Serpent and Nuclear Data: Needs, processing and verification

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IAEA TM on the Compilation of Nuclear Data Experiments for Radiation Characterization
Oct 10 – 14, 2022

Outline

- Serpent in a nutshell in 2022.
- Radiation transport and depletion capabilities of Serpent.
- Validation of Serpent at VTT.
- Validation of Serpent by users.
- Sensitivity calculations and nuclear data uncertainty propagation with Serpent.

Serpent overview

Serpent is a continuous-energy Monte Carlo neutron and photon transport code:

- Developed at VTT since 2004
- Physics models for neutron, photon and coupled neutron/photon transport simulations
- Originally developed for reactor physics calculations
- OpenMP/MPI parallelization
- Support for various geometry types (CSG, mesh, CAD, etc...)
- Built-in routines for group constant generation, burnup calculation and variance reduction
- Multi-physics interface for external coupling
- User-friendly, adaptable, no external dependencies, no wrappers

Serpent started out as a reactor physics code, but is currently used for a wide range of fission, fusion and other radiation and particle transport applications.

- Website: https://serpent.vtt.fi/serpent/
- Current base version Serpent 2.2 (May 2022).
- Over 1000 users in 250 organizations in 43 countries.

Neutron transport

- Based on a combination of surface tracking and delta tracking.
  - Complemented with additional rejection sampling to model density and temperature distributions separately from the geometry model.
- Multiple intercompatible geometry models:
  - Constructive Solid Geometry (surfaces, cells, universes)
  - CAD-geometry model based on STL solids (triangulated closed surfaces).
  - Unstructured mesh based geometry with support for OpenFOAM mesh format.
- Interaction physics modelled with ENDF laws and standard collision kinematics.
  - ACE libraries currently produced with NJOY.

Depletion

- Transmutation cross sections evaluated based on ACE format interaction cross sections.
  - Direct 1 group evaluation or spectrum collapse.
- Combined with ENDF NFY and decay data to construct the burnup matrix.
  - Branching ratios for reactions can have a major effect on results.
- Matrix exponential solved with CRAM.
  - Higher order predictor corrector methods with substeps to describe evolution of reaction rates during burnup step.
- Collision based domain decomposition for very large burnup problems.

Photon transport

- Uses ACE format interaction cross sections.
- Includes models for:
  - The photoelectric effect.
  - Rayleigh scattering.
  - Compton scattering.
  - Electron-positron pair production.
  - Atomic relaxation.
  - Thick target bremsstrahlung.
- Photon physics modelling between Monte Carlo codes differs much more than neutron physics modelling.
- Input data for models from multiple sources.

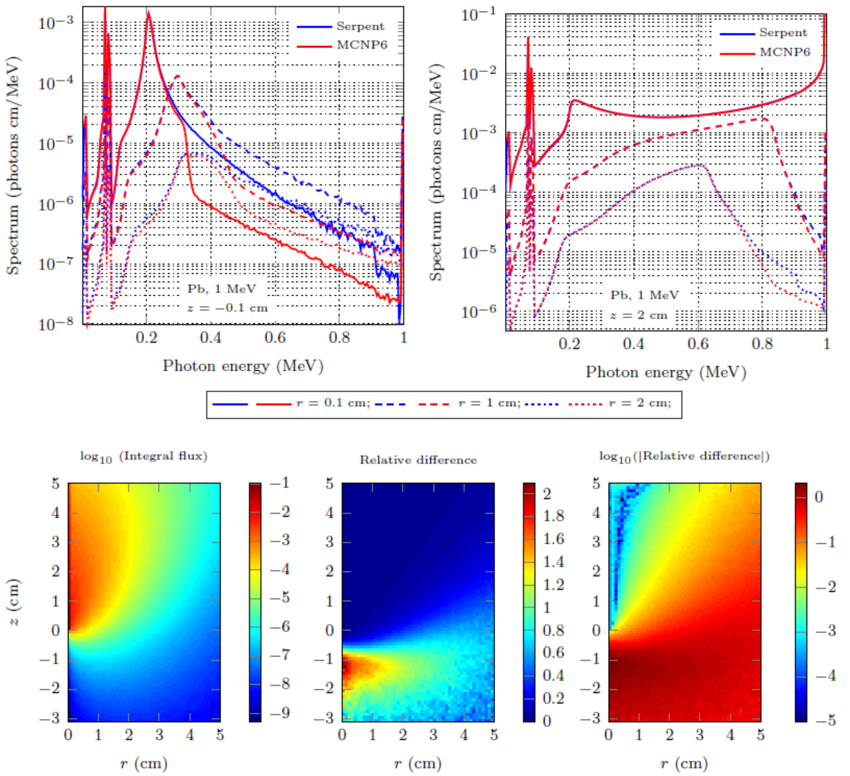

Figure 6.10: At the top row, the volume integrated photon energy spectrum for 1 MeV photon beam in a lead cylinder at six locations of the geometry. At the bottom row, the total integral flux given by Serpent in the cylinder and the relative difference (Eq. (6.1)) compared with MCNP6.

