Upcoming features in Serpent photon transport mode

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Outline

- Current photoatomic physics in Serpent
- Photonuclear mode
- Bremsstrahlung emitted by beta particles

Photon transport mode

- Photon transport mode was introduced in version 2.1.24 in 2015
- Photon transport can be used for elements Z = 1 to 99
- Energy range of photons from 1 keV to 100 MeV
- No electron transport, bremsstrahlung production is taken into account with the thick-target bremsstrahlung (TTB) approximation
- Data:
  - Most of the interaction data is from ENDF-B-VII.1 (form factors, incoherent scattering functions, photoelectric cross sections and atomic relaxation data)
  - Compton profiles and bremsstrahlung data from other sources
  - Total interaction cross sections are read from an ACE format library, e.g. MCNP's mcplib12 photon data library
- Serpent's photon physics are described in Ref. [1] (somewhat outdated)

Photo 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

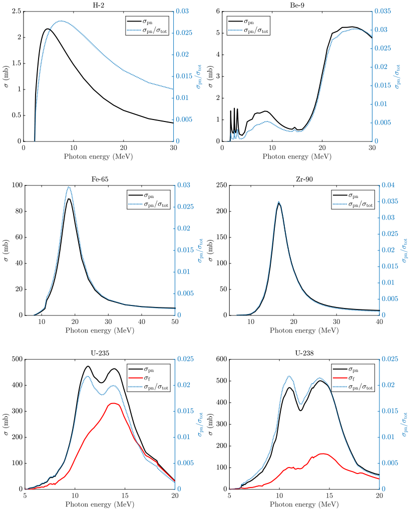
- Compton scattering and photoelectric effect cause vacancies in electron shells
- Relaxation cascade through radiative (fluorescence) and non-radiative (Auger, Coster–Kronig) transitions
- Transitions are sampled according to the probabilities given by ENDF/B-VII.1, all possible transitions are included

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

Photonuclear physics in a nutshell

- Giant dipole resonance (GDR)
  - Photon interacts with the dipole moment of the nucleus
  - For light nuclei, GDR is observed at 20-25 MeV. For heavy nuclei, GDR occurs at around 15 MeV.
  - One or two broad resonance peaks
- Quasi-deuteron absorption
  - Photon interacts with the dipole moment of a neutron-proton pair inside the nucleus
  - Smaller cross section than the GDR
- Interaction probability is always below 5-6%
- Neutrons, protons, gammas, alphas etc. can be produced in a photonuclear reaction
- Photofission is possible for heavy nuclides



Applications of photonuclear reactions

- Reactor physics, e.g. heavy water reactors, beryllium reflectors
- Shielding design
- Activation analysis
- Neutron source using electron accelerators
- Dose calculations in radiotherapy
- Nuclear security, e.g. non-destructive detection of nuclear materials

Photonuclear models in Model Carlo codes

- Data- and model-based approaches are used in Monte Carlo codes
- Data libraries in ENDF format:
  - IAEA Photonuclear Data Library (1999): 164 nuclides
  - KAERI Photonuclear Data Library (2000): 143 nuclides
  - ENDF/B-VIII.0 or ENDF/B-VII.0: 163 nuclides
  - JENDL/PD-2016: 181 nuclides in standard and 2681 in extended version
  - TENDL-2017: 2808 nuclides
- NJOY can be used for processing ENDF format photonuclear data into ACE format
- MCNP photonuclear data in ACE format:
  - 13 in LA150u library (.24u)
  - 157 nuclides in endf7u library (.70u), data available up to 20-150 MeV depending on nuclide
- Physics models are also used in some Monte Carlo codes, e.g. Geant4, Cascade-Exciton Model (CEM) in MCNP
- Serpent uses the ACE format photonuclear data

Photonuclear ACE data format

- Photonuclear ACE data [2]:
  - Total photonuclear and reaction cross sections are given in the XSS block as usual
  - All secondary particle information is given in the IXS block (which is stored in the XSS block)
  - A reaction can produce any set of secondary particle types, which have different energy and angular distributions
- Serpent routines were updated to read and process photonuclear data
  - Total photonuclear cross sections are added to total photon cross sections
  - Photonuclear energy grid points are added to the unionized photon energy grid
  - Secondary particles are added as “secondary reactions” under each photonuclear reaction
- xsdirconvert.pl script was updated to include photonuclear data in the Serpent directory file

