Status and recent progress in photon transport in Serpent 2

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Jaakko Leppänen

VTT Technical Research Center of Finland

Outline

Photon transport mode

- Background
- Interaction data and physics

Radioactive decay source mode

Coupled neutron-photon transport mode

Photon detectors

Future work

Photon transport mode: background

The main motivation for expanding to photon transport is to simulate gamma heating in multi-physics calculations, which becomes important especially in fast transients

Photon interaction physics routines were introduced in update 2.1.24[1]

Photon transport mode also enables running shielding and dose-rate calculations for problems involving gamma radiation

The simulation can be run using a user-defined source, but there are also two coupled modes under development:

1) Radioactive decay source mode, which combines burnup or activation calculation with radioactive decay data and photon emission spectra from ENDF data

2) Coupled neutron-photon transport simulation mode, in which fission, capture and inelastic scattering gammas are produced during the neutron transport simulation

These two modes account for the delayed and prompt gamma radiation produced by neutron reactions, respectively

[1] T. Kaltiaisenaho. "*Implementing a photon physics model in Serpent 2.*" M.Sc. Thesis, Aalto University. 2016.

Photon transport mode: interaction data

Photon interaction physics for elements from Z = 1 to 98 and photons from 1 keV to 100 MeV, with reaction cross sections read from ACE format libraries[2]

The physics model differs from MCNP, and all required interaction data is not available in the ACE format data libraries. Additional data is read from separate files:

- 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 included 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

The data scheme may be revised at some point

For questions, contact: Toni.Kaltiaisenaho@aalto.fi

[2] Currently recommended photon library: mcplib84 from MCNP6 distribution.

Photon transport mode: 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 (caused by the momentum distribution of the electron), important below 1 MeV

Photoelectric effect:

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

Pair production:

- The energies of the electron and positron are sampled from the theoretical differential cross section given by Davies, Bethe and Maximon, with some extensions and approximations used in PENELOPE and Geant4
- Positron annihilation at rest

Photon transport mode: 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:

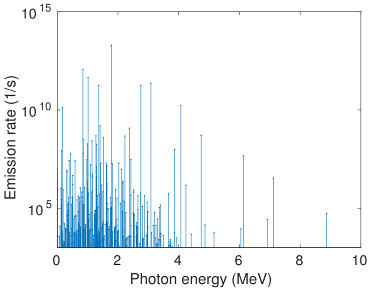
- Electrons are generated through Compton scattering, photoelectric effect, pair production and non-radiative transitions
- Bremsstrahlung photon production is important especially for high-Z atoms at energies above $\sim$1 MeV
- The number of bremsstrahlung photons and their energies are sampled from 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

Radioactive decay source mode

A radioactive decay source mode was implemented already in Serpent version 2.1.24, for the purpose of radiation transport calculations involving activated materials

The source term is determined by:

- Isotopic material compositions, either user-defined or obtained from a previous burnup / activation calculation
- Decay constants of radioactive nuclides, read from ENDF-format decay data file
- Photon emission line spectra, read from ENDF-format decay data file



Only (discrete) photon emitting reactions are included for now, but the methodology is planned to be extended to neutrons in the future.

Radioactive decay source mode

Sampling the emission energy from discrete line spectra is straightforward:

1) Sample decaying nuclide
2) Sample emission line

Two algorithms for sampling the position:

Analog sampling – Source points are sampled uniformly throughout the geometry and each point accepted or rejected based on the ratio of local to maximum emission rate.

Implicit sampling – Source points are sampled uniformly throughout the geometry and the weight of the emitted photon adjusted according to the ratio of local to average emission rate.

Efficiency of analog sampling becomes poor when most (but not all) of the activity is concentrated on local hot spots.

Implicit sampling allows covering the geometry uniformly with source points, but may lead to sparse distribution of weights and lead to problems with tally statistics.