From T. Kaltiaisenaho, “Implementing a photon physics model in Serpent 2”, MSc thesis, Aalto University, 2016.
https://aaltodoc.aalto.fi/bitstream/handle/123456789/21004/master_Kaltiaisenaho_Toni_2016.pdf?sequence=1&isAllowed=y

Coupled neutron photon transport

- Photons produced from neutron interactions.
  - Either analog or implicit sampling.
  - Banked in memory to wait for simulation after current neutron transport finishes.
- Utilized for shielding and accurate energy deposition calculations.
- Decay photons not included in the coupled neutron photon calculation.
- Photonuclear interactions included in a separate development branch.

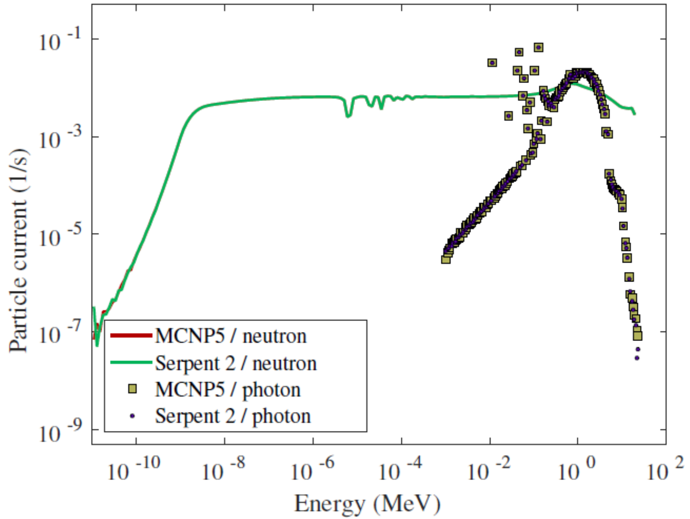

Fig. 1. Example of a "Broomstick" comparison calculation used for validating the photon production routine in Serpent 2 against MCNP5. Out-going neutron and photon current spectra calculated using the two codes. The example case is for ^{238}U from JENDL-4.0.

From J. Leppänen, T. Kaltiaisenaho, V. Valtavirta, and M. Metsälä, "Development of a coupled neutron / photon transport mode in the Serpent 2 Monte Carlo code," Proc. M&C 2017, Jeju, Korea, Apr. 16–20, 2017.

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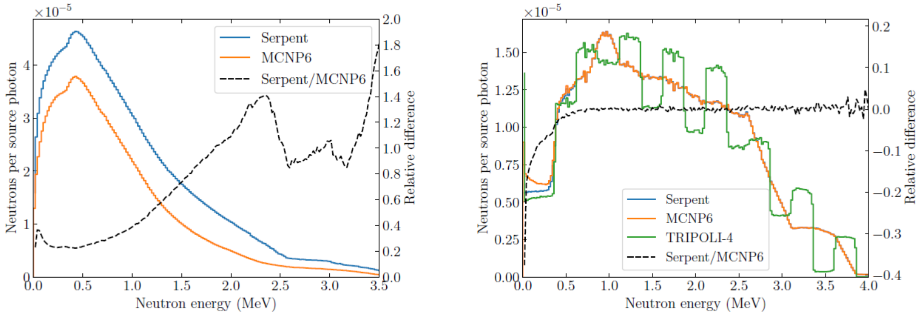


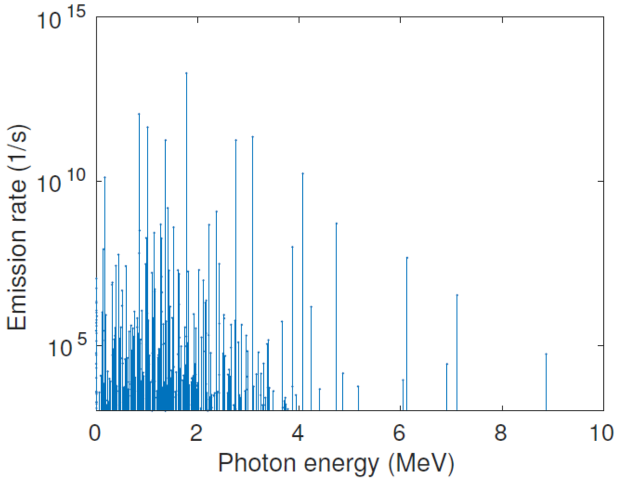
Figure 3: Photoneutron spectra on the surfaces of the tungsten and lead cubes.

