Some codes for calculating beta spectrum exist (RADLST, BTSPEC, BetaShape)
- Simple theoretical model for the spectrum is used in Serpent:

$$N(p)dp = \sum_i I_i F(Z,E) p^2 (E_i - E)^2 dp,$$

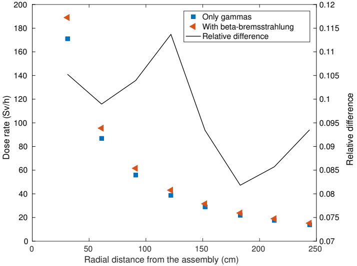
where I_i is the intensity and E_i is the end-point energy of the ith branch, $F(Z,E)$ is a Fermi function, E is the total energy and p is the momentum of a beta particle.

  - Fermi function approximation given by Venkataramaiah et al. [3] is used
  - Intensities and end-point energies are read from ENDF-format decay data library
  - Suitability for decay heat calculations may be limited
- User-defined beta spectrum can also be used in Serpent
- Beta bremsstrahlung photons are created with the TTB model
- TTB is also used for internal conversion and Auger electrons



Beta bremsstrahlung - test case

- Effective dose rate calculation[1] for 15x15 PWR assembly (28.43 MWd/kgU, 657 days of cooling)
- Dose rates were increased about 10% by including the beta bremsstrahlung source



Effective dose rates at different radial distances from the axial midpoint of the assembly

---

[1] Calculated by Silja Häkkinen and Antti Räty (VTT) as a part of a dose rate benchmark under the framework of NEA's Expert Group on Advanced Fuel Cycle Scenarios

Flux-to-Effective dose conversion factors

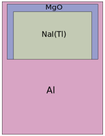
- Built-in ANSI/ANS 6.1.1-1977, ICRP-21 (1971), ICRP-74 (1996), and ICRP-116 (2010) conversion factors for photons and neutrons
- Different irradiation geometries included in the ICRP-74 and ICRP-116 data [4]
- Other conversion factors can be used by applying a user-defined response function (`dr -100` and `fun` card)

Detector modeling with Serpent

- Pulse-height detector (response function -27) was added in version 2.1.25
  - Calculates the energy deposited in a detector material by a photon (and possible secondary photons and electrons) which is scored into a pulse
  - The result is an ideal photon spectrum
- In reality, the spectrum is broadened due to statistical fluctuations in the production of light photons in the detector material (scintillators) and electrons in photomultiplier tube, and electronic noise
  - Results in a Gaussian shape of the photopeak
  - Energy resolution of a detector is defined as $R_E(E_0) = \frac{\mathrm{FWHM}}{E_0}$, where E_0 is the photopeak energy and FWHM is the full width at half maximum
- NEW: Two ways to include energy broadening effect in Serpent:
  1) Provide (E_0, FWHM) or $(E_0, R_E(E_0))$ data, and FWHM is interpolated from the data
  2) Provide constants a, b, c, which you obtain by fitting $(E_0, \mathrm{FWHM(E_0)})$ data into the equation $\mathrm{FWHM(E)} = a + b\sqrt{E + cE^2}$ (same as the `FT GEB` card in MCNP)

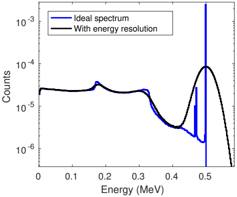
  $\Rightarrow$ Scored energy is sampled from a normal distribution $\mathcal{N}(E_{\mathrm{dep}}, \sigma^2)$, where E_{dep} is the energy deposited in the detector material and $\sigma = \frac{\mathrm{FWHM(E_{dep})}}{\sqrt{8 \ln 2}}$.

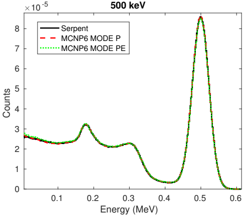
Example of a detector simulation

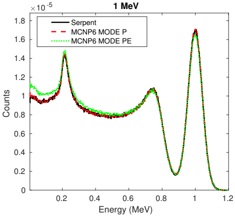


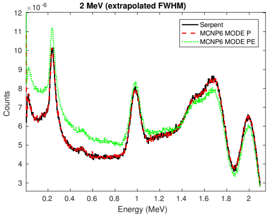
- NaI(Tl) detector (31 x 19 mm) simulation with 0.5, 1 and 2 MeV point sources located 5.45 cm from the front surface
- Detector geometry and constants a, b, c for equation $\mathrm{FWHM(E)} = a + b\sqrt{E + cE^2}$ obtained from Ref. [5]
- Spectra calculated with Serpent, MCNP6 mode P and mode PE (electron transport mode)

⇒ Electron transport needed above 1–2 MeV, depending on the size of the detector







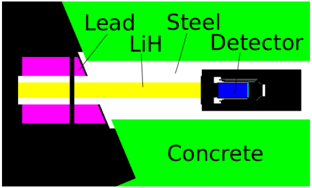


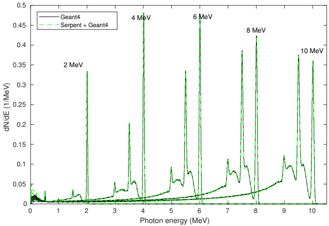
Source file creation for electron transport code

- Serpent is not suitable for detector modeling above photon energies of about 1–2 MeV
- One way to overcome this limitation is to do the detector modeling with an electron transport code:
  1) In Serpent calculation, create a surface source file for photons that pass a surface located around the detector (`df` and `ds` detector parameters)
  2) Model the detector and its surroundings with the electron transport code
  3) Read photons from the surface source file in the electron transport code
- Source file creation:
  - Setting the cell inside the surface located around the detector to be an outside cell (problem: doesn't work with coupled neutron-photon transport)
  - Using detector flagging so that primary photons are not double-counted (problem: secondary photons are included in the source file)
- How much of the detector surroundings should be included in the electron transport calculation?

Serpent + Geant4

- Geant4
  - General-purpose Monte Carlo particle simulation toolkit
  - Comprehensive selection of photon and electron physics models
  - Widely used for detector modeling
- Geant4 class (`G4VPrimaryGenerator`) implemented for reading Serpent source file and generating primary events
- Spectrum calculation for JET KM6T LaBr3(Ce) gamma detector with Geant4 and Serpent+Geant4:
  - Unidirectional and monoenergetic disk source in front of LiH neutron attenuator
  - Geant4 simulation for the whole geometry
  - Serpent photon simulation from the source to the detector + Geant4 detector simulation





Future work

- Photonuclear interactions
- (α,n)-reactions

References

[1] M. J. Berger, J. Coursey, M. Zucker, and J. Chang, “Stopping-power and range tables for electrons, protons, and helium ions,” NIST, http://www.nist.gov/pml/data/star/index.cfm

[2] R. M. Sternheimer, S. M. Seltzer, and M. J. Berger, “Density effect for the ionization loss of charged particles in various substances,” Phys. Rev. B, 26, 6067–6076 (1982).

[3] P. Venkataramaiah, K. Gopala, A. Basavaraju, S. S. Suryanarayana, and H. Sanjeeviah, “A simple relation for the Fermi function”, J. Phys. G, vol. 11, no. 3, p. 359, 1985

[4] "Conversion Coefficients for Radiological Protection Quantities for External Radiation Exposures", ICRP Publication 116, Ann. ICRP 40(2–5), (2010).

[5] Salgado, César Marques, et al. “Validation of a NaI (Tl) detector’s model developed with MCNP-X code”, Progress in Nuclear Energy 59 (2012): 19-25.