Discrete inelastic photonuclear reactions (MT=50-90)

- In ENDF/B-VIII.0, discrete two-body scattering (LAW=2) is used for discrete inelastic reactions in $^{2}\mathrm{H}$, $^{12}\mathrm{C}$, $^{16}\mathrm{O}$, $^{51}\mathrm{V}$, $^{180}\mathrm{W}$ and $^{183}\mathrm{W}$
- Only angular distribution is provided for calculating the cosine of the emission angle μ_{CM} in the CM frame (center-of-mass)
- Collision kinematics must be used to solve the energy of the emitted particle E'_{CM} and transform μ_{CM} and E'_{CM} to LAB frame
- Different collision kinematics approaches:
  - In MCNP, the CM energy is calculated as (according to Ref. [3])

    $$E'_{\mathrm{CM}} = \frac{A}{A+1}(E_\gamma + Q),$$

    where A is the ratio of the nuclide mass to neutron mass m_{n}, E_γ is the photon energy , and Q is the reaction Q value. No transformation from CM to LAB frame is made.
  - In TRIPOLI-4 [4], non-relativistic approach is used

    $$E'_{\mathrm{CM}} = \frac{A-1}{A}\left(E_\gamma + Q - \frac{E_\gamma^2}{2m_{\mathrm{n}}c^2A}\right).$$

    E'_{CM} and μ_{CM} are transformed into LAB frame using non-relativistic transformation.
  - In MC21[3], relativistic collision kinematics and transformation from CM to LAB frame is used.
- Serpent uses the relativistic collision kinematics presented in Ref. [3]. The kinematics used in MCNP and TRIPOLI-4 have also been implemented for testing purposes.

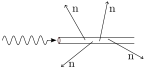
Other photonuclear reactions

- Complex reaction MT=5: Multiple reactions lumped together, any secondary particle type is possible. Particle production is defined by multiplicity.
- Continuum inelastic reaction MT=91
- Photofission MT=18
- (γ, xn), (γ, nx), (γ, 2nx) etc. reactions
- Other reactions which don't emit neutrons
- For most reactions, correlated energy-angular (energy law 44) or just energy distribution (law 4) is given. Maxwell-fission spectrum (law 7), evaporation spectrum (law 9) and energy-dependent Watt spectrum (law 11) are also used.
- Reaction outcome (energy and direction in CM or LAB) can be sampled with the already existing methods in Serpent
  - Some corrections required for energy-angular distributions (Kalbach-Mann systematics)
- If the energy or direction is in CM frame, relativistic transformation to LAB frame is used in Serpent
  - Non-relativistic transformation is used in TRIPOLI-4, no transformation in MCNP