From T. Kaltiaisenaho, “Photonuclear reactions in Serpent 2 Monte Carlo code,” Proc. M&C 2019, Portland, OR, USA, Aug. 25-29, 2019.

A very nice recent application of coupled neutron-photon transport for a shielding application:
Christoph Hauf (TUM) - Simulations of the new shielding at SR8 with Serpent 2

Radioactive decay source

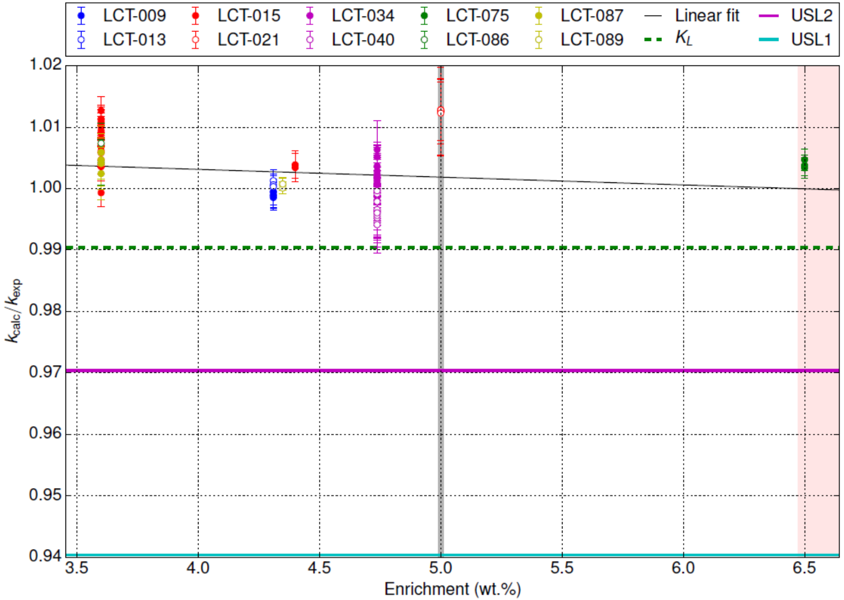
- Neutrons and photons produced from decay reactions are not included in coupled neutron photon calculations.
- The radioactive decay source definition in Serpent generates a fixed source of neutrons, photons and secondary bremsstrahlung from beta-decay based on depleted material compositions.
- Useful for spent fuel shielding calculations as well as other shielding applications.



Photon line spectrum from a Serpent decay source definition

Validation at VTT
Criticality safety

- Serpent used to evaluate subcriticality of wet spent nuclear fuel storage at Finnish NPPs.
- Validation based on specific target application:
  - Evaluation of Upper Safety Limit for k_{eff}.
  - Based on NRC *Guide for validation of nuclear critical safety calculational methodology* (Dean, Tayloe)
- Criticality safety validation package developed at VTT over the years:
  - Some 700 Serpent inputs for LCT cases from the ICSBEP handbook
  - Automated scripts for setting up, running and analyzing simulations.
  - Similarity analysis can be conducted utilizing sensitivity calculation capabilities of Serpent.



Linear trend analysis of the k_{eff} ratio as a function of mean fuel enrichment.

From V. Valtavirta, “Criticality safety validation of Serpent for nuclear fuel wet storage calculations”, VTT Customer Report, VTT-CR-02424-17, http://montecarlo.vtt.fi/download/VTT-CR-02424-17_web.pdf

Validation at VTT Dosimetry

- One of the applications of Serpent at the Finnish NPPs is the generation of dosimetry kernels for reduced order models.
  - Reactor pressure vessel and sample chains.
- Recent validation conducted at VTT based on U.S. NRC Regulatory Guide 1.190.
- Two PWR verification cases:
  - Standard Core Loading Pattern (STD)
  - Partial Length Shield Assembly (PLS)
- Two experimental validation cases:
  - PCA Pressure Vessel Facility
  - HBR-2 Vessel Dosimetry Benchmark