Radioactive decay source mode

The radioactive decay source mode is most conveniently used with burnup or activation calculation (radioactive material compositions read from a binary restart file)

The same input can be used in both calculations without major modifications:

- Isotopic material compositions automatically converted into elemental
- Source normalization done automatically based on total photon emission rate

Test applications:

- Radiation shielding calculations for CASTOR canister with spent nuclear fuel (carried out within the SAFIR2018/KATVE project)
- Shut-down dose-rate calculations for the ITER fusion reactor[3,4]

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[3] P. Siren and J. Leppänen. "*Expanding the Use of Serpent 2 to Fusion Applications: Development of a Plasma Neutron Source.*" In proc. PHYSOR 2016. Sun Valley, ID, May 1-6, 2016.

[4] J. Leppänen and T. Kaltiaisenaho. "*Expanding the Use of Serpent 2 to Fusion Applications: Shut-down Dose Rate Calculations.*" In proc. PHYSOR 2016. Sun Valley, ID, May 1-6, 2016.

Coupled neutron-photon transport mode

Work on a coupled neutron-photon transport is under way:

- Prompt gamma production reactions are now included in the physics models (data from standard ACE files)
- The sampling routines are being comprehensively tested by comparing against MCNP5:
  - Simple “Broomstick” problem: unidirectional neutron beam along a narrow cylinder, secondary neutron and photon spectra tallied
  - Carried out for all nuclides in ENDF/B-VII.1, JEFF-3.2, JENDL-4.0 and FENDL-3.0 evaluated nuclear data files (as part of testing new cross section libraries for Serpent 2)
- The coupling is not yet accomplished, but the methodology can be tested by writing the produced photons in a source file for second simulation

Coupled neutron-photon transport mode

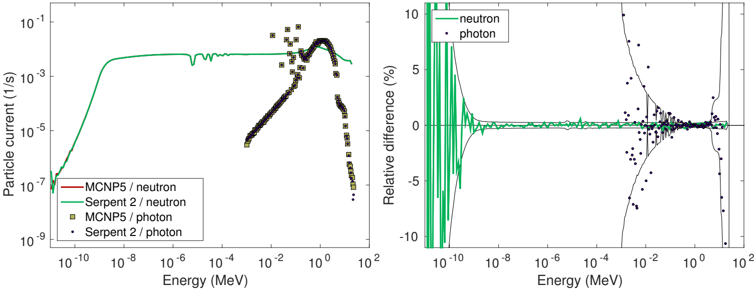

Figure 1 : Comparison of secondary neutron and photon spectra between Serpent 2 and MCNP5 (“broomstick” model, U-238 from JENDL-4.0). Left: outward current spectra, Right: relative differences between the codes.

Photon detectors

The conventional detectors (tallies) are available for photons as well. In addition there are three photon-specific detector types:[5]

1) Photon dose rate detector based on built-in photon mass-energy attenuation coefficients from NIST data:

    - Material-wise coefficients for 48 materials
    - Elemental data for calculating coefficients for arbitrary input materials (done automatically)

2) Photon pulse height detector

3) Analog photon heating detector equivalent with the *f8 tally in MCNP (implemented in 2.1.27)

The standard detector methodology in Serpent 2 also includes user-defined response functions, which can be used, for example, in the calculation of biological dose.

The coupled neutron/photon transport mode was tested by a summer student from Aalto University (the report is not completed yet)

[5] The response numbers are listed at Serpent Wiki: http://serpent.vtt.fi/mediawiki/index.php/ENDF_reaction_MT's_and_macroscopic_reaction_numbers

Future work

The coupled simulation mode is planned to be completed in update 2.1.28

The “broomstick” validation calculations will be completed and the results reported within the near future

The coupled mode enables more accurate calculation of heat deposition:

- Direct neutron and prompt gamma heating become important in fast transients?
- More accurate model for steady-state calculations as well

The contribution of delayed heating will be studied in slow transients and burnup calculations

Plans for extending the photon physics mode:

- Photonuclear reactions
- Electron transport mode for accurate physics of secondary particles

The work is planned to continue after we get Toni back in February 2017