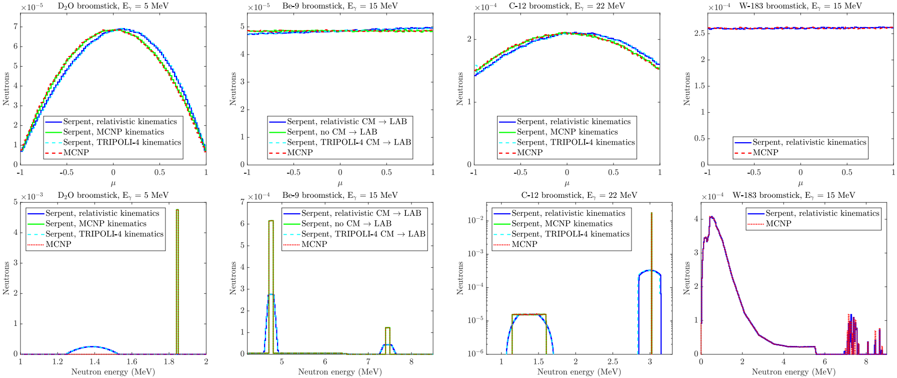
Photonuclear mode in Serpent

- Usage of photonuclear mode:
  - User can define which secondary particle types are included in the simulation (neutrons or gammas)
  - Photonuclear library can be defined for all the nuclides in the problem
  - Photonuclear data substitution for nuclides for which photonuclear data is not found in the library
- Analog mode:
  - Photonuclear reaction is selected with a probability given by its cross section, all reactions are included.
  - The number of emitted secondary particles is sampled based on the multiplicity given in the data.
- Forced collision mode:
  - In each collision, a photoatomic and a photonuclear reaction are sampled (if possible). The weight of both reaction outcomes are adjusted by the ratio of their cross sections to the total cross section.
  - Only those photonuclear reactions which produce secondary particles defined by the user are included. The weight of the secondary particle is multiplied by the multiplicity.
  - Weight cutoff with Russian roulette can be used.

Broomstick test case for photonuclear reactions

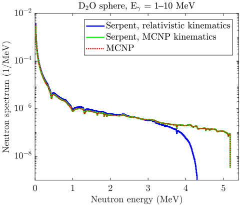


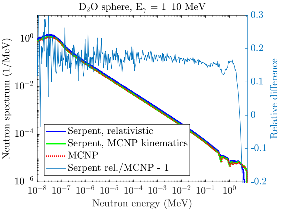
- Forced collisions in both Serpent and MCNP
- D_2O at 5 MeV: only MT=50 possible for ^2H
- ^9Be at 10 MeV: only MT=29 $(\gamma, n2\alpha)$ (ENDF/B-VIII.0: E_n in LAB, endfu: E_n in CM)
- ^{12}C at 22 MeV: MT=5 and MT=50 are possible
- ^{183}W at 15 MeV: continuum level MT=91 dominates, MT=50-69 also possible

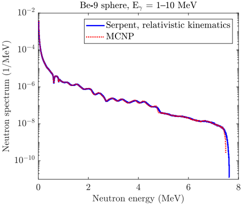


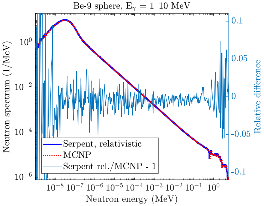
Sphere test case

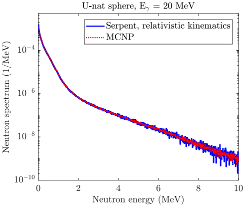
- Isotropic point source at the center of a sphere of radius 10 cm, source energy uniformly distributed between 1 and 10 MeV
- Neutron spectrum tallied on the surface of the sphere
- Tested materials: $\mathrm{D_2O}$, $^9\mathrm{Be}$ and U-nat
- In $\mathrm{D_2O}$, neutrons are created at lower energies with the relativistic kinematics used in Serpent
- Reasonably good agreement in $^9\mathrm{Be}$ and U-nat

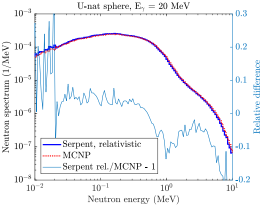










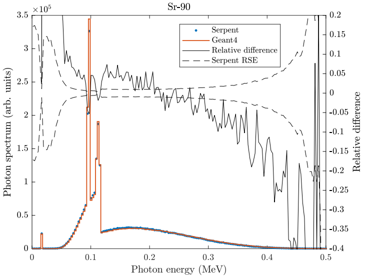


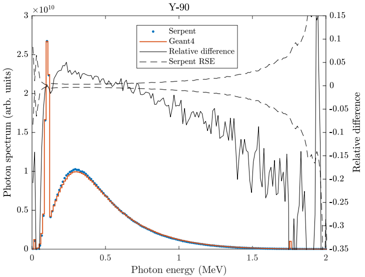
Bremsstrahlung emitted by beta particles