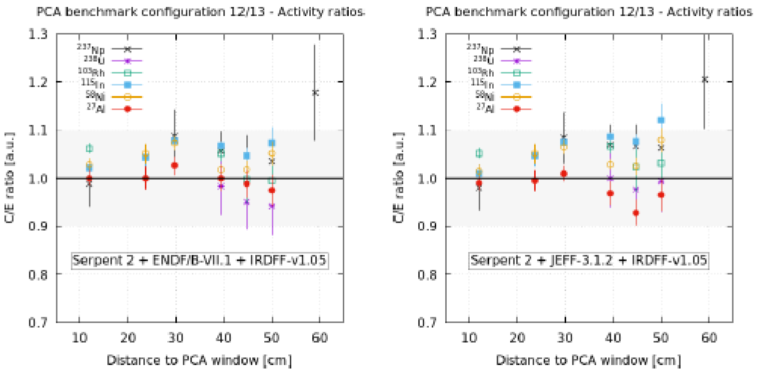


Figure 4: Specific activity C/E ratios for the PCA case. Calculations with Serpent 2 were conducted using transport XS data from ENDF/B-VII.1 (left) and JEFF-3.1.2 libraries (right). Both cases use the same dosimetry XS data (IRDFF version 1.05). Shaded areas represent a ± 10 % uncertainty range.

E. Dorval, "Validation of the Serpent 2 Monte Carlo code for reactor dosimetry applications", Submitted to 17th International symposium on reactor dosimetry

Validation at VTT Depletion

- Computational comparisons between codes are common.
  - Can be tricky due to different definitions of kappa and burnup.
  - Effect of (energy dependent) branching ratio data is obvious.

- Some experimental comparisons made against data from SFCOMPO.
- Participation in SKB blind benchmark.
- Future participation in project LAGER, with Studsvik.
  - Measurements of radial nuclide distributions for a low burnup gadolinium rod.

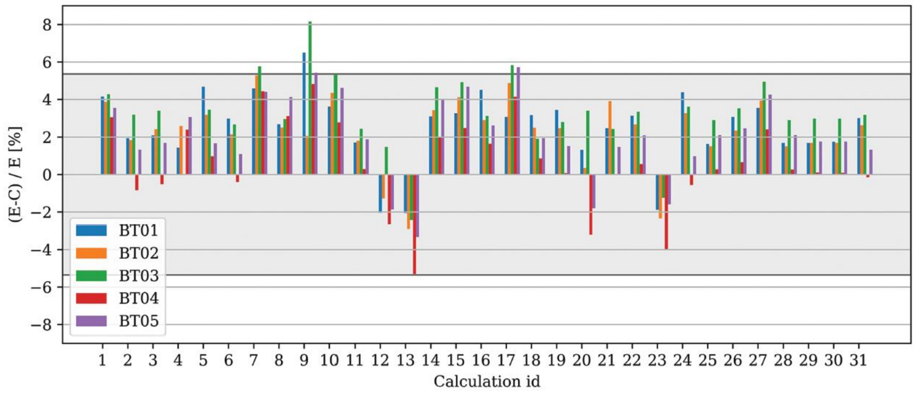


Fig. 8. Relative difference between measured (E) and calculated (C) decay heat rate values for the five different assemblies studied.

From P. Jansson *et al.*, “Blind Benchmark Exercise for Spent Nuclear Fuel Decay Heat”, Nuclear Science and Engineering, 2022

Validation at VTT
Photon transport

- Comparison against MCNP and GEANT-4 during development.
- Some general cases calculated:
  - Kansas skyshine experiment.
  - Hupmobile TLD measurements.
  - OKTAVIAN benchmarks.
  - ALARM benchmarks.
- Testing the CAD geometry in Serpent with photon transport:
  - VTT's experimental facilities.

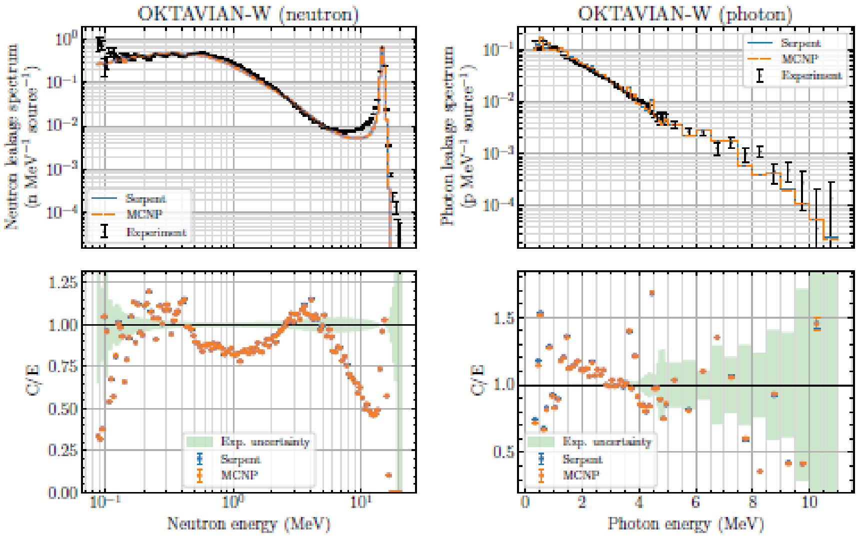


Figure 4. Neutron and photon spectra in tungsten (SINBAD OKTAVIAN benchmark).

T. Kaltiaisenaho, "Validation of the coupled neutron-photon transport in Serpent 2 with OKTAVIAN benchmarks", Research report, VTT-R-00005-20

Validation by users

- Users typically validate Serpent for their own applications.
- A fraction of pubished results are included in the Serpent Wiki
  - https://serpent.vtt.fi/mediawiki/index.php/Validation_and_verification
- Many presentations on the topic at Serpent User Group Meetings:
  - https://serpent.vtt.fi/serpent/users.htm
- In practice, much of user driven validation may not be public.
- Keeping track of even the published cases is difficult.

Sensitivity analyses

- Serpent includes collision history based sensitivity calculation capabilities.
- First order sensitivities of various responses such as k_{eff} and spectral indices to perturbations in etc. nuclear data simple to calculate.
- Useful for further investigations into modelled experiments.

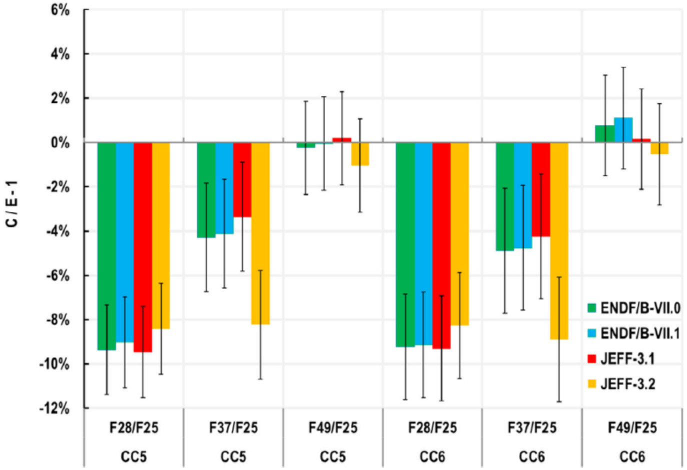


Fig. 6. C/E-1 for spectral indices in the CC5 and CC6 cores obtained with different data libraries. Error bars indicate experimental and statistical uncertainties combined[1].

From E. Fridman, V. Valtavirta, M. Aufiero,
Nuclear data sensitivity and uncertainty analysis of critical VENUS-F cores with the Serpent Monte Carlo code,
Annals of Nuclear Energy, 138, 2020.

Table 1
Summary of the estimated uncertainties.

Parameter	CC5		CC6	
	C-E, pcm	Data uncertainty, pcm	C-E, pcm	Data uncertainty, pcm
k-eff	860 ± 2	2193 ± 1	835 ± 2	2228 ± 2
	C/E-1, %	Data uncertainty, %	C-E, %	Data uncertainty, %
F28/F28	−9.0 + 2.1	7.9 + 0.8	−9.1 + 2.4	8.2 + 1.0
F37/F28	−4.1 + 2.5	4.9 + 0.5	−4.8 + 2.8	5.7 + 0.7
F49/F28	−0.1 + 2.1	1.1 + 0.1	1.1 + 2.3	2.2 + 0.5

Summary

- Serpent includes models for neutron, photon and coupled neutron photon transport.
- Source particles from a radioactive material composition can be emitted using the radioactive decay source definition.
- General validation at VTT conducted for:
  - Criticality safety.
  - Dosimetry.
  - Depletion.
  - Photon transport.
  - (General reactor modelling).
- Serpent users validate Serpent for their own applications.
- Sensitivity analyses and uncertainty propagation can offer further insight to modelled experiments.

beyond
the obvious

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