- Neutron-rich nuclides in spent fuel decay predominantly through beta decay
- Bremsstrahlung emitted by beta particles can contribute 10–20% to the total photon dose rate in spent fuel [5]
- Serpent has a radioactive decay source mode, which uses ENDF format decay data file
- The TTB approximation implemented in Serpent can be used for creating beta bremsstrahlung
- Available beta spectrum data:
  - 1000 nuclides in ICRP Publication 107 [6], the data can be downloaded from [7]. The beta spectrum file ICRP-07.BET can be directly used in Serpent.
  - 460 nuclides in RADAR [8]
  - 280 nuclides in ENDF-B-VII.1 decay library (mostly beta-delayed neutron emitters)
- User-defined beta spectrum can also be used in Serpent
- Theoretical model for beta spectrum has been implemented in Serpent [9]
- ICRP-107 and ENDF beta spectrum data can be used together with the built-in spectrum model

Beta bremsstrahlung: Comparison with Geant4

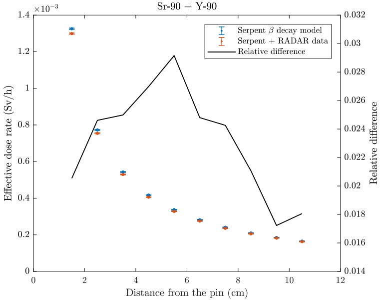
- Single fuel-pin (radius=0.4 cm, height=100 cm) surrounded by air
- Photon spectrum tallied outside the pin
- Built-in spectrum model used in Serpent calculations
- Beta source in the fuel
  - Sr-90: E_{max} = 546 keV, $T_{1/2} = 28.8$ years, decays into Y-90
  - Y-90: E_{max} = 2279 keV, $T_{1/2} = 2.67$ days
- Slight overestimation in the bremsstrahlung "peak" region is most likely due to leakage of electrons in the Geant4 simulation.
- Underestimation at the high end of the spectrum probably due to the failure of the CSDA used by the Serpent TTB approximation.

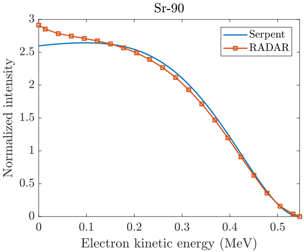


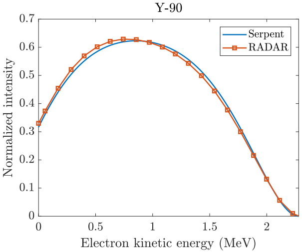


Beta bremsstrahlung: Comparison with RADAR data

- Same fuel-pin geometry as in the previous slide
- Combined Sr-90 and Y-90 decay
- Effective dose rate tallied as a function of radial distance from the pin
- Serpent result is 2–3% higher







Future work

- Photonuclear reactions:
  - Correction to energy-angular distribution
  - Heating numbers for energy deposition
  - Comparisons with TRIPOLI-4
  - ACE format cross section library
- Photoatomic cross section library based on the new ENDF/B-VIII.0 library
  - ENDF/B-VIII.0 photoatomic data is taken from EPICS2017 (Electron-Photon Interaction Cross Sections). Most importantly, the binding energies have been updated.
  - Photon data will also be updated (photoelectric effect cross sections, atomic relaxation data, form factors)
- (α,n)-reactions

Thank you for your attention!

References

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[4] O. Petit, N. Huot, and C. Jouanne, “Implementation of photonuclear reactions in the Monte Carlo transport code TRIPOLI-4 and its first validation in waste package field,” *Progress in Nuclear Science and Technology*, **2**, 798–802 (2011).

[5] O. Hermann and C. Alexander, “Review of spent-fuel photon and neutron source spectra,” Oak Ridge National Lab., TN (USA) (1986).

[6] “ICRP CD1 - Nuclear Decay Data for Dosimetric Calculations, Supplemental Material,” Annals of the ICRP, `http://journals.sagepub.com/doi/suppl/10.1177/ANIB_38_3`.

[7] K. Eckerman and A. Endo, “ICRP Publication 107. Nuclear decay data for dosimetric calculations.,” *Annals of the ICRP*, **38**, *3*, 7–96 (2008).

[8] “RADAR - The Decay Data,” RADAR - the RAdiation Dose Assessment Resource, `http://www.doseinfo-radar.com`.

[9] T. Kaltiaisenaho, “Implementing a beta bremsstrahlung source in Serpent,” VTT-R-00953-18, VTT Technical Research Centre of Finland Ltd. (2018).